



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:19 AM UTC

PDB ID : 3ZS2 / pdb_00003zs2
Title : TyrB25,NMePheB26,LysB28,ProB29-insulin analogue crystal structure
Authors : Antolikova, E.; Zakova, L.; Turkenburg, J.P.; Watson, C.J.; Hanclova, I.; Sanda, M.; Cooper, A.; Kraus, T.; Brzozowski, A.M.; Jiracek, J.A.
Deposited on : 2011-06-21
Resolution : 1.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

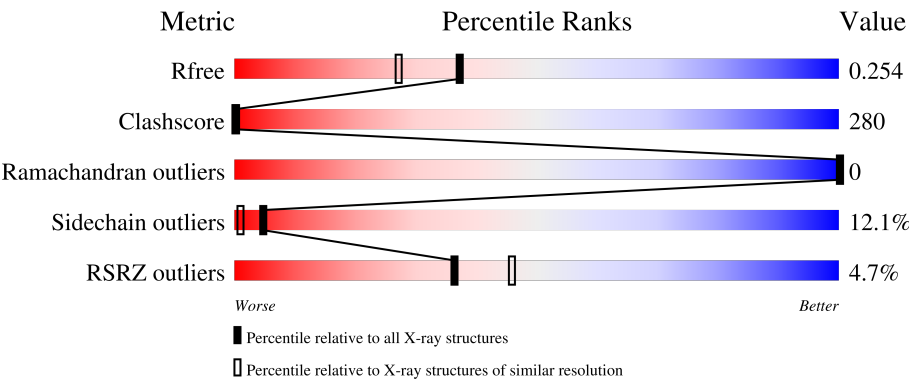
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	21	5% 86% 10% 5%
1	C	21	5% 90% 5%
1	E	21	5% 81% 19%
1	G	21	5% 14% 62% 19% 5%
1	I	21	5% 90% 5%

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Mol	Chain	Length	Quality of chain
1	K	21	
2	B	30	
2	D	30	
2	F	30	
2	H	30	
2	J	30	
2	L	30	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MEA	B	26	-	X	-	-
2	MEA	D	26	-	X	-	-
2	MEA	F	26	-	X	X	-
2	MEA	H	26	-	X	-	-
2	MEA	J	26	-	X	-	-
2	MEA	L	26	-	X	-	-
3	IPH	A	1022	-	X	-	-
3	IPH	C	1022	-	X	-	-
3	IPH	E	1022	-	X	-	-
3	IPH	G	1022	-	X	-	-
3	IPH	I	1022	-	X	-	-
3	IPH	K	1022	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2440 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called INSULIN A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	20	Total	C	N	O	S	0	0	0
			159	97	24	34	4			
1	C	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	E	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	G	20	Total	C	N	O	S	0	0	0
			159	97	24	34	4			
1	I	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	K	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

- Molecule 2 is a protein called INSULIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	27	Total	C	N	O	S	0	0	0
			219	144	36	37	2			
2	D	25	Total	C	N	O	S	0	0	0
			194	125	34	33	2			
2	F	25	Total	C	N	O	S	0	0	0
			194	125	34	33	2			
2	H	28	Total	C	N	O	S	0	0	1
			220	144	37	37	2			
2	J	29	Total	C	N	O	S	0	0	0
			235	155	39	39	2			
2	L	26	Total	C	N	O	S	0	0	0
			212	140	35	35	2			

There are 24 discrepancies between the modelled and reference sequences:

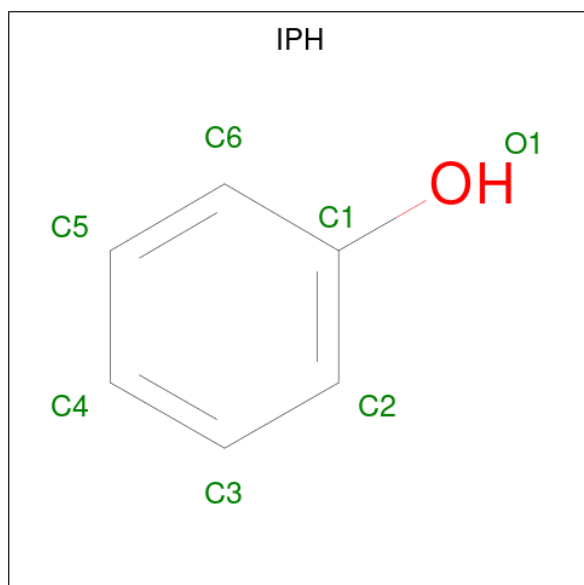
Chain	Residue	Modelled	Actual	Comment	Reference
B	25	TYR	PHE	engineered mutation	UNP P01308

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	MEA	TYR	engineered mutation	UNP P01308
B	28	LYS	PRO	engineered mutation	UNP P01308
B	29	PRO	LYS	engineered mutation	UNP P01308
D	25	TYR	PHE	engineered mutation	UNP P01308
D	26	MEA	TYR	engineered mutation	UNP P01308
D	28	LYS	PRO	engineered mutation	UNP P01308
D	29	PRO	LYS	engineered mutation	UNP P01308
F	25	TYR	PHE	engineered mutation	UNP P01308
F	26	MEA	TYR	engineered mutation	UNP P01308
F	28	LYS	PRO	engineered mutation	UNP P01308
F	29	PRO	LYS	engineered mutation	UNP P01308
H	25	TYR	PHE	engineered mutation	UNP P01308
H	26	MEA	TYR	engineered mutation	UNP P01308
H	28	LYS	PRO	engineered mutation	UNP P01308
H	29	PRO	LYS	engineered mutation	UNP P01308
J	25	TYR	PHE	engineered mutation	UNP P01308
J	26	MEA	TYR	engineered mutation	UNP P01308
J	28	LYS	PRO	engineered mutation	UNP P01308
J	29	PRO	LYS	engineered mutation	UNP P01308
L	25	TYR	PHE	engineered mutation	UNP P01308
L	26	MEA	TYR	engineered mutation	UNP P01308
L	28	LYS	PRO	engineered mutation	UNP P01308
L	29	PRO	LYS	engineered mutation	UNP P01308

- Molecule 3 is PHENOL (CCD ID: IPH) (formula: C₆H₆O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 6 1	0	0
3	C	1	Total C O 7 6 1	0	0
3	E	1	Total C O 7 6 1	0	0
3	G	1	Total C O 7 6 1	0	0
3	I	1	Total C O 7 6 1	0	0
3	K	1	Total C O 7 6 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Zn 1 1	0	0
5	D	1	Total Zn 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	B	17	Total O 17 17	0	0
6	C	17	Total O 17 17	0	0
6	D	10	Total O 10 10	0	0
6	E	7	Total O 7 7	0	0

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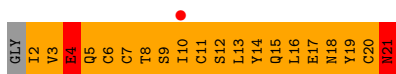
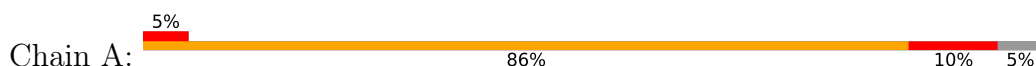
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	15	Total 15	O 15	0	0
6	G	17	Total 17	O 17	0	0
6	H	17	Total 17	O 17	0	0
6	I	19	Total 19	O 19	0	0
6	J	16	Total 16	O 16	0	0
6	K	9	Total 9	O 9	0	0
6	L	4	Total 4	O 4	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

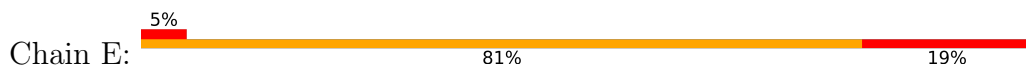
- Molecule 1: INSULIN A CHAIN



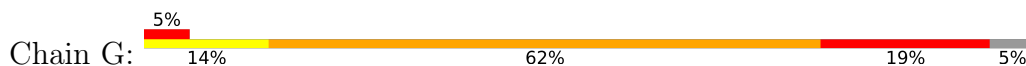
- Molecule 1: INSULIN A CHAIN



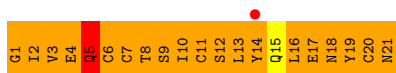
- Molecule 1: INSULIN A CHAIN



- Molecule 1: INSULIN A CHAIN



- Molecule 1: INSULIN A CHAIN

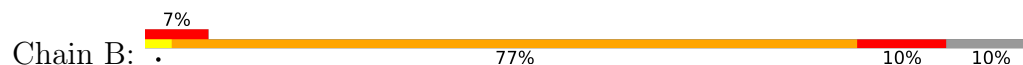


- Molecule 1: INSULIN A CHAIN

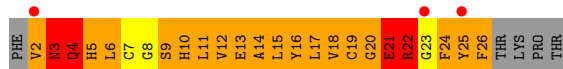
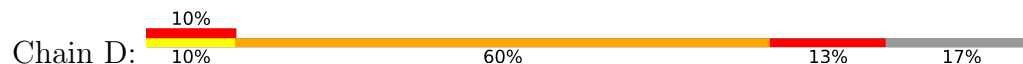




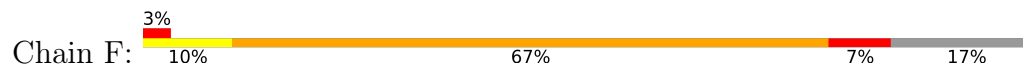
• Molecule 2: INSULIN B CHAIN



• Molecule 2: INSULIN B CHAIN



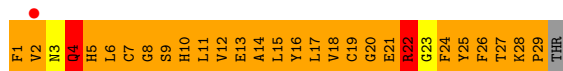
• Molecule 2: INSULIN B CHAIN



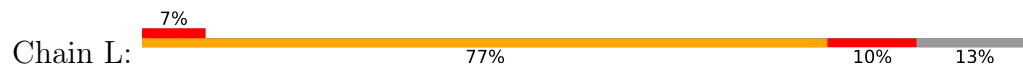
• Molecule 2: INSULIN B CHAIN



• Molecule 2: INSULIN B CHAIN



• Molecule 2: INSULIN B CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.66Å 62.17Å 46.68Å 90.00° 111.32° 90.00°	Depositor
Resolution (Å)	53.68 – 1.97 53.68 – 1.97	Depositor EDS
% Data completeness (in resolution range)	89.9 (53.68-1.97) 49.4 (53.68-1.97)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.193 , 0.252 0.201 , 0.254	Depositor DCC
R_{free} test set	617 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.035 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2440	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CL, MEA, IPH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	10.36	99/160 (61.9%)	6.51	112/215 (52.1%)
1	C	11.90	117/164 (71.3%)	6.55	103/220 (46.8%)
1	E	11.39	98/164 (59.8%)	6.95	117/220 (53.2%)
1	G	10.31	92/160 (57.5%)	6.25	95/215 (44.2%)
1	I	11.60	112/164 (68.3%)	6.61	105/220 (47.7%)
1	K	11.43	117/164 (71.3%)	6.88	100/220 (45.5%)
2	B	11.61	129/211 (61.1%)	7.02	140/283 (49.5%)
2	D	11.50	111/185 (60.0%)	7.06	122/249 (49.0%)
2	F	10.29	100/185 (54.1%)	7.75	141/249 (56.6%)
2	H	11.25	130/212 (61.3%)	6.81	132/285 (46.3%)
2	J	10.96	128/228 (56.1%)	6.78	147/306 (48.0%)
2	L	11.37	142/205 (69.3%)	6.90	141/276 (51.1%)
All	All	11.18	1375/2202 (62.4%)	6.86	1455/2958 (49.2%)

All (1375) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	20	CYS	CA-C	34.67	1.96	1.52
2	D	24	PHE	CA-C	32.68	1.92	1.52
1	C	9	SER	N-CA	31.72	1.86	1.45
2	J	10	HIS	CD2-NE2	31.71	1.72	1.37
2	F	12	VAL	CA-CB	31.36	1.93	1.54
2	L	5	HIS	CE1-NE2	31.13	1.63	1.32
2	D	9	SER	CA-C	31.01	1.93	1.52
2	D	12	VAL	CA-CB	30.78	1.91	1.54
2	B	6	LEU	CA-C	30.43	1.93	1.52
2	J	2	VAL	CA-CB	30.18	1.88	1.54
2	B	12	VAL	CA-CB	29.82	1.87	1.54
2	J	5	HIS	CE1-NE2	29.59	1.62	1.32
2	H	17	LEU	CA-C	29.44	1.89	1.52
2	H	18	VAL	N-CA	28.27	1.82	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	13	GLU	CA-C	28.16	1.90	1.52
2	B	14	ALA	N-CA	28.02	1.80	1.46
1	E	18	ASN	CA-C	27.74	1.90	1.52
2	H	10	HIS	ND1-CE1	27.37	1.59	1.32
1	C	19	TYR	N-CA	27.18	1.82	1.46
1	G	7	CYS	N-CA	27.18	1.80	1.45
2	D	17	LEU	N-CA	27.01	1.80	1.46
2	B	7	CYS	N-CA	26.96	1.80	1.46
1	C	8	THR	CA-C	26.96	1.88	1.52
1	E	8	THR	CA-C	26.76	1.87	1.53
1	C	14	TYR	CA-C	26.75	1.86	1.52
2	L	19	CYS	N-CA	26.72	1.81	1.46
1	K	5	GLN	CA-C	26.66	1.87	1.52
1	C	4	GLU	CA-C	26.61	1.88	1.52
2	J	12	VAL	C-N	26.54	1.67	1.33
1	A	10	ILE	CA-C	26.51	1.81	1.52
1	G	10	ILE	C-O	26.50	1.51	1.24
1	G	14	TYR	CA-C	-26.43	1.18	1.52
2	L	10	HIS	CD2-NE2	26.39	1.66	1.37
1	I	14	TYR	N-CA	26.18	1.78	1.46
2	H	14	ALA	N-CA	26.15	1.78	1.46
2	H	6	LEU	N-CA	-26.14	1.15	1.46
2	L	12	VAL	C-N	26.09	1.66	1.33
2	H	12	VAL	CA-C	-26.05	1.22	1.52
1	I	6	CYS	N-CA	25.93	1.76	1.46
1	I	17	GLU	CA-C	25.87	1.89	1.52
1	I	5	GLN	CA-C	25.82	1.87	1.52
2	B	17	LEU	CA-C	25.79	1.85	1.52
2	J	1	PHE	C-N	25.76	1.65	1.33
1	K	17	GLU	CA-C	25.73	1.89	1.52
1	G	6	CYS	CA-C	25.66	1.86	1.52
2	D	10	HIS	N-CA	25.55	1.79	1.46
2	L	14	ALA	CA-C	25.55	1.85	1.52
1	C	5	GLN	N-CA	25.48	1.77	1.46
1	I	13	LEU	CA-C	25.48	1.87	1.52
1	A	11	CYS	C-N	25.43	1.66	1.33
1	G	9	SER	CA-CB	25.40	1.88	1.53
2	H	11	LEU	N-CA	25.38	1.78	1.46
2	L	2	VAL	CA-CB	25.35	1.84	1.54
2	F	21	GLU	N-CA	25.33	1.78	1.46
2	D	16	TYR	CA-C	25.31	1.85	1.52
1	G	14	TYR	N-CA	25.19	1.77	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	18	VAL	CA-C	25.06	1.87	1.52
1	E	16	LEU	C-O	25.06	1.53	1.24
2	D	3	ASN	N-CA	25.05	1.77	1.46
2	L	15	LEU	N-CA	24.96	1.76	1.46
1	I	10	ILE	CA-C	24.90	1.79	1.52
1	G	11	CYS	CA-C	-24.85	1.21	1.52
2	H	7	CYS	N-CA	24.81	1.76	1.46
2	H	12	VAL	CA-CB	24.79	1.82	1.54
2	B	10	HIS	ND1-CE1	24.74	1.57	1.32
2	D	21	GLU	C-O	24.74	1.54	1.24
1	I	4	GLU	CA-CB	24.74	1.92	1.53
2	H	2	VAL	CA-CB	24.73	1.85	1.54
2	B	10	HIS	CG-ND1	-24.71	1.11	1.38
1	C	3	VAL	CA-CB	24.70	1.82	1.54
2	B	10	HIS	CG-CD2	24.66	1.62	1.35
1	C	15	GLN	N-CA	24.61	1.77	1.46
2	H	16	TYR	CA-CB	24.56	1.91	1.53
2	H	5	HIS	CA-C	-24.37	1.22	1.52
1	I	18	ASN	N-CA	24.36	1.78	1.46
1	I	2	ILE	N-CA	24.34	1.76	1.46
2	F	7	CYS	C-N	24.30	1.66	1.33
2	H	15	LEU	C-N	24.16	1.64	1.33
2	J	10	HIS	CB-CG	24.16	1.83	1.50
2	H	10	HIS	CA-C	24.13	1.83	1.52
2	J	13	GLU	CA-CB	24.07	1.91	1.53
2	B	10	HIS	CA-C	24.05	1.84	1.52
1	C	16	LEU	CA-C	-23.92	1.22	1.52
1	I	15	GLN	CA-C	-23.82	1.22	1.52
2	L	22	ARG	CZ-NH2	23.79	1.64	1.33
2	J	15	LEU	N-CA	23.75	1.76	1.46
2	L	24	PHE	CA-CB	23.67	1.95	1.53
1	K	10	ILE	CA-C	23.62	1.82	1.52
2	B	5	HIS	CA-CB	23.54	1.90	1.53
1	E	9	SER	N-CA	23.48	1.75	1.45
2	F	20	GLY	CA-C	23.47	1.83	1.51
1	E	2	ILE	C-O	23.40	1.51	1.24
2	J	5	HIS	CG-CD2	23.35	1.61	1.35
2	J	21	GLU	CA-C	23.30	1.83	1.52
2	L	1	PHE	C-N	23.28	1.62	1.33
2	D	4	GLN	N-CA	-23.19	1.17	1.46
1	E	19	TYR	N-CA	23.14	1.76	1.46
1	E	12	SER	C-O	23.09	1.53	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	11	CYS	CA-CB	23.04	1.86	1.53
2	F	21	GLU	C-O	22.95	1.52	1.24
1	E	5	GLN	C-O	22.91	1.52	1.24
1	E	10	ILE	CA-C	-22.91	1.26	1.52
2	L	13	GLU	CA-CB	22.79	1.89	1.53
1	E	15	GLN	C-O	22.74	1.52	1.24
2	D	7	CYS	C-N	22.68	1.62	1.33
2	H	4	GLN	C-N	22.66	1.64	1.33
2	B	4	GLN	C-N	22.63	1.61	1.33
1	I	16	LEU	N-CA	-22.62	1.18	1.46
1	I	6	CYS	CA-C	22.61	1.81	1.52
2	B	22	ARG	N-CA	-22.60	1.18	1.46
1	C	17	GLU	N-CA	-22.58	1.18	1.46
1	K	18	ASN	C-O	22.49	1.52	1.24
2	J	10	HIS	ND1-CE1	22.38	1.54	1.32
1	A	7	CYS	N-CA	22.31	1.75	1.46
2	H	6	LEU	CA-C	22.30	1.80	1.52
1	C	18	ASN	CA-C	22.19	1.82	1.52
2	H	13	GLU	CA-C	22.16	1.82	1.52
2	H	13	GLU	N-CA	-22.16	1.19	1.46
2	J	19	CYS	N-CA	22.11	1.75	1.46
2	H	21	GLU	CA-C	-22.09	1.24	1.52
2	D	3	ASN	CA-C	-22.04	1.22	1.52
2	L	5	HIS	C-N	22.04	1.62	1.33
2	J	14	ALA	CA-C	21.97	1.80	1.52
1	E	11	CYS	N-CA	-21.97	1.17	1.46
1	I	3	VAL	C-N	21.90	1.63	1.33
1	A	18	ASN	N-CA	-21.90	1.19	1.46
2	B	18	VAL	C-O	21.88	1.51	1.24
1	G	15	GLN	N-CA	-21.88	1.19	1.46
2	H	8	GLY	C-N	21.85	1.61	1.33
2	L	6	LEU	CA-CB	21.77	1.87	1.53
2	B	21	GLU	CA-C	-21.75	1.24	1.52
2	J	8	GLY	C-N	21.65	1.60	1.33
2	B	18	VAL	N-CA	21.53	1.73	1.46
1	G	18	ASN	C-N	21.51	1.64	1.33
1	K	14	TYR	C-O	21.50	1.50	1.24
1	E	2	ILE	N-CA	21.49	1.74	1.46
1	I	20	CYS	CA-C	21.40	1.81	1.52
2	J	10	HIS	CG-ND1	21.37	1.61	1.38
1	A	12	SER	CA-CB	21.33	1.86	1.53
1	A	16	LEU	C-N	21.19	1.60	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	4	GLU	N-CA	-21.12	1.20	1.46
2	J	11	LEU	N-CA	21.05	1.71	1.46
2	H	9	SER	CA-CB	21.02	1.86	1.53
2	J	22	ARG	C-N	21.01	1.64	1.33
2	F	8	GLY	C-O	-21.01	0.98	1.23
2	L	22	ARG	CD-NE	20.92	1.75	1.46
1	A	6	CYS	CA-C	20.87	1.79	1.52
2	B	2	VAL	N-CA	-20.87	1.22	1.46
1	K	2	ILE	CA-C	20.82	1.81	1.52
1	E	4	GLU	CA-C	20.82	1.80	1.52
2	L	5	HIS	N-CA	-20.82	1.21	1.46
1	E	10	ILE	CA-CB	20.81	1.80	1.54
2	J	10	HIS	CA-C	20.79	1.80	1.52
1	K	2	ILE	N-CA	20.76	1.72	1.46
1	E	14	TYR	C-N	-20.76	1.06	1.34
2	L	5	HIS	CG-ND1	20.72	1.61	1.38
2	H	5	HIS	CA-CB	20.71	1.86	1.53
2	F	11	LEU	C-N	20.64	1.59	1.33
2	L	11	LEU	C-N	-20.57	1.09	1.33
2	D	5	HIS	CA-C	20.56	1.80	1.52
2	D	2	VAL	CA-C	20.55	1.96	1.52
2	F	18	VAL	C-N	20.53	1.64	1.33
1	A	11	CYS	N-CA	20.51	1.73	1.46
2	D	19	CYS	CA-CB	20.47	1.87	1.53
2	J	3	ASN	C-N	20.46	1.60	1.33
2	F	15	LEU	C-O	-20.45	1.00	1.24
2	B	3	ASN	N-CA	20.43	1.71	1.46
2	H	3	ASN	CA-C	20.40	1.78	1.52
1	C	3	VAL	N-CA	-20.34	1.22	1.46
2	B	2	VAL	CA-CB	20.34	1.79	1.54
2	B	15	LEU	C-O	20.27	1.50	1.24
2	F	3	ASN	CA-C	-20.25	1.26	1.52
2	F	10	HIS	ND1-CE1	-20.20	1.12	1.32
2	D	11	LEU	C-N	20.18	1.59	1.34
1	E	5	GLN	CA-C	20.18	1.79	1.52
2	D	7	CYS	CA-C	-20.07	1.26	1.52
2	B	5	HIS	CA-C	-20.05	1.28	1.52
2	J	10	HIS	C-N	19.98	1.60	1.33
1	K	13	LEU	C-N	-19.97	1.07	1.34
2	D	15	LEU	N-CA	-19.94	1.22	1.46
1	C	16	LEU	C-O	19.93	1.47	1.24
2	D	14	ALA	CA-C	-19.87	1.26	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	10	HIS	N-CA	19.81	1.72	1.46
1	I	7	CYS	N-CA	19.80	1.72	1.46
1	K	21	ASN	N-CA	19.78	1.83	1.46
2	F	16	TYR	C-O	-19.74	1.00	1.24
1	A	5	GLN	CA-C	-19.72	1.27	1.52
1	K	13	LEU	CA-C	19.71	1.77	1.52
1	I	16	LEU	CA-CB	19.71	1.85	1.53
2	H	10	HIS	CE1-NE2	-19.70	1.12	1.32
1	E	4	GLU	C-N	-19.70	1.06	1.34
2	J	19	CYS	C-N	19.66	1.58	1.33
2	H	24	PHE	C-O	19.64	1.48	1.24
1	K	16	LEU	N-CA	-19.63	1.22	1.46
2	L	4	GLN	N-CA	19.61	1.70	1.46
1	I	6	CYS	C-O	19.59	1.52	1.24
1	E	17	GLU	N-CA	-19.59	1.22	1.46
2	B	11	LEU	CA-CB	-19.54	1.20	1.53
1	A	3	VAL	N-CA	19.52	1.70	1.46
2	B	10	HIS	C-N	-19.48	1.07	1.34
2	L	16	TYR	C-N	19.46	1.58	1.33
2	D	14	ALA	C-N	19.46	1.59	1.33
1	E	7	CYS	N-CA	-19.44	1.20	1.46
2	B	6	LEU	CB-CG	19.40	1.92	1.53
2	F	14	ALA	C-N	19.37	1.59	1.33
1	E	16	LEU	N-CA	19.36	1.69	1.46
1	K	16	LEU	CA-C	19.35	1.78	1.52
2	L	20	GLY	CA-C	19.28	1.79	1.51
1	K	6	CYS	N-CA	19.19	1.71	1.46
2	J	22	ARG	N-CA	19.19	1.70	1.46
2	D	15	LEU	CA-CB	19.09	1.83	1.53
2	J	25	TYR	CA-CB	19.08	1.91	1.53
2	F	24	PHE	CA-C	19.07	1.75	1.52
1	C	11	CYS	N-CA	-19.04	1.21	1.46
2	L	19	CYS	C-O	19.00	1.49	1.24
1	C	7	CYS	C-O	-18.96	1.00	1.23
1	C	2	ILE	C-N	18.96	1.56	1.33
2	F	24	PHE	C-O	18.93	1.46	1.23
1	C	7	CYS	CA-CB	18.92	1.80	1.54
2	D	6	LEU	N-CA	18.91	1.70	1.46
2	D	18	VAL	C-N	18.88	1.62	1.33
1	A	6	CYS	N-CA	-18.83	1.20	1.45
2	J	2	VAL	C-N	-18.79	1.08	1.33
2	D	10	HIS	CE1-NE2	18.78	1.51	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	3	VAL	N-CA	18.78	1.69	1.46
1	K	18	ASN	N-CA	18.76	1.69	1.46
2	L	22	ARG	C-O	18.75	1.48	1.24
1	C	17	GLU	CA-CB	18.75	1.82	1.53
1	C	12	SER	C-O	18.71	1.53	1.23
1	E	1	GLY	CA-C	18.69	1.85	1.52
1	I	12	SER	CB-OG	18.67	1.79	1.42
1	K	15	GLN	C-O	18.65	1.46	1.24
2	D	12	VAL	C-O	-18.64	1.02	1.24
1	A	19	TYR	CA-CB	18.63	1.84	1.53
1	K	1	GLY	CA-C	18.60	1.85	1.52
2	H	10	HIS	CG-ND1	-18.59	1.17	1.38
1	A	17	GLU	CA-C	-18.59	1.28	1.52
2	L	10	HIS	CB-CG	18.58	1.76	1.50
2	D	13	GLU	CA-C	18.57	1.76	1.52
1	G	10	ILE	CA-CB	-18.57	1.30	1.54
1	C	2	ILE	N-CA	18.53	1.70	1.46
2	F	22	ARG	C-O	18.49	1.47	1.24
2	J	11	LEU	C-N	-18.49	1.09	1.33
2	B	22	ARG	CA-C	18.48	1.77	1.52
2	J	5	HIS	CD2-NE2	-18.47	1.17	1.37
1	K	10	ILE	CA-CB	18.45	1.79	1.54
1	K	7	CYS	C-N	-18.40	1.08	1.33
2	D	16	TYR	C-O	-18.40	1.02	1.24
2	L	3	ASN	C-N	18.39	1.58	1.33
1	G	10	ILE	CA-C	18.38	1.74	1.52
2	J	4	GLN	CA-CB	18.34	1.82	1.53
2	J	3	ASN	CA-CB	-18.32	1.24	1.53
2	L	4	GLN	CA-C	-18.28	1.29	1.52
1	I	10	ILE	CA-CB	18.26	1.75	1.54
2	D	20	GLY	C-O	18.26	1.48	1.24
2	F	20	GLY	C-N	-18.24	1.09	1.34
2	H	18	VAL	C-O	18.21	1.46	1.24
1	A	3	VAL	C-N	-18.18	1.09	1.33
1	E	15	GLN	CA-C	18.17	1.77	1.52
1	K	8	THR	C-O	18.17	1.48	1.23
2	F	4	GLN	N-CA	-18.13	1.23	1.46
1	C	5	GLN	CA-CB	-18.13	1.24	1.53
1	A	8	THR	CA-CB	-18.12	1.25	1.53
2	B	11	LEU	N-CA	18.08	1.69	1.46
2	D	14	ALA	N-CA	18.08	1.69	1.46
2	F	3	ASN	N-CA	18.01	1.68	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	GLN	N-CA	17.99	1.68	1.46
1	G	11	CYS	C-N	17.96	1.58	1.33
2	F	12	VAL	C-O	-17.95	1.03	1.24
2	J	28	LYS	CA-CB	17.94	1.84	1.52
1	C	20	CYS	CA-CB	17.88	1.82	1.53
2	L	10	HIS	ND1-CE1	17.87	1.50	1.32
1	I	18	ASN	C-O	17.85	1.47	1.24
1	E	19	TYR	C-O	17.84	1.48	1.23
2	H	10	HIS	CB-CG	17.84	1.75	1.50
2	B	2	VAL	CA-C	17.83	1.75	1.52
1	C	19	TYR	C-O	17.83	1.48	1.24
1	I	14	TYR	CA-CB	-17.79	1.25	1.53
1	C	11	CYS	CA-C	17.79	1.74	1.52
2	L	2	VAL	C-N	-17.74	1.07	1.33
1	I	4	GLU	N-CA	-17.71	1.25	1.46
2	D	11	LEU	CA-C	-17.71	1.30	1.52
1	I	3	VAL	N-CA	17.69	1.69	1.46
1	K	11	CYS	N-CA	17.69	1.69	1.46
2	J	18	VAL	CA-C	17.64	1.77	1.52
2	B	4	GLN	CA-CB	-17.63	1.23	1.53
2	J	19	CYS	C-O	17.61	1.47	1.24
1	A	2	ILE	C-N	17.53	1.57	1.33
2	H	22	ARG	C-O	-17.53	1.02	1.24
1	E	2	ILE	CB-CG1	17.51	1.88	1.53
2	B	3	ASN	CA-C	17.49	1.78	1.52
1	C	12	SER	N-CA	17.48	1.70	1.45
1	G	12	SER	CA-CB	17.47	1.82	1.53
2	J	22	ARG	CA-CB	-17.44	1.24	1.53
1	K	3	VAL	CA-C	-17.44	1.30	1.52
1	K	15	GLN	CA-C	-17.44	1.30	1.52
2	L	22	ARG	CA-CB	-17.42	1.24	1.53
2	D	25	TYR	N-CA	17.41	1.79	1.46
2	F	21	GLU	CA-CB	-17.37	1.24	1.53
2	H	2	VAL	N-CA	-17.37	1.25	1.46
1	E	13	LEU	C-O	17.36	1.45	1.24
1	A	17	GLU	CA-CB	17.33	1.80	1.53
2	L	17	LEU	CA-CB	17.32	1.80	1.53
2	B	13	GLU	N-CA	-17.31	1.25	1.46
2	J	2	VAL	N-CA	17.31	1.66	1.46
1	I	8	THR	C-O	17.28	1.47	1.23
1	I	20	CYS	C-N	-17.28	1.09	1.33
2	F	4	GLN	C-O	-17.27	1.03	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2	ILE	CA-C	-17.24	1.27	1.52
1	A	9	SER	C-N	-17.23	1.13	1.33
2	F	19	CYS	C-O	-17.23	1.01	1.24
2	H	15	LEU	CA-CB	-17.16	1.25	1.53
1	G	12	SER	N-CA	-17.15	1.23	1.45
1	C	15	GLN	CA-CB	-17.13	1.25	1.53
2	B	10	HIS	N-CA	17.11	1.66	1.46
2	J	6	LEU	N-CA	17.10	1.67	1.46
2	F	15	LEU	CA-CB	17.06	1.80	1.53
1	G	13	LEU	C-N	17.04	1.57	1.33
1	E	6	CYS	CA-C	-17.04	1.29	1.52
1	E	18	ASN	N-CA	17.00	1.68	1.46
1	I	21	ASN	CA-CB	-17.00	1.19	1.53
2	B	4	GLN	N-CA	16.99	1.68	1.46
1	I	3	VAL	CA-C	-16.96	1.29	1.53
1	E	9	SER	C-O	16.95	1.46	1.23
2	J	9	SER	C-N	-16.94	1.10	1.34
1	K	3	VAL	C-O	16.92	1.44	1.24
1	E	5	GLN	CA-CB	-16.91	1.25	1.53
2	B	6	LEU	N-CA	-16.87	1.26	1.46
2	J	9	SER	CA-CB	16.84	1.79	1.53
2	L	13	GLU	C-N	-16.83	1.11	1.33
2	B	17	LEU	C-N	-16.83	1.13	1.34
1	K	4	GLU	CA-CB	16.79	1.79	1.53
1	G	5	GLN	C-N	16.74	1.56	1.33
1	E	7	CYS	C-O	-16.73	1.01	1.24
2	L	3	ASN	CA-C	16.72	1.75	1.52
1	I	7	CYS	C-O	16.71	1.47	1.23
2	B	22	ARG	C-O	-16.65	1.04	1.24
2	D	8	GLY	C-O	-16.62	1.04	1.23
2	B	11	LEU	C-O	16.55	1.45	1.24
1	C	2	ILE	CB-CG1	16.55	1.86	1.53
1	C	14	TYR	CA-CB	16.49	1.78	1.53
2	J	13	GLU	C-N	-16.47	1.12	1.33
1	C	6	CYS	CA-C	-16.47	1.31	1.52
1	E	14	TYR	CA-C	16.46	1.74	1.52
2	B	16	TYR	CA-CB	16.45	1.81	1.53
2	H	11	LEU	C-N	16.42	1.53	1.33
1	K	14	TYR	N-CA	16.42	1.66	1.46
1	E	8	THR	C-N	-16.39	1.10	1.33
1	G	8	THR	CB-OG1	16.39	1.70	1.43
1	A	18	ASN	C-N	16.38	1.59	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	GLN	CA-C	16.36	1.75	1.52
1	E	6	CYS	N-CA	16.35	1.69	1.45
2	L	11	LEU	N-CA	16.35	1.66	1.46
2	F	10	HIS	CG-CD2	-16.30	1.18	1.35
2	L	5	HIS	ND1-CE1	-16.30	1.16	1.32
1	G	11	CYS	C-O	16.29	1.42	1.23
2	D	22	ARG	NE-CZ	-16.28	1.15	1.33
2	H	23	GLY	C-O	16.27	1.53	1.23
2	D	8	GLY	N-CA	-16.27	1.26	1.45
1	K	12	SER	CB-OG	16.25	1.74	1.42
2	J	22	ARG	CZ-NH1	16.25	1.55	1.32
2	L	10	HIS	CG-ND1	16.23	1.56	1.38
2	F	9	SER	CA-C	16.22	1.74	1.52
2	H	6	LEU	CB-CG	16.18	1.85	1.53
1	K	7	CYS	N-CA	16.18	1.67	1.46
1	A	6	CYS	C-O	-16.17	1.02	1.24
2	D	18	VAL	CA-C	-16.11	1.31	1.52
1	E	5	GLN	N-CA	16.11	1.67	1.46
2	B	23	GLY	N-CA	16.09	1.72	1.45
2	J	5	HIS	N-CA	-16.06	1.26	1.46
2	J	22	ARG	NE-CZ	16.06	1.50	1.33
2	H	24	PHE	CB-CG	16.05	1.87	1.50
1	C	7	CYS	N-CA	-16.04	1.25	1.45
2	B	22	ARG	CZ-NH2	-16.04	1.12	1.33
1	C	6	CYS	N-CA	16.04	1.67	1.46
1	I	15	GLN	CD-OE1	15.98	1.53	1.23
2	F	11	LEU	C-O	-15.98	1.05	1.24
1	A	5	GLN	CA-CB	15.95	1.78	1.53
2	D	20	GLY	C-N	-15.95	1.12	1.34
1	G	10	ILE	N-CA	-15.95	1.28	1.46
1	K	14	TYR	CA-CB	-15.95	1.27	1.53
2	D	11	LEU	N-CA	-15.90	1.27	1.46
1	G	3	VAL	N-CA	15.86	1.65	1.46
1	C	13	LEU	CA-CB	15.84	1.78	1.53
2	D	22	ARG	CA-C	15.82	1.74	1.52
2	H	4	GLN	N-CA	15.82	1.66	1.46
2	H	25	TYR	CG-CD2	15.81	1.72	1.39
1	E	6	CYS	C-O	15.80	1.44	1.24
1	I	13	LEU	CB-CG	15.80	1.85	1.53
2	F	4	GLN	CD-OE1	15.73	1.53	1.23
2	J	4	GLN	CA-C	-15.71	1.31	1.52
1	I	14	TYR	CB-CG	15.70	1.86	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	12	SER	CA-CB	-15.67	1.30	1.53
1	C	16	LEU	CB-CG	-15.65	1.22	1.53
1	C	18	ASN	N-CA	15.64	1.66	1.46
2	B	7	CYS	CB-SG	15.64	2.32	1.81
2	J	29	PRO	CA-CB	-15.56	1.22	1.53
1	K	5	GLN	C-N	-15.56	1.12	1.33
2	H	22	ARG	N-CA	-15.55	1.26	1.46
2	D	10	HIS	ND1-CE1	-15.55	1.17	1.32
2	D	12	VAL	N-CA	-15.53	1.28	1.46
1	I	14	TYR	CZ-OH	15.49	1.70	1.38
1	G	11	CYS	N-CA	15.48	1.64	1.45
1	K	6	CYS	CA-C	15.47	1.72	1.52
1	A	13	LEU	CA-CB	-15.46	1.29	1.53
2	H	14	ALA	CA-C	15.42	1.72	1.52
2	B	12	VAL	CA-C	-15.42	1.34	1.52
1	K	10	ILE	C-O	-15.38	1.05	1.24
2	L	7	CYS	CA-C	15.36	1.73	1.52
1	I	2	ILE	CB-CG1	15.36	1.84	1.53
2	L	14	ALA	C-N	15.36	1.54	1.33
2	H	24	PHE	C-N	-15.32	1.11	1.33
1	E	2	ILE	CA-C	-15.31	1.32	1.53
1	K	17	GLU	CG-CD	15.22	1.90	1.52
2	D	10	HIS	CG-ND1	15.21	1.54	1.38
1	G	2	ILE	CB-CG1	-15.20	1.23	1.53
2	L	5	HIS	CB-CG	-15.14	1.28	1.50
1	E	19	TYR	CA-CB	-15.12	1.27	1.53
2	B	17	LEU	CB-CG	-15.09	1.23	1.53
1	C	10	ILE	CA-C	-15.08	1.33	1.52
1	K	20	CYS	CB-SG	15.05	2.31	1.81
2	B	11	LEU	C-N	15.04	1.52	1.33
1	G	13	LEU	CA-CB	-15.03	1.28	1.53
1	G	15	GLN	C-N	15.02	1.53	1.34
1	A	10	ILE	CA-CB	-14.99	1.36	1.54
1	I	11	CYS	N-CA	14.93	1.65	1.46
2	L	8	GLY	N-CA	14.86	1.67	1.45
1	K	9	SER	C-O	14.85	1.41	1.24
1	I	1	GLY	CA-C	14.83	1.78	1.52
1	K	15	GLN	CD-OE1	14.83	1.51	1.23
1	K	17	GLU	N-CA	14.81	1.65	1.46
2	F	9	SER	C-O	-14.78	1.06	1.24
2	F	10	HIS	CG-ND1	14.74	1.54	1.38
1	I	19	TYR	C-O	-14.74	1.04	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	15	GLN	C-O	14.73	1.41	1.24
2	B	9	SER	CA-CB	14.71	1.76	1.53
1	A	19	TYR	N-CA	14.71	1.67	1.46
1	C	8	THR	C-O	-14.69	1.06	1.24
2	F	9	SER	C-N	14.67	1.55	1.33
1	G	12	SER	C-O	-14.66	1.04	1.23
1	G	12	SER	C-N	-14.66	1.14	1.34
1	K	8	THR	CB-OG1	14.63	1.67	1.43
2	B	14	ALA	C-O	14.63	1.41	1.24
2	H	22	ARG	CA-CB	14.62	1.77	1.53
1	K	12	SER	C-O	14.62	1.43	1.23
2	J	1	PHE	CA-CB	14.61	1.82	1.53
1	I	13	LEU	C-N	-14.60	1.15	1.33
2	B	12	VAL	C-O	14.59	1.40	1.24
1	A	4	GLU	C-N	14.55	1.53	1.33
2	B	24	PHE	C-N	-14.55	1.12	1.33
1	A	8	THR	C-N	14.53	1.53	1.33
1	K	6	CYS	C-O	14.52	1.44	1.24
2	D	10	HIS	CA-C	-14.51	1.32	1.52
1	G	16	LEU	N-CA	14.51	1.64	1.46
2	J	3	ASN	CA-C	14.50	1.71	1.52
1	I	2	ILE	CA-C	14.47	1.72	1.52
1	A	17	GLU	N-CA	14.45	1.63	1.46
2	H	11	LEU	CA-CB	-14.44	1.29	1.53
2	B	3	ASN	C-N	-14.38	1.12	1.33
2	B	22	ARG	CD-NE	-14.27	1.26	1.46
2	L	3	ASN	CB-CG	14.26	1.87	1.52
1	A	3	VAL	CA-CB	14.23	1.73	1.54
1	E	17	GLU	CA-C	14.23	1.72	1.52
1	A	10	ILE	C-O	14.22	1.40	1.24
1	G	14	TYR	CA-CB	14.22	1.75	1.53
2	L	10	HIS	CA-C	14.19	1.72	1.52
1	G	14	TYR	CB-CG	-14.16	1.20	1.51
2	B	21	GLU	CA-CB	14.13	1.75	1.53
2	B	8	GLY	CA-C	-14.11	1.33	1.51
1	E	3	VAL	N-CA	-14.11	1.28	1.46
2	J	22	ARG	C-O	14.11	1.41	1.24
2	H	14	ALA	C-N	-14.08	1.13	1.33
1	G	20	CYS	CA-CB	-14.07	1.31	1.53
2	D	22	ARG	C-O	14.06	1.41	1.24
2	B	24	PHE	CA-C	14.02	1.69	1.52
2	D	25	TYR	CA-C	-14.01	1.23	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	18	ASN	CA-C	-14.01	1.33	1.52
2	L	10	HIS	C-N	14.00	1.52	1.33
1	K	16	LEU	CB-CG	13.99	1.81	1.53
1	G	13	LEU	CA-C	13.97	1.71	1.52
1	G	15	GLN	CD-OE1	13.94	1.50	1.23
1	A	4	GLU	CA-CB	-13.92	1.31	1.53
2	L	14	ALA	N-CA	-13.90	1.29	1.46
1	C	14	TYR	C-N	-13.89	1.15	1.34
2	F	2	VAL	C-N	13.89	1.52	1.33
2	D	23	GLY	C-N	13.89	1.50	1.33
1	C	16	LEU	C-N	13.88	1.51	1.33
2	B	15	LEU	CG-CD2	13.85	1.98	1.52
2	F	14	ALA	N-CA	13.82	1.63	1.46
1	A	14	TYR	CG-CD2	13.82	1.68	1.39
2	D	19	CYS	C-O	-13.79	1.05	1.24
1	E	19	TYR	CG-CD1	13.79	1.68	1.39
2	H	1	PHE	CA-CB	13.78	1.81	1.53
2	B	23	GLY	C-N	13.78	1.50	1.33
1	E	9	SER	CB-OG	-13.78	1.14	1.42
2	F	16	TYR	C-N	13.77	1.53	1.33
2	F	25	TYR	CA-C	-13.77	1.24	1.52
2	F	13	GLU	C-O	-13.76	1.07	1.24
2	J	11	LEU	CB-CG	-13.76	1.25	1.53
2	L	21	GLU	N-CA	13.73	1.65	1.46
1	I	19	TYR	N-CA	-13.73	1.27	1.46
2	F	6	LEU	N-CA	13.72	1.63	1.46
1	E	7	CYS	CA-CB	13.71	1.78	1.53
2	H	4	GLN	CA-CB	-13.70	1.30	1.53
2	F	5	HIS	C-O	-13.67	1.07	1.24
1	I	10	ILE	CB-CG1	13.66	1.80	1.53
2	H	22	ARG	CZ-NH1	-13.62	1.13	1.32
2	D	21	GLU	CA-C	13.61	1.71	1.52
2	F	22	ARG	NE-CZ	13.61	1.48	1.33
1	C	1	GLY	CA-C	13.61	1.76	1.52
1	G	15	GLN	C-O	-13.60	1.07	1.24
2	J	22	ARG	CZ-NH2	-13.59	1.15	1.33
1	C	19	TYR	CG-CD2	13.58	1.67	1.39
1	E	14	TYR	C-O	13.57	1.39	1.24
2	J	11	LEU	CA-CB	13.56	1.74	1.53
2	J	12	VAL	CA-C	13.56	1.71	1.52
1	A	10	ILE	CB-CG1	13.53	1.80	1.53
2	D	22	ARG	CB-CG	13.52	1.93	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	15	LEU	C-N	-13.51	1.16	1.33
2	B	13	GLU	CB-CG	13.51	1.93	1.52
2	F	16	TYR	CA-C	13.49	1.70	1.52
2	J	12	VAL	CA-CB	-13.48	1.35	1.54
1	K	17	GLU	C-O	13.46	1.41	1.24
2	D	13	GLU	CD-OE1	13.45	1.50	1.25
1	G	6	CYS	CB-SG	13.45	2.25	1.81
2	H	25	TYR	CE1-CZ	13.44	1.70	1.38
1	K	10	ILE	CB-CG1	13.43	1.80	1.53
1	G	19	TYR	CA-CB	13.38	1.76	1.53
2	J	22	ARG	CD-NE	-13.36	1.27	1.46
2	L	22	ARG	NE-CZ	-13.35	1.18	1.33
2	J	5	HIS	CA-C	13.34	1.70	1.52
2	B	15	LEU	C-N	13.31	1.52	1.33
2	J	5	HIS	CB-CG	-13.30	1.31	1.50
1	K	7	CYS	C-O	13.29	1.41	1.24
1	G	19	TYR	CG-CD2	-13.27	1.11	1.39
1	E	16	LEU	CB-CG	-13.26	1.26	1.53
1	A	15	GLN	CA-C	13.20	1.69	1.52
2	B	15	LEU	CA-CB	-13.19	1.31	1.53
1	A	19	TYR	C-O	13.18	1.43	1.24
2	B	9	SER	N-CA	-13.17	1.30	1.46
1	A	21	ASN	CA-CB	13.15	1.79	1.53
1	I	14	TYR	C-O	13.15	1.39	1.24
2	B	18	VAL	CA-CB	-13.12	1.35	1.54
2	B	23	GLY	CA-C	-13.05	1.34	1.52
2	L	1	PHE	CB-CG	13.02	1.80	1.50
1	G	6	CYS	C-N	-12.99	1.15	1.33
2	J	29	PRO	C-O	12.98	1.49	1.23
2	J	16	TYR	N-CA	-12.97	1.30	1.46
1	C	6	CYS	C-N	12.94	1.52	1.33
2	J	28	LYS	C-N	-12.94	1.13	1.34
2	J	25	TYR	C-O	-12.92	0.97	1.23
2	D	6	LEU	CA-CB	-12.90	1.32	1.53
2	F	19	CYS	CA-CB	12.89	1.73	1.53
2	L	23	GLY	C-O	-12.89	1.04	1.23
2	D	12	VAL	CA-C	12.88	1.69	1.52
2	L	21	GLU	C-O	12.88	1.43	1.24
1	A	14	TYR	CE1-CZ	12.85	1.69	1.38
1	E	16	LEU	CA-C	-12.83	1.36	1.52
2	J	4	GLN	N-CA	12.83	1.62	1.46
2	L	21	GLU	C-N	-12.83	1.13	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	GLU	CD-OE1	-12.78	1.01	1.25
1	A	4	GLU	CA-C	12.78	1.69	1.52
1	G	19	TYR	C-O	12.76	1.41	1.24
2	J	12	VAL	N-CA	-12.74	1.30	1.46
2	D	15	LEU	C-O	-12.71	1.09	1.24
2	F	17	LEU	C-O	-12.71	1.08	1.24
2	J	13	GLU	N-CA	12.70	1.61	1.46
1	G	14	TYR	CZ-OH	-12.70	1.11	1.38
2	H	27	THR	N-CA	-12.70	1.22	1.46
2	F	17	LEU	N-CA	12.67	1.62	1.46
1	A	14	TYR	CA-CB	12.66	1.73	1.53
2	D	5	HIS	CA-CB	12.63	1.73	1.53
1	E	20	CYS	CA-CB	12.63	1.74	1.53
1	C	13	LEU	N-CA	-12.62	1.30	1.46
2	D	23	GLY	N-CA	12.61	1.63	1.45
1	G	8	THR	CA-CB	-12.61	1.34	1.54
2	L	18	VAL	CA-CB	-12.61	1.37	1.54
1	I	21	ASN	N-CA	12.59	1.70	1.46
2	L	24	PHE	C-N	-12.59	1.15	1.33
2	D	10	HIS	CB-CG	-12.58	1.32	1.50
1	C	19	TYR	CA-CB	-12.57	1.33	1.53
2	L	4	GLN	CA-CB	12.56	1.72	1.53
1	E	3	VAL	CA-CB	12.53	1.72	1.54
2	F	17	LEU	CB-CG	12.50	1.78	1.53
1	I	4	GLU	CA-C	-12.50	1.37	1.52
2	F	22	ARG	CG-CD	12.48	1.89	1.52
2	F	5	HIS	CA-C	12.46	1.69	1.52
2	H	13	GLU	CB-CG	12.45	1.89	1.52
1	A	18	ASN	CA-C	12.43	1.69	1.52
1	A	2	ILE	CB-CG1	-12.43	1.28	1.53
2	D	3	ASN	CG-ND2	12.40	1.59	1.33
1	C	17	GLU	CD-OE2	12.39	1.48	1.25
1	A	21	ASN	CB-CG	12.38	1.83	1.52
1	E	21	ASN	CA-CB	12.37	1.78	1.53
2	J	25	TYR	CG-CD2	-12.36	1.13	1.39
2	H	16	TYR	CA-C	-12.36	1.36	1.52
1	K	9	SER	C-N	12.35	1.50	1.33
2	H	3	ASN	C-O	-12.35	1.09	1.24
1	I	15	GLN	C-N	12.33	1.50	1.34
2	L	4	GLN	C-N	-12.33	1.17	1.33
2	D	22	ARG	C-N	-12.30	1.13	1.33
2	F	10	HIS	CA-C	-12.30	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	19	CYS	CA-CB	-12.29	1.32	1.53
2	F	22	ARG	CA-CB	12.21	1.74	1.53
2	H	7	CYS	CB-SG	12.21	2.21	1.81
1	K	4	GLU	CD-OE2	12.21	1.48	1.25
1	A	19	TYR	CG-CD1	-12.20	1.13	1.39
2	D	5	HIS	C-O	-12.18	1.09	1.24
2	B	14	ALA	C-N	-12.17	1.16	1.33
2	J	16	TYR	CG-CD2	12.16	1.64	1.39
1	I	14	TYR	CD1-CE1	12.16	1.75	1.38
2	B	7	CYS	C-O	12.15	1.39	1.24
1	A	13	LEU	C-N	12.15	1.49	1.33
1	I	14	TYR	CD2-CE2	12.14	1.75	1.38
2	L	24	PHE	C-O	-12.14	1.09	1.23
1	G	21	ASN	CG-ND2	12.14	1.58	1.33
2	H	24	PHE	CD1-CE1	12.14	1.75	1.38
2	L	15	LEU	CA-CB	12.12	1.72	1.53
2	F	10	HIS	CB-CG	-12.11	1.33	1.50
1	C	4	GLU	C-N	-12.11	1.17	1.33
1	C	16	LEU	N-CA	12.10	1.61	1.46
2	F	10	HIS	CA-CB	12.10	1.73	1.53
1	G	5	GLN	CD-OE1	12.04	1.46	1.23
1	K	8	THR	N-CA	11.97	1.61	1.46
1	A	15	GLN	C-O	-11.97	1.10	1.24
2	B	25	TYR	CG-CD2	11.95	1.64	1.39
1	C	19	TYR	C-N	11.94	1.49	1.33
2	B	25	TYR	N-CA	11.94	1.69	1.46
1	C	6	CYS	C-O	11.94	1.40	1.24
1	E	14	TYR	CA-CB	11.93	1.72	1.53
1	C	15	GLN	C-O	11.92	1.39	1.24
1	I	3	VAL	C-O	11.91	1.38	1.24
2	B	24	PHE	CG-CD1	-11.90	1.13	1.38
2	H	1	PHE	CA-C	-11.90	1.27	1.52
2	B	1	PHE	CA-C	-11.88	1.27	1.52
2	J	29	PRO	N-CA	11.88	1.64	1.47
1	C	11	CYS	CA-CB	11.88	1.70	1.53
1	E	15	GLN	CA-CB	-11.86	1.33	1.53
1	I	19	TYR	CG-CD1	11.86	1.64	1.39
2	L	1	PHE	CG-CD2	11.86	1.63	1.38
1	I	9	SER	CB-OG	11.82	1.65	1.42
1	I	20	CYS	CB-SG	11.82	2.20	1.81
1	C	5	GLN	CA-C	11.80	1.68	1.52
1	K	21	ASN	C-O	-11.81	0.99	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	15	LEU	N-CA	11.80	1.61	1.46
2	J	15	LEU	CA-C	-11.80	1.36	1.52
2	L	5	HIS	CA-C	11.80	1.67	1.52
2	B	24	PHE	CG-CD2	11.77	1.63	1.38
1	A	2	ILE	N-CA	-11.76	1.24	1.46
2	H	1	PHE	C-N	11.76	1.48	1.33
1	I	19	TYR	CA-C	-11.75	1.36	1.52
1	I	3	VAL	CA-CB	-11.72	1.37	1.54
1	C	4	GLU	CA-CB	11.72	1.71	1.53
1	G	19	TYR	CE1-CZ	-11.70	1.10	1.38
2	L	23	GLY	CA-C	-11.70	1.33	1.52
2	L	24	PHE	N-CA	-11.69	1.31	1.45
2	D	20	GLY	CA-C	11.69	1.67	1.51
1	E	19	TYR	CE2-CZ	11.68	1.66	1.38
2	B	11	LEU	CG-CD2	11.65	1.91	1.52
1	C	14	TYR	CG-CD1	-11.65	1.14	1.39
1	G	10	ILE	CB-CG1	11.64	1.76	1.53
2	J	24	PHE	CB-CG	11.64	1.77	1.50
2	H	10	HIS	C-N	-11.62	1.18	1.34
1	K	13	LEU	CB-CG	-11.61	1.30	1.53
2	B	21	GLU	CD-OE2	-11.60	1.03	1.25
2	H	17	LEU	CG-CD1	11.59	1.90	1.52
2	H	21	GLU	C-N	11.56	1.49	1.34
2	H	15	LEU	CG-CD2	11.55	1.90	1.52
2	H	3	ASN	C-N	-11.52	1.18	1.34
2	L	6	LEU	N-CA	11.52	1.60	1.46
1	I	18	ASN	C-N	11.49	1.50	1.33
1	G	15	GLN	CA-C	11.47	1.67	1.52
2	J	24	PHE	C-O	-11.45	1.10	1.23
2	B	24	PHE	CB-CG	11.44	1.76	1.50
1	E	4	GLU	CD-OE1	-11.43	1.03	1.25
1	C	10	ILE	CA-CB	11.40	1.69	1.54
1	C	21	ASN	C-O	11.39	1.46	1.23
1	K	2	ILE	CB-CG1	11.37	1.76	1.53
1	G	11	CYS	CB-SG	-11.36	1.43	1.81
1	C	8	THR	CB-OG1	-11.36	1.25	1.43
1	C	14	TYR	CE2-CZ	-11.36	1.10	1.38
1	C	7	CYS	CA-C	-11.35	1.38	1.52
1	I	5	GLN	CD-OE1	-11.35	1.01	1.23
1	G	2	ILE	CB-CG2	11.34	1.90	1.52
1	K	5	GLN	CA-CB	11.33	1.71	1.53
1	C	21	ASN	N-CA	-11.33	1.24	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	13	LEU	CG-CD2	11.32	1.89	1.52
2	D	21	GLU	CG-CD	11.31	1.80	1.52
1	E	6	CYS	CA-CB	-11.29	1.38	1.54
1	E	21	ASN	C-OXT	11.27	1.46	1.23
1	E	15	GLN	N-CA	11.27	1.60	1.46
1	C	4	GLU	CD-OE2	-11.21	1.04	1.25
2	B	14	ALA	CA-C	11.17	1.67	1.52
1	A	7	CYS	CA-CB	11.14	1.73	1.53
1	C	11	CYS	C-N	11.13	1.47	1.33
1	K	13	LEU	C-O	11.13	1.36	1.24
2	D	16	TYR	N-CA	-11.12	1.32	1.46
1	C	17	GLU	C-O	-11.09	1.11	1.24
1	C	9	SER	C-N	11.09	1.61	1.33
1	K	16	LEU	CA-CB	11.09	1.70	1.53
2	L	9	SER	CA-CB	11.09	1.70	1.53
2	F	3	ASN	C-N	11.08	1.49	1.33
1	E	14	TYR	CG-CD1	-11.07	1.16	1.39
1	A	16	LEU	N-CA	11.07	1.60	1.46
2	J	16	TYR	CE1-CZ	11.01	1.64	1.38
2	B	4	GLN	CD-OE1	10.99	1.44	1.23
2	B	1	PHE	CB-CG	-10.99	1.25	1.50
1	G	5	GLN	CA-CB	10.97	1.71	1.53
2	H	9	SER	N-CA	-10.96	1.33	1.46
1	A	12	SER	CB-OG	-10.96	1.20	1.42
2	L	6	LEU	CG-CD1	10.93	1.88	1.52
1	C	12	SER	CA-C	-10.93	1.38	1.53
2	L	13	GLU	CA-C	-10.93	1.38	1.52
2	L	17	LEU	CB-CG	10.91	1.75	1.53
1	A	8	THR	CB-OG1	10.90	1.61	1.43
1	A	11	CYS	CB-SG	-10.89	1.45	1.81
2	L	16	TYR	N-CA	-10.89	1.33	1.46
2	B	9	SER	CA-C	10.89	1.67	1.52
2	L	13	GLU	CG-CD	-10.87	1.24	1.52
2	B	16	TYR	CG-CD2	-10.87	1.16	1.39
1	A	17	GLU	C-N	-10.86	1.19	1.33
2	J	6	LEU	CA-CB	10.86	1.70	1.53
2	H	6	LEU	C-O	-10.86	1.11	1.24
1	A	2	ILE	CA-C	10.84	1.75	1.52
2	H	24	PHE	CD2-CE2	10.84	1.71	1.38
2	B	23	GLY	C-O	10.82	1.42	1.23
2	D	11	LEU	CA-CB	10.82	1.70	1.53
2	D	13	GLU	N-CA	10.80	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	SER	CA-CB	10.78	1.76	1.54
2	H	18	VAL	CB-CG1	10.78	1.88	1.52
1	C	19	TYR	CE1-CZ	10.75	1.64	1.38
2	L	22	ARG	CG-CD	-10.75	1.20	1.52
1	A	16	LEU	CB-CG	10.73	1.75	1.53
2	J	25	TYR	CE1-CZ	-10.73	1.12	1.38
2	L	16	TYR	CG-CD1	10.73	1.61	1.39
2	F	11	LEU	N-CA	-10.72	1.33	1.46
2	B	8	GLY	C-O	10.71	1.36	1.24
1	I	8	THR	C-N	10.71	1.48	1.33
1	K	17	GLU	C-N	-10.71	1.19	1.34
2	D	3	ASN	C-N	10.70	1.49	1.33
2	L	6	LEU	C-N	-10.69	1.18	1.33
1	C	8	THR	CB-CG2	10.69	1.87	1.52
1	K	3	VAL	C-N	10.68	1.48	1.33
1	A	18	ASN	CB-CG	-10.65	1.25	1.52
1	C	17	GLU	CG-CD	10.65	1.78	1.52
1	E	1	GLY	C-O	10.63	1.44	1.23
2	F	21	GLU	CG-CD	10.63	1.78	1.52
2	F	20	GLY	C-O	10.62	1.38	1.24
1	G	4	GLU	N-CA	10.60	1.59	1.46
2	B	17	LEU	C-O	10.58	1.36	1.24
1	A	19	TYR	CE2-CZ	-10.56	1.12	1.38
2	J	28	LYS	CA-C	10.56	1.66	1.52
2	B	24	PHE	N-CA	-10.55	1.32	1.46
1	G	13	LEU	CB-CG	-10.55	1.32	1.53
1	E	4	GLU	CA-CB	10.54	1.69	1.53
2	B	4	GLN	C-O	10.54	1.38	1.24
2	D	22	ARG	N-CA	10.54	1.59	1.46
1	G	3	VAL	CA-CB	10.53	1.67	1.54
1	I	12	SER	CA-C	-10.52	1.38	1.53
1	A	6	CYS	CB-SG	10.50	2.15	1.81
1	E	4	GLU	C-O	10.50	1.36	1.24
1	I	10	ILE	C-N	-10.50	1.18	1.33
2	J	23	GLY	C-O	-10.45	1.09	1.23
1	C	14	TYR	N-CA	-10.45	1.33	1.46
2	B	16	TYR	CE1-CZ	-10.45	1.13	1.38
1	K	15	GLN	CB-CG	-10.44	1.21	1.52
1	G	18	ASN	N-CA	-10.43	1.32	1.46
2	H	17	LEU	N-CA	-10.42	1.34	1.46
1	I	5	GLN	N-CA	-10.42	1.32	1.46
2	J	4	GLN	CG-CD	10.40	1.78	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	7	CYS	N-CA	10.39	1.59	1.46
2	H	11	LEU	C-O	10.38	1.37	1.24
2	H	16	TYR	CG-CD2	-10.38	1.17	1.39
2	L	3	ASN	CA-CB	-10.35	1.36	1.53
2	H	21	GLU	CB-CG	-10.34	1.21	1.52
2	L	25	TYR	CA-CB	10.32	1.74	1.53
2	F	6	LEU	C-O	-10.30	1.11	1.24
2	J	28	LYS	CB-CG	-10.29	1.21	1.52
2	B	16	TYR	N-CA	-10.29	1.32	1.46
2	L	21	GLU	CA-C	10.29	1.70	1.52
1	I	4	GLU	C-O	-10.28	1.12	1.24
2	D	4	GLN	C-N	10.27	1.47	1.33
2	F	21	GLU	CA-C	10.27	1.67	1.52
1	E	17	GLU	CA-CB	10.24	1.69	1.53
1	I	20	CYS	N-CA	-10.24	1.32	1.45
1	I	7	CYS	C-N	-10.22	1.19	1.33
1	K	5	GLN	N-CA	-10.21	1.33	1.46
2	H	22	ARG	C-N	10.20	1.53	1.33
2	B	3	ASN	CB-CG	-10.19	1.26	1.52
2	D	24	PHE	C-O	10.18	1.36	1.23
2	B	10	HIS	CB-CG	10.18	1.64	1.50
1	A	10	ILE	N-CA	-10.16	1.33	1.46
2	J	14	ALA	C-N	10.16	1.47	1.34
2	L	4	GLN	CG-CD	10.15	1.77	1.52
1	K	5	GLN	CD-NE2	-10.12	1.11	1.33
1	K	18	ASN	CA-C	-10.12	1.39	1.52
2	L	10	HIS	CA-CB	10.11	1.69	1.53
2	B	16	TYR	C-O	10.10	1.36	1.24
1	K	21	ASN	CA-CB	-10.10	1.33	1.53
1	E	10	ILE	CB-CG1	-10.09	1.33	1.53
1	E	9	SER	C-N	10.05	1.55	1.33
2	F	3	ASN	CG-ND2	10.05	1.54	1.33
1	I	4	GLU	CG-CD	-10.04	1.26	1.52
2	B	8	GLY	C-N	10.04	1.46	1.33
1	I	7	CYS	CA-CB	-10.04	1.36	1.53
1	K	2	ILE	CA-CB	-10.02	1.40	1.54
1	I	21	ASN	C-OXT	10.01	1.43	1.23
1	I	5	GLN	CA-CB	10.00	1.69	1.53
2	F	3	ASN	CA-CB	10.00	1.68	1.53
1	I	9	SER	C-N	10.00	1.45	1.33
1	A	15	GLN	CD-NE2	-9.99	1.12	1.33
2	D	4	GLN	CD-OE1	9.99	1.42	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	13	GLU	CA-C	9.98	1.66	1.52
2	B	25	TYR	CE1-CZ	9.97	1.62	1.38
1	K	8	THR	C-N	9.97	1.46	1.33
1	C	9	SER	CB-OG	-9.97	1.22	1.42
2	D	13	GLU	CA-CB	-9.96	1.37	1.53
2	J	11	LEU	CA-C	-9.95	1.39	1.52
1	I	18	ASN	CA-CB	-9.95	1.36	1.53
2	L	16	TYR	CE1-CZ	9.95	1.62	1.38
2	L	19	CYS	CA-C	-9.95	1.38	1.52
1	A	21	ASN	CA-C	9.93	1.73	1.52
2	J	21	GLU	C-O	-9.93	1.11	1.24
2	D	5	HIS	CG-CD2	-9.92	1.25	1.35
2	H	5	HIS	ND1-CE1	9.91	1.42	1.32
2	J	19	CYS	CA-C	-9.91	1.39	1.52
1	E	20	CYS	C-N	9.91	1.47	1.33
1	A	15	GLN	C-N	-9.90	1.20	1.33
1	K	18	ASN	CB-CG	-9.87	1.27	1.52
1	K	7	CYS	CA-C	9.87	1.66	1.52
1	K	14	TYR	CZ-OH	9.87	1.58	1.38
2	J	13	GLU	CD-OE1	-9.84	1.06	1.25
2	L	17	LEU	C-N	-9.84	1.20	1.33
1	G	21	ASN	CA-CB	9.80	1.73	1.53
2	F	22	ARG	CZ-NH1	9.80	1.46	1.32
1	K	3	VAL	CA-CB	-9.77	1.41	1.54
1	A	14	TYR	C-N	9.77	1.46	1.33
2	F	15	LEU	CG-CD1	9.76	1.84	1.52
2	H	19	CYS	C-O	9.73	1.37	1.24
1	K	19	TYR	CA-CB	9.73	1.70	1.53
1	G	18	ASN	CB-CG	9.69	1.76	1.52
2	F	2	VAL	CA-C	9.68	1.73	1.52
2	L	16	TYR	CG-CD2	9.68	1.59	1.39
1	C	2	ILE	C-O	9.67	1.36	1.24
2	L	15	LEU	C-O	9.67	1.35	1.24
2	J	27	THR	C-O	-9.67	1.04	1.23
1	I	10	ILE	C-O	-9.67	1.13	1.24
2	B	4	GLN	CB-CG	9.66	1.81	1.52
1	I	19	TYR	CA-CB	9.66	1.70	1.53
1	K	11	CYS	CA-CB	9.66	1.68	1.53
1	I	16	LEU	CG-CD1	9.64	1.84	1.52
2	J	27	THR	CB-OG1	9.64	1.59	1.43
1	I	5	GLN	C-O	-9.64	1.11	1.24
2	D	19	CYS	CA-C	-9.62	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	7	CYS	C-O	9.62	1.35	1.23
1	G	16	LEU	CA-C	9.59	1.66	1.52
2	B	13	GLU	CD-OE2	-9.58	1.07	1.25
2	L	22	ARG	N-CA	9.54	1.58	1.46
2	B	22	ARG	CZ-NH1	-9.53	1.19	1.32
2	J	2	VAL	CA-C	-9.53	1.41	1.52
1	A	21	ASN	C-O	-9.52	1.04	1.23
1	C	17	GLU	CA-C	9.52	1.65	1.52
2	F	13	GLU	CD-OE2	-9.52	1.07	1.25
2	H	10	HIS	CG-CD2	9.50	1.46	1.35
1	C	19	TYR	CA-C	-9.50	1.40	1.52
1	I	12	SER	C-O	9.49	1.36	1.23
2	F	18	VAL	C-O	-9.47	1.12	1.23
1	C	12	SER	C-N	9.46	1.46	1.33
1	I	13	LEU	CA-CB	9.46	1.68	1.53
2	L	13	GLU	N-CA	9.46	1.57	1.46
2	L	7	CYS	CA-CB	-9.45	1.38	1.53
2	D	11	LEU	CG-CD2	9.44	1.83	1.52
2	J	21	GLU	C-N	-9.43	1.21	1.34
2	L	6	LEU	CG-CD2	-9.43	1.21	1.52
2	J	5	HIS	C-N	9.43	1.46	1.33
1	C	15	GLN	CG-CD	-9.41	1.28	1.52
1	G	6	CYS	N-CA	-9.41	1.33	1.46
2	B	22	ARG	CA-CB	9.40	1.68	1.53
1	C	20	CYS	CA-C	-9.40	1.40	1.52
1	I	16	LEU	CB-CG	9.39	1.72	1.53
1	C	6	CYS	CA-CB	-9.37	1.38	1.53
2	J	24	PHE	CA-C	-9.37	1.41	1.52
1	I	12	SER	CA-CB	-9.36	1.39	1.53
1	C	20	CYS	N-CA	-9.34	1.34	1.45
1	I	20	CYS	C-O	9.33	1.35	1.23
2	L	25	TYR	CB-CG	9.28	1.72	1.51
1	A	11	CYS	CA-C	-9.28	1.40	1.52
1	E	9	SER	CA-C	-9.27	1.41	1.52
1	C	13	LEU	C-O	9.27	1.35	1.24
2	B	1	PHE	CA-CB	9.27	1.72	1.53
2	L	4	GLN	CB-CG	-9.26	1.24	1.52
2	H	13	GLU	CA-CB	9.25	1.67	1.53
2	J	15	LEU	CA-CB	9.24	1.68	1.53
2	D	10	HIS	C-N	9.21	1.46	1.33
2	H	7	CYS	C-N	-9.20	1.20	1.33
2	F	2	VAL	C-O	-9.19	1.05	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	15	LEU	CA-C	-9.18	1.41	1.52
1	I	19	TYR	CE2-CZ	9.18	1.60	1.38
1	K	19	TYR	N-CA	-9.17	1.34	1.46
2	L	1	PHE	CD2-CE2	9.17	1.66	1.38
1	A	9	SER	CA-C	-9.17	1.41	1.52
1	C	8	THR	N-CA	-9.17	1.34	1.46
2	B	15	LEU	N-CA	9.14	1.58	1.46
1	K	1	GLY	C-N	-9.14	1.23	1.34
2	F	9	SER	CA-CB	-9.14	1.38	1.53
1	K	15	GLN	N-CA	9.14	1.57	1.46
2	D	19	CYS	N-CA	-9.13	1.33	1.46
2	H	4	GLN	CG-CD	-9.11	1.29	1.52
1	C	16	LEU	CG-CD2	9.11	1.82	1.52
2	D	2	VAL	C-N	9.10	1.46	1.34
2	F	5	HIS	C-N	9.09	1.46	1.33
2	D	6	LEU	CA-C	9.07	1.64	1.52
2	L	20	GLY	N-CA	-9.05	1.32	1.45
1	G	4	GLU	CA-C	-9.04	1.40	1.52
2	H	17	LEU	CB-CG	-9.04	1.35	1.53
1	E	18	ASN	CA-CB	-9.00	1.38	1.53
2	D	13	GLU	CB-CG	8.97	1.79	1.52
1	G	14	TYR	CD1-CE1	-8.97	1.11	1.38
1	A	7	CYS	C-O	8.96	1.35	1.24
2	D	4	GLN	C-O	-8.96	1.13	1.24
2	B	1	PHE	C-O	8.94	1.41	1.23
1	E	10	ILE	N-CA	-8.94	1.35	1.46
2	J	3	ASN	CB-CG	8.92	1.74	1.52
2	B	17	LEU	CG-CD1	8.91	1.81	1.52
1	E	14	TYR	CE2-CZ	-8.91	1.16	1.38
2	L	16	TYR	CB-CG	-8.90	1.32	1.51
1	E	6	CYS	CB-SG	-8.89	1.51	1.81
2	B	7	CYS	CA-C	8.87	1.65	1.52
1	E	18	ASN	C-O	8.88	1.35	1.24
2	H	10	HIS	C-O	-8.86	1.13	1.24
1	A	8	THR	CA-C	8.86	1.64	1.52
2	D	15	LEU	CG-CD1	8.83	1.81	1.52
1	K	18	ASN	CA-CB	-8.82	1.38	1.53
2	D	23	GLY	C-O	8.79	1.37	1.23
1	A	18	ASN	CG-ND2	8.78	1.51	1.33
2	L	5	HIS	CG-CD2	8.78	1.45	1.35
2	J	3	ASN	CG-ND2	8.76	1.51	1.33
2	J	22	ARG	CG-CD	-8.76	1.26	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	TYR	CG-CD1	-8.75	1.21	1.39
1	G	14	TYR	CD2-CE2	-8.74	1.12	1.38
1	I	9	SER	CA-C	-8.73	1.42	1.52
2	H	2	VAL	CB-CG1	-8.72	1.23	1.52
2	F	25	TYR	N-CA	8.71	1.62	1.46
2	F	16	TYR	CG-CD1	8.70	1.57	1.39
2	J	3	ASN	N-CA	-8.67	1.35	1.46
1	G	9	SER	CA-C	-8.66	1.42	1.52
2	D	9	SER	CA-CB	-8.66	1.39	1.53
2	F	2	VAL	CB-CG2	8.66	1.81	1.52
2	H	6	LEU	C-N	8.65	1.45	1.33
1	C	3	VAL	CA-C	-8.65	1.42	1.52
1	A	18	ASN	CG-OD1	8.64	1.40	1.23
2	B	9	SER	CB-OG	-8.63	1.24	1.42
2	L	1	PHE	CD1-CE1	8.63	1.64	1.38
2	J	21	GLU	N-CA	-8.62	1.35	1.46
2	H	15	LEU	C-O	8.59	1.35	1.24
1	E	19	TYR	CE1-CZ	8.58	1.58	1.38
2	B	19	CYS	C-O	8.58	1.35	1.24
2	L	12	VAL	CB-CG2	8.57	1.80	1.52
2	L	22	ARG	C-N	8.56	1.48	1.33
2	B	25	TYR	CG-CD1	-8.56	1.21	1.39
1	G	4	GLU	CG-CD	8.55	1.73	1.52
2	L	25	TYR	CG-CD1	-8.53	1.21	1.39
1	K	9	SER	N-CA	-8.52	1.35	1.46
1	A	2	ILE	CB-CG2	8.50	1.80	1.52
1	E	5	GLN	CD-OE1	-8.49	1.07	1.23
2	J	17	LEU	CA-C	8.49	1.64	1.52
2	F	13	GLU	N-CA	8.48	1.56	1.46
1	C	21	ASN	C-OXT	-8.47	1.06	1.23
2	B	24	PHE	C-O	8.46	1.33	1.23
2	D	8	GLY	C-N	-8.45	1.22	1.33
1	C	12	SER	CA-CB	8.45	1.66	1.53
1	G	18	ASN	CG-ND2	8.45	1.51	1.33
2	F	7	CYS	C-O	-8.45	1.14	1.24
1	A	16	LEU	CA-C	8.44	1.64	1.52
2	B	12	VAL	CB-CG2	-8.44	1.24	1.52
2	H	18	VAL	CA-CB	-8.44	1.42	1.54
2	L	1	PHE	CG-CD1	-8.44	1.21	1.38
2	F	19	CYS	CA-C	-8.41	1.40	1.52
2	L	12	VAL	CB-CG1	-8.40	1.24	1.52
2	H	20	GLY	C-O	-8.39	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	28	LYS	CE-NZ	8.39	1.74	1.49
1	I	18	ASN	CB-CG	-8.39	1.31	1.52
1	C	3	VAL	CB-CG1	-8.39	1.24	1.52
2	J	17	LEU	CA-CB	8.38	1.66	1.53
2	H	12	VAL	CB-CG2	-8.37	1.25	1.52
1	C	21	ASN	CA-C	8.37	1.70	1.52
2	L	1	PHE	CE1-CZ	8.36	1.63	1.38
2	H	16	TYR	CE1-CZ	-8.36	1.18	1.38
2	F	5	HIS	CG-CD2	8.36	1.45	1.35
2	B	2	VAL	CB-CG1	-8.35	1.25	1.52
2	J	27	THR	CA-C	8.34	1.70	1.52
1	K	19	TYR	C-O	-8.34	1.13	1.24
1	C	18	ASN	CA-CB	-8.34	1.39	1.53
1	I	13	LEU	N-CA	-8.34	1.36	1.46
2	F	14	ALA	C-O	-8.33	1.14	1.24
2	B	24	PHE	CE2-CZ	-8.31	1.13	1.38
2	J	28	LYS	CG-CD	8.28	1.77	1.52
1	G	16	LEU	CB-CG	8.27	1.70	1.53
2	L	11	LEU	CA-CB	8.27	1.66	1.53
2	J	4	GLN	CD-NE2	-8.27	1.15	1.33
2	D	5	HIS	CE1-NE2	-8.25	1.24	1.32
2	F	15	LEU	N-CA	-8.25	1.36	1.46
2	L	1	PHE	N-CA	8.25	1.61	1.46
1	C	5	GLN	CD-NE2	8.25	1.50	1.33
2	L	15	LEU	CA-C	-8.24	1.42	1.52
2	H	12	VAL	C-O	8.24	1.33	1.24
2	L	11	LEU	CB-CG	-8.22	1.37	1.53
1	C	10	ILE	C-N	-8.20	1.21	1.33
2	B	1	PHE	CD1-CE1	-8.19	1.14	1.38
1	K	21	ASN	CG-ND2	-8.17	1.16	1.33
2	H	15	LEU	CG-CD1	-8.16	1.25	1.52
1	A	13	LEU	CB-CG	8.14	1.69	1.53
2	J	12	VAL	CB-CG2	8.13	1.79	1.52
1	E	18	ASN	CB-CG	8.13	1.72	1.52
2	L	8	GLY	C-N	8.13	1.43	1.33
2	J	2	VAL	CB-CG1	8.11	1.79	1.52
1	K	2	ILE	C-N	-8.07	1.23	1.33
2	L	16	TYR	C-O	8.07	1.33	1.24
2	B	24	PHE	CD1-CE1	8.05	1.62	1.38
2	L	7	CYS	C-N	8.03	1.46	1.33
1	K	5	GLN	CG-CD	8.02	1.72	1.52
2	H	2	VAL	C-O	-8.02	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	9	SER	CB-OG	8.02	1.58	1.42
2	L	21	GLU	CG-CD	-8.01	1.32	1.52
2	L	25	TYR	C-O	7.98	1.39	1.23
1	I	6	CYS	CB-SG	7.97	2.07	1.81
1	C	9	SER	CA-C	-7.96	1.42	1.52
2	D	11	LEU	CG-CD1	7.96	1.78	1.52
1	E	4	GLU	CG-CD	7.96	1.72	1.52
1	C	19	TYR	CG-CD1	7.95	1.56	1.39
2	F	3	ASN	CG-OD1	7.95	1.38	1.23
1	I	10	ILE	CG1-CD1	7.95	1.82	1.51
1	E	19	TYR	CG-CD2	7.94	1.56	1.39
1	G	2	ILE	N-CA	-7.94	1.31	1.46
2	D	3	ASN	CG-OD1	7.93	1.38	1.23
1	A	14	TYR	CE2-CZ	-7.93	1.19	1.38
1	I	21	ASN	CG-OD1	-7.93	1.08	1.23
2	H	1	PHE	CB-CG	-7.93	1.32	1.50
1	G	3	VAL	CA-C	7.92	1.62	1.52
1	E	17	GLU	CG-CD	-7.92	1.32	1.52
1	G	18	ASN	C-O	-7.89	1.13	1.24
2	B	11	LEU	CG-CD1	-7.88	1.26	1.52
1	K	8	THR	CA-C	-7.87	1.42	1.52
2	J	24	PHE	CD2-CE2	7.86	1.62	1.38
2	L	24	PHE	CA-C	7.85	1.62	1.52
1	E	2	ILE	CA-CB	-7.84	1.43	1.54
1	G	17	GLU	C-N	-7.83	1.23	1.33
2	H	10	HIS	CD2-NE2	7.80	1.46	1.37
2	B	24	PHE	CE1-CZ	7.78	1.61	1.38
1	G	9	SER	N-CA	-7.76	1.34	1.46
1	A	4	GLU	CG-CD	7.75	1.71	1.52
2	D	21	GLU	CD-OE2	-7.75	1.10	1.25
2	L	18	VAL	N-CA	-7.72	1.36	1.46
1	G	12	SER	CB-OG	7.72	1.57	1.42
2	J	27	THR	CA-CB	7.72	1.75	1.54
2	H	21	GLU	CD-OE2	7.72	1.40	1.25
1	I	14	TYR	CA-C	7.66	1.63	1.52
1	G	15	GLN	CD-NE2	7.65	1.49	1.33
2	L	15	LEU	CB-CG	-7.65	1.38	1.53
1	G	2	ILE	CA-C	7.65	1.69	1.52
2	H	16	TYR	N-CA	-7.65	1.37	1.46
2	F	16	TYR	CE2-CZ	7.63	1.56	1.38
2	H	11	LEU	CG-CD1	-7.63	1.27	1.52
1	E	3	VAL	C-O	7.62	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	20	CYS	C-O	-7.61	1.14	1.23
2	H	24	PHE	CG-CD1	-7.61	1.22	1.38
1	K	2	ILE	C-O	7.59	1.33	1.24
1	G	9	SER	C-N	-7.59	1.22	1.33
1	C	18	ASN	CG-OD1	-7.57	1.09	1.23
1	A	14	TYR	CA-C	-7.57	1.43	1.52
2	F	23	GLY	N-CA	-7.56	1.31	1.45
2	L	4	GLN	CD-OE1	-7.56	1.09	1.23
2	H	13	GLU	CD-OE2	-7.55	1.11	1.25
2	B	10	HIS	CD2-NE2	-7.54	1.29	1.37
2	J	18	VAL	C-N	-7.54	1.22	1.33
1	C	8	THR	CA-CB	7.53	1.65	1.53
2	J	18	VAL	CB-CG1	7.51	1.77	1.52
2	F	16	TYR	N-CA	-7.51	1.37	1.46
1	K	15	GLN	CG-CD	7.50	1.70	1.52
1	E	2	ILE	CB-CG2	7.50	1.77	1.52
2	L	25	TYR	CZ-OH	7.50	1.53	1.38
2	H	25	TYR	CG-CD1	7.50	1.55	1.39
2	L	16	TYR	CE2-CZ	7.49	1.56	1.38
2	D	22	ARG	CA-CB	7.48	1.66	1.53
1	K	14	TYR	CB-CG	7.47	1.68	1.51
2	B	2	VAL	CB-CG2	7.47	1.77	1.52
1	E	13	LEU	C-N	7.45	1.43	1.33
2	L	21	GLU	CB-CG	7.43	1.74	1.52
2	J	14	ALA	CA-CB	-7.43	1.41	1.53
1	A	5	GLN	CG-CD	7.42	1.70	1.52
1	C	19	TYR	CE2-CZ	7.41	1.56	1.38
1	K	12	SER	CA-C	7.40	1.63	1.53
2	B	22	ARG	C-N	7.39	1.47	1.33
2	H	11	LEU	CG-CD2	7.37	1.76	1.52
1	K	14	TYR	CA-C	7.37	1.62	1.52
1	A	16	LEU	CG-CD1	-7.37	1.28	1.52
2	F	22	ARG	N-CA	7.36	1.55	1.46
1	C	11	CYS	CB-SG	7.35	2.05	1.81
2	L	20	GLY	C-N	7.33	1.45	1.33
2	L	12	VAL	CA-C	7.32	1.63	1.52
1	K	14	TYR	CD2-CE2	7.32	1.60	1.38
1	K	20	CYS	C-N	-7.27	1.23	1.33
1	K	16	LEU	CG-CD1	7.27	1.76	1.52
2	B	10	HIS	C-O	7.26	1.32	1.24
2	L	25	TYR	CE2-CZ	-7.26	1.20	1.38
1	I	14	TYR	CG-CD1	7.25	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	24	PHE	CD2-CE2	7.25	1.60	1.38
1	C	13	LEU	CG-CD2	7.24	1.76	1.52
2	L	14	ALA	CA-CB	-7.21	1.41	1.53
1	C	21	ASN	CB-CG	7.19	1.70	1.52
2	F	14	ALA	CA-C	-7.18	1.43	1.52
2	L	25	TYR	CA-C	7.18	1.68	1.52
1	E	20	CYS	N-CA	-7.15	1.37	1.46
2	F	5	HIS	ND1-CE1	7.14	1.39	1.32
2	L	8	GLY	CA-C	-7.12	1.43	1.51
1	G	18	ASN	CA-C	7.12	1.62	1.52
1	I	19	TYR	CB-CG	-7.12	1.35	1.51
2	B	1	PHE	CD2-CE2	-7.10	1.17	1.38
2	L	16	TYR	CA-CB	-7.10	1.42	1.53
1	I	19	TYR	CZ-OH	-7.10	1.23	1.38
2	J	14	ALA	N-CA	-7.09	1.38	1.46
2	F	23	GLY	C-O	7.09	1.35	1.23
2	J	12	VAL	CB-CG1	-7.09	1.29	1.52
2	L	9	SER	C-N	-7.08	1.24	1.34
2	L	2	VAL	CA-C	-7.08	1.44	1.52
1	A	15	GLN	CA-CB	7.06	1.64	1.53
1	C	4	GLU	CG-CD	7.06	1.69	1.52
2	B	15	LEU	CA-C	-7.06	1.43	1.52
2	H	21	GLU	CA-CB	7.04	1.64	1.53
1	I	8	THR	N-CA	-7.03	1.37	1.46
2	L	12	VAL	C-O	7.03	1.33	1.24
1	I	8	THR	CB-CG2	7.02	1.75	1.52
2	H	25	TYR	CE2-CZ	6.99	1.55	1.38
2	H	4	GLN	CB-CG	6.97	1.73	1.52
2	B	19	CYS	C-N	-6.97	1.23	1.33
1	K	10	ILE	CG1-CD1	6.97	1.78	1.51
2	F	15	LEU	CA-C	-6.96	1.44	1.52
2	F	22	ARG	C-N	-6.96	1.19	1.33
2	H	5	HIS	CG-CD2	6.96	1.43	1.35
2	L	7	CYS	N-CA	-6.95	1.37	1.46
2	H	8	GLY	CA-C	-6.95	1.42	1.51
2	H	13	GLU	C-O	-6.95	1.16	1.24
2	F	16	TYR	CG-CD2	6.92	1.53	1.39
2	F	4	GLN	CD-NE2	6.92	1.47	1.33
1	I	18	ASN	CG-ND2	-6.90	1.18	1.33
2	J	5	HIS	ND1-CE1	-6.90	1.25	1.32
1	K	14	TYR	CE1-CZ	6.89	1.54	1.38
1	E	11	CYS	CA-C	6.88	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2	ILE	C-N	6.88	1.42	1.34
1	E	17	GLU	CD-OE1	6.88	1.38	1.25
2	H	17	LEU	C-N	-6.87	1.25	1.34
1	A	11	CYS	C-O	-6.86	1.15	1.23
1	I	10	ILE	N-CA	-6.83	1.37	1.46
2	H	3	ASN	CG-OD1	-6.83	1.10	1.23
1	A	3	VAL	CB-CG1	6.82	1.75	1.52
1	A	5	GLN	CB-CG	6.82	1.72	1.52
1	G	7	CYS	C-N	6.81	1.44	1.33
1	K	17	GLU	CD-OE2	6.80	1.38	1.25
1	K	19	TYR	CA-C	-6.80	1.43	1.52
2	L	1	PHE	CA-CB	6.80	1.67	1.53
2	B	4	GLN	CG-CD	-6.80	1.35	1.52
2	L	25	TYR	CD2-CE2	6.80	1.59	1.38
1	C	5	GLN	CB-CG	6.78	1.72	1.52
2	F	16	TYR	CE1-CZ	6.77	1.54	1.38
2	B	21	GLU	CD-OE1	6.75	1.38	1.25
2	B	8	GLY	N-CA	6.75	1.54	1.45
2	H	19	CYS	CA-C	-6.74	1.43	1.52
1	G	15	GLN	CB-CG	6.73	1.72	1.52
2	D	7	CYS	C-O	6.72	1.32	1.24
1	C	2	ILE	CB-CG2	6.72	1.74	1.52
1	K	14	TYR	CG-CD2	6.72	1.53	1.39
2	H	2	VAL	CB-CG2	6.71	1.74	1.52
2	D	4	GLN	CD-NE2	6.71	1.47	1.33
1	K	3	VAL	CB-CG2	-6.71	1.30	1.52
2	J	3	ASN	CG-OD1	-6.70	1.10	1.23
1	G	16	LEU	C-O	-6.70	1.15	1.24
1	G	3	VAL	C-N	6.69	1.43	1.33
2	J	29	PRO	CB-CG	6.67	1.82	1.49
2	L	25	TYR	CG-CD2	6.67	1.53	1.39
2	J	24	PHE	CD1-CE1	6.67	1.58	1.38
1	K	2	ILE	CB-CG2	-6.66	1.30	1.52
2	J	13	GLU	CA-C	-6.65	1.44	1.52
1	K	15	GLN	CA-CB	6.64	1.63	1.53
2	B	25	TYR	CE2-CZ	-6.63	1.22	1.38
1	K	14	TYR	CD1-CE1	6.62	1.58	1.38
2	D	16	TYR	CG-CD1	6.58	1.53	1.39
1	A	8	THR	CB-CG2	6.57	1.74	1.52
1	G	21	ASN	CA-C	6.56	1.66	1.52
1	I	2	ILE	CB-CG2	-6.54	1.30	1.52
1	C	15	GLN	CD-NE2	-6.52	1.19	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	11	LEU	CG-CD1	6.52	1.74	1.52
2	J	13	GLU	CB-CG	6.51	1.72	1.52
2	B	16	TYR	CB-CG	-6.48	1.37	1.51
1	A	3	VAL	C-O	-6.48	1.16	1.24
2	D	4	GLN	CA-CB	6.47	1.64	1.53
2	F	4	GLN	CA-CB	6.45	1.64	1.53
1	I	16	LEU	C-O	-6.45	1.16	1.24
2	D	13	GLU	C-O	-6.44	1.16	1.24
1	K	14	TYR	C-N	6.44	1.42	1.33
2	D	3	ASN	CA-CB	6.43	1.63	1.53
2	D	9	SER	C-O	-6.39	1.16	1.24
1	A	17	GLU	CB-CG	6.38	1.71	1.52
1	G	2	ILE	C-O	-6.34	1.10	1.23
2	J	15	LEU	CB-CG	-6.29	1.40	1.53
2	H	2	VAL	C-N	6.28	1.41	1.33
2	H	24	PHE	N-CA	-6.28	1.38	1.46
2	H	25	TYR	C-O	6.28	1.36	1.23
1	C	18	ASN	CG-ND2	6.27	1.46	1.33
2	L	21	GLU	CD-OE1	-6.27	1.13	1.25
2	L	8	GLY	C-O	6.27	1.32	1.23
1	K	19	TYR	CG-CD2	6.26	1.52	1.39
1	K	20	CYS	N-CA	-6.25	1.38	1.46
2	J	18	VAL	CA-CB	-6.24	1.45	1.54
2	B	15	LEU	CB-CG	-6.23	1.41	1.53
2	J	1	PHE	CA-C	6.23	1.66	1.52
2	J	1	PHE	CG-CD1	-6.23	1.25	1.38
2	J	24	PHE	CG-CD1	6.20	1.51	1.38
2	J	24	PHE	C-N	6.20	1.42	1.33
2	D	24	PHE	CA-CB	-6.20	1.43	1.53
1	K	11	CYS	C-O	-6.19	1.16	1.23
1	E	10	ILE	CG1-CD1	6.17	1.75	1.51
1	K	7	CYS	CA-CB	-6.17	1.42	1.53
1	C	13	LEU	CA-C	-6.17	1.44	1.52
1	I	17	GLU	CD-OE1	-6.17	1.13	1.25
1	I	5	GLN	CB-CG	-6.17	1.33	1.52
1	E	19	TYR	CA-C	-6.14	1.44	1.52
2	D	12	VAL	C-N	-6.13	1.25	1.33
2	H	27	THR	CB-CG2	6.13	1.72	1.52
2	F	2	VAL	CA-CB	-6.12	1.38	1.54
1	A	13	LEU	CG-CD2	6.11	1.72	1.52
1	I	2	ILE	CA-CB	-6.08	1.45	1.54
1	E	3	VAL	CB-CG2	6.07	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	12	VAL	CA-CB	-6.06	1.46	1.54
1	K	19	TYR	CZ-OH	-6.06	1.25	1.38
2	D	17	LEU	CG-CD1	-6.05	1.32	1.52
1	E	17	GLU	C-N	-6.05	1.25	1.33
1	I	15	GLN	CB-CG	-6.05	1.34	1.52
2	D	6	LEU	CB-CG	6.03	1.65	1.53
2	D	12	VAL	CB-CG1	6.03	1.72	1.52
2	L	16	TYR	CZ-OH	-6.02	1.25	1.38
1	C	4	GLU	N-CA	-6.01	1.39	1.46
1	G	5	GLN	C-O	-6.01	1.16	1.24
1	I	12	SER	N-CA	5.97	1.52	1.45
1	I	11	CYS	CA-C	5.96	1.60	1.52
2	D	21	GLU	CA-CB	-5.96	1.43	1.53
2	F	10	HIS	C-O	-5.96	1.16	1.24
2	H	6	LEU	CA-CB	5.95	1.62	1.53
2	L	17	LEU	CG-CD1	-5.94	1.32	1.52
2	J	16	TYR	CA-CB	5.93	1.62	1.53
2	H	23	GLY	CA-C	-5.93	1.43	1.52
1	C	13	LEU	C-N	5.92	1.41	1.33
2	F	24	PHE	N-CA	-5.88	1.38	1.46
2	D	5	HIS	C-N	-5.87	1.25	1.33
2	L	1	PHE	CA-C	5.87	1.65	1.52
2	H	8	GLY	C-O	5.87	1.31	1.23
2	L	1	PHE	CE2-CZ	-5.87	1.21	1.38
2	J	2	VAL	CB-CG2	-5.85	1.33	1.52
2	D	15	LEU	CG-CD2	5.85	1.71	1.52
1	K	3	VAL	CB-CG1	5.84	1.71	1.52
1	E	15	GLN	CG-CD	-5.84	1.37	1.52
1	G	9	SER	C-O	5.84	1.30	1.23
2	J	6	LEU	CG-CD1	5.80	1.71	1.52
2	L	13	GLU	CD-OE2	5.79	1.36	1.25
1	A	9	SER	CB-OG	-5.79	1.30	1.42
2	H	1	PHE	CD1-CE1	-5.79	1.21	1.38
2	D	3	ASN	C-O	5.78	1.31	1.24
2	H	27	THR	CA-CB	5.78	1.70	1.54
1	G	5	GLN	CG-CD	5.78	1.66	1.52
2	H	25	TYR	CA-CB	-5.77	1.42	1.53
1	C	18	ASN	CB-CG	5.75	1.66	1.52
2	J	15	LEU	C-O	5.74	1.31	1.24
2	H	7	CYS	CA-CB	5.74	1.62	1.53
1	A	12	SER	C-N	-5.74	1.25	1.33
2	L	9	SER	N-CA	-5.73	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	4	GLU	CB-CG	5.73	1.69	1.52
1	E	18	ASN	CG-OD1	-5.72	1.12	1.23
2	F	8	GLY	C-N	-5.72	1.25	1.33
2	F	10	HIS	CE1-NE2	5.71	1.38	1.32
1	I	4	GLU	CD-OE2	-5.71	1.14	1.25
1	I	11	CYS	CB-SG	5.71	2.00	1.81
1	I	7	CYS	CA-C	-5.69	1.44	1.52
1	G	19	TYR	N-CA	5.68	1.53	1.46
2	D	14	ALA	C-O	5.67	1.30	1.24
2	B	3	ASN	CG-OD1	-5.67	1.12	1.23
2	J	1	PHE	CB-CG	5.67	1.63	1.50
1	G	16	LEU	CA-CB	5.66	1.62	1.53
1	E	21	ASN	CA-C	-5.64	1.41	1.52
1	K	11	CYS	C-N	-5.63	1.24	1.33
1	K	19	TYR	CE2-CZ	5.63	1.51	1.38
1	K	17	GLU	CD-OE1	-5.63	1.14	1.25
2	H	19	CYS	N-CA	5.63	1.53	1.46
2	B	7	CYS	C-N	-5.59	1.27	1.34
2	L	5	HIS	CA-CB	-5.59	1.44	1.53
2	J	19	CYS	CA-CB	5.59	1.63	1.53
2	F	7	CYS	CA-C	-5.58	1.45	1.52
1	K	9	SER	CB-OG	-5.58	1.30	1.42
2	H	1	PHE	N-CA	-5.57	1.35	1.46
1	G	3	VAL	C-O	-5.57	1.17	1.24
1	G	21	ASN	CG-OD1	-5.56	1.12	1.23
2	H	13	GLU	CG-CD	5.55	1.66	1.52
1	C	17	GLU	CD-OE1	-5.54	1.14	1.25
1	A	6	CYS	C-N	5.54	1.42	1.33
1	K	16	LEU	C-O	5.54	1.30	1.24
1	C	6	CYS	CB-SG	-5.53	1.62	1.81
2	F	4	GLN	C-N	5.52	1.41	1.33
2	J	24	PHE	CA-CB	5.52	1.62	1.53
1	C	19	TYR	CB-CG	-5.51	1.39	1.51
1	A	21	ASN	CG-ND2	-5.51	1.21	1.33
2	D	21	GLU	CB-CG	5.50	1.69	1.52
2	B	25	TYR	C-O	5.47	1.34	1.23
2	J	13	GLU	CD-OE2	5.45	1.35	1.25
2	L	16	TYR	CD1-CE1	-5.45	1.22	1.38
2	H	27	THR	CB-OG1	-5.44	1.35	1.43
1	C	3	VAL	C-N	5.41	1.41	1.33
1	C	17	GLU	CB-CG	5.40	1.68	1.52
1	A	5	GLN	CD-NE2	-5.40	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	17	GLU	CA-C	-5.39	1.45	1.52
1	I	1	GLY	C-O	-5.39	1.12	1.23
1	E	19	TYR	CB-CG	-5.38	1.39	1.51
1	C	19	TYR	CZ-OH	-5.38	1.26	1.38
1	C	21	ASN	CA-CB	5.38	1.64	1.53
2	H	15	LEU	CA-C	-5.38	1.45	1.52
1	A	7	CYS	CA-C	-5.37	1.45	1.52
1	C	14	TYR	CB-CG	-5.37	1.39	1.51
2	B	16	TYR	CZ-OH	-5.36	1.26	1.38
2	B	21	GLU	C-N	5.36	1.41	1.33
2	L	16	TYR	CD2-CE2	-5.34	1.22	1.38
1	E	18	ASN	C-N	-5.33	1.25	1.33
2	B	18	VAL	CB-CG1	5.32	1.70	1.52
2	H	10	HIS	N-CA	-5.31	1.39	1.46
1	I	15	GLN	N-CA	5.30	1.52	1.46
1	K	13	LEU	CG-CD2	5.30	1.70	1.52
2	H	27	THR	C-N	-5.30	1.25	1.33
1	I	17	GLU	CG-CD	-5.29	1.38	1.52
2	L	25	TYR	CE1-CZ	5.29	1.50	1.38
2	D	4	GLN	CG-CD	-5.29	1.38	1.52
1	C	17	GLU	C-N	-5.28	1.26	1.33
2	L	25	TYR	CD1-CE1	5.28	1.54	1.38
1	E	13	LEU	CG-CD2	5.27	1.70	1.52
2	D	17	LEU	CA-CB	-5.27	1.44	1.53
1	I	14	TYR	CE2-CZ	5.26	1.50	1.38
1	A	16	LEU	CA-CB	-5.26	1.44	1.53
2	H	22	ARG	CZ-NH2	-5.24	1.26	1.33
1	K	10	ILE	N-CA	-5.24	1.39	1.46
1	C	10	ILE	N-CA	-5.23	1.40	1.46
2	D	6	LEU	CG-CD1	-5.23	1.35	1.52
2	H	9	SER	C-O	-5.22	1.18	1.24
1	K	19	TYR	CE1-CZ	5.22	1.50	1.38
1	A	13	LEU	CG-CD1	-5.21	1.35	1.52
1	A	15	GLN	N-CA	-5.21	1.40	1.46
1	G	6	CYS	C-O	-5.21	1.16	1.24
2	D	24	PHE	CG-CD2	5.20	1.49	1.38
1	I	17	GLU	C-N	-5.18	1.26	1.33
2	L	5	HIS	CD2-NE2	-5.18	1.32	1.37
1	E	16	LEU	CG-CD2	5.17	1.69	1.52
2	F	11	LEU	CB-CG	5.17	1.63	1.53
2	D	16	TYR	CE2-CZ	5.16	1.50	1.38
2	J	10	HIS	CA-CB	-5.15	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	19	CYS	CB-SG	-5.14	1.64	1.81
2	H	12	VAL	C-N	5.14	1.40	1.33
2	F	12	VAL	CB-CG2	-5.14	1.35	1.52
1	I	7	CYS	CB-SG	-5.13	1.64	1.81
1	K	21	ASN	C-OXT	-5.13	1.13	1.23
2	H	1	PHE	C-O	5.12	1.33	1.23
1	G	21	ASN	C-OXT	-5.11	1.13	1.23
1	A	15	GLN	CD-OE1	-5.10	1.13	1.23
1	K	9	SER	CA-C	-5.10	1.46	1.52
1	K	19	TYR	CB-CG	-5.10	1.40	1.51
1	E	7	CYS	CA-C	-5.09	1.45	1.52
1	E	10	ILE	CB-CG2	-5.09	1.35	1.52
2	B	19	CYS	CA-CB	-5.07	1.45	1.53
1	A	7	CYS	CB-SG	-5.05	1.64	1.81
1	G	19	TYR	C-N	-5.04	1.26	1.33
1	I	8	THR	CA-C	-5.01	1.45	1.52
1	I	3	VAL	CB-CG2	-5.01	1.36	1.52

All (1455) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	10	HIS	CE1-NE2-CD2	-23.99	85.01	109.00
2	F	7	CYS	N-CA-C	-22.58	86.66	111.28
1	A	14	TYR	N-CA-C	-22.48	87.02	111.07
2	F	7	CYS	CA-C-O	-22.31	96.90	120.55
2	J	4	GLN	OE1-CD-NE2	-21.00	101.60	122.60
2	L	22	ARG	NE-CZ-NH1	-20.78	100.72	121.50
1	K	20	CYS	O-C-N	-20.76	97.33	122.87
1	A	11	CYS	CA-C-O	-20.73	97.08	120.92
2	L	10	HIS	CA-CB-CG	20.67	134.47	113.80
1	C	14	TYR	O-C-N	-20.42	101.04	122.07
2	L	1	PHE	CA-CB-CG	20.41	134.21	113.80
1	G	5	GLN	N-CA-C	-20.11	86.96	111.69
1	C	4	GLU	O-C-N	-20.10	100.81	122.12
2	H	2	VAL	N-CA-C	-19.80	90.43	110.62
2	F	11	LEU	CA-C-O	-19.75	99.42	120.55
2	J	18	VAL	N-CA-C	19.74	132.52	111.00
2	H	10	HIS	CG-CD2-NE2	19.63	126.83	107.20
2	J	24	PHE	CA-CB-CG	19.57	133.37	113.80
2	H	3	ASN	O-C-N	-19.51	101.98	122.07
2	D	18	VAL	CA-C-O	-19.48	98.84	120.46
1	I	13	LEU	O-C-N	-19.35	101.61	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	5	HIS	CG-CD2-NE2	-19.15	88.05	107.20
2	F	18	VAL	CA-C-O	-19.09	99.27	120.46
2	B	10	HIS	ND1-CE1-NE2	19.03	127.43	108.40
1	K	5	GLN	O-C-N	-18.90	100.61	122.15
1	C	9	SER	CA-C-O	-18.66	100.32	121.40
1	K	7	CYS	N-CA-C	18.62	135.99	113.28
1	G	6	CYS	O-C-N	-18.40	99.97	122.24
2	D	16	TYR	O-C-N	-18.36	102.66	122.12
2	J	5	HIS	ND1-CG-CD2	18.32	124.42	106.10
2	D	11	LEU	CA-C-O	-18.28	101.87	120.70
2	H	10	HIS	O-C-N	-18.20	101.41	122.15
2	L	5	HIS	ND1-CG-CD2	18.07	124.17	106.10
1	E	14	TYR	CA-C-O	17.96	140.12	120.90
1	C	8	THR	O-C-N	-17.93	98.92	122.23
1	G	18	ASN	N-CA-C	-17.92	90.68	112.54
1	I	10	ILE	O-C-N	-17.91	103.14	122.67
2	L	4	GLN	OE1-CD-NE2	-17.91	104.69	122.60
2	B	6	LEU	O-C-N	-17.88	103.50	122.09
1	I	5	GLN	O-C-N	-17.85	100.31	122.27
2	F	14	ALA	CA-C-O	-17.84	101.52	120.42
2	B	17	LEU	N-CA-C	17.77	130.34	111.14
2	D	7	CYS	CA-C-O	-17.77	101.58	120.42
2	D	5	HIS	O-C-N	-17.73	103.32	122.12
1	C	16	LEU	O-C-N	17.69	142.31	122.15
2	J	1	PHE	CA-CB-CG	17.53	131.33	113.80
1	K	13	LEU	CA-C-O	17.48	139.17	120.82
1	E	4	GLU	CA-C-O	17.43	139.54	120.90
2	H	10	HIS	ND1-CG-CD2	-17.38	88.72	106.10
2	D	10	HIS	CG-CD2-NE2	-17.27	89.93	107.20
1	A	18	ASN	OD1-CG-ND2	17.17	139.77	122.60
2	H	10	HIS	CE1-NE2-CD2	-17.04	91.96	109.00
2	L	3	ASN	OD1-CG-ND2	-16.90	105.70	122.60
2	B	10	HIS	N-CA-C	16.88	131.37	111.11
2	B	10	HIS	CG-CD2-NE2	16.83	124.03	107.20
1	C	21	ASN	CA-CB-CG	16.82	129.42	112.60
2	D	9	SER	O-C-N	-16.80	104.31	122.12
2	F	18	VAL	N-CA-C	-16.68	93.90	111.58
2	B	17	LEU	CA-C-O	16.58	137.78	120.70
2	L	18	VAL	N-CA-C	16.58	129.07	111.00
2	B	10	HIS	CA-C-O	16.56	138.62	120.90
1	A	21	ASN	OD1-CG-ND2	-16.47	106.13	122.60
2	H	9	SER	N-CA-C	-16.46	91.36	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	15	GLN	O-C-N	16.31	140.75	122.15
1	I	4	GLU	N-CA-C	-16.19	93.66	111.14
1	I	7	CYS	CA-C-N	-16.05	94.76	122.36
1	I	7	CYS	C-N-CA	-16.05	94.76	122.36
1	K	5	GLN	CA-C-O	16.03	137.41	120.42
2	D	21	GLU	N-CA-CB	-16.00	84.87	110.14
1	C	12	SER	N-CA-C	-15.95	89.75	110.33
2	D	12	VAL	O-C-N	-15.94	106.27	121.89
2	D	7	CYS	O-C-N	15.84	140.21	122.15
1	K	15	GLN	O-C-N	15.82	138.89	122.12
2	H	17	LEU	O-C-N	-15.73	105.67	122.03
1	C	2	ILE	O-C-N	15.61	139.44	121.80
2	J	14	ALA	N-CA-C	15.60	127.77	111.07
2	F	12	VAL	N-CA-C	-15.59	94.72	110.62
2	H	22	ARG	N-CA-C	-15.58	93.79	111.71
2	L	5	HIS	CA-CB-CG	-15.55	98.25	113.80
1	K	3	VAL	O-C-N	15.53	137.82	121.83
1	G	11	CYS	O-C-N	15.50	140.93	123.10
1	K	7	CYS	CA-C-O	15.47	137.59	119.18
2	F	6	LEU	CB-CA-C	-15.31	85.06	110.79
2	L	24	PHE	CA-CB-CG	15.26	129.06	113.80
1	K	5	GLN	OE1-CD-NE2	-15.21	107.39	122.60
1	E	16	LEU	O-C-N	15.15	138.18	122.12
2	J	21	GLU	O-C-N	-15.03	102.69	122.23
1	K	10	ILE	O-C-N	-15.00	103.82	122.57
2	F	3	ASN	N-CA-C	-14.98	94.95	111.28
2	F	3	ASN	CA-C-O	-14.96	104.69	120.55
2	F	14	ALA	N-CA-C	-14.94	95.08	111.36
2	D	7	CYS	N-CA-C	-14.82	95.20	111.36
2	H	17	LEU	N-CA-C	14.78	127.08	110.97
1	A	15	GLN	OE1-CD-NE2	-14.67	107.93	122.60
2	D	14	ALA	CA-C-O	-14.61	104.02	120.24
2	J	7	CYS	N-CA-C	14.61	126.91	111.14
1	E	21	ASN	CA-CB-CG	14.58	127.18	112.60
2	F	24	PHE	CA-CB-CG	-14.57	99.22	113.80
1	E	5	GLN	N-CA-C	14.53	128.67	111.82
2	F	10	HIS	CE1-NE2-CD2	14.50	123.50	109.00
2	D	24	PHE	CA-CB-CG	-14.47	99.33	113.80
2	J	8	GLY	N-CA-C	-14.47	94.03	113.27
2	L	21	GLU	N-CA-C	14.44	130.37	113.19
2	B	2	VAL	CB-CA-C	14.43	130.94	112.04
2	D	3	ASN	O-C-N	14.41	139.08	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	20	CYS	CA-C-O	14.33	137.18	121.56
2	L	11	LEU	N-CA-C	14.29	126.57	111.14
2	B	23	GLY	O-C-N	14.23	136.43	122.91
2	F	10	HIS	CG-CD2-NE2	-14.22	92.98	107.20
2	F	12	VAL	N-CA-CB	14.22	129.88	110.54
1	K	17	GLU	CA-C-O	14.08	136.53	119.49
2	H	22	ARG	CA-C-O	-14.05	104.22	120.10
2	F	7	CYS	CA-C-N	14.05	135.57	119.98
2	F	7	CYS	C-N-CA	14.05	135.57	119.98
2	F	16	TYR	N-CA-C	-14.00	96.10	111.36
2	J	5	HIS	ND1-CE1-NE2	13.99	122.39	108.40
1	K	21	ASN	CA-CB-CG	-13.95	98.65	112.60
2	B	4	GLN	CG-CD-NE2	-13.93	95.51	116.40
2	J	10	HIS	CA-CB-CG	13.87	127.67	113.80
2	B	3	ASN	O-C-N	-13.83	106.21	122.11
2	J	2	VAL	N-CA-CB	13.75	125.77	110.51
2	J	24	PHE	CA-C-O	-13.74	106.53	121.23
2	D	10	HIS	ND1-CG-CD2	13.71	119.81	106.10
1	E	8	THR	CA-C-O	13.71	137.45	120.31
1	E	6	CYS	O-C-N	13.70	138.17	122.27
1	E	8	THR	O-C-N	-13.68	103.84	122.30
1	A	14	TYR	CG-CD1-CE1	-13.66	100.71	121.20
1	G	4	GLU	CB-CA-C	-13.66	85.71	110.70
2	H	21	GLU	O-C-N	13.56	137.61	122.15
2	F	3	ASN	O-C-N	13.53	136.46	122.12
2	B	21	GLU	O-C-N	13.52	136.15	122.09
2	F	4	GLN	OE1-CD-NE2	13.52	136.12	122.60
2	F	20	GLY	CA-C-O	13.50	138.69	121.68
1	K	15	GLN	CA-C-N	-13.45	101.95	120.38
1	K	15	GLN	C-N-CA	-13.45	101.95	120.38
2	B	13	GLU	O-C-N	-13.45	108.11	122.09
2	J	22	ARG	NE-CZ-NH1	13.42	134.92	121.50
2	J	7	CYS	CB-CA-C	-13.42	89.70	110.90
1	E	12	SER	CA-C-N	-13.41	100.81	120.38
1	E	12	SER	C-N-CA	-13.41	100.81	120.38
2	J	28	LYS	CA-C-O	13.38	130.63	119.66
1	E	17	GLU	N-CA-CB	-13.29	90.12	110.06
2	F	10	HIS	N-CA-C	-13.29	95.49	112.23
2	D	20	GLY	CA-C-O	13.27	138.40	121.68
1	A	14	TYR	CB-CG-CD1	-13.23	100.95	120.80
2	F	3	ASN	N-CA-CB	13.22	129.55	110.12
2	B	10	HIS	O-C-N	-13.18	108.38	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	18	ASN	OD1-CG-ND2	-13.16	109.44	122.60
1	C	14	TYR	CA-C-O	13.15	134.63	120.82
2	D	11	LEU	O-C-N	13.12	136.26	122.09
2	D	4	GLN	CA-C-O	-13.11	106.53	120.55
1	I	7	CYS	N-CA-C	13.10	129.68	113.17
1	A	15	GLN	O-C-N	-13.09	108.59	122.07
1	C	3	VAL	N-CA-C	-13.06	98.14	110.42
2	H	24	PHE	CD1-CG-CD2	-12.94	99.19	118.60
2	B	14	ALA	CA-C-O	12.91	134.57	120.63
2	F	5	HIS	CA-CB-CG	12.89	126.69	113.80
2	H	12	VAL	O-C-N	12.78	135.61	121.94
1	K	18	ASN	N-CA-C	12.76	126.38	111.71
1	E	16	LEU	CA-C-N	-12.75	102.91	120.38
1	E	16	LEU	C-N-CA	-12.75	102.91	120.38
2	B	4	GLN	OE1-CD-NE2	12.73	135.33	122.60
1	E	8	THR	OG1-CB-CG2	-12.71	83.88	109.30
1	G	14	TYR	O-C-N	12.71	136.63	122.15
2	J	18	VAL	CB-CA-C	-12.69	95.24	112.24
1	C	6	CYS	O-C-N	12.67	137.57	122.24
2	D	14	ALA	O-C-N	12.65	138.68	122.23
2	F	20	GLY	O-C-N	-12.65	108.32	122.61
1	C	4	GLU	CA-C-O	12.64	134.28	120.63
2	F	19	CYS	N-CA-CB	12.62	129.26	110.33
2	D	10	HIS	CE1-NE2-CD2	12.61	121.61	109.00
1	A	21	ASN	CA-CB-CG	12.58	125.18	112.60
2	F	10	HIS	N-CA-CB	12.57	129.66	110.30
1	I	13	LEU	CA-C-O	12.55	134.19	120.63
1	E	2	ILE	CA-C-N	-12.52	100.69	120.47
1	E	2	ILE	C-N-CA	-12.52	100.69	120.47
2	J	17	LEU	N-CA-C	-12.51	96.20	111.33
2	F	17	LEU	N-CA-CB	12.48	128.80	110.20
2	J	29	PRO	N-CD-CG	-12.47	84.49	103.20
2	F	13	GLU	CB-CA-C	-12.37	88.06	110.70
1	C	12	SER	O-C-N	12.36	137.27	122.68
2	B	24	PHE	CA-C-O	12.34	134.67	121.10
1	I	17	GLU	O-C-N	-12.32	106.37	122.39
2	L	22	ARG	NH1-CZ-NH2	12.29	135.28	119.30
2	H	24	PHE	CA-C-N	-12.29	99.58	121.70
2	H	24	PHE	C-N-CA	-12.29	99.58	121.70
2	J	5	HIS	CG-ND1-CE1	-12.28	88.42	109.30
2	L	11	LEU	CA-C-O	12.25	133.32	120.70
2	H	25	TYR	N-CA-CB	-12.24	89.69	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	18	ASN	CA-C-O	-12.22	104.35	119.38
2	B	12	VAL	O-C-N	12.21	134.15	121.94
1	E	5	GLN	N-CA-CB	-12.21	91.36	110.28
2	J	5	HIS	CB-CG-ND1	-12.19	104.41	122.70
1	G	8	THR	CA-CB-CG2	-12.17	89.82	110.50
2	J	28	LYS	N-CA-CB	12.15	128.30	110.32
2	H	2	VAL	CB-CA-C	12.11	128.49	112.14
2	J	8	GLY	CA-C-O	-12.11	108.10	120.45
1	G	5	GLN	CA-C-O	-12.10	106.81	120.24
1	C	10	ILE	CA-CB-CG1	12.09	130.96	110.40
1	K	16	LEU	N-CA-CB	-12.07	91.95	110.06
2	F	13	GLU	CB-CG-CD	-12.07	92.09	112.60
1	E	15	GLN	N-CA-CB	-12.06	91.64	110.22
2	L	11	LEU	CB-CA-C	-12.04	91.88	110.90
1	I	12	SER	CB-CA-C	-12.03	87.55	111.60
1	K	18	ASN	CA-CB-CG	-12.01	100.59	112.60
2	J	28	LYS	N-CA-C	-11.99	94.73	109.72
1	I	16	LEU	N-CA-C	-11.98	97.93	111.71
2	B	19	CYS	N-CA-C	11.90	127.98	113.23
1	K	3	VAL	CA-C-N	-11.85	104.41	120.28
1	K	3	VAL	C-N-CA	-11.85	104.41	120.28
2	D	3	ASN	N-CA-CB	11.84	128.46	110.22
2	H	21	GLU	CA-C-O	-11.81	107.90	120.42
2	H	14	ALA	CA-C-O	11.80	133.06	120.55
2	D	10	HIS	CA-CB-CG	-11.80	102.00	113.80
1	G	9	SER	CA-C-N	-11.79	106.79	123.06
1	G	9	SER	C-N-CA	-11.79	106.79	123.06
2	D	10	HIS	N-CA-CB	11.79	128.45	110.30
1	G	6	CYS	CA-C-O	11.79	133.35	119.32
1	I	18	ASN	O-C-N	11.77	138.71	122.46
1	E	12	SER	N-CA-C	-11.76	85.74	110.80
2	D	17	LEU	N-CA-CB	11.71	127.65	110.20
2	J	5	HIS	CG-CD2-NE2	-11.71	95.49	107.20
1	I	3	VAL	O-C-N	11.70	139.59	122.04
1	G	3	VAL	N-CA-CB	11.70	125.09	110.47
2	D	4	GLN	OE1-CD-NE2	11.69	134.29	122.60
1	I	13	LEU	N-CA-C	11.69	125.47	111.33
1	I	3	VAL	CA-C-O	-11.68	107.65	119.92
2	B	8	GLY	O-C-N	11.66	135.75	122.34
2	B	9	SER	CB-CA-C	11.66	129.47	110.81
1	I	18	ASN	CA-CB-CG	-11.66	100.94	112.60
2	F	6	LEU	N-CA-CB	11.63	127.34	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4	GLU	O-C-N	-11.62	110.00	122.09
2	H	27	THR	CA-CB-OG1	-11.62	92.17	109.60
2	J	16	TYR	CB-CG-CD1	-11.57	103.45	120.80
1	E	13	LEU	N-CA-CB	-11.54	91.90	110.14
1	K	13	LEU	N-CA-C	11.54	123.41	111.07
2	D	22	ARG	CA-C-O	11.53	137.00	120.51
2	B	9	SER	N-CA-C	-11.52	97.28	111.11
2	F	16	TYR	CA-C-N	11.52	140.28	120.58
2	F	16	TYR	C-N-CA	11.52	140.28	120.58
2	F	13	GLU	CA-C-N	11.51	136.63	120.29
2	F	13	GLU	C-N-CA	11.51	136.63	120.29
2	B	12	VAL	CA-C-N	-11.50	105.01	120.54
2	B	12	VAL	C-N-CA	-11.50	105.01	120.54
2	J	24	PHE	N-CA-CB	-11.47	93.78	111.56
2	B	3	ASN	CA-C-O	11.46	133.76	120.92
1	E	2	ILE	O-C-N	11.46	139.23	122.04
2	H	6	LEU	O-C-N	-11.45	109.73	122.09
2	H	16	TYR	N-CA-C	-11.41	97.41	111.11
2	B	5	HIS	O-C-N	11.40	133.89	122.03
1	I	20	CYS	O-C-N	-11.40	109.41	122.86
1	C	19	TYR	O-C-N	11.39	136.03	122.24
2	J	16	TYR	CG-CD1-CE1	-11.39	104.11	121.20
2	L	21	GLU	CA-C-O	11.37	137.10	118.91
2	D	19	CYS	N-CA-C	-11.34	99.17	113.23
2	L	10	HIS	CB-CA-C	11.33	131.59	110.63
1	A	14	TYR	CZ-CE2-CD2	-11.32	99.22	119.60
1	K	18	ASN	O-C-N	11.31	135.46	122.22
1	E	19	TYR	CA-C-N	-11.30	103.68	120.75
1	E	19	TYR	C-N-CA	-11.30	103.68	120.75
2	L	5	HIS	CE1-NE2-CD2	11.30	120.30	109.00
2	J	12	VAL	CA-C-O	-11.30	108.62	120.71
1	A	18	ASN	CA-C-O	-11.29	108.44	120.63
2	H	14	ALA	N-CA-C	11.29	123.59	111.28
1	K	7	CYS	CA-C-N	-11.26	102.99	122.36
1	K	7	CYS	C-N-CA	-11.26	102.99	122.36
2	H	24	PHE	CE1-CZ-CE2	-11.26	99.73	120.00
2	L	12	VAL	N-CA-C	-11.22	97.06	111.09
1	G	18	ASN	CA-CB-CG	11.21	123.81	112.60
1	C	11	CYS	N-CA-CB	-11.20	91.69	110.16
1	A	6	CYS	O-C-N	-11.19	108.58	122.35
2	B	10	HIS	CB-CG-CD2	11.14	145.69	131.20
2	B	13	GLU	N-CA-CB	-11.13	93.35	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2	ILE	CA-C-O	-11.12	108.46	120.47
2	B	27	THR	N-CA-CB	-11.11	92.61	111.50
2	L	23	GLY	CA-C-O	-11.11	108.43	122.65
2	L	9	SER	N-CA-C	11.09	123.06	110.97
1	K	1	GLY	O-C-N	-11.09	105.26	123.00
2	H	18	VAL	CA-C-N	-11.08	103.09	122.26
2	H	18	VAL	C-N-CA	-11.08	103.09	122.26
2	L	10	HIS	N-CA-C	-11.07	98.98	111.71
2	B	24	PHE	CG-CD2-CE2	11.07	139.51	120.70
2	L	16	TYR	CD1-CG-CD2	11.07	134.70	118.10
2	H	24	PHE	CA-C-O	11.06	136.33	120.51
1	G	14	TYR	N-CA-CB	11.06	126.53	110.16
2	H	13	GLU	O-C-N	-11.06	110.59	122.09
2	L	8	GLY	N-CA-C	-11.05	98.57	113.27
1	E	4	GLU	CB-CG-CD	11.05	131.39	112.60
1	I	8	THR	CB-CA-C	11.04	126.92	109.03
2	H	17	LEU	CA-C-O	10.98	132.53	121.00
1	K	2	ILE	CA-C-O	10.98	132.32	120.57
2	B	17	LEU	O-C-N	-10.97	110.24	122.09
2	H	5	HIS	CA-CB-CG	10.93	124.73	113.80
2	H	10	HIS	CA-C-O	10.91	131.98	120.42
1	I	19	TYR	N-CA-C	-10.90	99.65	113.16
2	F	10	HIS	ND1-CE1-NE2	-10.88	97.52	108.40
2	F	2	VAL	CA-C-N	10.88	134.86	120.28
2	F	2	VAL	C-N-CA	10.88	134.86	120.28
2	H	7	CYS	N-CA-CB	10.88	126.37	110.06
2	F	22	ARG	CA-C-N	-10.87	101.86	121.32
2	F	22	ARG	C-N-CA	-10.87	101.86	121.32
2	B	24	PHE	CB-CG-CD2	10.84	139.13	120.70
2	F	24	PHE	CB-CA-C	10.84	130.77	110.62
1	I	8	THR	N-CA-CB	-10.81	96.22	110.59
1	A	14	TYR	CA-C-O	-10.81	109.47	120.82
2	L	12	VAL	CB-CA-C	10.79	129.73	112.26
2	D	18	VAL	CB-CA-C	-10.77	98.37	111.94
2	H	23	GLY	O-C-N	10.75	134.12	123.05
2	H	27	THR	N-CA-CB	-10.75	93.22	111.50
2	H	5	HIS	O-C-N	10.74	133.69	122.09
1	A	4	GLU	CB-CA-C	-10.74	92.59	110.85
2	B	6	LEU	N-CA-C	10.72	123.98	111.11
1	A	16	LEU	N-CA-C	-10.70	99.49	112.54
1	A	12	SER	N-CA-CB	10.69	125.03	110.38
2	L	3	ASN	CA-CB-CG	10.62	123.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	24	PHE	O-C-N	-10.59	111.18	123.25
1	C	7	CYS	N-CA-C	-10.58	100.42	113.97
1	C	18	ASN	O-C-N	-10.58	108.52	122.59
2	H	10	HIS	CB-CG-CD2	10.57	144.95	131.20
2	J	3	ASN	CB-CG-ND2	10.56	132.25	116.40
1	K	9	SER	N-CA-CB	-10.54	92.96	110.68
2	J	17	LEU	CB-CA-C	10.53	128.59	110.68
2	H	23	GLY	N-CA-C	-10.52	90.36	112.45
2	F	15	LEU	N-CA-CB	10.51	125.31	110.07
2	H	14	ALA	O-C-N	-10.48	111.01	122.12
1	C	11	CYS	CB-CA-C	10.47	126.97	109.80
1	K	14	TYR	CA-C-N	-10.46	106.27	120.28
1	K	14	TYR	C-N-CA	-10.46	106.27	120.28
1	C	15	GLN	N-CA-C	10.45	123.73	111.71
2	H	10	HIS	N-CA-C	10.45	122.75	111.36
2	J	10	HIS	ND1-CG-CD2	-10.43	95.67	106.10
1	K	8	THR	O-C-N	10.42	136.32	122.36
2	D	19	CYS	CA-C-O	-10.41	107.09	119.27
2	H	22	ARG	NE-CZ-NH2	10.40	128.56	119.20
2	H	4	GLN	CA-C-O	-10.38	108.03	119.97
1	A	9	SER	N-CA-CB	10.36	130.81	111.53
2	F	9	SER	CA-C-N	10.35	138.28	120.68
2	F	9	SER	C-N-CA	10.35	138.28	120.68
1	K	18	ASN	CA-C-N	-10.34	101.42	121.58
1	K	18	ASN	C-N-CA	-10.34	101.42	121.58
2	J	29	PRO	CA-N-CD	10.33	126.46	112.00
1	E	20	CYS	CB-CA-C	10.33	128.11	109.62
2	B	5	HIS	CA-C-N	-10.32	106.61	120.54
2	B	5	HIS	C-N-CA	-10.32	106.61	120.54
2	F	16	TYR	CA-C-O	-10.31	109.49	120.42
1	G	16	LEU	CD1-CG-CD2	-10.31	88.12	110.80
1	A	5	GLN	OE1-CD-NE2	-10.30	112.30	122.60
1	C	5	GLN	N-CA-C	10.28	122.57	111.36
1	E	9	SER	N-CA-C	-10.28	95.03	110.14
2	D	16	TYR	CA-C-N	10.27	138.15	120.58
2	D	16	TYR	C-N-CA	10.27	138.15	120.58
1	A	20	CYS	CB-CA-C	-10.26	91.97	109.51
1	K	2	ILE	N-CA-C	10.24	123.85	111.05
2	B	22	ARG	O-C-N	-10.23	111.27	122.12
1	I	19	TYR	CB-CG-CD2	-10.23	105.45	120.80
2	L	5	HIS	CA-C-O	-10.22	110.17	120.70
2	F	13	GLU	N-CA-CB	10.21	125.42	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	25	TYR	CA-CB-CG	10.21	132.27	113.90
2	B	1	PHE	CA-C-N	-10.20	106.15	120.53
2	B	1	PHE	C-N-CA	-10.20	106.15	120.53
2	B	2	VAL	CA-CB-CG2	10.19	127.72	110.40
2	L	15	LEU	CA-C-N	-10.19	107.19	120.44
2	L	15	LEU	C-N-CA	-10.19	107.19	120.44
2	D	11	LEU	N-CA-C	-10.18	100.15	111.14
2	L	18	VAL	O-C-N	-10.16	108.43	121.84
2	B	24	PHE	O-C-N	-10.16	113.41	123.46
1	C	10	ILE	N-CA-CB	10.15	124.57	110.56
2	D	5	HIS	CA-CB-CG	10.13	123.93	113.80
2	D	6	LEU	CB-CA-C	-10.13	92.16	110.70
1	G	19	TYR	N-CA-C	10.13	125.17	113.02
2	F	10	HIS	CB-CG-CD2	-10.13	118.04	131.20
1	G	12	SER	O-C-N	-10.12	111.31	122.85
1	G	20	CYS	CB-CA-C	-10.13	92.93	110.45
2	H	3	ASN	CA-C-O	10.12	131.45	120.82
2	B	16	TYR	CB-CA-C	10.12	130.55	110.42
1	A	5	GLN	O-C-N	10.10	133.67	122.15
1	K	6	CYS	N-CA-CB	-10.10	95.36	110.61
1	G	15	GLN	CA-C-N	10.07	135.08	120.38
1	G	15	GLN	C-N-CA	10.07	135.08	120.38
1	I	7	CYS	CA-C-O	10.06	131.12	119.35
1	E	3	VAL	CB-CA-C	10.06	127.75	112.16
2	J	21	GLU	N-CA-C	10.05	124.05	111.69
2	B	27	THR	CA-CB-CG2	-10.04	93.43	110.50
2	L	19	CYS	O-C-N	10.04	136.31	122.46
1	E	11	CYS	CB-CA-C	10.03	126.26	109.80
2	B	25	TYR	CB-CG-CD1	-10.03	105.76	120.80
2	J	27	THR	CA-CB-OG1	10.02	124.62	109.60
1	A	14	TYR	CG-CD2-CE2	10.01	136.22	121.20
2	L	1	PHE	CG-CD2-CE2	10.01	137.72	120.70
2	B	25	TYR	CG-CD1-CE1	-9.99	106.22	121.20
1	C	12	SER	CA-CB-OG	-9.99	91.13	111.10
1	G	15	GLN	CA-C-O	-9.99	109.86	120.55
1	K	11	CYS	N-CA-CB	9.97	125.11	110.06
2	L	8	GLY	O-C-N	9.97	132.46	122.19
1	A	10	ILE	N-CA-C	9.96	121.75	109.30
2	D	15	LEU	N-CA-C	-9.96	100.38	111.14
2	H	9	SER	CB-CA-C	9.96	126.74	110.81
1	G	17	GLU	CB-CA-C	-9.95	89.19	109.99
1	E	8	THR	N-CA-C	9.95	126.36	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	PHE	CB-CG-CD2	9.93	137.58	120.70
1	G	21	ASN	CA-CB-CG	9.93	122.53	112.60
2	F	4	GLN	CG-CD-NE2	-9.92	101.52	116.40
2	D	20	GLY	CA-C-N	-9.91	105.92	120.38
2	D	20	GLY	C-N-CA	-9.91	105.92	120.38
2	B	24	PHE	CD1-CE1-CZ	9.90	137.81	120.00
1	E	14	TYR	N-CA-C	9.89	122.98	111.11
1	G	13	LEU	CB-CA-C	-9.88	92.35	110.63
2	J	10	HIS	ND1-CE1-NE2	-9.88	98.52	108.40
1	G	6	CYS	N-CA-C	9.88	126.53	113.30
2	J	6	LEU	N-CA-C	-9.87	99.39	111.33
2	F	5	HIS	N-CA-CB	9.86	124.85	110.06
1	I	19	TYR	CG-CD2-CE2	-9.85	106.43	121.20
1	E	5	GLN	CA-C-O	9.84	131.28	119.97
2	J	4	GLN	O-C-N	9.83	132.54	122.12
1	I	6	CYS	CA-C-O	9.82	130.04	119.34
2	F	11	LEU	CA-C-N	9.82	133.91	120.46
2	F	11	LEU	C-N-CA	9.82	133.91	120.46
2	B	19	CYS	N-CA-CB	-9.79	95.17	110.44
1	I	8	THR	CA-CB-OG1	-9.79	94.92	109.60
1	K	20	CYS	CA-C-O	9.77	131.94	121.19
1	E	18	ASN	O-C-N	-9.77	109.60	122.59
2	L	4	GLN	CG-CD-NE2	9.76	131.03	116.40
2	J	27	THR	O-C-N	-9.74	107.42	123.00
1	K	17	GLU	N-CA-C	9.73	124.26	112.38
1	A	14	TYR	CB-CG-CD2	9.73	135.40	120.80
2	F	11	LEU	CB-CA-C	-9.73	94.44	110.79
2	J	18	VAL	O-C-N	-9.72	109.00	121.84
1	I	17	GLU	CA-C-O	9.69	131.21	119.49
1	A	15	GLN	N-CA-C	9.69	121.43	111.07
2	L	25	TYR	CB-CG-CD2	9.68	135.32	120.80
1	I	6	CYS	N-CA-C	9.68	127.44	113.02
1	E	12	SER	CA-CB-OG	-9.67	91.76	111.10
1	E	9	SER	O-C-N	9.67	136.41	122.97
1	K	13	LEU	O-C-N	-9.66	112.12	122.07
2	F	5	HIS	N-CA-C	-9.65	99.66	111.33
1	C	18	ASN	CB-CG-ND2	9.64	130.85	116.40
1	I	1	GLY	O-C-N	-9.62	107.60	123.00
1	K	16	LEU	CB-CA-C	9.61	127.01	110.68
2	B	3	ASN	N-CA-C	9.60	127.20	111.37
2	J	3	ASN	CA-C-O	-9.59	110.25	120.42
2	J	1	PHE	CA-C-N	9.58	132.96	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	PHE	C-N-CA	9.58	132.96	120.60
2	H	24	PHE	CG-CD2-CE2	9.56	136.96	120.70
2	H	1	PHE	O-C-N	9.56	138.30	123.00
2	F	7	CYS	O-C-N	9.55	132.25	122.12
1	K	17	GLU	CB-CG-CD	9.56	128.84	112.60
2	H	6	LEU	CA-C-N	9.55	133.46	120.38
2	H	6	LEU	C-N-CA	9.55	133.46	120.38
2	J	19	CYS	O-C-N	9.54	136.36	122.43
2	F	3	ASN	OD1-CG-ND2	9.54	132.14	122.60
1	G	13	LEU	CA-C-N	9.52	133.81	120.29
1	G	13	LEU	C-N-CA	9.52	133.81	120.29
2	B	21	GLU	CA-C-O	-9.49	110.75	120.90
2	J	22	ARG	O-C-N	9.48	133.01	122.20
2	J	18	VAL	CA-C-O	9.48	130.86	120.71
2	L	7	CYS	CB-CA-C	-9.48	93.35	110.70
2	D	18	VAL	N-CA-C	-9.48	101.54	111.58
2	J	21	GLU	CB-CG-CD	-9.47	96.50	112.60
1	E	16	LEU	N-CA-C	9.45	121.58	111.28
2	L	1	PHE	CD1-CE1-CZ	9.42	136.95	120.00
1	K	14	TYR	CA-CB-CG	-9.40	96.97	113.90
2	B	2	VAL	O-C-N	-9.40	112.68	121.89
1	A	11	CYS	O-C-N	9.40	134.06	123.16
2	H	24	PHE	CB-CG-CD2	9.37	136.63	120.70
1	A	16	LEU	CD1-CG-CD2	-9.37	90.19	110.80
1	G	3	VAL	N-CA-C	-9.36	99.95	110.62
2	J	11	LEU	CA-C-O	9.35	130.46	120.55
2	L	6	LEU	N-CA-C	-9.35	100.02	111.33
1	G	16	LEU	N-CA-C	-9.34	99.80	111.75
2	L	17	LEU	CB-CA-C	9.34	125.75	110.81
1	K	12	SER	CB-CA-C	-9.33	92.93	111.60
2	L	16	TYR	CA-C-O	-9.33	111.03	120.82
2	J	28	LYS	CB-CA-C	9.30	122.93	109.08
2	L	22	ARG	N-CA-CB	-9.30	95.93	110.44
2	J	16	TYR	CZ-CE2-CD2	-9.28	102.90	119.60
1	A	8	THR	CA-CB-CG2	-9.27	94.74	110.50
2	F	22	ARG	CA-C-O	9.27	133.76	120.51
2	F	17	LEU	CB-CA-C	-9.26	93.75	110.70
2	H	6	LEU	N-CA-C	-9.26	101.14	111.14
2	D	17	LEU	CB-CA-C	-9.25	93.78	110.70
2	B	22	ARG	N-CA-C	-9.23	100.16	111.33
2	D	12	VAL	CA-C-N	9.23	133.40	120.29
2	D	12	VAL	C-N-CA	9.23	133.40	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	11	LEU	N-CA-C	-9.22	100.15	111.40
2	B	1	PHE	O-C-N	9.21	137.74	123.00
2	F	4	GLN	CA-C-O	-9.21	110.69	120.55
1	A	20	CYS	CA-C-N	9.20	138.26	121.70
1	A	20	CYS	C-N-CA	9.20	138.26	121.70
2	L	2	VAL	N-CA-C	9.20	119.25	110.42
2	D	22	ARG	CA-C-N	-9.19	108.11	121.44
2	D	22	ARG	C-N-CA	-9.19	108.11	121.44
2	J	22	ARG	NE-CZ-NH2	-9.17	110.95	119.20
2	J	4	GLN	CB-CG-CD	9.16	128.18	112.60
2	D	2	VAL	CA-C-N	9.16	133.47	120.28
2	D	2	VAL	C-N-CA	9.16	133.47	120.28
1	G	4	GLU	N-CA-C	9.14	122.94	111.69
1	G	8	THR	CB-CA-C	-9.12	94.23	109.55
2	J	18	VAL	CG1-CB-CG2	9.12	130.86	110.80
2	H	24	PHE	N-CA-C	-9.11	91.40	110.80
2	B	15	LEU	O-C-N	9.10	134.52	122.33
1	E	11	CYS	N-CA-C	-9.09	94.37	109.46
1	A	7	CYS	N-CA-CB	9.09	124.73	110.46
2	J	13	GLU	N-CA-CB	9.09	123.48	109.94
1	A	11	CYS	N-CA-C	9.08	125.21	109.96
1	C	10	ILE	CA-C-N	-9.08	109.39	122.19
1	C	10	ILE	C-N-CA	-9.08	109.39	122.19
2	B	25	TYR	CB-CG-CD2	9.05	134.38	120.80
2	J	15	LEU	N-CA-C	-9.05	101.30	111.71
2	F	21	GLU	N-CA-C	9.04	123.32	111.75
1	E	20	CYS	N-CA-CB	-9.04	96.75	110.04
2	F	4	GLN	CA-C-N	9.03	132.75	120.38
2	F	4	GLN	C-N-CA	9.03	132.75	120.38
2	D	24	PHE	O-C-N	-9.03	113.76	123.42
2	J	1	PHE	CB-CA-C	9.02	127.25	110.10
2	B	14	ALA	N-CA-C	9.01	122.23	111.33
2	F	24	PHE	CA-C-O	9.01	130.87	121.23
1	G	11	CYS	CA-C-O	-9.01	110.65	121.28
2	D	24	PHE	N-CA-CB	-9.00	97.60	111.56
1	E	20	CYS	CA-C-O	-9.00	112.01	121.55
1	E	10	ILE	O-C-N	8.99	133.65	122.59
1	A	17	GLU	O-C-N	8.99	131.44	122.09
1	K	14	TYR	N-CA-CB	-8.98	96.39	110.22
2	B	18	VAL	CA-C-N	-8.96	105.90	121.66
2	B	18	VAL	C-N-CA	-8.96	105.90	121.66
2	D	2	VAL	O-C-N	-8.94	108.69	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	9	SER	N-CA-CB	-8.94	96.55	110.85
2	D	14	ALA	N-CA-C	-8.94	100.70	111.69
1	E	2	ILE	CB-CA-C	-8.92	99.08	111.65
1	E	18	ASN	CA-C-O	8.92	133.26	120.51
2	L	16	TYR	N-CA-C	8.91	120.60	111.07
2	H	17	LEU	CD1-CG-CD2	8.90	130.38	110.80
2	F	15	LEU	CA-C-O	-8.90	111.54	120.70
1	I	19	TYR	CD1-CE1-CZ	-8.90	103.58	119.60
1	I	3	VAL	CB-CA-C	-8.88	99.12	111.65
1	E	19	TYR	CD1-CG-CD2	8.87	131.41	118.10
2	B	17	LEU	N-CA-CB	-8.86	97.22	110.07
1	G	14	TYR	CA-C-O	-8.86	111.03	120.42
2	D	21	GLU	N-CA-C	8.86	123.09	111.75
2	H	4	GLN	OE1-CD-NE2	8.86	131.46	122.60
2	H	13	GLU	N-CA-C	-8.85	100.49	111.11
2	H	15	LEU	O-C-N	8.85	134.18	122.33
2	H	24	PHE	CD1-CE1-CZ	8.85	135.92	120.00
1	A	6	CYS	CA-C-N	8.84	138.51	122.06
1	A	6	CYS	C-N-CA	8.84	138.51	122.06
2	B	22	ARG	NH1-CZ-NH2	-8.84	107.81	119.30
1	C	13	LEU	N-CA-C	-8.84	100.64	111.33
2	B	20	GLY	CA-C-N	8.82	132.44	120.54
2	B	20	GLY	C-N-CA	8.82	132.44	120.54
1	I	15	GLN	CB-CG-CD	-8.82	97.61	112.60
2	B	25	TYR	CG-CD2-CE2	8.81	134.42	121.20
1	C	1	GLY	O-C-N	-8.81	108.90	123.00
1	G	21	ASN	CB-CG-ND2	8.81	129.62	116.40
1	I	19	TYR	CA-C-O	-8.81	108.62	119.28
2	D	13	GLU	O-C-N	-8.79	112.13	122.15
1	G	14	TYR	CD1-CG-CD2	8.79	131.29	118.10
1	E	20	CYS	CA-CB-SG	8.76	134.56	114.40
1	E	16	LEU	CA-C-O	8.76	129.83	120.55
1	E	5	GLN	CA-CB-CG	-8.75	96.59	114.10
2	J	9	SER	N-CA-C	8.75	120.51	110.97
1	C	14	TYR	CB-CA-C	8.75	124.62	110.88
2	D	10	HIS	O-C-N	8.74	134.04	122.33
2	B	22	ARG	CA-C-N	8.74	136.96	121.32
2	B	22	ARG	C-N-CA	8.74	136.96	121.32
1	K	18	ASN	OD1-CG-ND2	8.74	131.34	122.60
1	I	5	GLN	CG-CD-NE2	8.72	129.48	116.40
2	J	16	TYR	N-CA-C	8.72	120.56	111.14
1	A	16	LEU	CA-C-N	8.71	132.30	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	LEU	C-N-CA	8.71	132.30	120.54
2	L	15	LEU	N-CA-CB	8.71	122.93	110.12
2	L	25	TYR	CG-CD2-CE2	8.71	134.27	121.20
2	D	3	ASN	CA-C-O	-8.71	110.26	120.10
2	F	22	ARG	CB-CG-CD	8.70	131.31	111.30
1	I	15	GLN	CG-CD-NE2	-8.70	103.35	116.40
2	L	10	HIS	ND1-CG-CD2	-8.69	97.41	106.10
1	A	10	ILE	N-CA-CB	-8.68	99.63	110.31
1	K	16	LEU	O-C-N	-8.68	112.92	122.12
1	G	16	LEU	N-CA-CB	8.67	123.84	110.14
2	J	18	VAL	CA-CB-CG2	-8.65	95.69	110.40
1	K	2	ILE	O-C-N	-8.64	113.14	121.87
1	E	13	LEU	CA-C-N	-8.63	108.89	120.54
1	E	13	LEU	C-N-CA	-8.63	108.89	120.54
1	C	15	GLN	CA-C-O	8.62	129.84	120.10
1	E	15	GLN	CA-C-O	8.61	129.82	120.10
2	B	25	TYR	CZ-CE2-CD2	-8.59	104.14	119.60
2	F	9	SER	CA-C-O	-8.58	110.71	120.24
2	F	12	VAL	O-C-N	-8.58	113.55	121.87
1	E	19	TYR	N-CA-C	8.58	123.98	113.17
2	D	16	TYR	N-CA-C	-8.57	101.94	111.28
2	H	12	VAL	CA-CB-CG2	-8.56	95.84	110.40
1	C	10	ILE	O-C-N	8.55	132.75	122.83
2	D	12	VAL	CA-CB-CG1	8.55	124.94	110.40
1	I	18	ASN	CB-CG-ND2	-8.54	103.59	116.40
2	L	18	VAL	CA-CB-CG2	-8.54	95.88	110.40
1	G	15	GLN	OE1-CD-NE2	8.54	131.14	122.60
1	A	5	GLN	N-CA-CB	8.53	122.79	110.16
2	F	5	HIS	CA-C-N	8.52	134.93	120.71
2	F	5	HIS	C-N-CA	8.52	134.93	120.71
2	J	12	VAL	CA-CB-CG1	-8.52	95.92	110.40
2	L	14	ALA	CA-C-N	8.50	131.67	120.28
2	L	14	ALA	C-N-CA	8.50	131.67	120.28
2	D	6	LEU	CB-CG-CD1	-8.50	85.21	110.70
2	J	28	LYS	O-C-N	-8.49	109.23	121.54
2	L	16	TYR	CB-CA-C	-8.49	97.55	110.88
2	F	13	GLU	O-C-N	-8.46	111.24	122.23
1	C	8	THR	CA-C-N	8.45	135.90	122.21
1	C	8	THR	C-N-CA	8.45	135.90	122.21
2	D	22	ARG	CG-CD-NE	8.45	130.58	112.00
2	L	12	VAL	CA-C-O	-8.44	111.35	120.47
2	J	22	ARG	CA-C-O	-8.44	110.75	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	25	TYR	CA-C-O	-8.42	106.49	120.80
2	B	27	THR	CA-CB-OG1	8.42	122.23	109.60
2	L	3	ASN	CA-C-N	8.39	131.52	120.28
2	L	3	ASN	C-N-CA	8.39	131.52	120.28
1	G	7	CYS	N-CA-CB	8.38	122.32	110.67
2	L	17	LEU	N-CA-C	-8.38	101.05	111.11
2	L	5	HIS	CB-CG-CD2	-8.38	120.31	131.20
2	D	8	GLY	O-C-N	-8.37	113.84	122.13
2	F	10	HIS	ND1-CG-CD2	8.36	114.46	106.10
2	D	3	ASN	OD1-CG-ND2	8.36	130.96	122.60
2	B	2	VAL	N-CA-CB	-8.36	100.03	110.47
1	E	19	TYR	O-C-N	8.35	132.78	122.34
2	D	18	VAL	O-C-N	8.35	137.78	121.91
2	H	13	GLU	CA-CB-CG	8.35	130.79	114.10
1	I	14	TYR	N-CA-C	8.34	121.42	111.33
2	D	23	GLY	O-C-N	8.34	130.69	122.77
2	L	4	GLN	CA-C-N	-8.33	109.11	120.44
2	L	4	GLN	C-N-CA	-8.33	109.11	120.44
2	F	14	ALA	N-CA-CB	8.33	122.49	110.16
2	J	11	LEU	CA-C-N	-8.33	107.22	120.55
2	J	11	LEU	C-N-CA	-8.33	107.22	120.55
2	D	19	CYS	CA-C-N	8.33	136.31	120.07
2	D	19	CYS	C-N-CA	8.33	136.31	120.07
2	J	21	GLU	CA-C-O	8.32	129.48	120.24
2	F	18	VAL	CB-CA-C	-8.32	101.45	111.94
1	I	2	ILE	O-C-N	-8.32	113.50	121.90
1	G	11	CYS	CA-CB-SG	-8.32	95.27	114.40
1	G	21	ASN	CB-CG-OD1	-8.32	104.17	120.80
1	G	9	SER	N-CA-CB	8.32	125.56	110.76
2	L	4	GLN	O-C-N	8.31	130.93	122.12
2	H	2	VAL	CG1-CB-CG2	-8.30	92.53	110.80
2	H	12	VAL	CB-CA-C	-8.30	101.16	111.87
2	J	12	VAL	N-CA-C	-8.30	101.96	111.00
1	I	7	CYS	CA-CB-SG	-8.29	95.32	114.40
1	I	15	GLN	OE1-CD-NE2	8.29	130.89	122.60
1	E	15	GLN	CA-C-N	-8.29	109.17	120.28
1	E	15	GLN	C-N-CA	-8.29	109.17	120.28
1	K	10	ILE	CA-C-N	8.29	133.28	121.42
1	K	10	ILE	C-N-CA	8.29	133.28	121.42
1	A	14	TYR	CD1-CE1-CZ	8.29	134.52	119.60
2	D	3	ASN	N-CA-C	-8.28	102.18	111.71
2	F	13	GLU	CA-CB-CG	-8.28	97.54	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	15	LEU	CA-C-O	-8.27	110.03	119.79
2	D	21	GLU	CA-C-O	8.27	129.46	120.20
1	E	13	LEU	O-C-N	8.26	131.61	122.20
2	L	2	VAL	N-CA-CB	8.24	120.20	110.55
2	H	3	ASN	N-CA-C	8.23	119.88	111.07
2	J	5	HIS	CA-C-N	8.22	131.64	120.38
2	J	5	HIS	C-N-CA	8.22	131.64	120.38
1	E	17	GLU	O-C-N	-8.22	113.41	122.12
2	F	14	ALA	O-C-N	8.21	131.51	122.15
2	H	13	GLU	CB-CA-C	8.21	123.94	110.81
1	G	9	SER	N-CA-C	-8.20	98.11	108.45
2	J	28	LYS	CG-CD-CE	8.21	130.17	111.30
1	C	19	TYR	CD1-CG-CD2	8.20	130.40	118.10
1	K	19	TYR	N-CA-CB	-8.20	96.63	110.41
2	H	21	GLU	CB-CA-C	-8.19	96.93	110.85
1	K	6	CYS	N-CA-C	8.19	124.27	113.30
2	B	13	GLU	CA-C-O	8.17	129.65	120.90
1	E	19	TYR	CA-CB-CG	-8.16	99.21	113.90
2	J	17	LEU	CD1-CG-CD2	-8.16	92.85	110.80
2	F	15	LEU	CA-C-N	8.15	131.86	120.29
2	F	15	LEU	C-N-CA	8.15	131.86	120.29
1	I	10	ILE	CA-C-O	8.15	130.33	121.04
2	L	9	SER	CB-CA-C	-8.15	98.41	110.96
2	B	1	PHE	CD1-CG-CD2	8.14	130.81	118.60
2	F	21	GLU	CA-C-O	8.12	129.29	120.20
2	F	5	HIS	CA-C-O	-8.11	111.88	120.63
2	B	1	PHE	CB-CG-CD2	-8.10	106.92	120.70
2	H	27	THR	OG1-CB-CG2	8.10	125.51	109.30
1	G	10	ILE	CA-C-O	8.10	130.15	120.67
2	J	3	ASN	OD1-CG-ND2	-8.09	114.51	122.60
2	B	6	LEU	N-CA-CB	-8.08	97.90	109.94
2	F	6	LEU	CB-CG-CD1	-8.07	86.48	110.70
2	H	13	GLU	CA-C-N	8.07	131.10	120.28
2	H	13	GLU	C-N-CA	8.07	131.10	120.28
1	K	8	THR	CB-CA-C	8.05	122.07	109.03
2	L	12	VAL	N-CA-CB	-8.04	96.21	110.77
2	F	14	ALA	CA-C-N	8.04	131.38	120.44
2	F	14	ALA	C-N-CA	8.04	131.38	120.44
2	B	3	ASN	OD1-CG-ND2	8.03	130.63	122.60
2	J	16	TYR	CD1-CG-CD2	8.03	130.15	118.10
1	C	20	CYS	N-CA-C	-8.03	99.18	110.50
1	I	18	ASN	OD1-CG-ND2	8.03	130.62	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	13	GLU	CB-CA-C	-8.02	97.21	110.85
2	J	5	HIS	CA-CB-CG	-8.01	105.79	113.80
1	E	6	CYS	CA-C-N	-8.01	107.88	122.38
1	E	6	CYS	C-N-CA	-8.01	107.88	122.38
1	A	13	LEU	CA-C-O	-8.01	110.23	119.60
1	I	9	SER	CA-C-O	-8.00	112.12	121.16
2	J	4	GLN	N-CA-C	-7.99	101.66	111.33
2	B	15	LEU	CD1-CG-CD2	7.99	128.38	110.80
2	H	11	LEU	O-C-N	7.99	131.57	122.22
2	J	11	LEU	N-CA-C	7.99	119.99	111.28
2	F	25	TYR	CA-C-O	-7.98	107.23	120.80
2	D	19	CYS	N-CA-CB	7.97	122.88	110.44
2	H	16	TYR	CB-CA-C	7.97	123.56	110.81
1	C	13	LEU	O-C-N	7.96	130.56	122.12
2	L	25	TYR	CB-CA-C	7.95	125.20	110.10
2	F	24	PHE	N-CA-C	-7.95	96.63	108.79
2	J	11	LEU	N-CA-CB	7.95	121.80	110.12
1	K	8	THR	CA-C-N	-7.94	111.79	122.99
1	K	8	THR	C-N-CA	-7.94	111.79	122.99
1	I	8	THR	OG1-CB-CG2	7.94	125.17	109.30
2	J	12	VAL	N-CA-CB	-7.91	97.35	110.56
2	L	25	TYR	CD1-CE1-CZ	7.91	133.83	119.60
1	I	15	GLN	CA-CB-CG	-7.91	98.29	114.10
1	C	21	ASN	CB-CA-C	7.90	125.12	110.10
2	H	19	CYS	N-CA-CB	-7.90	98.76	110.53
1	A	18	ASN	CA-CB-CG	-7.89	104.71	112.60
2	F	15	LEU	CB-CA-C	-7.89	98.43	110.90
1	I	8	THR	O-C-N	7.88	132.92	122.36
1	K	9	SER	CA-CB-OG	-7.88	95.34	111.10
2	L	4	GLN	CB-CG-CD	-7.87	99.22	112.60
2	F	16	TYR	N-CA-CB	7.87	121.81	110.16
1	E	21	ASN	CA-C-O	-7.86	97.41	121.00
2	L	16	TYR	CE1-CZ-CE2	7.86	136.03	120.30
2	B	1	PHE	CG-CD2-CE2	-7.86	107.33	120.70
1	C	7	CYS	CA-C-O	-7.86	110.56	118.97
1	E	3	VAL	CA-CB-CG1	7.86	123.75	110.40
2	B	25	TYR	CB-CA-C	7.84	125.00	110.10
2	H	8	GLY	CA-C-O	-7.84	106.93	120.57
2	D	9	SER	CA-C-N	7.83	134.00	120.68
2	D	9	SER	C-N-CA	7.83	134.00	120.68
2	H	10	HIS	CA-CB-CG	-7.83	105.97	113.80
1	E	5	GLN	CA-C-N	-7.83	109.94	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	5	GLN	C-N-CA	-7.83	109.94	122.23
1	K	19	TYR	CD1-CG-CD2	7.82	129.84	118.10
2	F	22	ARG	N-CA-CB	-7.82	97.27	110.49
2	B	25	TYR	CD1-CE1-CZ	7.82	133.68	119.60
2	L	14	ALA	N-CA-CB	-7.82	98.59	110.16
2	L	22	ARG	O-C-N	7.81	133.16	122.46
2	J	10	HIS	N-CA-C	-7.81	102.76	111.82
2	H	17	LEU	CB-CG-CD2	-7.80	87.29	110.70
2	F	23	GLY	CA-C-N	-7.80	107.34	121.62
2	F	23	GLY	C-N-CA	-7.80	107.34	121.62
1	G	18	ASN	CB-CA-C	7.79	126.59	110.31
1	K	3	VAL	CA-CB-CG2	-7.78	97.18	110.40
1	I	10	ILE	CA-CB-CG1	7.77	123.60	110.40
1	G	5	GLN	CB-CA-C	7.76	124.91	110.70
2	L	20	GLY	O-C-N	-7.76	112.61	122.70
2	L	21	GLU	CA-C-N	-7.76	108.01	121.66
2	L	21	GLU	C-N-CA	-7.76	108.01	121.66
2	D	10	HIS	CB-CG-CD2	-7.75	121.12	131.20
2	D	24	PHE	CB-CA-C	7.75	125.04	110.62
1	E	10	ILE	N-CA-C	-7.75	98.86	109.55
1	E	5	GLN	OE1-CD-NE2	-7.75	114.85	122.60
2	L	16	TYR	N-CA-CB	-7.75	98.77	110.01
2	F	12	VAL	CA-C-N	7.71	133.76	120.58
2	F	12	VAL	C-N-CA	7.71	133.76	120.58
1	K	10	ILE	CA-CB-CG1	7.71	123.50	110.40
2	L	15	LEU	CA-C-O	7.70	128.72	120.55
1	K	6	CYS	CA-C-O	7.69	128.47	119.32
1	C	12	SER	CA-C-N	-7.68	109.86	120.38
1	C	12	SER	C-N-CA	-7.68	109.86	120.38
1	K	4	GLU	N-CA-C	-7.68	102.91	111.28
2	J	16	TYR	CB-CA-C	-7.68	98.77	110.90
1	A	14	TYR	CB-CA-C	7.66	122.91	110.88
2	H	18	VAL	CA-C-O	7.66	128.77	120.57
2	J	8	GLY	O-C-N	7.65	130.07	122.19
1	I	13	LEU	N-CA-CB	-7.65	98.58	110.06
1	E	14	TYR	N-CA-CB	-7.65	98.54	109.94
1	I	14	TYR	CD1-CG-CD2	-7.65	106.63	118.10
1	E	15	GLN	N-CA-C	7.64	120.50	111.71
1	I	8	THR	CA-C-N	-7.63	110.58	122.87
1	I	8	THR	C-N-CA	-7.63	110.58	122.87
1	C	5	GLN	CB-CA-C	-7.62	97.89	110.85
1	G	13	LEU	CD1-CG-CD2	7.62	127.57	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	20	GLY	N-CA-C	-7.62	98.24	111.50
2	L	4	GLN	N-CA-CB	7.61	121.31	110.12
1	A	8	THR	CA-C-O	-7.61	110.81	119.41
1	K	4	GLU	CB-CA-C	7.60	123.41	110.79
1	C	9	SER	O-C-N	7.60	132.37	123.17
1	G	19	TYR	CB-CG-CD1	7.58	132.18	120.80
1	I	10	ILE	N-CA-CB	7.57	119.63	110.31
1	E	21	ASN	CB-CA-C	7.57	124.47	110.10
2	J	14	ALA	CA-C-N	7.54	131.14	120.28
2	J	14	ALA	C-N-CA	7.54	131.14	120.28
2	H	3	ASN	CA-CB-CG	7.54	120.14	112.60
1	A	3	VAL	CA-C-O	7.54	130.20	120.78
1	E	21	ASN	N-CA-C	-7.53	89.91	111.00
1	A	11	CYS	CA-C-N	7.53	135.21	121.06
1	A	11	CYS	C-N-CA	7.53	135.21	121.06
2	L	12	VAL	CG1-CB-CG2	7.53	127.36	110.80
2	L	1	PHE	CB-CA-C	7.53	124.40	110.10
1	I	3	VAL	CA-CB-CG2	-7.52	97.61	110.40
1	I	11	CYS	N-CA-C	-7.51	97.34	109.96
2	H	8	GLY	O-C-N	7.51	132.46	122.70
2	J	14	ALA	CB-CA-C	-7.50	99.10	110.88
2	L	5	HIS	CA-C-N	7.49	130.64	120.38
2	L	5	HIS	C-N-CA	7.49	130.64	120.38
2	L	1	PHE	CA-C-O	-7.49	108.07	120.80
1	G	10	ILE	CA-CB-CG2	-7.48	97.78	110.50
2	L	6	LEU	N-CA-CB	7.48	121.28	110.06
2	J	20	GLY	N-CA-C	-7.48	98.79	111.73
1	G	19	TYR	CG-CD1-CE1	7.47	132.41	121.20
1	G	21	ASN	N-CA-CB	-7.47	97.79	110.50
2	H	4	GLN	N-CA-C	-7.47	103.15	111.82
2	H	12	VAL	CA-C-N	-7.47	110.45	120.54
2	H	12	VAL	C-N-CA	-7.47	110.45	120.54
1	E	19	TYR	CG-CD2-CE2	-7.47	110.00	121.20
1	K	3	VAL	CB-CA-C	-7.46	101.92	112.22
2	D	12	VAL	N-CA-CB	7.46	119.80	110.47
2	H	2	VAL	CA-CB-CG2	7.46	123.08	110.40
1	K	17	GLU	O-C-N	-7.46	112.69	122.39
2	B	18	VAL	O-C-N	7.46	129.40	121.87
1	I	18	ASN	CA-C-N	-7.45	108.89	122.38
1	I	18	ASN	C-N-CA	-7.45	108.89	122.38
1	G	17	GLU	N-CA-C	7.45	122.13	112.89
1	G	15	GLN	CG-CD-NE2	-7.45	105.23	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	13	LEU	CA-C-O	-7.44	111.69	120.10
1	I	10	ILE	N-CA-C	-7.44	100.00	109.30
2	J	6	LEU	CD1-CG-CD2	-7.42	94.47	110.80
2	B	22	ARG	CB-CA-C	7.42	123.29	110.68
1	G	10	ILE	N-CA-CB	-7.42	98.49	111.39
2	B	1	PHE	CA-CB-CG	-7.41	106.39	113.80
1	A	13	LEU	CA-CB-CG	-7.41	90.36	116.30
2	B	15	LEU	CA-C-N	-7.40	107.40	121.54
2	B	15	LEU	C-N-CA	-7.40	107.40	121.54
1	A	14	TYR	O-C-N	7.40	129.69	122.07
2	D	16	TYR	CB-CG-CD2	-7.39	109.71	120.80
2	J	22	ARG	CD-NE-CZ	-7.39	114.05	124.40
1	A	14	TYR	OH-CZ-CE2	-7.38	97.77	119.90
2	F	4	GLN	CA-CB-CG	-7.38	99.34	114.10
1	G	14	TYR	CG-CD2-CE2	-7.37	110.14	121.20
1	I	2	ILE	N-CA-C	7.37	121.34	111.17
1	E	18	ASN	CB-CG-ND2	7.37	127.46	116.40
1	I	1	GLY	CA-C-N	7.37	132.71	120.62
1	I	1	GLY	C-N-CA	7.37	132.71	120.62
2	J	14	ALA	O-C-N	-7.37	114.48	122.07
1	A	16	LEU	CA-C-O	-7.36	110.32	119.38
2	D	15	LEU	CA-C-O	-7.36	113.12	120.70
1	C	13	LEU	N-CA-CB	-7.35	99.04	110.06
1	G	12	SER	CA-CB-OG	7.34	125.78	111.10
2	F	6	LEU	CA-CB-CG	-7.34	90.62	116.30
2	D	18	VAL	CG1-CB-CG2	-7.34	94.66	110.80
2	B	21	GLU	CG-CD-OE1	7.32	135.24	118.40
1	K	15	GLN	CG-CD-NE2	-7.32	105.42	116.40
2	J	13	GLU	CG-CD-OE1	-7.31	101.58	118.40
1	K	7	CYS	N-CA-CB	-7.31	98.99	110.46
2	B	8	GLY	CA-C-N	-7.30	110.68	120.54
2	B	8	GLY	C-N-CA	-7.30	110.68	120.54
2	L	2	VAL	CB-CA-C	-7.30	102.62	111.97
2	B	17	LEU	CB-CG-CD1	-7.29	88.84	110.70
1	E	16	LEU	CB-CG-CD2	-7.27	88.88	110.70
1	I	19	TYR	CD1-CG-CD2	7.27	129.01	118.10
2	B	1	PHE	CD1-CE1-CZ	-7.27	106.91	120.00
2	F	19	CYS	CA-C-O	-7.27	111.10	119.60
2	J	4	GLN	N-CA-CB	7.26	120.95	110.06
2	D	2	VAL	CA-CB-CG2	7.26	122.75	110.40
2	H	25	TYR	CA-C-O	-7.25	108.48	120.80
2	L	18	VAL	CG1-CB-CG2	-7.24	94.88	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	11	LEU	O-C-N	7.23	131.17	122.27
2	J	1	PHE	CA-C-O	-7.23	108.51	120.80
1	I	16	LEU	CB-CA-C	7.23	124.00	110.63
2	J	13	GLU	CA-C-O	7.22	128.63	120.90
2	L	5	HIS	CG-ND1-CE1	-7.22	97.03	109.30
1	E	14	TYR	CA-C-N	-7.22	109.89	120.28
1	E	14	TYR	C-N-CA	-7.22	109.89	120.28
2	L	7	CYS	N-CA-C	7.21	120.56	111.69
2	J	10	HIS	CA-C-N	7.20	129.93	120.28
2	J	10	HIS	C-N-CA	7.20	129.93	120.28
2	H	3	ASN	N-CA-CB	7.20	120.44	110.01
2	B	22	ARG	NE-CZ-NH1	7.20	128.70	121.50
2	L	7	CYS	CA-C-N	7.19	129.19	120.13
2	L	7	CYS	C-N-CA	7.19	129.19	120.13
1	C	21	ASN	OD1-CG-ND2	-7.18	115.42	122.60
2	J	10	HIS	CG-ND1-CE1	7.17	121.50	109.30
1	C	15	GLN	OE1-CD-NE2	7.17	129.77	122.60
1	E	19	TYR	CB-CA-C	-7.17	98.12	110.09
2	F	17	LEU	CB-CG-CD2	7.17	132.20	110.70
2	J	27	THR	CB-CA-C	7.17	124.86	109.10
2	D	18	VAL	CA-CB-CG2	-7.16	98.22	110.40
2	J	15	LEU	CA-C-N	-7.16	110.70	120.44
2	J	15	LEU	C-N-CA	-7.16	110.70	120.44
1	C	20	CYS	CA-CB-SG	7.16	130.87	114.40
1	A	8	THR	OG1-CB-CG2	7.15	123.60	109.30
1	G	20	CYS	CA-CB-SG	-7.14	97.98	114.40
1	C	19	TYR	CG-CD1-CE1	-7.13	110.50	121.20
2	H	5	HIS	N-CA-CB	7.13	120.40	110.07
1	A	5	GLN	CA-C-N	-7.12	110.93	122.26
1	A	5	GLN	C-N-CA	-7.12	110.93	122.26
2	B	10	HIS	CB-CG-ND1	-7.12	112.01	122.70
1	A	17	GLU	CA-CB-CG	7.12	128.34	114.10
1	I	18	ASN	CB-CA-C	-7.11	95.14	109.99
1	A	15	GLN	CB-CA-C	-7.10	99.73	110.88
2	J	21	GLU	CA-C-N	7.10	130.74	120.38
2	J	21	GLU	C-N-CA	7.10	130.74	120.38
1	A	13	LEU	CB-CA-C	-7.09	95.41	109.67
2	B	6	LEU	CA-C-N	7.09	130.73	120.38
2	B	6	LEU	C-N-CA	7.09	130.73	120.38
2	L	13	GLU	CA-C-O	7.09	128.48	120.90
1	C	18	ASN	CA-CB-CG	7.08	119.68	112.60
1	E	4	GLU	N-CA-C	7.07	119.59	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	12	SER	O-C-N	7.06	131.33	122.43
2	J	25	TYR	CB-CG-CD1	7.06	131.39	120.80
1	I	9	SER	CA-CB-OG	7.06	125.21	111.10
1	E	7	CYS	CA-C-O	-7.05	110.74	119.28
1	C	20	CYS	CB-CA-C	7.05	122.51	109.54
1	K	8	THR	N-CA-CB	-7.04	101.22	110.59
2	J	6	LEU	CB-CA-C	7.03	122.63	110.68
2	F	18	VAL	CG1-CB-CG2	-7.03	95.34	110.80
1	E	14	TYR	O-C-N	-7.02	114.79	122.09
1	G	3	VAL	CA-CB-CG1	-7.01	98.48	110.40
2	B	6	LEU	CA-C-O	7.01	128.40	120.90
1	G	19	TYR	CA-C-O	6.99	127.89	119.43
1	C	21	ASN	N-CA-C	-6.99	91.43	111.00
2	D	6	LEU	CA-CB-CG	-6.97	91.91	116.30
2	J	24	PHE	N-CA-C	6.97	119.45	108.79
1	G	4	GLU	N-CA-CB	6.96	120.57	110.20
2	J	11	LEU	CB-CA-C	-6.96	99.24	110.79
2	H	19	CYS	O-C-N	6.96	131.53	122.42
1	A	20	CYS	CA-C-O	-6.96	113.01	121.36
1	K	5	GLN	CG-CD-OE1	6.95	134.70	120.80
1	A	10	ILE	CA-C-O	6.93	128.94	121.04
2	D	10	HIS	CB-CA-C	-6.93	96.25	110.38
1	A	21	ASN	N-CA-CB	-6.92	98.73	110.50
2	B	4	GLN	O-C-N	6.92	132.01	122.46
1	E	17	GLU	CG-CD-OE2	-6.92	102.48	118.40
2	L	16	TYR	O-C-N	6.92	129.20	122.07
1	E	17	GLU	N-CA-C	6.92	119.70	111.33
2	D	21	GLU	CB-CG-CD	6.91	124.34	112.60
1	A	3	VAL	CA-CB-CG1	6.90	122.13	110.40
1	A	5	GLN	CA-CB-CG	6.88	127.86	114.10
2	F	22	ARG	NE-CZ-NH1	6.88	128.38	121.50
1	C	19	TYR	CB-CA-C	-6.88	98.54	110.17
2	B	13	GLU	CB-CA-C	6.87	121.81	110.81
1	A	19	TYR	N-CA-CB	6.86	122.49	110.42
2	B	5	HIS	N-CA-C	-6.86	103.50	110.97
1	E	10	ILE	CA-C-N	-6.85	112.53	122.19
1	E	10	ILE	C-N-CA	-6.85	112.53	122.19
1	K	4	GLU	N-CA-CB	-6.85	100.05	110.12
2	B	24	PHE	CB-CA-C	-6.85	98.93	110.43
2	F	22	ARG	CA-CB-CG	6.84	127.79	114.10
2	B	7	CYS	CA-C-O	6.84	127.86	120.20
1	C	19	TYR	CA-C-N	-6.83	110.21	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	19	TYR	C-N-CA	-6.83	110.21	120.94
2	H	16	TYR	O-C-N	6.83	129.19	122.09
1	C	17	GLU	O-C-N	-6.83	114.88	122.12
1	E	4	GLU	CG-CD-OE2	6.82	134.10	118.40
1	K	9	SER	O-C-N	6.82	131.42	123.30
1	K	21	ASN	N-CA-CB	6.82	122.10	110.50
1	A	19	TYR	CB-CG-CD2	6.82	131.03	120.80
2	L	2	VAL	CA-C-O	6.82	128.40	121.17
2	J	25	TYR	CG-CD1-CE1	6.81	131.41	121.20
1	C	17	GLU	CG-CD-OE2	6.81	134.06	118.40
2	J	15	LEU	O-C-N	6.79	130.17	122.22
1	G	14	TYR	CE1-CZ-CE2	6.79	133.88	120.30
1	A	17	GLU	N-CA-CB	6.79	120.06	109.94
2	L	3	ASN	N-CA-C	-6.78	103.69	112.23
1	E	8	THR	CA-CB-OG1	6.78	119.77	109.60
2	H	25	TYR	CG-CD1-CE1	-6.78	111.04	121.20
1	E	17	GLU	CB-CA-C	6.77	122.19	110.68
2	D	13	GLU	N-CA-CB	6.76	120.17	110.16
1	E	13	LEU	CB-CA-C	6.76	123.57	110.46
2	H	25	TYR	CB-CG-CD1	-6.75	110.67	120.80
2	F	16	TYR	CD1-CG-CD2	6.75	128.23	118.10
2	B	13	GLU	N-CA-C	6.75	119.21	111.11
1	G	3	VAL	CB-CA-C	6.75	120.88	112.04
2	J	3	ASN	CA-C-N	6.74	129.62	120.38
2	J	3	ASN	C-N-CA	6.74	129.62	120.38
1	C	19	TYR	N-CA-CB	6.74	120.78	110.61
2	L	11	LEU	N-CA-CB	6.73	119.83	110.07
2	H	6	LEU	CB-CA-C	6.73	121.54	110.90
2	H	16	TYR	CA-C-N	-6.73	111.76	120.65
2	H	16	TYR	C-N-CA	-6.73	111.76	120.65
2	J	6	LEU	N-CA-CB	6.73	120.16	110.06
1	C	8	THR	CA-C-O	6.73	127.71	120.24
2	L	13	GLU	CA-C-N	-6.72	110.74	120.29
2	L	13	GLU	C-N-CA	-6.72	110.74	120.29
1	A	2	ILE	CA-CB-CG1	-6.71	98.99	110.40
2	J	2	VAL	CA-CB-CG1	6.71	121.80	110.40
1	C	4	GLU	CB-CA-C	6.70	122.06	110.68
1	E	21	ASN	N-CA-CB	6.70	121.88	110.50
2	F	2	VAL	CB-CA-C	-6.70	98.68	111.40
2	L	13	GLU	OE1-CD-OE2	6.70	138.97	122.90
1	E	12	SER	CA-C-O	6.69	130.08	120.51
1	A	10	ILE	CA-CB-CG1	-6.69	99.03	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	6	CYS	CB-CA-C	6.69	121.47	110.17
1	K	19	TYR	CB-CA-C	6.69	123.26	109.95
2	B	24	PHE	N-CA-CB	6.67	121.70	111.56
2	J	10	HIS	CB-CG-ND1	6.67	132.70	122.70
2	B	22	ARG	CA-CB-CG	6.67	127.44	114.10
1	I	5	GLN	CA-C-O	6.67	127.64	119.97
1	I	7	CYS	O-C-N	6.66	130.67	122.34
1	I	12	SER	N-CA-C	-6.66	100.11	110.17
1	A	19	TYR	CG-CD2-CE2	6.66	131.19	121.20
1	E	4	GLU	CB-CA-C	6.66	121.46	110.81
1	C	19	TYR	CB-CG-CD1	-6.65	110.82	120.80
1	A	14	TYR	N-CA-CB	6.65	119.65	110.01
1	A	3	VAL	N-CA-CB	6.65	122.20	111.23
2	H	22	ARG	CB-CA-C	6.65	122.93	110.63
2	B	8	GLY	CA-C-O	-6.64	112.98	120.09
2	L	10	HIS	ND1-CE1-NE2	-6.64	101.76	108.40
2	H	10	HIS	ND1-CE1-NE2	6.64	115.04	108.40
1	C	10	ILE	CB-CA-C	-6.64	102.12	111.21
2	B	11	LEU	N-CA-CB	-6.63	100.01	110.28
1	C	1	GLY	CA-C-N	6.62	131.16	120.30
1	C	1	GLY	C-N-CA	6.62	131.16	120.30
2	D	5	HIS	CA-C-N	6.62	131.91	120.58
2	D	5	HIS	C-N-CA	6.62	131.91	120.58
2	H	22	ARG	CD-NE-CZ	6.62	133.67	124.40
2	H	1	PHE	CD1-CG-CD2	6.62	128.53	118.60
2	B	15	LEU	N-CA-CB	-6.62	100.11	110.30
2	B	1	PHE	CE1-CZ-CE2	6.62	131.91	120.00
1	C	17	GLU	CA-CB-CG	6.62	127.33	114.10
1	G	2	ILE	CA-C-N	6.62	129.86	120.53
1	G	2	ILE	C-N-CA	6.62	129.86	120.53
1	E	7	CYS	CB-CA-C	6.61	121.92	110.01
1	A	15	GLN	CB-CG-CD	-6.60	101.37	112.60
2	F	10	HIS	CA-C-O	-6.60	112.00	119.79
1	E	17	GLU	CA-C-O	6.59	127.75	120.63
1	E	3	VAL	CG1-CB-CG2	-6.58	96.33	110.80
1	C	14	TYR	CG-CD1-CE1	-6.58	111.33	121.20
1	K	16	LEU	CA-C-O	6.57	127.73	120.63
2	D	6	LEU	N-CA-CB	6.57	119.99	110.20
2	D	4	GLN	N-CA-C	-6.56	103.39	111.40
2	J	9	SER	CA-C-O	6.56	127.89	121.00
1	A	9	SER	CA-C-N	-6.56	112.06	120.98
1	A	9	SER	C-N-CA	-6.56	112.06	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	GLN	OE1-CD-NE2	6.56	129.16	122.60
2	H	22	ARG	CA-C-N	6.56	136.14	120.99
2	H	22	ARG	C-N-CA	6.56	136.14	120.99
1	I	2	ILE	CA-C-O	6.55	127.78	120.64
2	D	2	VAL	N-CA-C	6.54	129.32	111.00
1	E	3	VAL	N-CA-CB	-6.54	99.47	110.65
1	A	13	LEU	CB-CG-CD1	-6.53	91.11	110.70
1	I	6	CYS	CA-C-N	-6.52	111.78	122.54
1	I	6	CYS	C-N-CA	-6.52	111.78	122.54
2	F	18	VAL	CA-CB-CG1	6.52	121.49	110.40
2	B	12	VAL	CA-CB-CG1	6.51	121.46	110.40
1	C	19	TYR	CE1-CZ-CE2	6.50	133.31	120.30
2	L	11	LEU	CB-CG-CD1	-6.50	91.19	110.70
2	J	20	GLY	CA-C-O	-6.50	113.44	121.56
1	K	9	SER	CB-CA-C	-6.49	97.84	109.71
1	K	6	CYS	CA-C-N	-6.49	110.00	122.06
1	K	6	CYS	C-N-CA	-6.49	110.00	122.06
2	L	5	HIS	N-CA-CB	-6.47	100.69	110.07
2	D	12	VAL	N-CA-C	-6.47	103.25	110.62
1	G	19	TYR	CA-C-N	-6.47	111.48	122.67
1	G	19	TYR	C-N-CA	-6.47	111.48	122.67
1	A	4	GLU	N-CA-C	6.47	118.41	111.36
2	D	4	GLN	CG-CD-NE2	-6.45	106.72	116.40
2	F	9	SER	N-CA-CB	6.45	119.81	110.20
1	A	20	CYS	CA-CB-SG	-6.44	99.60	114.40
1	C	2	ILE	N-CA-C	-6.43	103.05	111.09
2	D	6	LEU	N-CA-C	6.43	119.60	111.69
2	D	22	ARG	N-CA-CB	-6.43	99.62	110.49
2	H	5	HIS	CA-C-O	-6.43	114.08	120.70
1	G	14	TYR	CB-CG-CD2	-6.43	111.16	120.80
2	H	17	LEU	N-CA-CB	-6.42	100.53	109.91
1	A	8	THR	N-CA-C	6.42	121.24	113.41
1	K	17	GLU	CG-CD-OE2	6.41	133.15	118.40
1	E	12	SER	CB-CA-C	6.41	123.17	110.42
2	J	10	HIS	CB-CA-C	6.41	122.97	110.67
2	F	8	GLY	CA-C-N	6.40	131.52	120.58
2	F	8	GLY	C-N-CA	6.40	131.52	120.58
1	I	17	GLU	N-CA-C	6.39	120.18	112.38
2	J	2	VAL	CA-C-O	6.39	127.92	121.27
2	F	21	GLU	N-CA-CB	-6.38	100.06	110.14
1	C	19	TYR	CA-CB-CG	-6.38	102.42	113.90
2	B	16	TYR	CG-CD2-CE2	-6.38	111.64	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	16	TYR	N-CA-CB	-6.37	99.72	110.49
1	K	13	LEU	N-CA-CB	-6.37	100.77	110.01
1	G	19	TYR	CZ-CE2-CD2	6.37	131.06	119.60
2	B	14	ALA	CA-C-N	-6.36	109.86	120.68
2	B	14	ALA	C-N-CA	-6.36	109.86	120.68
2	J	4	GLN	CG-CD-NE2	6.36	125.94	116.40
2	H	3	ASN	CA-C-N	6.35	129.96	120.31
2	H	3	ASN	C-N-CA	6.35	129.96	120.31
1	G	3	VAL	CG1-CB-CG2	6.34	124.75	110.80
2	L	21	GLU	CA-CB-CG	-6.33	101.43	114.10
1	E	3	VAL	CA-CB-CG2	6.33	121.16	110.40
2	L	11	LEU	CA-CB-CG	-6.33	94.14	116.30
2	F	6	LEU	N-CA-C	6.33	119.12	111.40
2	H	23	GLY	CA-C-N	-6.33	109.45	121.54
2	H	23	GLY	C-N-CA	-6.33	109.45	121.54
2	H	22	ARG	NH1-CZ-NH2	-6.33	111.08	119.30
1	G	2	ILE	CA-CB-CG2	6.32	121.25	110.50
2	J	3	ASN	N-CA-C	6.31	118.24	111.36
2	J	13	GLU	CG-CD-OE2	6.31	132.92	118.40
1	K	17	GLU	OE1-CD-OE2	-6.31	107.75	122.90
2	H	12	VAL	CA-C-O	-6.31	113.86	121.18
1	G	19	TYR	CB-CA-C	-6.30	99.15	110.37
2	B	16	TYR	CB-CG-CD2	-6.30	111.35	120.80
1	I	10	ILE	CB-CG1-CD1	6.29	127.02	113.80
1	E	3	VAL	N-CA-C	-6.29	103.19	111.05
1	C	12	SER	N-CA-CB	6.29	118.84	110.29
2	B	2	VAL	CA-CB-CG1	-6.29	99.71	110.40
1	I	16	LEU	O-C-N	-6.29	114.86	122.22
2	H	4	GLN	CA-C-N	6.28	128.98	120.44
2	H	4	GLN	C-N-CA	6.28	128.98	120.44
1	A	2	ILE	CA-C-N	6.28	133.27	121.97
1	A	2	ILE	C-N-CA	6.28	133.27	121.97
2	H	13	GLU	CB-CG-CD	6.27	123.26	112.60
1	I	2	ILE	CA-CB-CG1	6.27	121.06	110.40
1	C	6	CYS	CA-C-O	-6.27	111.86	119.32
2	L	1	PHE	CD1-CG-CD2	-6.27	109.20	118.60
2	B	24	PHE	CD1-CG-CD2	-6.26	109.20	118.60
2	H	18	VAL	N-CA-C	6.26	118.87	111.05
1	I	20	CYS	N-CA-CB	6.26	119.18	110.17
2	J	3	ASN	CA-CB-CG	-6.26	106.34	112.60
2	B	18	VAL	CA-C-O	6.25	127.26	120.57
1	E	9	SER	CB-CA-C	6.25	121.48	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	21	GLU	CB-CA-C	-6.25	100.82	110.81
2	L	25	TYR	CD1-CG-CD2	-6.24	108.74	118.10
1	C	4	GLU	CG-CD-OE1	6.24	132.74	118.40
1	C	10	ILE	CG1-CB-CG2	-6.24	91.99	110.70
2	B	18	VAL	CA-CB-CG1	-6.23	99.81	110.40
1	A	10	ILE	CB-CA-C	-6.23	102.05	111.33
2	J	5	HIS	CB-CA-C	-6.22	100.34	110.79
1	C	14	TYR	CG-CD2-CE2	6.21	130.52	121.20
2	L	16	TYR	CG-CD1-CE1	-6.21	111.89	121.20
2	L	22	ARG	CA-CB-CG	-6.21	101.69	114.10
1	A	18	ASN	CA-C-N	6.20	136.03	121.52
1	A	18	ASN	C-N-CA	6.20	136.03	121.52
1	E	19	TYR	CE1-CZ-CE2	6.19	132.68	120.30
1	I	10	ILE	CB-CA-C	6.18	120.54	111.33
2	F	11	LEU	CB-CG-CD1	-6.18	92.16	110.70
2	F	2	VAL	CA-C-O	-6.18	110.30	120.80
2	F	2	VAL	N-CA-CB	6.17	121.99	111.50
2	J	9	SER	CB-CA-C	-6.17	101.45	110.96
2	B	15	LEU	N-CA-C	6.17	120.00	112.23
2	D	22	ARG	N-CA-C	6.16	123.92	110.80
1	I	13	LEU	CB-CA-C	6.16	121.15	110.68
2	F	18	VAL	CA-C-N	6.16	132.84	121.52
2	F	18	VAL	C-N-CA	6.16	132.84	121.52
1	A	4	GLU	CA-C-N	6.15	129.03	120.29
1	A	4	GLU	C-N-CA	6.15	129.03	120.29
1	A	17	GLU	CB-CA-C	-6.15	100.97	110.81
2	L	15	LEU	O-C-N	6.15	128.64	122.12
1	C	15	GLN	CG-CD-NE2	-6.15	107.18	116.40
1	A	18	ASN	N-CA-CB	-6.14	100.85	110.06
2	B	19	CYS	CA-C-O	6.14	126.45	119.27
2	H	7	CYS	CA-C-O	6.14	127.26	120.63
2	B	18	VAL	N-CA-CB	-6.13	100.16	110.65
2	J	16	TYR	OH-CZ-CE2	-6.13	101.52	119.90
1	G	10	ILE	CA-C-N	-6.12	112.24	122.64
1	G	10	ILE	C-N-CA	-6.12	112.24	122.64
2	D	5	HIS	CA-C-O	6.10	127.22	120.63
2	H	5	HIS	CB-CA-C	-6.09	101.27	110.90
1	E	16	LEU	N-CA-CB	-6.09	101.17	110.12
2	L	8	GLY	CA-C-O	-6.09	114.24	120.45
2	H	1	PHE	CA-CB-CG	6.08	119.88	113.80
2	F	6	LEU	CA-C-N	6.07	128.42	120.28
2	F	6	LEU	C-N-CA	6.07	128.42	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	19	CYS	N-CA-C	-6.07	105.84	113.18
2	D	12	VAL	CB-CA-C	6.06	119.98	112.04
1	E	4	GLU	OE1-CD-OE2	-6.05	108.39	122.90
1	C	2	ILE	CB-CA-C	-6.04	102.47	112.26
1	I	9	SER	CA-C-N	6.04	129.19	120.98
1	I	9	SER	C-N-CA	6.04	129.19	120.98
2	B	20	GLY	N-CA-C	6.03	123.24	112.02
2	L	16	TYR	CB-CG-CD1	-6.03	111.75	120.80
1	G	14	TYR	N-CA-C	-6.03	104.79	111.36
2	J	15	LEU	CD1-CG-CD2	-6.03	97.55	110.80
1	C	18	ASN	OD1-CG-ND2	-6.01	116.58	122.60
1	C	19	TYR	CZ-CE2-CD2	-6.01	108.78	119.60
1	A	19	TYR	N-CA-C	6.01	120.34	113.19
2	F	8	GLY	O-C-N	-6.01	116.42	122.19
1	K	18	ASN	N-CA-CB	-6.01	100.97	110.22
1	G	18	ASN	CB-CG-ND2	6.00	125.41	116.40
2	F	21	GLU	O-C-N	6.00	129.04	122.20
2	J	10	HIS	CA-C-O	-6.00	113.07	119.97
2	B	4	GLN	CA-C-O	-6.00	111.88	119.31
2	D	24	PHE	CA-C-O	5.99	127.64	121.23
2	D	11	LEU	CD1-CG-CD2	5.99	123.97	110.80
2	J	6	LEU	CB-CG-CD1	5.99	128.66	110.70
2	F	9	SER	O-C-N	-5.98	114.46	122.23
2	L	18	VAL	N-CA-CB	-5.98	100.58	110.56
1	E	9	SER	CA-C-O	-5.98	114.13	121.78
1	A	18	ASN	CB-CG-ND2	-5.97	107.44	116.40
2	H	25	TYR	CZ-CE2-CD2	-5.97	108.85	119.60
2	J	16	TYR	CE1-CZ-CE2	5.96	132.23	120.30
2	H	1	PHE	CA-C-O	-5.96	110.67	120.80
2	B	2	VAL	N-CA-C	-5.96	103.83	110.62
1	K	2	ILE	CA-CB-CG2	-5.95	100.38	110.50
2	J	5	HIS	N-CA-C	5.94	118.64	111.40
1	I	19	TYR	CE1-CZ-CE2	5.93	132.16	120.30
1	C	10	ILE	CB-CG1-CD1	5.92	126.24	113.80
2	D	13	GLU	N-CA-C	5.91	117.81	111.36
1	E	19	TYR	CB-CG-CD2	-5.91	111.93	120.80
1	C	4	GLU	CA-C-N	5.91	128.68	120.29
1	C	4	GLU	C-N-CA	5.91	128.68	120.29
2	D	4	GLN	CA-CB-CG	-5.89	102.31	114.10
2	F	19	CYS	CA-CB-SG	-5.89	100.85	114.40
1	I	2	ILE	N-CA-CB	5.89	119.79	110.54
1	I	11	CYS	N-CA-CB	5.87	119.74	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	12	VAL	CA-C-N	5.87	128.46	120.54
2	J	12	VAL	C-N-CA	5.87	128.46	120.54
2	B	12	VAL	CB-CA-C	5.87	119.39	111.88
1	G	5	GLN	CB-CG-CD	5.87	122.57	112.60
1	G	2	ILE	O-C-N	-5.86	113.63	123.00
2	L	3	ASN	CB-CA-C	5.86	122.33	110.38
2	H	2	VAL	CA-C-O	-5.85	114.87	120.95
2	F	4	GLN	CB-CA-C	-5.84	100.97	110.79
1	K	19	TYR	CE1-CZ-CE2	5.84	131.98	120.30
2	F	8	GLY	N-CA-C	-5.84	105.72	112.73
2	D	21	GLU	CG-CD-OE1	5.84	131.83	118.40
1	I	14	TYR	CB-CA-C	-5.84	100.76	110.68
2	B	7	CYS	N-CA-C	5.83	119.21	111.75
2	J	15	LEU	N-CA-CB	5.83	119.19	110.22
1	I	20	CYS	N-CA-C	-5.82	102.29	110.50
1	C	14	TYR	N-CA-CB	-5.82	101.57	110.01
1	I	2	ILE	CA-CB-CG2	-5.82	100.61	110.50
1	K	10	ILE	CB-CA-C	5.82	120.83	111.29
2	J	28	LYS	CD-CE-NZ	5.81	130.49	111.90
1	A	2	ILE	N-CA-CB	-5.81	101.63	111.50
2	F	4	GLN	N-CA-CB	5.81	118.72	110.13
1	A	6	CYS	N-CA-CB	-5.80	102.12	110.65
2	H	25	TYR	CD1-CG-CD2	5.80	126.81	118.10
2	J	4	GLN	CG-CD-OE1	5.80	132.41	120.80
2	B	22	ARG	CA-C-O	-5.79	114.37	120.63
1	G	19	TYR	CA-CB-CG	-5.79	103.47	113.90
1	E	19	TYR	CD1-CE1-CZ	-5.79	109.17	119.60
1	E	6	CYS	CA-CB-SG	-5.79	101.09	114.40
1	E	12	SER	O-C-N	5.79	130.28	122.59
2	F	5	HIS	O-C-N	-5.79	115.99	122.12
2	J	14	ALA	N-CA-CB	-5.78	101.63	110.01
1	G	3	VAL	CA-C-N	5.77	130.44	120.58
1	G	3	VAL	C-N-CA	5.77	130.44	120.58
1	C	4	GLU	CB-CG-CD	-5.76	102.80	112.60
2	J	25	TYR	CA-C-O	-5.76	111.00	120.80
1	E	15	GLN	CB-CA-C	5.76	121.29	110.63
2	L	10	HIS	CG-ND1-CE1	5.76	119.09	109.30
2	J	1	PHE	CG-CD2-CE2	5.76	130.49	120.70
1	G	4	GLU	CB-CG-CD	-5.76	102.81	112.60
1	A	9	SER	CA-C-O	5.75	127.73	121.06
1	A	10	ILE	O-C-N	-5.75	116.41	122.67
2	L	24	PHE	CA-C-O	5.75	127.54	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	15	LEU	CA-C-N	5.75	127.98	120.28
2	D	15	LEU	C-N-CA	5.75	127.98	120.28
2	B	12	VAL	CA-CB-CG2	-5.74	100.64	110.40
1	C	18	ASN	CA-C-O	5.74	128.71	120.51
1	E	14	TYR	CG-CD2-CE2	5.72	129.79	121.20
1	A	10	ILE	CG1-CB-CG2	5.72	127.85	110.70
1	I	21	ASN	CA-CB-CG	-5.71	106.89	112.60
2	L	3	ASN	CB-CG-OD1	5.71	132.22	120.80
2	L	16	TYR	CG-CD2-CE2	-5.70	112.65	121.20
2	D	13	GLU	CG-CD-OE2	-5.69	105.30	118.40
2	D	16	TYR	CG-CD2-CE2	-5.68	112.68	121.20
1	K	10	ILE	CB-CG1-CD1	5.68	125.73	113.80
2	F	22	ARG	O-C-N	5.68	130.14	122.59
1	A	15	GLN	CA-CB-CG	-5.67	102.76	114.10
1	I	11	CYS	CB-CA-C	5.66	118.87	109.53
2	B	15	LEU	CB-CG-CD1	-5.66	93.72	110.70
1	E	2	ILE	CG1-CB-CG2	5.66	127.67	110.70
2	B	18	VAL	CA-CB-CG2	5.65	120.01	110.40
2	F	6	LEU	CA-C-O	-5.65	114.50	120.55
2	D	10	HIS	CA-C-O	-5.65	113.12	119.79
1	A	8	THR	CB-CA-C	-5.65	99.36	109.24
2	D	21	GLU	OE1-CD-OE2	-5.64	109.35	122.90
1	E	2	ILE	N-CA-C	5.64	120.31	112.35
2	J	2	VAL	CA-C-N	-5.63	112.29	120.29
2	J	2	VAL	C-N-CA	-5.63	112.29	120.29
2	L	19	CYS	CA-C-N	-5.63	110.36	121.41
2	L	19	CYS	C-N-CA	-5.63	110.36	121.41
1	C	9	SER	N-CA-C	5.63	117.74	109.24
1	A	19	TYR	CD1-CE1-CZ	5.62	129.72	119.60
1	K	3	VAL	N-CA-C	5.62	116.40	110.72
2	D	22	ARG	O-C-N	-5.62	115.12	122.59
2	J	8	GLY	CA-C-N	5.61	128.05	120.65
2	J	8	GLY	C-N-CA	5.61	128.05	120.65
2	D	2	VAL	CG1-CB-CG2	-5.60	98.47	110.80
2	H	22	ARG	CA-CB-CG	5.60	125.30	114.10
2	J	25	TYR	CZ-CE2-CD2	5.60	129.68	119.60
2	F	7	CYS	N-CA-CB	5.60	118.35	110.12
1	E	7	CYS	N-CA-CB	-5.58	101.89	110.44
1	G	11	CYS	CB-CA-C	-5.58	100.06	109.50
1	I	15	GLN	CA-C-N	-5.58	112.25	120.28
1	I	15	GLN	C-N-CA	-5.58	112.25	120.28
1	K	21	ASN	CB-CA-C	-5.57	99.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7	CYS	CA-CB-SG	5.57	127.21	114.40
2	D	17	LEU	CA-CB-CG	-5.57	96.81	116.30
1	K	20	CYS	CA-C-N	5.57	131.72	121.70
1	K	20	CYS	C-N-CA	5.57	131.72	121.70
2	B	13	GLU	CB-CG-CD	5.57	122.06	112.60
1	C	8	THR	CA-CB-OG1	-5.57	101.25	109.60
1	I	5	GLN	CA-C-N	5.57	130.93	122.08
1	I	5	GLN	C-N-CA	5.57	130.93	122.08
2	D	21	GLU	CB-CA-C	5.56	121.25	110.46
2	F	2	VAL	CA-CB-CG2	-5.56	100.95	110.40
2	H	4	GLN	O-C-N	5.56	129.10	122.27
1	A	14	TYR	CE1-CZ-OH	5.55	136.56	119.90
1	G	14	TYR	CD1-CE1-CZ	-5.55	109.60	119.60
1	A	6	CYS	N-CA-C	-5.55	106.50	113.72
2	J	13	GLU	N-CA-C	-5.55	104.45	111.11
1	E	6	CYS	CB-CA-C	-5.54	100.06	109.38
2	H	23	GLY	CA-C-O	5.53	130.44	122.58
2	F	9	SER	N-CA-C	-5.53	104.89	111.69
1	K	11	CYS	N-CA-C	-5.53	101.47	110.20
2	F	16	TYR	O-C-N	-5.53	115.85	122.15
1	A	4	GLU	OE1-CD-OE2	-5.52	109.66	122.90
1	A	21	ASN	CB-CG-OD1	5.52	131.83	120.80
1	E	1	GLY	CA-C-O	5.52	132.39	120.80
2	D	22	ARG	CB-CA-C	5.52	121.40	110.42
1	C	2	ILE	CG1-CB-CG2	5.51	127.23	110.70
2	D	16	TYR	N-CA-CB	5.51	118.22	110.12
1	A	14	TYR	CA-C-N	5.50	127.60	120.44
1	A	14	TYR	C-N-CA	5.50	127.60	120.44
1	A	21	ASN	N-CA-C	5.50	126.39	111.00
2	F	12	VAL	CB-CA-C	5.49	119.55	112.14
1	I	4	GLU	CA-C-O	-5.49	115.05	120.70
1	A	9	SER	CB-CA-C	-5.48	97.40	109.56
2	H	16	TYR	CG-CD1-CE1	5.48	129.41	121.20
1	C	6	CYS	N-CA-CB	5.47	118.88	110.61
1	C	16	LEU	CA-C-N	-5.47	112.88	120.38
1	C	16	LEU	C-N-CA	-5.47	112.88	120.38
2	L	3	ASN	CA-C-O	-5.47	113.33	119.79
1	K	12	SER	N-CA-C	-5.47	101.92	110.17
2	J	24	PHE	CA-C-N	5.46	131.53	121.70
2	J	24	PHE	C-N-CA	5.46	131.53	121.70
2	J	9	SER	CA-CB-OG	5.46	122.02	111.10
1	G	8	THR	OG1-CB-CG2	5.46	120.21	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	18	ASN	CA-C-O	5.46	126.27	120.10
2	D	13	GLU	CB-CG-CD	-5.45	103.33	112.60
1	G	2	ILE	CB-CA-C	-5.45	100.70	111.60
2	D	5	HIS	CB-CA-C	5.44	119.92	110.68
1	C	11	CYS	CA-C-N	5.43	130.62	120.95
1	C	11	CYS	C-N-CA	5.43	130.62	120.95
2	L	10	HIS	CA-C-N	5.43	127.82	120.44
2	L	10	HIS	C-N-CA	5.43	127.82	120.44
1	C	2	ILE	CA-C-N	-5.42	114.10	120.72
1	C	2	ILE	C-N-CA	-5.42	114.10	120.72
2	F	21	GLU	CB-CG-CD	5.42	121.82	112.60
2	D	14	ALA	CB-CA-C	-5.42	100.79	110.70
1	A	4	GLU	CA-C-O	-5.41	114.69	120.42
1	I	2	ILE	CB-CA-C	-5.41	104.15	112.05
2	H	17	LEU	CA-CB-CG	-5.41	97.38	116.30
2	H	14	ALA	N-CA-CB	5.41	118.07	110.12
2	F	19	CYS	CB-CA-C	-5.40	98.81	109.67
1	C	4	GLU	OE1-CD-OE2	-5.40	109.93	122.90
1	G	21	ASN	CB-CA-C	5.40	120.36	110.10
2	J	9	SER	N-CA-CB	5.40	117.79	109.91
1	G	13	LEU	N-CA-CB	5.39	118.52	110.22
2	B	24	PHE	N-CA-C	-5.38	100.13	108.42
2	J	1	PHE	CB-CG-CD2	5.38	129.85	120.70
1	K	5	GLN	CB-CA-C	5.37	119.98	110.85
2	H	24	PHE	N-CA-CB	5.36	119.55	110.49
2	F	2	VAL	CA-CB-CG1	5.36	119.51	110.40
1	A	19	TYR	O-C-N	5.35	130.96	122.41
1	I	21	ASN	CB-CG-ND2	5.34	124.42	116.40
2	F	16	TYR	CA-CB-CG	5.34	123.52	113.90
1	A	15	GLN	CG-CD-OE1	5.34	131.48	120.80
1	I	14	TYR	CA-C-O	5.34	126.40	120.63
2	L	22	ARG	NE-CZ-NH2	5.33	124.00	119.20
2	H	3	ASN	CB-CA-C	-5.33	102.52	110.88
2	L	10	HIS	CB-CG-ND1	5.32	130.69	122.70
1	K	8	THR	CA-CB-CG2	5.32	119.55	110.50
2	B	24	PHE	CB-CG-CD1	-5.32	111.66	120.70
1	K	18	ASN	CB-CG-OD1	-5.32	110.17	120.80
2	B	12	VAL	N-CA-CB	-5.31	104.61	110.51
2	L	18	VAL	CA-C-N	5.31	130.43	121.14
2	L	18	VAL	C-N-CA	5.31	130.43	121.14
2	B	16	TYR	CD1-CE1-CZ	-5.30	110.06	119.60
1	C	14	TYR	CB-CG-CD2	5.30	128.75	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	19	CYS	N-CA-CB	5.30	119.03	110.40
1	I	4	GLU	CG-CD-OE2	-5.29	106.24	118.40
2	H	12	VAL	CA-CB-CG1	5.29	119.39	110.40
2	F	10	HIS	CB-CA-C	-5.29	99.60	110.38
2	J	1	PHE	CD1-CE1-CZ	5.28	129.51	120.00
1	E	1	GLY	O-C-N	-5.28	114.56	123.00
2	F	18	VAL	CA-CB-CG2	-5.28	101.43	110.40
2	L	6	LEU	CB-CA-C	5.28	119.65	110.68
2	L	14	ALA	O-C-N	-5.28	116.14	122.15
1	A	17	GLU	CA-C-N	-5.27	113.16	120.38
1	A	17	GLU	C-N-CA	-5.27	113.16	120.38
2	F	10	HIS	CA-CB-CG	-5.27	108.53	113.80
2	H	9	SER	CA-C-O	-5.27	115.26	120.90
1	A	13	LEU	CD1-CG-CD2	5.27	122.39	110.80
2	L	4	GLN	CB-CA-C	-5.27	102.04	110.79
1	E	14	TYR	CA-CB-CG	-5.25	104.45	113.90
1	K	19	TYR	N-CA-C	-5.25	106.83	113.18
1	E	13	LEU	CB-CG-CD1	5.24	126.43	110.70
1	C	14	TYR	CB-CG-CD1	-5.24	112.94	120.80
2	D	25	TYR	N-CA-CB	5.23	119.39	110.50
2	L	1	PHE	CE1-CZ-CE2	-5.23	110.58	120.00
2	F	6	LEU	CB-CG-CD2	5.23	126.39	110.70
2	L	2	VAL	CA-C-N	-5.23	111.79	120.68
2	L	2	VAL	C-N-CA	-5.23	111.79	120.68
2	H	24	PHE	CB-CA-C	-5.22	100.03	110.42
1	C	14	TYR	N-CA-C	5.22	116.66	111.07
2	L	17	LEU	CA-CB-CG	5.21	134.55	116.30
2	B	24	PHE	CG-CD1-CE1	-5.21	111.84	120.70
1	I	9	SER	O-C-N	5.21	129.72	123.16
1	C	2	ILE	CB-CG1-CD1	5.20	124.73	113.80
1	I	5	GLN	CB-CA-C	5.20	120.66	110.67
2	L	15	LEU	CD1-CG-CD2	-5.19	99.38	110.80
2	L	18	VAL	CA-C-O	5.19	126.26	120.71
1	E	14	TYR	CB-CA-C	5.18	119.09	110.81
1	K	15	GLN	N-CA-CB	-5.17	102.51	110.12
2	B	16	TYR	CG-CD1-CE1	5.17	128.95	121.20
1	K	19	TYR	CB-CG-CD1	-5.17	113.05	120.80
2	B	16	TYR	CB-CG-CD1	5.17	128.55	120.80
1	G	2	ILE	CA-CB-CG1	-5.17	101.62	110.40
2	B	16	TYR	CA-C-O	5.16	127.89	120.51
1	G	20	CYS	N-CA-CB	-5.16	102.47	110.46
2	B	13	GLU	CA-CB-CG	5.15	124.40	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	5	GLN	N-CA-CB	5.14	117.86	110.20
1	C	17	GLU	CB-CA-C	5.13	119.39	110.68
2	L	7	CYS	N-CA-CB	-5.12	102.56	110.20
2	D	18	VAL	CA-CB-CG1	5.12	119.11	110.40
2	F	13	GLU	CG-CD-OE1	5.12	130.19	118.40
2	L	13	GLU	CA-CB-CG	5.12	124.35	114.10
2	L	22	ARG	N-CA-C	5.12	119.58	113.23
1	C	13	LEU	CB-CA-C	5.12	119.38	110.68
1	G	15	GLN	CA-CB-CG	-5.12	103.86	114.10
1	A	5	GLN	CB-CG-CD	5.12	121.30	112.60
2	H	16	TYR	CB-CG-CD1	5.11	128.47	120.80
2	B	24	PHE	CE1-CZ-CE2	-5.11	110.81	120.00
2	D	21	GLU	CA-C-N	-5.11	111.78	121.54
2	D	21	GLU	C-N-CA	-5.11	111.78	121.54
2	B	24	PHE	CZ-CE2-CD2	-5.11	110.81	120.00
1	I	19	TYR	CA-C-N	5.10	128.95	120.94
1	I	19	TYR	C-N-CA	5.10	128.95	120.94
1	I	14	TYR	CE1-CZ-CE2	-5.10	110.10	120.30
1	K	1	GLY	CA-C-O	5.09	131.50	120.80
2	L	16	TYR	CA-CB-CG	-5.09	104.73	113.90
2	H	7	CYS	O-C-N	-5.09	116.72	122.12
2	F	18	VAL	N-CA-CB	5.09	119.81	110.40
1	E	15	GLN	OE1-CD-NE2	5.08	127.68	122.60
2	H	21	GLU	CA-CB-CG	-5.08	103.94	114.10
2	D	13	GLU	CA-C-N	5.08	129.26	120.58
2	D	13	GLU	C-N-CA	5.08	129.26	120.58
2	D	16	TYR	CD1-CE1-CZ	-5.08	110.46	119.60
1	K	13	LEU	CA-C-N	-5.08	112.97	120.28
1	K	13	LEU	C-N-CA	-5.08	112.97	120.28
2	H	14	ALA	CB-CA-C	-5.07	102.37	110.79
1	K	18	ASN	CB-CA-C	-5.07	101.25	110.63
2	H	19	CYS	CB-CA-C	-5.06	100.84	109.65
2	L	2	VAL	CA-CB-CG2	-5.06	101.80	110.40
1	K	12	SER	CA-C-O	5.05	128.44	121.88
1	C	21	ASN	CA-C-O	5.05	136.14	121.00
1	I	19	TYR	CE1-CZ-OH	-5.05	104.76	119.90
2	L	21	GLU	CB-CG-CD	-5.04	104.02	112.60
1	A	3	VAL	O-C-N	-5.04	116.27	122.57
1	C	18	ASN	CB-CA-C	-5.04	100.39	110.42
2	D	22	ARG	NH1-CZ-NH2	5.04	125.85	119.30
1	G	19	TYR	N-CA-CB	5.03	117.77	110.47
2	L	11	LEU	CA-C-N	-5.03	112.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	11	LEU	C-N-CA	-5.03	112.06	120.30
2	F	11	LEU	O-C-N	5.03	128.25	122.17
2	F	22	ARG	N-CA-C	5.01	121.48	110.80
1	G	12	SER	CA-C-N	5.01	127.49	120.28
1	G	12	SER	C-N-CA	5.01	127.49	120.28
1	A	11	CYS	N-CA-CB	-5.01	102.12	110.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	159	0	144	91	0
1	C	163	0	149	112	0
1	E	163	0	148	134	0
1	G	159	0	143	74	0
1	I	163	0	149	116	0
1	K	163	0	147	126	0
2	B	219	0	207	152	0
2	D	194	0	181	101	0
2	F	194	0	180	65	0
2	H	220	0	207	101	0
2	J	235	0	225	137	0
2	L	212	0	197	121	0
3	A	7	0	5	2	0
3	C	7	0	6	0	0
3	E	7	0	5	0	0
3	G	7	0	6	2	0
3	I	7	0	5	1	0
3	K	7	0	5	2	0
4	B	1	0	0	0	0
4	C	1	0	0	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	17	0	0	5	0
6	C	17	0	0	3	0
6	D	10	0	0	6	0
6	E	7	0	0	1	0
6	F	15	0	0	5	0
6	G	17	0	0	6	0
6	H	17	0	0	3	0
6	I	19	0	0	6	0
6	J	16	0	0	1	0
6	K	9	0	0	1	0
6	L	4	0	0	0	0
All	All	2440	0	2109	1226	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 280.

All (1226) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:10:HIS:CG	2:H:10:HIS:CB	1.75	1.70
1:I:14:TYR:CE1	1:I:14:TYR:CD1	1.75	1.70
2:B:24:PHE:CG	2:B:24:PHE:CB	1.77	1.68
1:I:14:TYR:CD2	1:I:14:TYR:CE2	1.75	1.68
2:H:24:PHE:CE1	2:H:24:PHE:CD1	1.75	1.65
1:I:8:THR:CG2	1:I:8:THR:CB	1.75	1.65
2:L:10:HIS:CB	2:L:10:HIS:CG	1.76	1.63
2:H:22:ARG:CB	2:H:22:ARG:CA	1.77	1.62
1:A:9:SER:CA	1:A:9:SER:CB	1.76	1.62
1:C:2:ILE:CG2	1:C:2:ILE:CB	1.74	1.62
1:G:14:TYR:CA	1:G:14:TYR:CB	1.75	1.62
1:K:2:ILE:CG1	1:K:2:ILE:CB	1.76	1.62
2:B:2:VAL:CB	2:B:2:VAL:CG2	1.77	1.61
1:C:13:LEU:CB	1:C:13:LEU:CA	1.78	1.61
2:J:24:PHE:CG	2:J:24:PHE:CB	1.77	1.61
2:L:17:LEU:CG	2:L:17:LEU:CB	1.75	1.61
2:J:11:LEU:CB	2:J:11:LEU:CA	1.74	1.61
2:J:28:LYS:CD	2:J:28:LYS:CG	1.77	1.61
1:K:10:ILE:CD1	1:K:10:ILE:CG1	1.78	1.61
2:D:11:LEU:CG	2:D:11:LEU:CD1	1.78	1.61
2:D:13:GLU:CG	2:D:13:GLU:CB	1.79	1.61
1:E:10:ILE:CD1	1:E:10:ILE:CG1	1.75	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:ASN:CB	1:E:21:ASN:CA	1.78	1.61
1:G:10:ILE:CB	1:G:10:ILE:CG1	1.76	1.60
2:L:1:PHE:CB	2:L:1:PHE:CG	1.80	1.60
2:J:10:HIS:CG	2:J:10:HIS:CB	1.84	1.60
2:B:2:VAL:CB	2:B:2:VAL:CA	1.79	1.60
2:J:2:VAL:CB	2:J:2:VAL:CG1	1.79	1.60
1:A:5:GLN:CA	1:A:5:GLN:CB	1.78	1.59
1:C:14:TYR:CB	1:C:14:TYR:CA	1.78	1.59
2:J:9:SER:CB	2:J:9:SER:CA	1.79	1.59
2:J:18:VAL:CB	2:J:18:VAL:CG1	1.77	1.59
1:K:10:ILE:CB	1:K:10:ILE:CA	1.79	1.59
1:A:3:VAL:CB	1:A:3:VAL:CG1	1.75	1.59
1:C:11:CYS:C	1:C:11:CYS:CA	1.74	1.59
1:C:15:GLN:C	1:C:15:GLN:CA	1.74	1.59
1:K:10:ILE:CG1	1:K:10:ILE:CB	1.80	1.59
1:E:7:CYS:CB	1:E:7:CYS:CA	1.78	1.59
2:F:2:VAL:CB	2:F:2:VAL:CG2	1.81	1.59
1:I:10:ILE:CB	1:I:10:ILE:CG1	1.80	1.59
1:I:10:ILE:CB	1:I:10:ILE:CA	1.75	1.59
1:C:13:LEU:CG	1:C:13:LEU:CD2	1.76	1.59
1:G:19:TYR:CA	1:G:19:TYR:CB	1.76	1.59
2:H:2:VAL:CG2	2:H:2:VAL:CB	1.74	1.59
1:A:17:GLU:CB	1:A:17:GLU:CA	1.80	1.58
1:A:10:ILE:CB	1:A:10:ILE:CG1	1.80	1.58
2:F:17:LEU:CB	2:F:17:LEU:CG	1.78	1.58
2:L:17:LEU:CB	2:L:17:LEU:CA	1.80	1.58
1:A:2:ILE:C	1:A:2:ILE:CA	1.75	1.58
2:B:2:VAL:CA	2:B:2:VAL:C	1.75	1.58
2:L:12:VAL:CG2	2:L:12:VAL:CB	1.80	1.58
1:K:16:LEU:CG	1:K:16:LEU:CB	1.81	1.57
1:K:16:LEU:CG	1:K:16:LEU:CD1	1.76	1.57
2:F:15:LEU:CB	2:F:15:LEU:CA	1.80	1.57
2:H:11:LEU:CD2	2:H:11:LEU:CG	1.76	1.57
1:G:12:SER:CB	1:G:12:SER:CA	1.82	1.57
1:E:10:ILE:CB	1:E:10:ILE:CA	1.80	1.57
1:E:15:GLN:C	1:E:15:GLN:CA	1.77	1.57
2:L:4:GLN:CG	2:L:4:GLN:CD	1.77	1.57
1:C:16:LEU:CD2	1:C:16:LEU:CG	1.82	1.56
1:C:17:GLU:CD	1:C:17:GLU:CG	1.78	1.56
2:J:27:THR:CB	2:J:27:THR:CA	1.75	1.56
1:A:2:ILE:CG2	1:A:2:ILE:CB	1.80	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:VAL:CB	2:H:12:VAL:CA	1.82	1.56
2:J:1:PHE:CA	2:J:1:PHE:CB	1.82	1.56
2:B:25:TYR:N	2:B:25:TYR:CA	1.68	1.56
1:E:14:TYR:C	1:E:14:TYR:CA	1.74	1.56
2:H:24:PHE:CG	2:H:24:PHE:CB	1.87	1.56
1:I:1:GLY:C	1:I:1:GLY:CA	1.78	1.56
2:J:4:GLN:CA	2:J:4:GLN:CB	1.82	1.56
1:K:13:LEU:C	1:K:13:LEU:CA	1.77	1.56
2:B:21:GLU:CB	2:B:21:GLU:CA	1.75	1.56
1:E:20:CYS:CB	1:E:20:CYS:CA	1.74	1.56
2:L:2:VAL:CB	2:L:2:VAL:CA	1.84	1.56
1:A:16:LEU:CG	1:A:16:LEU:CB	1.74	1.55
2:F:26:MEA:C	2:F:26:MEA:CA	1.84	1.55
1:I:10:ILE:CG1	1:I:10:ILE:CD1	1.82	1.55
1:K:18:ASN:N	1:K:18:ASN:CA	1.69	1.55
2:H:3:ASN:C	2:H:3:ASN:CA	1.78	1.55
1:I:14:TYR:CG	1:I:14:TYR:CB	1.86	1.55
2:B:16:TYR:CB	2:B:16:TYR:CA	1.81	1.55
2:F:15:LEU:CG	2:F:15:LEU:CD1	1.84	1.55
2:J:12:VAL:CB	2:J:12:VAL:CG2	1.79	1.55
2:J:18:VAL:C	2:J:18:VAL:CA	1.77	1.55
1:K:4:GLU:CB	1:K:4:GLU:CA	1.79	1.55
1:K:16:LEU:C	1:K:16:LEU:CA	1.78	1.55
2:B:4:GLN:CB	2:B:4:GLN:CG	1.81	1.55
2:B:9:SER:CB	2:B:9:SER:CA	1.76	1.55
2:B:17:LEU:CG	2:B:17:LEU:CD1	1.82	1.55
1:C:17:GLU:CA	1:C:17:GLU:CB	1.83	1.55
1:E:5:GLN:C	1:E:5:GLN:CA	1.80	1.55
1:I:13:LEU:CG	1:I:13:LEU:CB	1.85	1.55
1:I:16:LEU:CB	1:I:16:LEU:CA	1.85	1.55
1:E:16:LEU:N	1:E:16:LEU:CA	1.69	1.54
2:H:6:LEU:CB	2:H:6:LEU:CG	1.85	1.54
2:J:28:LYS:CB	2:J:28:LYS:CA	1.84	1.54
1:A:12:SER:CA	1:A:12:SER:CB	1.86	1.54
1:A:21:ASN:CB	1:A:21:ASN:CA	1.79	1.54
1:C:1:GLY:C	1:C:1:GLY:CA	1.76	1.54
1:C:3:VAL:CB	1:C:3:VAL:CA	1.82	1.54
1:K:11:CYS:N	1:K:11:CYS:CA	1.69	1.54
2:D:5:HIS:C	2:D:5:HIS:CA	1.80	1.54
1:E:2:ILE:CB	1:E:2:ILE:CG2	1.77	1.54
1:I:21:ASN:N	1:I:21:ASN:CA	1.70	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:21:GLU:CB	2:L:21:GLU:CG	1.74	1.54
2:F:21:GLU:CD	2:F:21:GLU:CG	1.78	1.54
2:H:9:SER:CB	2:H:9:SER:CA	1.86	1.54
2:J:4:GLN:CD	2:J:4:GLN:CG	1.78	1.54
1:K:6:CYS:CA	1:K:6:CYS:N	1.71	1.54
1:A:10:ILE:C	1:A:10:ILE:CA	1.81	1.54
1:I:2:ILE:CG1	1:I:2:ILE:CB	1.84	1.54
1:K:2:ILE:C	1:K:2:ILE:CA	1.81	1.54
1:C:20:CYS:CB	1:C:20:CYS:CA	1.83	1.53
2:D:14:ALA:N	2:D:14:ALA:CA	1.69	1.53
1:E:11:CYS:CB	1:E:11:CYS:CA	1.86	1.53
1:C:12:SER:N	1:C:12:SER:CA	1.70	1.53
2:H:2:VAL:CB	2:H:2:VAL:CA	1.85	1.53
2:H:5:HIS:CB	2:H:5:HIS:CA	1.86	1.53
2:B:11:LEU:N	2:B:11:LEU:CA	1.69	1.53
2:D:13:GLU:C	2:D:13:GLU:CA	1.76	1.53
2:D:19:CYS:CB	2:D:19:CYS:CA	1.87	1.53
1:G:18:ASN:CB	1:G:18:ASN:CG	1.76	1.53
2:L:4:GLN:N	2:L:4:GLN:CA	1.70	1.53
2:B:22:ARG:C	2:B:22:ARG:CA	1.77	1.53
2:J:10:HIS:C	2:J:10:HIS:CA	1.80	1.53
2:H:1:PHE:CB	2:H:1:PHE:CA	1.81	1.52
2:J:14:ALA:C	2:J:14:ALA:CA	1.80	1.52
2:L:20:GLY:CA	2:L:20:GLY:C	1.79	1.52
1:G:9:SER:CB	1:G:9:SER:CA	1.87	1.52
1:I:7:CYS:N	1:I:7:CYS:CA	1.72	1.52
1:A:11:CYS:CA	1:A:11:CYS:N	1.73	1.52
1:I:6:CYS:C	1:I:6:CYS:CA	1.81	1.52
1:I:16:LEU:CD1	1:I:16:LEU:CG	1.84	1.52
2:J:22:ARG:N	2:J:22:ARG:CA	1.70	1.52
2:B:3:ASN:C	2:B:3:ASN:CA	1.78	1.52
1:E:18:ASN:N	1:E:18:ASN:CA	1.68	1.52
1:I:3:VAL:N	1:I:3:VAL:CA	1.69	1.52
1:K:2:ILE:CA	1:K:2:ILE:N	1.72	1.52
2:B:18:VAL:CA	2:B:18:VAL:N	1.73	1.52
2:D:11:LEU:CG	2:D:11:LEU:CD2	1.83	1.52
2:F:3:ASN:CA	2:F:3:ASN:N	1.68	1.52
2:F:10:HIS:N	2:F:10:HIS:CA	1.72	1.52
2:F:24:PHE:C	2:F:24:PHE:CA	1.75	1.52
1:I:10:ILE:CA	1:I:10:ILE:C	1.79	1.52
2:J:2:VAL:CB	2:J:2:VAL:CA	1.87	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:VAL:CA	2:B:12:VAL:CB	1.87	1.51
1:C:7:CYS:CA	1:C:7:CYS:CB	1.80	1.51
2:D:6:LEU:N	2:D:6:LEU:CA	1.70	1.51
1:I:20:CYS:C	1:I:20:CYS:CA	1.81	1.51
1:C:2:ILE:N	1:C:2:ILE:CA	1.70	1.51
2:D:15:LEU:CG	2:D:15:LEU:CD1	1.81	1.51
2:L:6:LEU:CB	2:L:6:LEU:CA	1.87	1.51
2:L:13:GLU:CA	2:L:13:GLU:CB	1.89	1.51
1:A:6:CYS:C	1:A:6:CYS:CA	1.79	1.51
2:D:21:GLU:CD	2:D:21:GLU:CG	1.80	1.51
1:E:2:ILE:CB	1:E:2:ILE:CG1	1.88	1.51
1:E:6:CYS:N	1:E:6:CYS:CA	1.69	1.51
1:K:10:ILE:CA	1:K:10:ILE:C	1.82	1.51
2:L:3:ASN:C	2:L:3:ASN:CA	1.75	1.51
1:A:21:ASN:CB	1:A:21:ASN:CG	1.83	1.51
2:D:15:LEU:CA	2:D:15:LEU:CB	1.83	1.51
2:H:13:GLU:C	2:H:13:GLU:CA	1.82	1.51
1:A:3:VAL:CA	1:A:3:VAL:N	1.70	1.50
1:E:4:GLU:C	1:E:4:GLU:CA	1.80	1.50
2:J:11:LEU:CA	2:J:11:LEU:N	1.71	1.50
2:L:6:LEU:CD1	2:L:6:LEU:CG	1.88	1.50
2:F:20:GLY:C	2:F:20:GLY:CA	1.83	1.50
1:K:7:CYS:N	1:K:7:CYS:CA	1.67	1.50
1:E:9:SER:N	1:E:9:SER:CA	1.75	1.50
2:F:22:ARG:CD	2:F:22:ARG:CG	1.89	1.50
1:A:5:GLN:CA	1:A:5:GLN:N	1.68	1.50
2:B:4:GLN:N	2:B:4:GLN:CA	1.68	1.50
2:J:21:GLU:C	2:J:21:GLU:CA	1.83	1.50
2:L:14:ALA:C	2:L:14:ALA:CA	1.85	1.50
1:A:19:TYR:CB	1:A:19:TYR:CA	1.84	1.49
2:B:5:HIS:CB	2:B:5:HIS:CA	1.90	1.49
1:C:8:THR:CB	1:C:8:THR:CG2	1.87	1.49
2:B:11:LEU:CD2	2:B:11:LEU:CG	1.91	1.49
2:H:18:VAL:CB	2:H:18:VAL:CG1	1.88	1.49
2:L:22:ARG:CD	2:L:22:ARG:NE	1.75	1.49
1:A:7:CYS:N	1:A:7:CYS:CA	1.75	1.49
1:C:2:ILE:CB	1:C:2:ILE:CG1	1.86	1.49
1:C:18:ASN:C	1:C:18:ASN:CA	1.82	1.49
2:H:10:HIS:C	2:H:10:HIS:CA	1.83	1.49
2:H:13:GLU:CG	2:H:13:GLU:CB	1.89	1.49
2:H:17:LEU:CD1	2:H:17:LEU:CG	1.90	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:13:GLU:CA	2:J:13:GLU:CB	1.91	1.49
1:E:19:TYR:N	1:E:19:TYR:CA	1.76	1.48
2:H:15:LEU:CG	2:H:15:LEU:CD2	1.90	1.48
2:J:25:TYR:CB	2:J:25:TYR:CA	1.91	1.48
2:B:10:HIS:C	2:B:10:HIS:CA	1.84	1.48
2:D:26:MEA:N	2:D:26:MEA:C1	1.74	1.48
2:J:19:CYS:N	2:J:19:CYS:CA	1.75	1.48
2:J:28:LYS:CE	2:J:28:LYS:NZ	1.74	1.48
2:D:16:TYR:C	2:D:16:TYR:CA	1.85	1.48
2:H:6:LEU:CA	2:H:6:LEU:C	1.80	1.48
2:H:16:TYR:CB	2:H:16:TYR:CA	1.91	1.48
2:H:7:CYS:N	2:H:7:CYS:CA	1.76	1.48
1:E:1:GLY:C	1:E:1:GLY:CA	1.85	1.48
1:G:2:ILE:CB	1:G:2:ILE:CG2	1.90	1.48
1:K:3:VAL:CA	1:K:3:VAL:N	1.69	1.48
1:K:5:GLN:C	1:K:5:GLN:CA	1.87	1.48
2:B:6:LEU:CG	2:B:6:LEU:CB	1.92	1.47
1:G:13:LEU:CD2	1:G:13:LEU:CG	1.89	1.47
2:H:14:ALA:N	2:H:14:ALA:CA	1.78	1.47
2:B:23:GLY:N	2:B:23:GLY:CA	1.72	1.47
1:E:2:ILE:N	1:E:2:ILE:CA	1.74	1.47
2:L:3:ASN:CG	2:L:3:ASN:CB	1.87	1.47
1:K:1:GLY:C	1:K:1:GLY:CA	1.85	1.47
2:B:3:ASN:CA	2:B:3:ASN:N	1.71	1.47
2:J:15:LEU:N	2:J:15:LEU:CA	1.76	1.47
2:B:17:LEU:C	2:B:17:LEU:CA	1.85	1.46
1:C:15:GLN:CA	1:C:15:GLN:N	1.77	1.46
2:D:22:ARG:CB	2:D:22:ARG:CG	1.93	1.46
1:I:2:ILE:N	1:I:2:ILE:CA	1.76	1.46
2:L:18:VAL:C	2:L:18:VAL:CA	1.87	1.46
2:D:3:ASN:N	2:D:3:ASN:CA	1.77	1.46
1:G:6:CYS:C	1:G:6:CYS:CA	1.86	1.46
1:C:4:GLU:C	1:C:4:GLU:CA	1.88	1.46
1:I:13:LEU:C	1:I:13:LEU:CA	1.87	1.46
2:H:11:LEU:N	2:H:11:LEU:CA	1.78	1.46
1:I:4:GLU:CB	1:I:4:GLU:CA	1.92	1.46
2:J:26:MEA:CB	2:J:26:MEA:CA	1.93	1.46
1:I:5:GLN:C	1:I:5:GLN:CA	1.87	1.45
1:K:17:GLU:C	1:K:17:GLU:CA	1.88	1.45
1:C:14:TYR:CA	1:C:14:TYR:C	1.86	1.45
1:E:18:ASN:CA	1:E:18:ASN:C	1.89	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:GLU:N	2:F:21:GLU:CA	1.78	1.45
1:C:8:THR:CA	1:C:8:THR:C	1.88	1.45
1:I:6:CYS:CA	1:I:6:CYS:N	1.77	1.45
2:B:13:GLU:CB	2:B:13:GLU:CG	1.93	1.45
1:C:5:GLN:CA	1:C:5:GLN:N	1.77	1.45
2:D:12:VAL:CB	2:D:12:VAL:CA	1.91	1.45
1:K:17:GLU:CD	1:K:17:GLU:CG	1.90	1.45
2:L:15:LEU:N	2:L:15:LEU:CA	1.76	1.45
1:E:8:THR:C	1:E:8:THR:CA	1.87	1.44
2:L:24:PHE:CB	2:L:24:PHE:CA	1.95	1.44
2:B:13:GLU:C	2:B:13:GLU:CA	1.90	1.43
1:I:14:TYR:CA	1:I:14:TYR:N	1.78	1.43
1:I:14:TYR:CZ	1:I:14:TYR:OH	1.70	1.43
1:I:17:GLU:C	1:I:17:GLU:CA	1.89	1.43
2:F:12:VAL:CB	2:F:12:VAL:CA	1.93	1.43
2:H:17:LEU:C	2:H:17:LEU:CA	1.89	1.43
2:B:14:ALA:N	2:B:14:ALA:CA	1.80	1.43
2:D:25:TYR:N	2:D:25:TYR:CA	1.79	1.43
2:H:18:VAL:N	2:H:18:VAL:CA	1.82	1.43
2:L:19:CYS:N	2:L:19:CYS:CA	1.81	1.43
1:I:18:ASN:N	1:I:18:ASN:CA	1.78	1.43
2:D:24:PHE:C	2:D:24:PHE:CA	1.92	1.43
1:G:14:TYR:CA	1:G:14:TYR:N	1.77	1.43
1:C:11:CYS:SG	1:C:11:CYS:CB	2.05	1.42
1:I:9:SER:CB	1:I:9:SER:OG	1.65	1.42
2:B:7:CYS:N	2:B:7:CYS:CA	1.80	1.42
1:G:7:CYS:N	1:G:7:CYS:CA	1.81	1.42
1:K:8:THR:OG1	1:K:8:THR:CB	1.67	1.42
2:B:6:LEU:C	2:B:6:LEU:CA	1.93	1.41
2:D:17:LEU:N	2:D:17:LEU:CA	1.80	1.41
2:D:9:SER:C	2:D:9:SER:CA	1.93	1.41
2:B:15:LEU:CD2	2:B:15:LEU:CG	1.98	1.41
1:I:6:CYS:CB	1:I:6:CYS:SG	2.07	1.40
2:D:10:HIS:CA	2:D:10:HIS:N	1.79	1.40
1:C:19:TYR:N	1:C:19:TYR:CA	1.82	1.40
2:D:2:VAL:C	2:D:2:VAL:CA	1.96	1.39
1:K:20:CYS:C	1:K:20:CYS:CA	1.96	1.39
1:K:21:ASN:N	1:K:21:ASN:CA	1.83	1.38
1:C:9:SER:N	1:C:9:SER:CA	1.86	1.37
1:G:8:THR:OG1	1:G:8:THR:CB	1.70	1.36
2:J:29:PRO:CG	2:J:29:PRO:CB	1.83	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:12:SER:CB	1:K:12:SER:OG	1.74	1.33
1:A:6:CYS:CB	1:A:6:CYS:SG	2.15	1.32
1:I:12:SER:OG	1:I:12:SER:CB	1.79	1.31
1:I:20:CYS:SG	1:I:20:CYS:CB	2.20	1.29
2:H:7:CYS:CB	2:H:7:CYS:SG	2.21	1.28
2:J:10:HIS:NE2	2:J:10:HIS:CD2	1.72	1.27
1:G:6:CYS:CB	1:G:6:CYS:SG	2.25	1.23
2:H:2:VAL:CG2	2:H:2:VAL:CG1	2.18	1.22
2:B:17:LEU:CD1	2:B:17:LEU:CB	2.17	1.21
1:K:20:CYS:CB	1:K:20:CYS:SG	2.30	1.19
2:B:7:CYS:SG	2:B:7:CYS:CB	2.32	1.16
1:E:3:VAL:HG22	6:E:2001:HOH:O	1.46	1.12
2:B:17:LEU:CD1	2:B:17:LEU:HB2	1.80	1.09
2:H:12:VAL:CA	2:H:12:VAL:CG2	2.31	1.09
1:I:8:THR:HG23	6:I:2011:HOH:O	1.53	1.08
2:B:18:VAL:HA	1:G:13:LEU:HD21	1.29	1.07
1:G:18:ASN:HB3	6:G:2010:HOH:O	1.53	1.07
2:B:2:VAL:CA	2:B:2:VAL:CG1	2.34	1.04
2:F:26:MEA:C	2:F:26:MEA:HC3	1.88	1.03
2:L:18:VAL:C	2:L:18:VAL:HG22	1.83	1.03
2:L:4:GLN:CD	2:L:4:GLN:CB	2.32	1.03
2:B:21:GLU:CB	2:B:21:GLU:C	2.32	1.02
1:C:12:SER:N	1:C:12:SER:C	2.18	1.01
2:F:2:VAL:N	6:F:2001:HOH:O	1.93	1.01
2:J:28:LYS:CB	2:J:28:LYS:HA	1.87	1.01
2:F:3:ASN:N	2:F:3:ASN:C	2.18	1.00
1:G:14:TYR:CA	1:G:14:TYR:CG	2.45	1.00
2:B:24:PHE:CB	2:B:24:PHE:CD1	2.42	1.00
1:C:16:LEU:CD2	1:C:16:LEU:CB	2.39	1.00
2:J:28:LYS:HD2	2:L:20:GLY:HA2	1.44	0.99
1:A:10:ILE:C	1:A:10:ILE:HG22	1.86	0.99
2:F:26:MEA:C	2:F:26:MEA:C1	2.38	0.99
2:B:11:LEU:N	2:B:11:LEU:CB	2.24	0.99
2:D:26:MEA:C1	2:D:26:MEA:C	2.40	0.99
1:E:14:TYR:CA	1:E:15:GLN:N	2.26	0.99
1:G:14:TYR:CB	1:G:14:TYR:C	2.34	0.99
2:J:18:VAL:CG1	2:J:18:VAL:C	2.35	0.99
2:D:13:GLU:CB	2:D:13:GLU:C	2.36	0.98
2:D:26:MEA:C1	2:D:26:MEA:CA	2.40	0.98
2:H:11:LEU:CD2	2:H:11:LEU:CD1	2.40	0.98
2:B:6:LEU:HD22	2:J:10:HIS:CG	1.98	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:HIS:C	2:B:11:LEU:CA	2.36	0.98
2:J:12:VAL:HG12	2:L:12:VAL:HG13	1.44	0.97
1:A:10:ILE:CG1	1:A:10:ILE:CA	2.42	0.97
2:H:12:VAL:CB	2:H:12:VAL:C	2.38	0.97
2:B:12:VAL:CA	2:B:12:VAL:CG2	2.43	0.97
1:E:21:ASN:CB	1:E:21:ASN:HA	1.93	0.96
1:I:21:ASN:N	1:I:21:ASN:CB	2.28	0.96
2:B:24:PHE:C	2:B:25:TYR:CA	2.39	0.96
1:I:20:CYS:C	1:I:21:ASN:CA	2.38	0.96
2:J:28:LYS:CD	2:J:28:LYS:CB	2.44	0.95
1:A:10:ILE:C	1:A:10:ILE:CG2	2.39	0.95
2:J:27:THR:CA	2:J:27:THR:HB	1.94	0.95
1:A:9:SER:CB	1:A:9:SER:C	2.39	0.94
2:J:18:VAL:CB	2:J:18:VAL:C	2.39	0.94
2:J:11:LEU:CB	2:J:11:LEU:C	2.40	0.94
2:H:5:HIS:CB	2:H:5:HIS:C	2.41	0.93
1:A:17:GLU:CB	1:A:17:GLU:C	2.40	0.93
2:F:2:VAL:CG2	2:F:2:VAL:CA	2.47	0.93
1:G:21:ASN:HA	6:G:2016:HOH:O	1.68	0.92
2:H:17:LEU:CD1	2:H:17:LEU:HG	2.00	0.92
1:K:14:TYR:CD1	1:K:14:TYR:C	2.45	0.92
2:L:21:GLU:CB	2:L:21:GLU:CD	2.43	0.92
2:F:10:HIS:N	2:F:10:HIS:C	2.29	0.91
1:K:4:GLU:CB	1:K:4:GLU:N	2.33	0.91
1:I:10:ILE:CB	1:I:10:ILE:HA	2.00	0.91
2:L:12:VAL:CG2	2:L:12:VAL:HB	2.00	0.91
2:B:2:VAL:CB	2:B:2:VAL:N	2.33	0.91
2:L:18:VAL:C	2:L:18:VAL:CG2	2.44	0.91
1:E:7:CYS:CB	1:E:7:CYS:N	2.34	0.91
1:A:16:LEU:CB	1:A:16:LEU:HG	1.98	0.91
2:D:14:ALA:N	2:D:14:ALA:C	2.29	0.91
1:G:19:TYR:CA	1:G:19:TYR:CG	2.54	0.90
1:K:13:LEU:CA	1:K:14:TYR:N	2.34	0.90
1:G:4:GLU:CD	1:G:4:GLU:H	1.79	0.90
1:I:10:ILE:CA	1:I:10:ILE:HB	2.01	0.90
2:J:1:PHE:CB	2:J:1:PHE:HA	1.97	0.90
2:F:21:GLU:N	2:F:21:GLU:CB	2.34	0.90
2:L:1:PHE:CB	2:L:1:PHE:CD1	2.53	0.90
2:B:2:VAL:O	2:B:6:LEU:HG	1.71	0.90
2:B:17:LEU:C	2:B:18:VAL:CA	2.45	0.90
1:C:15:GLN:C	1:C:15:GLN:CB	2.43	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:12:VAL:CB	2:F:12:VAL:HA	2.00	0.90
1:I:2:ILE:CG1	1:I:2:ILE:CG2	2.49	0.90
1:A:21:ASN:ND2	2:B:22:ARG:HE	1.69	0.89
2:B:2:VAL:CG2	2:B:2:VAL:CG1	2.47	0.89
1:E:20:CYS:CB	1:E:20:CYS:N	2.34	0.89
2:J:25:TYR:OH	1:K:21:ASN:ND2	2.05	0.89
1:K:7:CYS:N	1:K:7:CYS:CB	2.36	0.89
1:I:8:THR:CG2	1:I:8:THR:HB	1.99	0.89
1:C:3:VAL:O	1:C:7:CYS:HB2	1.73	0.89
1:K:6:CYS:C	1:K:7:CYS:CA	2.46	0.89
2:B:22:ARG:C	2:B:22:ARG:N	2.30	0.89
2:F:19:CYS:O	2:F:22:ARG:HD3	1.73	0.89
2:H:22:ARG:CB	2:H:22:ARG:HA	2.02	0.89
2:L:6:LEU:CD1	2:L:6:LEU:CD2	2.50	0.89
1:C:3:VAL:CA	1:C:3:VAL:CG1	2.50	0.89
1:K:10:ILE:CG1	1:K:10:ILE:HB	2.03	0.89
2:J:12:VAL:CG2	2:J:12:VAL:CG1	2.49	0.88
2:D:19:CYS:O	2:D:22:ARG:HG3	1.73	0.88
2:L:22:ARG:NE	2:L:22:ARG:CG	2.36	0.88
2:D:11:LEU:CD2	2:D:11:LEU:HG	2.02	0.88
2:H:6:LEU:C	2:H:6:LEU:N	2.32	0.88
2:B:9:SER:OG	2:D:13:GLU:OE1	1.90	0.88
1:G:10:ILE:CG1	1:G:10:ILE:CA	2.52	0.88
1:K:2:ILE:CG1	1:K:2:ILE:CG2	2.52	0.88
1:E:10:ILE:CG1	1:E:10:ILE:CA	2.52	0.88
1:C:13:LEU:CB	1:C:13:LEU:N	2.37	0.88
1:K:6:CYS:N	1:K:6:CYS:CB	2.35	0.88
2:F:20:GLY:C	2:F:21:GLU:CA	2.47	0.87
1:C:13:LEU:CB	1:C:13:LEU:CD2	2.51	0.87
2:F:15:LEU:CB	2:F:15:LEU:C	2.46	0.87
2:J:14:ALA:C	2:J:14:ALA:CB	2.46	0.87
1:E:14:TYR:C	1:E:14:TYR:HA	1.96	0.87
2:J:25:TYR:CZ	1:K:21:ASN:ND2	2.43	0.87
2:B:3:ASN:C	2:B:4:GLN:CA	2.48	0.87
2:B:3:ASN:N	2:B:3:ASN:HA	1.86	0.87
2:H:6:LEU:HD22	2:L:10:HIS:CD2	2.10	0.87
2:D:26:MEA:C	2:D:26:MEA:HC3	2.04	0.86
2:F:17:LEU:CB	2:F:17:LEU:HG	2.05	0.86
1:E:2:ILE:HD12	1:E:19:TYR:CD1	2.10	0.86
2:B:4:GLN:CG	2:B:4:GLN:CA	2.53	0.86
2:D:11:LEU:CD1	2:D:11:LEU:CB	2.53	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:13:LEU:C	1:I:13:LEU:HA	1.98	0.86
1:A:10:ILE:CB	1:A:10:ILE:C	2.48	0.86
2:B:10:HIS:O	2:B:11:LEU:CA	2.24	0.86
2:L:2:VAL:CA	2:L:2:VAL:CG2	2.53	0.86
1:K:18:ASN:N	1:K:18:ASN:CB	2.38	0.86
2:B:18:VAL:N	2:B:18:VAL:CB	2.38	0.86
2:J:18:VAL:C	2:J:18:VAL:HG12	1.98	0.86
1:K:17:GLU:C	1:K:18:ASN:CA	2.49	0.85
2:H:13:GLU:C	2:H:13:GLU:N	2.35	0.85
1:E:1:GLY:C	1:E:4:GLU:HG2	2.00	0.85
1:C:2:ILE:N	1:C:2:ILE:C	2.34	0.85
1:C:18:ASN:C	1:C:18:ASN:CB	2.48	0.85
1:E:9:SER:N	1:E:9:SER:C	2.34	0.85
1:E:15:GLN:C	1:E:16:LEU:CA	2.49	0.85
2:H:9:SER:CB	2:H:9:SER:HA	2.05	0.85
1:I:14:TYR:CG	1:I:14:TYR:CA	2.57	0.85
2:J:11:LEU:CA	2:J:11:LEU:CG	2.53	0.85
2:L:21:GLU:CG	2:L:21:GLU:CA	2.54	0.85
1:I:2:ILE:HD13	2:J:15:LEU:HD11	1.58	0.84
2:D:3:ASN:N	2:D:3:ASN:C	2.36	0.84
1:E:5:GLN:C	1:E:6:CYS:CA	2.49	0.84
1:I:14:TYR:CG	1:I:14:TYR:C	2.55	0.84
1:K:12:SER:OG	1:K:12:SER:C	2.19	0.84
2:B:16:TYR:CA	2:B:16:TYR:CG	2.60	0.84
2:J:27:THR:CB	2:J:27:THR:HA	2.04	0.84
1:A:5:GLN:NE2	1:A:19:TYR:OH	2.11	0.84
1:C:2:ILE:CG1	1:C:2:ILE:HB	2.05	0.84
1:E:2:ILE:CG2	1:E:2:ILE:HB	2.06	0.84
1:E:2:ILE:HD12	1:E:19:TYR:CG	2.12	0.84
2:B:2:VAL:C	2:B:2:VAL:N	2.36	0.84
1:C:2:ILE:CG2	1:C:2:ILE:CA	2.56	0.84
1:C:14:TYR:CA	1:C:14:TYR:CG	2.60	0.84
1:K:16:LEU:C	1:K:16:LEU:HA	2.03	0.84
2:F:24:PHE:C	2:F:24:PHE:N	2.35	0.83
2:B:16:TYR:CB	2:B:16:TYR:N	2.42	0.83
1:I:2:ILE:CD1	2:J:15:LEU:HD11	2.09	0.83
1:K:5:GLN:OE1	1:K:19:TYR:OH	1.96	0.83
2:J:18:VAL:CG1	2:J:18:VAL:HB	2.02	0.83
1:E:4:GLU:C	1:E:4:GLU:HA	2.02	0.83
1:E:8:THR:C	1:E:8:THR:HA	2.00	0.83
1:G:19:TYR:CB	1:G:19:TYR:C	2.51	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:PHE:C	2:B:2:VAL:C	2.46	0.83
1:C:17:GLU:CB	1:C:17:GLU:N	2.40	0.83
2:H:2:VAL:CA	2:H:2:VAL:CG1	2.56	0.83
1:E:5:GLN:C	1:E:5:GLN:HA	2.02	0.82
1:G:2:ILE:CG2	1:G:2:ILE:CG1	2.57	0.82
2:H:12:VAL:C	2:H:13:GLU:C	2.46	0.82
2:D:9:SER:HA	2:D:12:VAL:HG22	1.60	0.82
1:G:14:TYR:N	1:G:14:TYR:C	2.37	0.82
1:E:15:GLN:C	1:E:15:GLN:HA	1.99	0.82
2:L:6:LEU:CB	2:L:6:LEU:HA	2.09	0.82
1:K:16:LEU:CD1	1:K:16:LEU:HG	2.08	0.82
1:C:14:TYR:CB	1:C:14:TYR:N	2.43	0.81
2:H:5:HIS:HB2	1:K:10:ILE:HD11	1.63	0.81
2:H:10:HIS:CG	2:H:10:HIS:CA	2.62	0.81
1:I:6:CYS:C	1:I:7:CYS:CA	2.53	0.81
2:J:2:VAL:CG1	2:J:2:VAL:CG2	2.57	0.81
1:E:6:CYS:N	1:E:7:CYS:N	2.27	0.81
1:E:19:TYR:N	1:E:19:TYR:CD1	2.48	0.81
2:B:4:GLN:CB	2:B:4:GLN:N	2.40	0.81
1:K:16:LEU:CB	1:K:16:LEU:CD2	2.58	0.80
2:B:9:SER:CB	2:B:9:SER:N	2.43	0.80
1:E:10:ILE:CB	1:E:10:ILE:C	2.53	0.80
2:L:22:ARG:CD	2:L:22:ARG:HH11	1.94	0.80
1:A:21:ASN:HB3	2:B:22:ARG:HB3	1.64	0.80
1:E:8:THR:C	1:E:9:SER:CA	2.52	0.80
1:A:10:ILE:CB	1:A:10:ILE:CD1	2.60	0.80
1:E:4:GLU:CA	1:E:5:GLN:N	2.39	0.80
1:K:2:ILE:C	1:K:3:VAL:CA	2.54	0.80
1:A:2:ILE:C	1:A:2:ILE:N	2.40	0.79
1:A:5:GLN:CB	1:A:5:GLN:C	2.52	0.79
1:E:6:CYS:N	1:E:6:CYS:CB	2.43	0.79
2:D:3:ASN:N	2:D:4:GLN:N	2.29	0.79
2:J:28:LYS:CG	2:J:28:LYS:CA	2.57	0.79
2:D:25:TYR:N	2:D:25:TYR:C	2.39	0.79
1:A:21:ASN:CB	1:A:21:ASN:N	2.45	0.79
2:D:13:GLU:CB	2:D:13:GLU:CD	2.54	0.79
1:I:7:CYS:N	1:I:7:CYS:CB	2.43	0.79
2:J:11:LEU:N	2:J:11:LEU:HA	1.94	0.79
1:K:10:ILE:CA	1:K:10:ILE:CG2	2.60	0.79
2:D:6:LEU:N	2:D:6:LEU:HA	1.96	0.78
1:K:17:GLU:C	1:K:17:GLU:HA	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:19:CYS:C	2:L:20:GLY:C	2.52	0.78
1:E:13:LEU:O	1:E:17:GLU:HG3	1.82	0.78
2:J:2:VAL:CA	2:J:2:VAL:CG2	2.61	0.78
2:J:9:SER:CB	2:J:9:SER:C	2.55	0.78
2:J:12:VAL:CG2	2:J:12:VAL:CA	2.58	0.78
2:J:15:LEU:N	2:J:16:TYR:N	2.30	0.78
1:C:4:GLU:O	1:C:8:THR:HG23	1.82	0.78
1:E:11:CYS:CB	1:E:11:CYS:N	2.45	0.78
2:J:22:ARG:N	2:J:22:ARG:CB	2.44	0.78
2:L:17:LEU:CB	2:L:17:LEU:HA	2.08	0.78
1:G:10:ILE:CG1	1:G:10:ILE:CG2	2.59	0.78
2:J:25:TYR:CE2	1:K:21:ASN:ND2	2.52	0.78
1:A:3:VAL:CG1	1:A:3:VAL:CG2	2.60	0.78
2:B:9:SER:CB	2:B:9:SER:HA	2.11	0.78
1:A:5:GLN:N	1:A:5:GLN:C	2.39	0.77
1:C:15:GLN:N	1:C:15:GLN:CB	2.43	0.77
2:J:13:GLU:OE1	2:L:9:SER:OG	2.02	0.77
2:H:2:VAL:CG2	2:H:2:VAL:HG11	2.15	0.77
2:D:17:LEU:N	2:D:17:LEU:HA	1.97	0.77
2:F:24:PHE:CA	2:F:25:TYR:N	2.48	0.77
1:I:10:ILE:CG1	1:I:10:ILE:CG2	2.62	0.77
1:K:8:THR:OG1	1:K:8:THR:CG2	2.32	0.77
1:I:17:GLU:HA	1:I:20:CYS:SG	2.24	0.77
1:G:12:SER:CB	1:G:12:SER:N	2.46	0.77
1:I:20:CYS:O	1:I:21:ASN:CA	2.33	0.77
1:K:3:VAL:N	1:K:3:VAL:CB	2.45	0.76
2:L:2:VAL:CB	2:L:2:VAL:C	2.57	0.76
1:A:6:CYS:C	1:A:6:CYS:N	2.42	0.76
1:E:6:CYS:N	1:E:7:CYS:H	1.82	0.76
2:F:15:LEU:CB	2:F:15:LEU:CD1	2.62	0.76
2:J:28:LYS:HD2	2:L:20:GLY:CA	2.16	0.76
1:A:2:ILE:CG2	1:A:2:ILE:CG1	2.61	0.76
2:B:2:VAL:CG2	2:B:2:VAL:HB	2.08	0.76
2:H:1:PHE:CB	2:H:1:PHE:C	2.57	0.76
1:I:10:ILE:C	1:I:10:ILE:N	2.44	0.76
1:E:2:ILE:CG2	1:E:2:ILE:CA	2.64	0.76
2:F:9:SER:HA	2:F:12:VAL:HG22	1.67	0.76
1:I:3:VAL:N	1:I:3:VAL:C	2.41	0.76
2:J:12:VAL:CG1	2:L:12:VAL:HG13	2.14	0.76
1:E:2:ILE:HB	1:E:19:TYR:CD2	2.20	0.76
2:F:17:LEU:HD23	2:L:17:LEU:HD12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:LEU:CD2	1:G:13:LEU:CB	2.60	0.76
2:H:2:VAL:CB	2:H:2:VAL:HA	2.07	0.76
1:I:6:CYS:C	1:I:6:CYS:HA	2.09	0.76
1:C:16:LEU:HA	1:C:16:LEU:HD23	1.68	0.75
2:F:17:LEU:CB	2:F:17:LEU:CD1	2.62	0.75
1:I:6:CYS:CB	1:I:11:CYS:SG	2.75	0.75
2:B:18:VAL:CA	1:G:13:LEU:HD21	2.11	0.75
1:C:14:TYR:C	1:C:14:TYR:HA	2.08	0.75
1:E:1:GLY:C	1:E:2:ILE:CA	2.59	0.75
2:J:15:LEU:N	2:J:15:LEU:C	2.42	0.74
2:B:25:TYR:N	2:B:25:TYR:CB	2.48	0.74
2:H:7:CYS:N	2:H:7:CYS:HA	1.99	0.74
1:K:2:ILE:CG1	1:K:2:ILE:CA	2.62	0.74
1:C:11:CYS:C	1:C:11:CYS:HA	2.03	0.74
2:F:20:GLY:O	2:F:21:GLU:CA	2.34	0.74
2:L:17:LEU:CB	2:L:17:LEU:CD2	2.64	0.74
2:H:5:HIS:HB2	1:K:10:ILE:CD1	2.18	0.74
1:K:5:GLN:O	1:K:6:CYS:CA	2.35	0.74
1:C:2:ILE:N	1:C:3:VAL:N	2.35	0.74
1:A:10:ILE:CG1	1:A:10:ILE:N	2.50	0.74
1:K:2:ILE:CB	1:K:2:ILE:CD1	2.64	0.74
1:E:18:ASN:N	1:E:18:ASN:CB	2.47	0.73
2:D:12:VAL:CA	2:D:12:VAL:HB	2.15	0.73
1:I:16:LEU:CB	1:I:16:LEU:N	2.46	0.73
1:A:12:SER:CB	1:A:12:SER:C	2.61	0.73
1:I:20:CYS:C	1:I:20:CYS:N	2.46	0.73
2:L:4:GLN:N	2:L:4:GLN:HA	1.99	0.73
1:A:10:ILE:C	1:A:11:CYS:CA	2.61	0.73
1:C:5:GLN:N	1:C:5:GLN:CB	2.49	0.73
1:E:10:ILE:CD1	2:J:2:VAL:HA	2.18	0.73
1:I:7:CYS:N	1:I:7:CYS:SG	2.62	0.73
1:I:2:ILE:C	1:I:3:VAL:CA	2.58	0.73
2:J:18:VAL:CG1	2:J:18:VAL:CA	2.65	0.73
1:K:5:GLN:C	1:K:6:CYS:CA	2.52	0.73
1:A:2:ILE:CA	1:A:2:ILE:CG2	2.65	0.73
1:G:4:GLU:HG2	6:G:2001:HOH:O	1.88	0.73
1:E:2:ILE:CG1	1:E:2:ILE:C	2.61	0.73
2:H:24:PHE:HE2	2:H:26:MEA:HB2	1.54	0.72
2:B:21:GLU:C	2:B:22:ARG:C	2.57	0.72
1:C:7:CYS:CB	1:C:7:CYS:C	2.61	0.72
2:B:2:VAL:C	2:B:2:VAL:HA	2.10	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:HIS:CA	2:B:11:LEU:N	2.46	0.72
1:E:9:SER:N	1:E:9:SER:O	2.22	0.72
1:E:17:GLU:C	1:E:18:ASN:CA	2.57	0.72
2:J:8:GLY:HA3	2:L:16:TYR:OH	1.89	0.72
2:B:17:LEU:C	2:B:17:LEU:HA	2.12	0.72
1:E:5:GLN:C	1:E:5:GLN:HG3	2.15	0.72
2:H:6:LEU:HD22	2:L:10:HIS:CG	2.24	0.72
1:I:20:CYS:CA	1:I:21:ASN:N	2.45	0.72
2:J:8:GLY:HA3	2:L:16:TYR:CZ	2.25	0.72
1:C:12:SER:N	1:C:12:SER:O	2.23	0.72
1:K:15:GLN:C	1:K:16:LEU:C	2.57	0.72
1:E:5:GLN:C	1:E:5:GLN:CB	2.56	0.72
1:K:17:GLU:HA	1:K:20:CYS:SG	2.30	0.72
1:A:19:TYR:CB	1:A:19:TYR:C	2.63	0.72
2:B:7:CYS:HB2	2:F:6:LEU:HD11	1.72	0.71
2:B:17:LEU:O	2:B:18:VAL:CA	2.38	0.71
2:D:15:LEU:CD1	2:D:15:LEU:CB	2.67	0.71
2:J:13:GLU:CB	2:J:13:GLU:HA	2.12	0.71
2:L:22:ARG:CD	2:L:22:ARG:NH1	2.52	0.71
1:C:20:CYS:CB	1:C:20:CYS:N	2.51	0.71
2:F:3:ASN:N	2:F:4:GLN:N	2.39	0.71
2:B:23:GLY:N	2:B:23:GLY:C	2.46	0.71
2:F:20:GLY:CA	2:F:21:GLU:N	2.47	0.71
1:G:21:ASN:ND2	2:H:25:TYR:CE2	2.58	0.71
1:K:13:LEU:C	1:K:13:LEU:HA	2.06	0.71
2:B:9:SER:CA	2:B:9:SER:OG	2.36	0.71
2:F:20:GLY:O	6:F:2010:HOH:O	2.09	0.71
2:H:3:ASN:C	2:H:3:ASN:CB	2.63	0.71
1:E:5:GLN:CA	1:E:6:CYS:N	2.54	0.70
1:E:16:LEU:N	1:E:16:LEU:CB	2.52	0.70
1:A:11:CYS:N	1:A:11:CYS:CB	2.51	0.70
1:A:2:ILE:C	1:A:2:ILE:CB	2.63	0.70
2:B:24:PHE:O	2:B:25:TYR:CA	2.39	0.70
2:H:10:HIS:CB	2:H:10:HIS:C	2.63	0.70
1:I:13:LEU:CB	1:I:13:LEU:CD1	2.69	0.70
2:J:4:GLN:CB	2:J:4:GLN:HA	2.11	0.70
2:B:3:ASN:O	2:B:4:GLN:CA	2.39	0.70
2:D:12:VAL:CB	2:D:12:VAL:HA	2.15	0.70
1:K:10:ILE:C	1:K:10:ILE:HA	2.10	0.70
2:L:19:CYS:O	2:L:20:GLY:C	2.34	0.70
2:B:6:LEU:HD22	2:J:10:HIS:CD2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:THR:O	1:E:9:SER:CA	2.39	0.70
2:F:10:HIS:N	2:F:11:LEU:N	2.40	0.70
2:L:10:HIS:CG	2:L:10:HIS:HB3	2.19	0.69
1:C:8:THR:HA	6:C:2007:HOH:O	1.93	0.69
1:G:9:SER:CB	1:G:9:SER:C	2.65	0.69
1:I:14:TYR:CE2	6:I:2012:HOH:O	2.45	0.69
2:B:17:LEU:HB2	2:B:17:LEU:HD13	1.74	0.69
2:L:5:HIS:C	2:L:5:HIS:CD2	2.71	0.69
1:E:10:ILE:HD11	2:J:2:VAL:HA	1.75	0.69
2:L:3:ASN:C	2:L:3:ASN:N	2.49	0.69
1:I:13:LEU:C	1:I:14:TYR:CA	2.60	0.69
1:K:11:CYS:N	1:K:11:CYS:C	2.51	0.69
1:E:2:ILE:CG1	1:E:2:ILE:CA	2.68	0.69
1:E:2:ILE:HB	1:E:19:TYR:CE2	2.28	0.68
1:K:2:ILE:CB	1:K:2:ILE:C	2.62	0.68
2:H:1:PHE:CA	2:H:1:PHE:CG	2.72	0.68
1:E:15:GLN:CA	1:E:16:LEU:N	2.55	0.68
1:E:18:ASN:C	1:E:19:TYR:CA	2.64	0.68
2:J:21:GLU:C	2:J:21:GLU:CB	2.66	0.68
2:J:18:VAL:C	2:J:19:CYS:CA	2.60	0.68
2:D:2:VAL:C	2:D:2:VAL:HA	2.13	0.68
2:B:11:LEU:N	2:B:11:LEU:HB2	2.09	0.68
2:B:24:PHE:CG	2:B:24:PHE:C	2.70	0.68
2:F:26:MEA:C	2:F:26:MEA:N	2.50	0.68
1:I:13:LEU:O	1:I:14:TYR:CA	2.42	0.68
2:H:14:ALA:N	2:H:14:ALA:HA	2.00	0.68
2:J:6:LEU:O	2:J:9:SER:HB3	1.94	0.68
1:K:7:CYS:N	1:K:7:CYS:SG	2.67	0.68
2:L:10:HIS:CG	2:L:10:HIS:HB2	2.19	0.68
1:G:6:CYS:O	1:G:7:CYS:CA	2.40	0.68
1:G:12:SER:CB	1:G:12:SER:C	2.67	0.67
2:J:10:HIS:C	2:J:10:HIS:N	2.52	0.67
2:B:13:GLU:C	2:B:13:GLU:HA	2.12	0.67
1:E:19:TYR:N	1:E:19:TYR:CG	2.62	0.67
1:C:11:CYS:C	1:C:11:CYS:N	2.45	0.67
1:K:6:CYS:O	1:K:7:CYS:HA	1.95	0.67
1:A:13:LEU:HD11	2:H:18:VAL:HA	1.75	0.67
1:E:11:CYS:C	1:E:12:SER:O	2.36	0.67
2:B:3:ASN:C	2:B:3:ASN:CB	2.66	0.67
2:B:6:LEU:CB	2:B:6:LEU:HG	2.18	0.67
1:C:15:GLN:CA	1:C:16:LEU:N	2.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LEU:CD2	1:C:16:LEU:CA	2.72	0.67
2:H:2:VAL:O	2:H:6:LEU:HG	1.94	0.67
2:L:20:GLY:C	2:L:20:GLY:N	2.50	0.67
1:G:14:TYR:CB	1:G:14:TYR:HA	2.15	0.67
1:A:5:GLN:N	1:A:6:CYS:N	2.41	0.67
1:I:18:ASN:N	1:I:19:TYR:N	2.43	0.67
1:K:3:VAL:N	1:K:3:VAL:HG23	2.08	0.67
1:G:21:ASN:ND2	2:H:25:TYR:CD2	2.63	0.67
2:L:22:ARG:CD	2:L:22:ARG:CZ	2.65	0.67
1:A:16:LEU:CB	1:A:16:LEU:CD1	2.62	0.66
1:I:2:ILE:N	1:I:2:ILE:HA	1.99	0.66
2:D:16:TYR:C	2:D:16:TYR:N	2.49	0.66
1:K:2:ILE:HD13	2:L:15:LEU:HD11	1.76	0.66
1:K:12:SER:O	1:K:16:LEU:HG	1.96	0.66
2:B:26:MEA:HC2	2:D:24:PHE:O	1.96	0.66
1:G:14:TYR:N	1:G:15:GLN:N	2.43	0.66
1:G:3:VAL:O	1:G:7:CYS:N	2.28	0.66
1:E:10:ILE:CD1	1:E:10:ILE:CB	2.65	0.66
2:D:6:LEU:N	2:D:6:LEU:HG	2.11	0.66
2:B:6:LEU:C	2:B:6:LEU:HA	2.11	0.66
2:D:15:LEU:O	2:D:19:CYS:HB2	1.96	0.66
1:C:11:CYS:C	1:C:12:SER:O	2.39	0.66
2:H:6:LEU:CB	2:H:6:LEU:HG	2.18	0.66
1:A:5:GLN:CB	1:A:5:GLN:HA	2.15	0.65
1:A:17:GLU:O	1:A:18:ASN:C	2.39	0.65
2:D:19:CYS:CB	2:D:19:CYS:C	2.67	0.65
1:C:2:ILE:HG23	1:C:3:VAL:N	2.11	0.65
2:H:15:LEU:CD2	2:H:15:LEU:HG	2.20	0.65
6:B:2015:HOH:O	1:G:13:LEU:HG	1.96	0.65
1:C:13:LEU:O	1:C:17:GLU:HG3	1.97	0.65
1:K:17:GLU:CA	1:K:18:ASN:N	2.56	0.65
1:G:9:SER:CB	1:G:10:ILE:N	2.59	0.65
1:K:7:CYS:CB	2:L:7:CYS:SG	2.83	0.65
1:G:17:GLU:O	1:G:17:GLU:HG2	1.95	0.65
2:H:24:PHE:CG	2:H:24:PHE:C	2.74	0.65
1:K:16:LEU:CD1	1:K:16:LEU:CD2	2.67	0.65
1:E:5:GLN:C	1:E:5:GLN:CG	2.70	0.65
2:J:9:SER:OG	2:L:13:GLU:OE2	2.15	0.65
2:J:16:TYR:CZ	2:L:8:GLY:HA3	2.32	0.65
2:B:11:LEU:CD2	2:B:11:LEU:CD1	2.69	0.65
2:J:2:VAL:CG1	2:J:2:VAL:HB	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:19:CYS:N	2:J:20:GLY:N	2.45	0.65
2:L:18:VAL:C	2:L:18:VAL:CB	2.66	0.65
2:D:2:VAL:CA	6:D:2002:HOH:O	2.45	0.65
1:I:17:GLU:C	1:I:17:GLU:CB	2.68	0.65
1:K:7:CYS:CA	2:L:7:CYS:SG	2.85	0.65
2:J:29:PRO:O	2:L:21:GLU:OE1	2.14	0.64
2:B:24:PHE:CG	2:B:24:PHE:CA	2.75	0.64
1:A:21:ASN:HB3	2:B:22:ARG:CB	2.26	0.64
2:F:15:LEU:CA	2:F:15:LEU:CG	2.74	0.64
1:I:12:SER:O	1:I:16:LEU:HG	1.97	0.64
1:C:14:TYR:O	1:C:15:GLN:CA	2.45	0.64
1:E:7:CYS:SG	2:F:11:LEU:CD1	2.85	0.64
1:K:12:SER:OG	1:K:12:SER:CA	2.41	0.64
2:B:17:LEU:CA	2:B:18:VAL:N	2.50	0.64
2:D:2:VAL:HA	6:D:2002:HOH:O	1.98	0.64
2:D:6:LEU:N	2:D:6:LEU:CG	2.61	0.64
1:A:21:ASN:ND2	2:B:22:ARG:NE	2.45	0.64
2:D:15:LEU:CB	2:D:15:LEU:C	2.65	0.64
2:H:4:GLN:NE2	6:H:2005:HOH:O	2.27	0.64
2:B:15:LEU:CD2	2:B:15:LEU:HG	2.21	0.63
1:E:10:ILE:CD1	1:E:10:ILE:HG23	2.28	0.63
6:B:2015:HOH:O	1:G:13:LEU:N	2.30	0.63
1:C:2:ILE:HD12	1:C:19:TYR:CB	2.27	0.63
2:B:10:HIS:C	2:B:10:HIS:CB	2.69	0.63
1:C:14:TYR:C	1:C:15:GLN:CA	2.62	0.63
1:I:16:LEU:CD1	1:I:16:LEU:HG	2.14	0.63
2:B:20:GLY:O	2:B:23:GLY:N	2.31	0.63
1:C:4:GLU:O	1:C:8:THR:CG2	2.47	0.63
1:I:9:SER:CB	1:I:9:SER:HG	2.09	0.63
1:E:1:GLY:H3	1:E:4:GLU:CD	2.07	0.63
1:I:2:ILE:O	1:I:6:CYS:N	2.32	0.63
2:D:3:ASN:N	2:D:4:GLN:H	1.96	0.63
1:E:1:GLY:O	1:E:4:GLU:HG2	1.98	0.63
1:E:16:LEU:N	1:E:17:GLU:N	2.46	0.63
1:G:3:VAL:HG23	1:G:7:CYS:HB2	1.81	0.63
1:E:10:ILE:HD13	2:J:2:VAL:HG22	1.81	0.63
2:H:16:TYR:CB	2:H:16:TYR:HA	2.21	0.63
2:B:4:GLN:N	2:B:4:GLN:C	2.55	0.62
1:C:14:TYR:O	1:C:17:GLU:HB2	1.98	0.62
1:E:19:TYR:N	1:E:19:TYR:CB	2.54	0.62
2:J:15:LEU:N	2:J:16:TYR:H	1.95	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:LEU:HD11	2:H:7:CYS:HB2	1.80	0.62
2:D:13:GLU:CG	2:D:13:GLU:C	2.72	0.62
2:F:14:ALA:O	2:F:18:VAL:N	2.26	0.62
4:C:1028:CL:CL	2:H:6:LEU:HB3	2.36	0.62
1:G:2:ILE:N	6:G:2001:HOH:O	2.32	0.62
1:G:10:ILE:CB	1:G:10:ILE:CD1	2.67	0.62
1:G:6:CYS:C	1:G:6:CYS:CB	2.72	0.62
1:I:3:VAL:N	1:I:3:VAL:CB	2.55	0.62
1:E:12:SER:O	1:E:13:LEU:C	2.39	0.62
2:F:12:VAL:CA	2:F:12:VAL:CG2	2.72	0.62
1:G:13:LEU:CD2	1:G:13:LEU:HG	2.22	0.62
1:G:4:GLU:CD	1:G:4:GLU:N	2.52	0.62
1:C:7:CYS:CA	1:C:7:CYS:SG	2.86	0.61
1:G:6:CYS:C	1:G:7:CYS:CA	2.64	0.61
2:H:1:PHE:CB	2:H:1:PHE:N	2.57	0.61
2:L:4:GLN:CD	2:L:4:GLN:HB3	2.24	0.61
2:B:17:LEU:HD12	6:B:2007:HOH:O	1.99	0.61
1:I:16:LEU:HB3	2:J:15:LEU:HD23	1.81	0.61
1:I:6:CYS:C	1:I:6:CYS:CB	2.70	0.61
1:A:14:TYR:O	1:A:17:GLU:HB3	2.00	0.61
1:C:3:VAL:CB	1:C:3:VAL:N	2.52	0.61
1:I:14:TYR:CD1	1:I:14:TYR:O	2.54	0.61
1:C:10:ILE:HD11	6:C:2011:HOH:O	2.01	0.61
2:J:2:VAL:CB	2:J:2:VAL:C	2.68	0.61
1:K:3:VAL:N	1:K:3:VAL:CG2	2.63	0.61
1:I:6:CYS:CA	1:I:7:CYS:N	2.59	0.61
1:K:8:THR:N	1:K:8:THR:HG1	1.99	0.61
1:A:10:ILE:N	1:A:10:ILE:HG13	2.16	0.61
3:A:1022:IPH:C5	2:B:11:LEU:HG	2.31	0.61
2:H:15:LEU:CD2	2:H:15:LEU:CD1	2.69	0.61
2:L:21:GLU:CG	2:L:21:GLU:N	2.64	0.61
1:A:3:VAL:N	1:A:3:VAL:C	2.56	0.61
2:H:16:TYR:HA	2:H:24:PHE:CE1	2.36	0.61
1:I:6:CYS:N	1:I:6:CYS:CB	2.60	0.61
1:I:8:THR:HG22	6:I:2005:HOH:O	2.00	0.61
1:C:19:TYR:N	1:C:19:TYR:CD1	2.69	0.60
2:L:19:CYS:N	2:L:20:GLY:N	2.49	0.60
1:E:2:ILE:N	1:E:3:VAL:N	2.49	0.60
1:I:14:TYR:CD1	1:I:14:TYR:C	2.79	0.60
2:J:19:CYS:N	2:J:19:CYS:C	2.51	0.60
1:K:2:ILE:CD1	2:L:15:LEU:HD11	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:GLU:CG	1:C:17:GLU:OE1	2.40	0.60
2:J:21:GLU:OE1	2:J:21:GLU:N	2.20	0.60
1:K:1:GLY:C	1:K:2:ILE:CA	2.64	0.60
2:L:17:LEU:CB	2:L:17:LEU:CD1	2.66	0.60
1:E:1:GLY:N	1:E:4:GLU:CG	2.65	0.60
1:E:14:TYR:O	1:E:17:GLU:HB2	2.02	0.60
2:L:18:VAL:C	2:L:18:VAL:HA	2.15	0.60
1:E:10:ILE:HG23	1:E:10:ILE:HD12	1.82	0.60
2:H:18:VAL:CG1	2:H:18:VAL:CA	2.73	0.60
1:I:5:GLN:HG2	6:I:2015:HOH:O	2.00	0.60
2:H:12:VAL:CB	2:H:13:GLU:N	2.65	0.60
1:C:10:ILE:HG13	1:C:11:CYS:O	2.03	0.59
1:E:18:ASN:O	1:E:19:TYR:HA	2.02	0.59
1:I:6:CYS:O	1:I:7:CYS:HA	2.02	0.59
1:K:5:GLN:C	1:K:5:GLN:HA	2.17	0.59
2:B:1:PHE:O	2:B:2:VAL:C	2.45	0.59
2:B:2:VAL:C	2:B:3:ASN:CA	2.71	0.59
1:C:8:THR:CG2	1:C:8:THR:HB	2.19	0.59
1:A:9:SER:CB	1:A:10:ILE:N	2.64	0.59
1:A:21:ASN:HA	2:B:23:GLY:O	2.01	0.59
1:K:19:TYR:O	2:L:24:PHE:HA	2.03	0.59
2:H:10:HIS:O	2:H:11:LEU:CA	2.50	0.59
1:E:2:ILE:CG1	1:E:2:ILE:HB	2.22	0.59
2:J:4:GLN:CB	2:J:4:GLN:C	2.67	0.59
1:A:5:GLN:HG2	1:A:11:CYS:SG	2.42	0.59
2:H:18:VAL:CG1	2:H:18:VAL:CG2	2.78	0.59
1:I:4:GLU:OE2	2:J:29:PRO:HB3	2.03	0.59
1:I:18:ASN:N	1:I:19:TYR:H	2.01	0.59
1:K:2:ILE:CB	1:K:2:ILE:N	2.60	0.59
1:I:13:LEU:CB	1:I:13:LEU:CD2	2.73	0.58
1:K:10:ILE:CB	1:K:10:ILE:N	2.57	0.58
1:A:20:CYS:SG	2:B:19:CYS:HA	2.43	0.58
1:K:16:LEU:HD13	2:L:14:ALA:HB1	1.83	0.58
2:L:22:ARG:NE	2:L:22:ARG:CB	2.65	0.58
2:J:16:TYR:OH	2:L:8:GLY:HA3	2.03	0.58
2:D:22:ARG:HG3	2:D:22:ARG:HH11	1.68	0.58
1:I:14:TYR:CB	1:I:14:TYR:N	2.53	0.58
1:C:3:VAL:CA	1:C:3:VAL:CG2	2.74	0.58
2:L:1:PHE:CG	2:L:1:PHE:HB3	2.24	0.58
2:B:9:SER:CA	2:B:9:SER:HG	2.15	0.58
1:C:4:GLU:O	1:C:5:GLN:CA	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:HIS:C	2:H:6:LEU:C	2.70	0.58
2:L:21:GLU:CB	2:L:21:GLU:OE1	2.50	0.58
1:C:2:ILE:HB	1:C:19:TYR:CD2	2.39	0.58
2:H:16:TYR:HA	2:H:24:PHE:HE1	1.69	0.58
2:D:14:ALA:N	2:D:15:LEU:N	2.51	0.58
2:J:26:MEA:O	2:L:23:GLY:HA2	2.04	0.58
1:A:19:TYR:CA	1:A:19:TYR:CG	2.78	0.57
2:J:28:LYS:CD	2:J:28:LYS:HB2	2.34	0.57
2:L:22:ARG:HH11	2:L:22:ARG:HD2	1.67	0.57
1:E:10:ILE:CB	1:E:10:ILE:N	2.62	0.57
1:E:10:ILE:CA	1:E:10:ILE:CG2	2.72	0.57
1:A:2:ILE:HD13	2:B:15:LEU:HD11	1.85	0.57
2:B:3:ASN:CA	2:B:4:GLN:N	2.53	0.57
2:B:17:LEU:C	2:B:17:LEU:CB	2.73	0.57
2:J:18:VAL:HG12	2:J:19:CYS:N	2.19	0.57
2:L:25:TYR:C	2:L:26:MEA:HD1	2.30	0.57
2:D:24:PHE:C	2:D:24:PHE:HA	2.19	0.57
1:E:6:CYS:N	1:E:6:CYS:SG	2.77	0.57
1:C:10:ILE:HG21	2:L:1:PHE:HB3	1.86	0.57
1:E:7:CYS:SG	2:F:11:LEU:HD12	2.45	0.57
1:E:10:ILE:HD13	1:E:10:ILE:HA	1.87	0.57
2:H:24:PHE:CG	2:H:24:PHE:CA	2.84	0.57
1:G:6:CYS:O	1:G:7:CYS:HA	2.04	0.57
2:H:2:VAL:CA	2:H:2:VAL:HB	2.16	0.57
1:C:19:TYR:N	1:C:20:CYS:N	2.53	0.57
1:K:2:ILE:CA	1:K:3:VAL:N	2.58	0.57
1:E:2:ILE:CB	1:E:2:ILE:N	2.61	0.57
2:B:15:LEU:C	2:B:17:LEU:N	2.59	0.56
2:L:21:GLU:N	2:L:21:GLU:HG2	2.19	0.56
2:B:10:HIS:C	2:B:10:HIS:HA	2.15	0.56
2:H:10:HIS:C	2:H:11:LEU:CA	2.66	0.56
1:C:2:ILE:CG2	1:C:2:ILE:C	2.77	0.56
1:C:15:GLN:O	1:C:18:ASN:HB3	2.05	0.56
1:C:16:LEU:HD23	1:C:16:LEU:CA	2.36	0.56
2:L:17:LEU:CB	2:L:17:LEU:HG	2.17	0.56
2:J:21:GLU:C	2:J:22:ARG:CA	2.66	0.56
1:K:11:CYS:N	3:K:1022:IPH:O1	2.33	0.56
2:H:2:VAL:CG2	2:H:2:VAL:HG13	2.30	0.56
1:I:21:ASN:N	1:I:21:ASN:CG	2.64	0.56
2:D:13:GLU:C	2:D:13:GLU:HG3	2.31	0.56
1:E:2:ILE:HG23	1:E:3:VAL:HG13	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2:ILE:HD13	1:G:2:ILE:HG21	1.88	0.56
2:L:6:LEU:O	2:L:9:SER:HB3	2.06	0.56
1:C:4:GLU:C	1:C:5:GLN:CA	2.67	0.56
2:J:22:ARG:HB2	2:J:22:ARG:CZ	2.36	0.56
1:C:20:CYS:SG	2:D:19:CYS:HA	2.46	0.55
2:D:9:SER:CA	2:D:12:VAL:HG22	2.34	0.55
2:D:2:VAL:HG12	1:G:8:THR:O	2.07	0.55
1:I:20:CYS:O	1:I:21:ASN:HA	2.05	0.55
1:C:14:TYR:CA	1:C:14:TYR:CD1	2.88	0.55
1:I:3:VAL:N	1:I:4:GLU:N	2.54	0.55
1:C:2:ILE:HD12	1:C:19:TYR:HB2	1.87	0.55
2:L:19:CYS:N	2:L:20:GLY:H	2.03	0.55
1:E:19:TYR:N	1:E:19:TYR:HA	2.06	0.55
1:E:20:CYS:CA	1:E:20:CYS:HB3	2.18	0.55
2:F:7:CYS:O	2:F:11:LEU:N	2.40	0.55
1:E:2:ILE:CG1	1:E:2:ILE:O	2.54	0.55
2:D:3:ASN:ND2	2:D:4:GLN:N	2.55	0.55
2:B:22:ARG:CA	2:B:22:ARG:O	2.40	0.55
1:G:9:SER:CB	1:G:10:ILE:H	2.19	0.55
2:J:28:LYS:CG	2:L:20:GLY:O	2.55	0.55
1:C:1:GLY:C	1:C:1:GLY:N	2.58	0.55
1:C:2:ILE:N	1:C:3:VAL:H	2.05	0.55
2:D:24:PHE:CD2	2:D:24:PHE:N	2.69	0.55
1:A:21:ASN:HD22	2:B:22:ARG:HE	1.50	0.54
2:F:2:VAL:CG2	2:F:2:VAL:HA	2.33	0.54
1:K:17:GLU:O	1:K:18:ASN:CA	2.54	0.54
2:L:4:GLN:N	2:L:5:HIS:N	2.54	0.54
2:L:13:GLU:CB	2:L:13:GLU:C	2.71	0.54
1:E:3:VAL:O	1:E:7:CYS:HB2	2.08	0.54
2:H:17:LEU:C	2:H:17:LEU:HA	2.18	0.54
2:L:11:LEU:O	2:L:12:VAL:C	2.42	0.54
2:J:26:MEA:CB	2:J:26:MEA:HA	2.24	0.54
1:K:6:CYS:HB2	2:L:11:LEU:HD11	1.88	0.54
1:K:7:CYS:HA	2:L:7:CYS:SG	2.47	0.54
2:B:25:TYR:N	2:B:25:TYR:CG	2.75	0.54
1:E:10:ILE:CD1	1:E:10:ILE:CG2	2.85	0.54
2:D:15:LEU:CB	2:D:15:LEU:N	2.59	0.54
1:I:18:ASN:N	1:I:18:ASN:CB	2.61	0.54
2:D:19:CYS:O	2:D:22:ARG:CG	2.51	0.54
1:I:2:ILE:HA	1:I:5:GLN:HB3	1.89	0.54
2:F:21:GLU:N	2:F:21:GLU:OE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:2001:HOH:O	1:K:10:ILE:HG13	2.08	0.54
1:K:2:ILE:C	1:K:2:ILE:HG23	2.33	0.54
2:D:10:HIS:N	2:D:10:HIS:C	2.56	0.54
2:B:12:VAL:CB	2:B:12:VAL:N	2.64	0.54
1:E:20:CYS:CA	1:E:20:CYS:HB2	2.18	0.54
1:G:9:SER:HB2	1:G:10:ILE:H	1.71	0.53
2:H:12:VAL:CA	2:H:12:VAL:HG23	2.35	0.53
2:D:25:TYR:C	2:D:26:MEA:C1	2.75	0.53
1:E:10:ILE:CG1	2:J:2:VAL:HA	2.39	0.53
2:J:25:TYR:HE1	2:J:27:THR:HG1	1.55	0.53
2:J:7:CYS:O	2:J:8:GLY:C	2.50	0.53
2:B:5:HIS:HB2	1:I:10:ILE:HD11	1.91	0.53
2:B:15:LEU:O	2:B:16:TYR:C	2.50	0.53
1:G:10:ILE:CG1	1:G:10:ILE:N	2.72	0.53
2:J:24:PHE:CG	2:J:24:PHE:HB3	2.21	0.53
2:B:8:GLY:O	2:B:9:SER:C	2.47	0.53
1:C:7:CYS:SG	2:D:11:LEU:CD1	2.96	0.53
1:G:9:SER:CB	1:G:9:SER:HA	2.22	0.53
1:A:12:SER:OG	1:A:15:GLN:HG3	2.08	0.53
2:F:5:HIS:HD2	6:H:2007:HOH:O	1.90	0.53
1:G:2:ILE:CG2	1:G:2:ILE:HD13	2.39	0.53
1:G:6:CYS:O	3:G:1022:IPH:O1	2.27	0.53
2:B:19:CYS:HB3	2:B:23:GLY:O	2.09	0.53
2:J:7:CYS:C	2:J:9:SER:N	2.65	0.53
1:E:12:SER:C	1:E:14:TYR:N	2.61	0.52
1:I:16:LEU:CD1	1:I:16:LEU:CD2	2.79	0.52
1:C:2:ILE:CG2	1:C:3:VAL:N	2.72	0.52
2:D:12:VAL:CA	2:D:12:VAL:CG2	2.78	0.52
2:H:24:PHE:CE2	2:H:26:MEA:HB2	2.40	0.52
1:I:10:ILE:CA	1:I:10:ILE:CG2	2.78	0.52
1:K:6:CYS:C	1:K:7:CYS:HA	2.30	0.52
1:C:18:ASN:C	1:C:19:TYR:CA	2.74	0.52
1:C:2:ILE:HD12	1:C:19:TYR:CG	2.44	0.52
1:C:2:ILE:HD13	2:D:15:LEU:HD11	1.90	0.52
2:D:16:TYR:HA	6:D:2007:HOH:O	2.09	0.52
1:C:21:ASN:HA	6:C:2017:HOH:O	2.09	0.52
2:D:24:PHE:C	2:D:24:PHE:CD1	2.87	0.52
1:A:21:ASN:HD22	2:B:22:ARG:NE	2.07	0.51
2:L:12:VAL:CG2	2:L:12:VAL:CA	2.76	0.51
1:A:20:CYS:SG	2:B:19:CYS:CA	2.98	0.51
1:E:1:GLY:H2	1:E:4:GLU:CG	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ASN:C	1:E:18:ASN:CB	2.75	0.51
2:D:3:ASN:HD22	2:D:4:GLN:N	2.08	0.51
2:J:18:VAL:O	2:J:19:CYS:CA	2.57	0.51
1:A:21:ASN:CB	2:B:22:ARG:HB3	2.38	0.51
2:D:3:ASN:HD22	2:D:4:GLN:H	1.58	0.51
1:E:10:ILE:HG12	2:J:2:VAL:HA	1.92	0.51
1:C:12:SER:C	1:C:14:TYR:N	2.63	0.51
1:C:19:TYR:N	1:C:20:CYS:H	2.08	0.51
1:E:16:LEU:O	1:E:17:GLU:C	2.54	0.51
1:G:8:THR:CB	1:G:8:THR:HG1	2.13	0.51
2:B:15:LEU:CD2	2:B:15:LEU:CB	2.82	0.51
2:H:12:VAL:O	2:H:13:GLU:C	2.54	0.51
1:A:10:ILE:CG1	1:A:10:ILE:H	2.22	0.51
1:C:4:GLU:C	1:C:4:GLU:HA	2.17	0.51
1:E:7:CYS:SG	2:F:11:LEU:HD11	2.51	0.51
2:L:15:LEU:N	2:L:16:TYR:N	2.59	0.51
2:J:28:LYS:HG3	2:L:20:GLY:O	2.11	0.50
1:K:1:GLY:O	1:K:2:ILE:CA	2.59	0.50
1:K:15:GLN:O	1:K:16:LEU:C	2.54	0.50
1:K:18:ASN:N	1:K:18:ASN:CG	2.69	0.50
2:B:21:GLU:C	2:B:21:GLU:HB2	2.31	0.50
2:D:18:VAL:O	2:D:18:VAL:CG1	2.59	0.50
1:E:2:ILE:HG23	1:E:3:VAL:N	2.27	0.50
2:F:2:VAL:O	2:F:6:LEU:N	2.41	0.50
2:H:18:VAL:CG1	2:H:18:VAL:C	2.83	0.50
2:J:25:TYR:CA	2:J:25:TYR:CG	2.83	0.50
2:B:11:LEU:O	2:B:14:ALA:N	2.45	0.50
2:D:21:GLU:HB3	6:D:2010:HOH:O	2.11	0.50
1:I:5:GLN:C	1:I:5:GLN:HA	2.20	0.50
2:J:21:GLU:O	2:J:22:ARG:CA	2.59	0.50
2:D:13:GLU:CG	2:D:13:GLU:CA	2.73	0.50
2:D:19:CYS:CB	2:D:19:CYS:HA	2.22	0.50
6:D:2009:HOH:O	1:I:13:LEU:HG	2.11	0.50
2:F:10:HIS:N	2:F:11:LEU:H	2.10	0.50
1:G:6:CYS:C	1:G:6:CYS:HA	2.19	0.50
1:E:2:ILE:O	1:E:3:VAL:C	2.54	0.50
2:B:21:GLU:CA	2:B:21:GLU:CG	2.81	0.50
1:E:6:CYS:HA	1:E:11:CYS:SG	2.52	0.50
1:G:2:ILE:CG2	1:G:2:ILE:CD1	2.89	0.50
1:I:6:CYS:C	1:I:7:CYS:HA	2.36	0.50
1:K:3:VAL:N	1:K:3:VAL:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:CYS:CA	2:D:19:CYS:SG	2.97	0.49
2:H:12:VAL:CA	2:H:12:VAL:HG22	2.35	0.49
1:I:10:ILE:HA	3:I:1022:IPH:O1	2.12	0.49
1:C:7:CYS:SG	2:D:11:LEU:HD12	2.53	0.49
1:E:2:ILE:CB	1:E:19:TYR:CE2	2.95	0.49
2:B:11:LEU:CD2	2:B:11:LEU:CB	2.84	0.49
1:E:11:CYS:CB	1:E:11:CYS:HA	2.21	0.49
2:J:12:VAL:HG12	2:L:12:VAL:CG1	2.31	0.49
1:A:2:ILE:C	1:A:2:ILE:CG1	2.86	0.49
1:C:15:GLN:C	1:C:15:GLN:HA	2.14	0.49
2:J:15:LEU:HD13	2:J:24:PHE:CD2	2.48	0.49
1:C:15:GLN:N	1:C:15:GLN:HG3	2.27	0.49
2:F:15:LEU:O	2:F:19:CYS:HB2	2.12	0.49
2:H:19:CYS:HB3	2:H:23:GLY:O	2.13	0.49
2:J:26:MEA:HC3	2:L:24:PHE:H	1.77	0.49
1:K:2:ILE:C	1:K:2:ILE:CG2	2.86	0.49
1:K:20:CYS:HA	2:L:23:GLY:O	2.12	0.49
2:D:20:GLY:O	2:D:21:GLU:C	2.55	0.49
1:A:5:GLN:N	1:A:6:CYS:H	2.09	0.49
1:A:7:CYS:N	1:A:8:THR:N	2.59	0.49
1:C:11:CYS:HA	1:C:15:GLN:HE21	1.78	0.49
1:E:2:ILE:CD1	1:E:19:TYR:CD1	2.91	0.49
1:E:16:LEU:N	1:E:17:GLU:H	2.10	0.49
2:J:25:TYR:HE2	1:K:21:ASN:CG	2.21	0.49
2:B:15:LEU:CD2	2:B:15:LEU:CA	2.90	0.48
1:E:1:GLY:H2	1:E:4:GLU:HG3	1.78	0.48
1:I:2:ILE:HG13	1:I:6:CYS:SG	2.53	0.48
1:A:9:SER:HB2	1:A:10:ILE:N	2.28	0.48
2:D:10:HIS:N	2:D:10:HIS:HA	2.07	0.48
2:F:20:GLY:HA2	6:F:2011:HOH:O	2.12	0.48
1:K:8:THR:CB	1:K:8:THR:HG1	2.10	0.48
2:L:25:TYR:HA	2:L:26:MEA:HC1	1.66	0.48
1:E:5:GLN:O	1:E:6:CYS:HA	2.13	0.48
1:I:17:GLU:C	1:I:18:ASN:CA	2.72	0.48
1:K:16:LEU:C	1:K:16:LEU:N	2.53	0.48
2:L:25:TYR:O	2:L:26:MEA:HB2	2.13	0.48
1:C:2:ILE:CD1	2:D:15:LEU:HD11	2.44	0.48
2:D:10:HIS:N	2:D:11:LEU:N	2.61	0.48
1:K:2:ILE:O	1:K:3:VAL:CA	2.62	0.48
1:K:3:VAL:N	1:K:4:GLU:N	2.61	0.48
2:B:6:LEU:HD22	2:J:10:HIS:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:2:ILE:N	1:K:2:ILE:HA	2.04	0.48
2:L:15:LEU:N	2:L:15:LEU:HA	2.10	0.48
2:B:7:CYS:N	2:B:7:CYS:HA	2.12	0.48
2:J:19:CYS:N	2:J:20:GLY:H	2.10	0.48
2:L:2:VAL:C	2:L:3:ASN:C	2.81	0.48
2:B:15:LEU:CD2	2:B:15:LEU:HA	2.44	0.48
1:C:2:ILE:CG2	1:C:2:ILE:HB	2.19	0.48
1:K:5:GLN:OE1	1:K:19:TYR:CZ	2.66	0.47
2:L:1:PHE:CG	2:L:1:PHE:HB2	2.24	0.47
2:B:2:VAL:CB	2:B:2:VAL:HA	2.18	0.47
1:I:4:GLU:OE2	2:J:29:PRO:CB	2.62	0.47
1:I:8:THR:CG2	1:I:8:THR:N	2.78	0.47
1:K:21:ASN:N	1:K:21:ASN:CG	2.72	0.47
2:L:2:VAL:O	2:L:3:ASN:C	2.56	0.47
2:J:25:TYR:HE2	1:K:21:ASN:OD1	1.96	0.47
2:B:12:VAL:C	2:B:13:GLU:C	2.82	0.47
2:D:15:LEU:O	2:D:19:CYS:CB	2.62	0.47
1:E:12:SER:OG	1:E:14:TYR:HB3	2.13	0.47
2:L:18:VAL:HG22	2:L:18:VAL:O	2.10	0.47
2:B:18:VAL:HG22	1:G:13:LEU:CD2	2.45	0.47
1:C:3:VAL:CB	1:C:3:VAL:HA	2.22	0.47
2:J:20:GLY:HA3	6:J:2012:HOH:O	2.14	0.47
1:K:14:TYR:CD1	1:K:14:TYR:O	2.67	0.47
1:A:17:GLU:CB	1:A:18:ASN:N	2.75	0.47
1:E:6:CYS:H	1:E:7:CYS:H	1.61	0.47
2:B:17:LEU:HD11	3:G:1022:IPH:H3	1.96	0.47
1:C:12:SER:H	1:C:15:GLN:NE2	2.13	0.47
1:E:10:ILE:CD1	1:E:10:ILE:HA	2.45	0.47
1:K:20:CYS:O	1:K:21:ASN:CA	2.62	0.47
2:D:13:GLU:CB	6:D:2006:HOH:O	2.63	0.47
1:E:4:GLU:HA	2:F:4:GLN:HE22	1.79	0.47
2:J:5:HIS:C	2:J:5:HIS:CD2	2.91	0.47
2:L:9:SER:O	2:L:10:HIS:C	2.56	0.47
2:L:17:LEU:CG	2:L:17:LEU:HB3	2.19	0.47
1:E:2:ILE:N	1:E:3:VAL:H	2.12	0.47
1:K:5:GLN:O	1:K:6:CYS:HA	2.14	0.47
1:K:13:LEU:O	1:K:14:TYR:C	2.56	0.47
1:A:7:CYS:N	1:A:7:CYS:HA	2.06	0.47
2:H:11:LEU:CD2	2:H:11:LEU:CB	2.80	0.47
3:K:1022:IPH:H4	2:L:10:HIS:HB3	1.97	0.47
2:J:11:LEU:CA	2:J:11:LEU:CD2	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:CYS:O	3:A:1022:IPH:O1	2.33	0.46
2:B:4:GLN:CG	2:B:4:GLN:C	2.87	0.46
1:C:10:ILE:CG2	2:L:1:PHE:CB	2.93	0.46
1:I:12:SER:OG	1:I:12:SER:C	2.57	0.46
1:A:20:CYS:SG	2:B:18:VAL:HG12	2.55	0.46
2:B:9:SER:O	2:B:13:GLU:HG3	2.14	0.46
2:B:18:VAL:N	2:B:18:VAL:HB	2.28	0.46
2:J:24:PHE:CB	2:J:24:PHE:CD2	2.76	0.46
1:K:6:CYS:HB2	2:L:11:LEU:CD1	2.45	0.46
2:B:15:LEU:HA	2:B:15:LEU:HD23	1.96	0.46
1:G:2:ILE:O	1:G:6:CYS:HB2	2.16	0.46
2:J:15:LEU:HB2	2:J:24:PHE:CZ	2.50	0.46
1:E:2:ILE:CG2	1:E:3:VAL:N	2.79	0.46
1:G:21:ASN:HB2	2:H:22:ARG:O	2.16	0.46
2:H:6:LEU:O	2:H:10:HIS:CD2	2.69	0.46
1:I:14:TYR:CG	1:I:14:TYR:O	2.69	0.46
1:K:4:GLU:CB	1:K:4:GLU:H	2.24	0.46
1:G:13:LEU:O	1:G:17:GLU:N	2.48	0.46
2:J:24:PHE:CG	2:J:24:PHE:HB2	2.21	0.46
2:B:16:TYR:OH	2:D:5:HIS:HA	2.16	0.46
1:A:2:ILE:HG12	2:B:11:LEU:HD22	1.98	0.46
2:B:9:SER:HB2	2:D:16:TYR:CE1	2.51	0.46
1:I:14:TYR:CZ	6:I:2012:HOH:O	2.66	0.46
2:J:26:MEA:CB	2:J:26:MEA:HC2	2.46	0.46
1:C:13:LEU:CB	1:C:13:LEU:H	2.26	0.45
1:C:15:GLN:O	1:C:18:ASN:CB	2.63	0.45
2:F:26:MEA:HZ	2:H:16:TYR:HE1	1.80	0.45
1:I:4:GLU:CB	1:I:4:GLU:C	2.76	0.45
1:I:7:CYS:HA	2:J:7:CYS:SG	2.56	0.45
2:D:13:GLU:HG3	2:D:13:GLU:O	2.16	0.45
1:I:14:TYR:N	1:I:14:TYR:HA	2.12	0.45
2:J:22:ARG:N	2:J:22:ARG:C	2.63	0.45
1:A:9:SER:CB	1:A:9:SER:HA	2.20	0.45
2:B:14:ALA:O	2:B:17:LEU:HB3	2.15	0.45
2:D:5:HIS:O	2:D:6:LEU:CA	2.65	0.45
2:H:17:LEU:C	2:H:17:LEU:CB	2.79	0.45
1:K:1:GLY:C	1:K:1:GLY:N	2.64	0.45
1:K:2:ILE:N	1:K:2:ILE:HG22	2.32	0.45
1:C:18:ASN:O	1:C:19:TYR:HA	2.17	0.45
1:E:8:THR:CA	1:E:9:SER:N	2.59	0.45
2:F:2:VAL:CA	6:F:2001:HOH:O	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:CYS:C	2:L:9:SER:N	2.74	0.45
1:I:8:THR:CG2	1:I:8:THR:CA	2.83	0.45
2:J:2:VAL:CB	2:J:2:VAL:HA	2.23	0.45
2:J:9:SER:C	2:J:10:HIS:C	2.83	0.45
2:L:17:LEU:CG	2:L:17:LEU:HB2	2.19	0.45
2:H:12:VAL:CA	2:H:12:VAL:CG1	2.77	0.45
2:J:18:VAL:CG1	2:J:18:VAL:O	2.64	0.45
2:J:27:THR:CB	2:J:27:THR:N	2.71	0.45
1:C:7:CYS:CB	1:C:7:CYS:N	2.60	0.45
1:C:10:ILE:HG13	1:C:11:CYS:C	2.41	0.45
2:D:22:ARG:CG	2:D:22:ARG:HH11	2.28	0.45
1:I:2:ILE:O	1:I:3:VAL:CA	2.64	0.45
1:A:2:ILE:CG2	1:A:2:ILE:N	2.78	0.45
2:J:22:ARG:N	2:J:22:ARG:HB2	2.32	0.45
1:G:17:GLU:O	1:G:18:ASN:C	2.53	0.44
2:H:16:TYR:CA	2:H:24:PHE:CE1	3.00	0.44
1:K:7:CYS:N	6:K:2004:HOH:O	2.49	0.44
2:D:15:LEU:CG	2:D:15:LEU:CA	2.83	0.44
1:E:2:ILE:C	1:E:4:GLU:N	2.62	0.44
2:J:16:TYR:HB2	2:L:12:VAL:HG11	1.98	0.44
2:L:10:HIS:O	2:L:13:GLU:HB3	2.17	0.44
2:B:5:HIS:CB	2:B:5:HIS:C	2.70	0.44
1:A:19:TYR:HB2	2:B:15:LEU:HD22	1.99	0.44
1:C:8:THR:C	1:C:8:THR:N	2.65	0.44
1:A:2:ILE:CG2	1:A:2:ILE:HB	2.22	0.44
2:L:22:ARG:NE	2:L:22:ARG:HB2	2.32	0.44
1:K:10:ILE:CG1	1:K:10:ILE:CG2	2.82	0.44
1:A:10:ILE:HG13	1:A:10:ILE:H	1.79	0.44
2:B:16:TYR:CB	2:B:16:TYR:HA	2.22	0.44
1:K:5:GLN:HG2	1:K:6:CYS:SG	2.57	0.44
2:B:23:GLY:N	2:B:23:GLY:O	2.50	0.44
2:H:12:VAL:C	2:H:12:VAL:CG1	2.87	0.44
2:J:18:VAL:CA	2:J:19:CYS:N	2.60	0.44
2:D:5:HIS:C	2:D:5:HIS:N	2.62	0.43
1:I:3:VAL:O	1:I:3:VAL:CG1	2.65	0.43
2:J:11:LEU:CA	2:J:11:LEU:HD23	2.48	0.43
1:A:10:ILE:HG22	1:A:10:ILE:O	2.18	0.43
1:G:6:CYS:SG	1:G:6:CYS:N	2.91	0.43
2:L:4:GLN:N	2:L:4:GLN:C	2.54	0.43
1:A:12:SER:CB	1:A:13:LEU:N	2.80	0.43
2:J:16:TYR:O	2:J:17:LEU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:GLN:CB	2:B:4:GLN:CD	2.71	0.43
1:C:15:GLN:N	1:C:15:GLN:CG	2.81	0.43
2:D:9:SER:C	2:D:9:SER:CB	2.81	0.43
2:F:21:GLU:CD	2:F:21:GLU:N	2.77	0.43
2:L:21:GLU:OE1	2:L:21:GLU:HB3	2.19	0.43
2:B:21:GLU:CB	2:B:22:ARG:N	2.78	0.43
1:E:2:ILE:H	1:E:2:ILE:HG22	1.84	0.43
1:E:17:GLU:O	1:E:18:ASN:CA	2.66	0.43
1:K:6:CYS:HB3	2:L:11:LEU:HD21	2.00	0.43
1:A:2:ILE:O	1:A:6:CYS:HB2	2.19	0.43
1:A:3:VAL:HG22	2:B:26:MEA:HZ	2.01	0.43
2:B:26:MEA:C1	2:D:24:PHE:O	2.66	0.43
2:L:24:PHE:CB	2:L:24:PHE:N	2.68	0.43
1:C:2:ILE:CA	1:C:2:ILE:CG1	2.86	0.43
1:E:2:ILE:O	1:E:2:ILE:HG12	2.19	0.43
1:C:3:VAL:CB	1:C:3:VAL:C	2.76	0.43
1:E:1:GLY:O	1:E:2:ILE:CA	2.67	0.43
1:K:2:ILE:CG1	1:K:2:ILE:C	2.92	0.43
2:L:14:ALA:C	2:L:14:ALA:CB	2.78	0.43
1:E:1:GLY:CA	1:E:2:ILE:N	2.65	0.43
1:E:18:ASN:O	1:E:19:TYR:CA	2.63	0.43
1:I:16:LEU:HD13	2:J:14:ALA:HB1	2.01	0.43
1:K:5:GLN:OE1	1:K:19:TYR:CE2	2.72	0.43
1:K:12:SER:C	1:K:16:LEU:HD12	2.43	0.43
1:E:1:GLY:N	1:E:4:GLU:HG3	2.33	0.42
1:I:5:GLN:O	1:I:6:CYS:CA	2.67	0.42
1:K:8:THR:OG1	1:K:8:THR:CA	2.56	0.42
2:B:9:SER:OG	2:D:13:GLU:CD	2.61	0.42
2:B:17:LEU:O	2:B:18:VAL:C	2.62	0.42
1:C:11:CYS:HA	1:C:15:GLN:NE2	2.34	0.42
1:E:16:LEU:HA	1:E:16:LEU:HD23	1.55	0.42
1:K:18:ASN:N	1:K:19:TYR:N	2.67	0.42
2:D:13:GLU:C	2:D:14:ALA:CA	2.73	0.42
1:G:13:LEU:CD2	1:G:13:LEU:HB3	2.47	0.42
1:K:2:ILE:HA	1:K:5:GLN:HB3	2.01	0.42
1:K:12:SER:CB	1:K:12:SER:HG	2.17	0.42
1:A:10:ILE:CA	1:A:11:CYS:N	2.65	0.42
1:E:1:GLY:N	1:E:4:GLU:CD	2.77	0.42
2:F:26:MEA:HE2	2:H:16:TYR:CD1	2.55	0.42
2:H:2:VAL:HG11	2:H:2:VAL:HG21	1.97	0.42
1:I:5:GLN:HE21	1:I:5:GLN:HB2	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:GLU:O	1:I:18:ASN:CA	2.67	0.42
1:A:2:ILE:N	1:A:4:GLU:OE1	2.53	0.42
1:G:2:ILE:N	6:G:2002:HOH:O	2.52	0.42
2:D:5:HIS:C	2:D:6:LEU:CA	2.70	0.42
1:A:2:ILE:C	1:A:4:GLU:OE1	2.62	0.42
2:F:9:SER:O	2:F:13:GLU:HG3	2.20	0.42
2:F:15:LEU:O	2:F:19:CYS:CB	2.67	0.42
2:F:26:MEA:HE2	2:H:16:TYR:HD1	1.84	0.42
1:A:21:ASN:HD21	2:B:22:ARG:HE	1.63	0.42
2:H:8:GLY:C	2:H:10:HIS:N	2.73	0.42
2:D:6:LEU:HG	2:D:6:LEU:H	1.83	0.41
1:K:17:GLU:O	1:K:20:CYS:CB	2.68	0.41
6:B:2015:HOH:O	1:G:12:SER:HA	2.19	0.41
2:B:4:GLN:CG	2:B:4:GLN:O	2.68	0.41
2:B:21:GLU:CB	2:B:21:GLU:N	2.68	0.41
2:F:10:HIS:ND1	6:F:2006:HOH:O	2.35	0.41
1:G:2:ILE:CG2	1:G:2:ILE:HB	2.27	0.41
2:H:6:LEU:O	2:H:10:HIS:HD2	2.02	0.41
2:J:8:GLY:CA	2:L:16:TYR:CZ	2.98	0.41
2:D:13:GLU:HA	2:D:16:TYR:HB3	2.02	0.41
1:E:10:ILE:HG22	1:E:11:CYS:O	2.20	0.41
2:H:9:SER:O	2:H:13:GLU:HG3	2.20	0.41
1:I:14:TYR:C	1:I:17:GLU:H	2.27	0.41
1:A:13:LEU:C	1:A:15:GLN:N	2.75	0.41
6:B:2015:HOH:O	1:G:12:SER:CA	2.69	0.41
1:E:19:TYR:O	1:E:20:CYS:C	2.63	0.41
1:G:21:ASN:HB3	6:G:2017:HOH:O	2.20	0.41
1:I:1:GLY:O	1:I:5:GLN:HB2	2.20	0.41
2:J:11:LEU:C	2:J:11:LEU:HB3	2.41	0.41
2:J:15:LEU:CD1	2:J:24:PHE:CD2	3.03	0.41
1:E:1:GLY:O	1:E:2:ILE:HA	2.21	0.41
2:B:10:HIS:O	2:B:11:LEU:C	2.63	0.41
1:E:2:ILE:CG2	1:E:2:ILE:N	2.84	0.41
2:F:2:VAL:HA	2:F:5:HIS:HB3	2.01	0.41
1:G:5:GLN:NE2	1:G:19:TYR:OH	2.53	0.41
1:I:8:THR:CG2	6:I:2011:HOH:O	2.36	0.41
1:K:2:ILE:N	1:K:2:ILE:CG2	2.83	0.41
1:K:18:ASN:HD22	1:K:18:ASN:HA	1.24	0.41
2:L:21:GLU:CG	2:L:21:GLU:H	2.33	0.41
2:B:6:LEU:HG	2:B:6:LEU:H	1.85	0.41
2:F:21:GLU:N	2:F:21:GLU:HB2	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:VAL:HG23	1:K:10:ILE:N	2.36	0.41
2:H:17:LEU:C	2:H:18:VAL:CA	2.76	0.41
2:J:19:CYS:C	2:J:20:GLY:O	2.59	0.41
1:A:2:ILE:HG23	1:A:3:VAL:N	2.36	0.40
2:H:1:PHE:HB3	2:H:3:ASN:OD1	2.21	0.40
1:I:2:ILE:HG23	1:I:3:VAL:N	2.33	0.40
2:F:15:LEU:HD13	2:F:24:PHE:HB2	2.02	0.40
2:L:11:LEU:HA	2:L:11:LEU:HD23	1.39	0.40
1:C:15:GLN:O	1:C:18:ASN:N	2.54	0.40
2:D:2:VAL:CG1	1:G:8:THR:O	2.69	0.40
2:F:20:GLY:O	2:F:21:GLU:C	2.64	0.40
1:A:15:GLN:O	1:A:18:ASN:HB3	2.22	0.40
1:I:13:LEU:HD22	2:J:18:VAL:CG2	2.51	0.40
2:J:9:SER:O	2:J:10:HIS:C	2.64	0.40
2:L:3:ASN:CA	2:L:3:ASN:O	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	18/21 (86%)	17 (94%)	1 (6%)	0	100	100
1	C	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	E	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	G	18/21 (86%)	17 (94%)	1 (6%)	0	100	100
1	I	19/21 (90%)	19 (100%)	0	0	100	100
1	K	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
2	B	24/30 (80%)	24 (100%)	0	0	100	100
2	D	23/30 (77%)	22 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	23/30 (77%)	22 (96%)	1 (4%)	0	100	100
2	H	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
2	J	26/30 (87%)	24 (92%)	2 (8%)	0	100	100
2	L	24/30 (80%)	23 (96%)	1 (4%)	0	100	100
All	All	257/306 (84%)	244 (95%)	13 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	20/20 (100%)	18 (90%)	2 (10%)	7	1
1	C	20/20 (100%)	19 (95%)	1 (5%)	22	10
1	E	20/20 (100%)	16 (80%)	4 (20%)	1	0
1	G	20/20 (100%)	16 (80%)	4 (20%)	1	0
1	I	20/20 (100%)	19 (95%)	1 (5%)	22	10
1	K	20/20 (100%)	18 (90%)	2 (10%)	7	1
2	B	22/25 (88%)	19 (86%)	3 (14%)	3	1
2	D	19/25 (76%)	15 (79%)	4 (21%)	1	0
2	F	19/25 (76%)	17 (90%)	2 (10%)	6	1
2	H	22/25 (88%)	20 (91%)	2 (9%)	9	2
2	J	24/25 (96%)	22 (92%)	2 (8%)	10	3
2	L	21/25 (84%)	18 (86%)	3 (14%)	3	1
All	All	247/270 (92%)	217 (88%)	30 (12%)	5	1

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU

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Mol	Chain	Res	Type
1	A	21	ASN
2	B	12	VAL
2	B	17	LEU
2	B	21	GLU
1	C	10	ILE
2	D	3	ASN
2	D	4	GLN
2	D	21	GLU
2	D	22	ARG
1	E	4	GLU
1	E	5	GLN
1	E	8	THR
1	E	10	ILE
2	F	2	VAL
2	F	3	ASN
1	G	2	ILE
1	G	3	VAL
1	G	4	GLU
1	G	13	LEU
2	H	17	LEU
2	H	27	THR
1	I	5	GLN
2	J	4	GLN
2	J	22	ARG
1	K	8	THR
1	K	17	GLU
2	L	12	VAL
2	L	17	LEU
2	L	21	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	21	ASN
2	B	10	HIS
1	C	5	GLN
1	C	15	GLN
2	D	3	ASN
2	D	4	GLN
1	E	5	GLN
1	E	21	ASN

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Mol	Chain	Res	Type
2	F	4	GLN
1	G	5	GLN
1	I	5	GLN
1	I	21	ASN
1	K	18	ASN
1	K	21	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEA	D	26	2	11,12,13	10.52	8 (72%)	13,14,16	9.05	12 (92%)
2	MEA	F	26	2	11,12,13	9.74	8 (72%)	13,14,16	8.13	11 (84%)
2	MEA	H	26	2	11,12,13	6.57	6 (54%)	13,14,16	4.76	11 (84%)
2	MEA	B	26	2	11,12,13	7.05	8 (72%)	13,14,16	5.63	10 (76%)
2	MEA	J	26	2	11,12,13	7.08	5 (45%)	13,14,16	4.95	10 (76%)
2	MEA	L	26	2	11,12,13	6.14	10 (90%)	13,14,16	5.99	10 (76%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEA	D	26	2	-	3/5/8/10	0/1/1/1
2	MEA	F	26	2	-	2/5/8/10	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEA	H	26	2	-	3/5/8/10	0/1/1/1
2	MEA	B	26	2	-	1/5/8/10	0/1/1/1
2	MEA	J	26	2	-	1/5/8/10	0/1/1/1
2	MEA	L	26	2	-	1/5/8/10	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	26	MEA	CA-N	-17.74	1.16	1.47
2	J	26	MEA	CB-CA	17.70	1.93	1.54
2	D	26	MEA	CA-N	-16.87	1.18	1.47
2	D	26	MEA	CD1-CG	16.64	1.71	1.38
2	D	26	MEA	CE2-CZ	15.72	1.72	1.38
2	F	26	MEA	CE2-CZ	14.16	1.69	1.38
2	F	26	MEA	CD1-CG	13.80	1.66	1.38
2	B	26	MEA	CD1-CG	13.14	1.64	1.38
2	B	26	MEA	CE2-CZ	11.93	1.64	1.38
2	D	26	MEA	C1-N	11.18	1.74	1.46
2	H	26	MEA	CD1-CG	10.85	1.60	1.38
2	F	26	MEA	CE2-CD2	-10.36	1.21	1.38
2	D	26	MEA	CE1-CD1	-10.25	1.21	1.38
2	L	26	MEA	CB-CA	-9.85	1.32	1.54
2	D	26	MEA	CE2-CD2	-9.83	1.22	1.38
2	F	26	MEA	CE1-CD1	-9.75	1.22	1.38
2	F	26	MEA	CB-CG	-9.44	1.29	1.51
2	L	26	MEA	C1-N	-9.10	1.24	1.46
2	J	26	MEA	C1-N	-9.08	1.24	1.46
2	H	26	MEA	CD2-CG	8.85	1.56	1.38
2	H	26	MEA	CE2-CZ	8.84	1.57	1.38
2	H	26	MEA	O-C	8.66	1.52	1.20
2	J	26	MEA	CD1-CG	-8.57	1.22	1.38
2	D	26	MEA	CB-CG	-8.53	1.31	1.51
2	H	26	MEA	CZ-CE1	8.14	1.56	1.38
2	B	26	MEA	O-C	8.11	1.50	1.20
2	B	26	MEA	CA-N	7.85	1.60	1.47
2	J	26	MEA	CE2-CZ	-7.77	1.21	1.38
2	H	26	MEA	C1-N	7.54	1.65	1.46
2	B	26	MEA	CB-CA	-7.00	1.38	1.54
2	L	26	MEA	CD1-CG	6.48	1.51	1.38
2	F	26	MEA	C1-N	6.44	1.62	1.46
2	L	26	MEA	CE2-CZ	6.17	1.51	1.38
2	L	26	MEA	CE1-CD1	5.94	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	26	MEA	CE2-CD2	5.92	1.49	1.38
2	L	26	MEA	CD2-CG	-5.54	1.28	1.38
2	L	26	MEA	CB-CG	5.05	1.63	1.51
2	B	26	MEA	CD2-CG	4.95	1.48	1.38
2	L	26	MEA	CZ-CE1	-4.51	1.28	1.38
2	B	26	MEA	CZ-CE1	4.13	1.47	1.38
2	D	26	MEA	CB-CA	-3.07	1.47	1.54
2	J	26	MEA	O-C	-2.83	1.09	1.20
2	L	26	MEA	O-C	-2.72	1.09	1.20
2	F	26	MEA	O-C	2.25	1.28	1.20
2	B	26	MEA	CE1-CD1	2.24	1.42	1.38

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	26	MEA	CZ-CE1-CD1	-18.08	97.94	120.24
2	F	26	MEA	CZ-CE1-CD1	-16.37	100.04	120.24
2	D	26	MEA	CE2-CD2-CG	-15.50	98.82	120.61
2	F	26	MEA	CE2-CD2-CG	-13.73	101.30	120.61
2	B	26	MEA	CB-CA-C	-12.90	86.14	111.81
2	L	26	MEA	CG-CB-CA	-12.36	95.91	113.51
2	D	26	MEA	CB-CG-CD2	-11.75	99.04	120.90
2	D	26	MEA	CE2-CZ-CE1	11.42	135.50	119.87
2	D	26	MEA	CD2-CG-CD1	11.01	134.60	118.23
2	F	26	MEA	CB-CG-CD2	-10.94	100.56	120.90
2	F	26	MEA	CD2-CG-CD1	10.52	133.86	118.23
2	H	26	MEA	CB-CA-C	-10.41	91.10	111.81
2	F	26	MEA	CE2-CZ-CE1	10.35	134.04	119.87
2	L	26	MEA	CB-CA-C	-9.90	92.13	111.81
2	H	26	MEA	CB-CA-N	8.12	122.43	110.48
2	J	26	MEA	CB-CA-N	7.75	121.90	110.48
2	J	26	MEA	CG-CB-CA	7.50	124.20	113.51
2	B	26	MEA	CZ-CE1-CD1	-7.24	111.31	120.24
2	J	26	MEA	CZ-CE2-CD2	-7.06	111.53	120.24
2	L	26	MEA	CZ-CE2-CD2	6.94	128.80	120.24
2	L	26	MEA	O-C-CA	-6.62	107.74	124.77
2	L	26	MEA	CE1-CD1-CG	6.44	129.67	120.61
2	B	26	MEA	CB-CA-N	6.34	119.82	110.48
2	B	26	MEA	CE2-CD2-CG	-6.04	112.12	120.61
2	H	26	MEA	CD2-CG-CD1	5.59	126.55	118.23
2	H	26	MEA	CE2-CZ-CE1	5.56	127.49	119.87
2	D	26	MEA	CG-CB-CA	-5.55	105.61	113.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	26	MEA	CE1-CD1-CG	-5.53	112.83	120.61
2	J	26	MEA	CZ-CE1-CD1	5.48	127.00	120.24
2	J	26	MEA	CE2-CD2-CG	5.42	128.23	120.61
2	L	26	MEA	CZ-CE1-CD1	-4.93	114.15	120.24
2	B	26	MEA	O-C-CA	4.89	137.34	124.77
2	D	26	MEA	CE1-CD1-CG	4.76	127.30	120.61
2	B	26	MEA	CB-CG-CD2	-4.70	112.16	120.90
2	B	26	MEA	CE2-CZ-CE1	4.54	126.09	119.87
2	D	26	MEA	CZ-CE2-CD2	4.52	125.82	120.24
2	L	26	MEA	CB-CG-CD1	4.45	129.19	120.90
2	B	26	MEA	CD2-CG-CD1	4.39	124.76	118.23
2	J	26	MEA	CB-CG-CD1	-4.29	112.91	120.90
2	B	26	MEA	CG-CB-CA	4.12	119.37	113.51
2	F	26	MEA	C1-N-CA	-4.02	101.70	113.70
2	F	26	MEA	CE1-CD1-CG	3.96	126.19	120.61
2	L	26	MEA	CE2-CD2-CG	-3.93	115.08	120.61
2	J	26	MEA	C1-N-CA	-3.89	102.09	113.70
2	J	26	MEA	CB-CG-CD2	3.85	128.06	120.90
2	F	26	MEA	CZ-CE2-CD2	3.50	124.56	120.24
2	H	26	MEA	CE2-CD2-CG	-3.41	115.82	120.61
2	J	26	MEA	O-C-CA	-3.35	116.16	124.77
2	D	26	MEA	O-C-CA	-3.27	116.36	124.77
2	L	26	MEA	CB-CG-CD2	-3.26	114.85	120.90
2	H	26	MEA	CZ-CE1-CD1	-3.23	116.25	120.24
2	F	26	MEA	CB-CA-N	-2.98	106.09	110.48
2	D	26	MEA	CB-CG-CD1	2.89	126.28	120.90
2	H	26	MEA	CB-CG-CD2	-2.80	115.69	120.90
2	H	26	MEA	CZ-CE2-CD2	-2.77	116.82	120.24
2	H	26	MEA	CE1-CD1-CG	-2.54	117.04	120.61
2	F	26	MEA	CB-CG-CD1	2.50	125.55	120.90
2	D	26	MEA	CB-CA-C	2.46	116.70	111.81
2	L	26	MEA	CE2-CZ-CE1	-2.45	116.52	119.87
2	B	26	MEA	C1-N-CA	-2.44	106.41	113.70
2	H	26	MEA	C1-N-CA	-2.44	106.42	113.70
2	D	26	MEA	CB-CA-N	-2.40	106.95	110.48
2	H	26	MEA	O-C-CA	2.35	130.82	124.77
2	F	26	MEA	CB-CA-C	2.25	116.28	111.81

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	26	MEA	O-C-CA-CB
2	D	26	MEA	O-C-CA-CB
2	D	26	MEA	C-CA-CB-CG
2	F	26	MEA	N-CA-CB-CG
2	F	26	MEA	C-CA-CB-CG
2	H	26	MEA	O-C-CA-CB
2	H	26	MEA	C-CA-CB-CG
2	J	26	MEA	O-C-CA-CB
2	L	26	MEA	O-C-CA-CB
2	H	26	MEA	N-CA-CB-CG
2	D	26	MEA	N-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	26	MEA	5	0
2	F	26	MEA	7	0
2	H	26	MEA	2	0
2	B	26	MEA	3	0
2	J	26	MEA	5	0
2	L	26	MEA	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	IPH	E	1022	-	7,7,7	2.46	2 (28%)	8,8,8	2.84	6 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IPH	A	1022	-	7,7,7	9.16	5 (71%)	8,8,8	8.40	8 (100%)
3	IPH	C	1022	-	7,7,7	5.07	4 (57%)	8,8,8	4.23	6 (75%)
3	IPH	G	1022	-	7,7,7	8.70	7 (100%)	8,8,8	8.82	7 (87%)
3	IPH	I	1022	-	7,7,7	2.66	6 (85%)	8,8,8	3.38	5 (62%)
3	IPH	K	1022	-	7,7,7	7.66	5 (71%)	8,8,8	5.39	7 (87%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IPH	E	1022	-	-	-	0/1/1/1
3	IPH	A	1022	-	-	-	0/1/1/1
3	IPH	C	1022	-	-	-	0/1/1/1
3	IPH	G	1022	-	-	-	0/1/1/1
3	IPH	I	1022	-	-	-	0/1/1/1
3	IPH	K	1022	-	-	-	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1022	IPH	C6-C1	18.19	1.73	1.39
3	A	1022	IPH	C4-C3	15.40	1.72	1.38
3	G	1022	IPH	C6-C1	13.61	1.64	1.39
3	G	1022	IPH	C4-C3	12.28	1.65	1.38
3	K	1022	IPH	C3-C2	-11.76	1.18	1.38
3	K	1022	IPH	C5-C6	-11.42	1.19	1.38
3	C	1022	IPH	C6-C1	8.86	1.55	1.39
3	C	1022	IPH	C4-C3	8.18	1.56	1.38
3	K	1022	IPH	O1-C1	-8.11	1.18	1.37
3	G	1022	IPH	C3-C2	7.48	1.51	1.38
3	G	1022	IPH	C2-C1	-7.01	1.25	1.39
3	G	1022	IPH	C5-C6	6.47	1.50	1.38
3	K	1022	IPH	C4-C3	-6.16	1.24	1.38
3	K	1022	IPH	C6-C1	-6.14	1.27	1.39
3	G	1022	IPH	C5-C4	-6.10	1.24	1.38
3	E	1022	IPH	C2-C1	-5.40	1.28	1.39
3	C	1022	IPH	C2-C1	4.06	1.46	1.39
3	I	1022	IPH	C6-C1	-3.81	1.31	1.39
3	C	1022	IPH	C5-C4	3.32	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1022	IPH	C5-C4	-3.25	1.31	1.38
3	I	1022	IPH	C5-C4	3.08	1.45	1.38
3	I	1022	IPH	C4-C3	-3.06	1.31	1.38
3	G	1022	IPH	O1-C1	3.05	1.43	1.37
3	A	1022	IPH	O1-C1	-2.59	1.31	1.37
3	A	1022	IPH	C5-C6	-2.56	1.34	1.38
3	A	1022	IPH	C3-C2	-2.47	1.34	1.38
3	I	1022	IPH	C2-C1	2.28	1.43	1.39
3	I	1022	IPH	C5-C6	-2.24	1.35	1.38
3	I	1022	IPH	C3-C2	-2.05	1.35	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1022	IPH	C4-C5-C6	-13.92	103.07	120.24
3	G	1022	IPH	C4-C5-C6	-13.26	103.88	120.24
3	A	1022	IPH	C3-C2-C1	-12.47	102.45	119.29
3	G	1022	IPH	C3-C2-C1	-12.29	102.69	119.29
3	G	1022	IPH	C4-C3-C2	11.01	133.82	120.24
3	G	1022	IPH	C5-C6-C1	10.78	133.85	119.29
3	K	1022	IPH	C5-C6-C1	-8.82	107.37	119.29
3	K	1022	IPH	C4-C3-C2	-8.56	109.68	120.24
3	C	1022	IPH	C4-C5-C6	-8.11	110.23	120.24
3	A	1022	IPH	C5-C4-C3	7.82	130.58	119.87
3	A	1022	IPH	C6-C1-C2	6.93	130.80	119.77
3	A	1022	IPH	O1-C1-C2	-6.63	101.54	120.00
3	C	1022	IPH	C5-C4-C3	5.71	127.69	119.87
3	G	1022	IPH	O1-C1-C2	-5.55	104.53	120.00
3	A	1022	IPH	C4-C3-C2	5.41	126.91	120.24
3	I	1022	IPH	C5-C6-C1	-5.24	112.21	119.29
3	I	1022	IPH	C4-C3-C2	-5.08	113.98	120.24
3	A	1022	IPH	C5-C6-C1	5.07	126.14	119.29
3	K	1022	IPH	C6-C1-C2	5.02	127.75	119.77
3	K	1022	IPH	C5-C4-C3	4.84	126.49	119.87
3	G	1022	IPH	O1-C1-C6	4.36	132.16	120.00
3	C	1022	IPH	C3-C2-C1	-4.35	113.41	119.29
3	E	1022	IPH	C4-C5-C6	-4.34	114.88	120.24
3	I	1022	IPH	C4-C5-C6	4.14	125.35	120.24
3	E	1022	IPH	C5-C6-C1	4.03	124.73	119.29
3	K	1022	IPH	C4-C5-C6	3.80	124.93	120.24
3	I	1022	IPH	C3-C2-C1	3.40	123.89	119.29
3	E	1022	IPH	C4-C3-C2	3.35	124.38	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1022	IPH	C5-C6-C1	3.28	123.72	119.29
3	K	1022	IPH	C3-C2-C1	3.26	123.69	119.29
3	C	1022	IPH	C6-C1-C2	2.85	124.29	119.77
3	K	1022	IPH	O1-C1-C6	-2.81	112.16	120.00
3	A	1022	IPH	O1-C1-C6	2.75	127.66	120.00
3	E	1022	IPH	O1-C1-C6	2.58	127.18	120.00
3	E	1022	IPH	O1-C1-C2	-2.53	112.96	120.00
3	C	1022	IPH	O1-C1-C2	-2.45	113.18	120.00
3	E	1022	IPH	C3-C2-C1	-2.25	116.24	119.29
3	I	1022	IPH	C6-C1-C2	2.21	123.28	119.77
3	G	1022	IPH	C6-C1-C2	2.18	123.23	119.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1022	IPH	2	0
3	G	1022	IPH	2	0
3	I	1022	IPH	1	0
3	K	1022	IPH	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	L	11
2	J	10
2	H	9
2	B	8
1	A	5
1	I	5
2	F	4

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Mol	Chain	Number of breaks
2	D	4
1	K	4
1	G	3
1	C	3
1	E	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	25:TYR	C	26:MEA	N	1.68
1	J	12:VAL	C	13:GLU	N	1.67
1	A	11:CYS	C	12:SER	N	1.66
1	L	12:VAL	C	13:GLU	N	1.66
1	F	7:CYS	C	8:GLY	N	1.65
1	J	1:PHE	C	2:VAL	N	1.65
1	F	18:VAL	C	19:CYS	N	1.64
1	G	18:ASN	C	19:TYR	N	1.64
1	H	4:GLN	C	5:HIS	N	1.64
1	H	15:LEU	C	16:TYR	N	1.64
1	H	25:TYR	C	26:MEA	N	1.64
1	J	22:ARG	C	23:GLY	N	1.64
1	D	18:VAL	C	19:CYS	N	1.63
1	I	3:VAL	C	4:GLU	N	1.63
1	L	1:PHE	C	2:VAL	N	1.63
1	D	7:CYS	C	8:GLY	N	1.62
1	L	5:HIS	C	6:LEU	N	1.62
1	B	4:GLN	C	5:HIS	N	1.61
1	C	9:SER	C	10:ILE	N	1.61
1	H	8:GLY	C	9:SER	N	1.61
1	J	3:ASN	C	4:GLN	N	1.60
1	J	8:GLY	C	9:SER	N	1.60
1	A	15:GLN	C	16:LEU	N	1.20
1	H	7:CYS	C	8:GLY	N	1.20
1	A	17:GLU	C	18:ASN	N	1.19
1	F	22:ARG	C	23:GLY	N	1.19
1	I	7:CYS	C	8:THR	N	1.19
1	K	17:GLU	C	18:ASN	N	1.19
1	H	3:ASN	C	4:GLN	N	1.18
1	H	10:HIS	C	11:LEU	N	1.18
1	I	10:ILE	C	11:CYS	N	1.18
1	L	6:LEU	C	7:CYS	N	1.18
1	C	4:GLU	C	5:GLN	N	1.17
1	L	4:GLN	C	5:HIS	N	1.17

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	14:ALA	C	15:LEU	N	1.16
1	L	15:LEU	C	16:TYR	N	1.16
1	B	26:MEA	C	27:THR	N	1.15
1	C	14:TYR	C	15:GLN	N	1.15
1	G	6:CYS	C	7:CYS	N	1.15
1	I	13:LEU	C	14:TYR	N	1.15
1	L	24:PHE	C	25:TYR	N	1.15
1	G	12:SER	C	13:LEU	N	1.14
1	A	9:SER	C	10:ILE	N	1.13
1	B	17:LEU	C	18:VAL	N	1.13
1	B	24:PHE	C	25:TYR	N	1.13
1	D	22:ARG	C	23:GLY	N	1.13
1	H	14:ALA	C	15:LEU	N	1.13
1	J	13:GLU	C	14:ALA	N	1.13
1	J	28:LYS	C	29:PRO	N	1.13
1	L	21:GLU	C	22:ARG	N	1.13
1	B	3:ASN	C	4:GLN	N	1.12
1	D	20:GLY	C	21:GLU	N	1.12
1	K	5:GLN	C	6:CYS	N	1.12
1	H	24:PHE	C	25:TYR	N	1.11
1	L	13:GLU	C	14:ALA	N	1.11
1	E	8:THR	C	9:SER	N	1.10
1	J	9:SER	C	10:HIS	N	1.10
1	A	3:VAL	C	4:GLU	N	1.09
1	F	20:GLY	C	21:GLU	N	1.09
1	I	20:CYS	C	21:ASN	N	1.09
1	J	11:LEU	C	12:VAL	N	1.09
1	L	11:LEU	C	12:VAL	N	1.09
1	J	2:VAL	C	3:ASN	N	1.08
1	K	7:CYS	C	8:THR	N	1.08
1	L	2:VAL	C	3:ASN	N	1.08
1	B	10:HIS	C	11:LEU	N	1.07
1	K	13:LEU	C	14:TYR	N	1.07
1	E	4:GLU	C	5:GLN	N	1.06
1	E	14:TYR	C	15:GLN	N	1.06

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	20/21 (95%)	0.85	1 (5%) 34 44	39, 54, 68, 70	0
1	C	21/21 (100%)	0.30	0 100 100	27, 36, 48, 55	0
1	E	21/21 (100%)	0.40	1 (4%) 35 45	28, 39, 57, 73	0
1	G	20/21 (95%)	0.59	1 (5%) 34 44	31, 36, 57, 66	0
1	I	21/21 (100%)	0.25	1 (4%) 35 45	27, 32, 44, 59	0
1	K	21/21 (100%)	0.70	0 100 100	27, 37, 53, 59	0
2	B	26/30 (86%)	0.42	2 (7%) 19 26	24, 30, 69, 94	0
2	D	24/30 (80%)	0.87	3 (12%) 8 11	21, 30, 59, 64	0
2	F	24/30 (80%)	0.26	1 (4%) 40 50	24, 30, 52, 66	0
2	H	27/30 (90%)	0.40	0 100 100	23, 30, 62, 76	0
2	J	28/30 (93%)	0.38	1 (3%) 46 56	24, 29, 55, 73	0
2	L	25/30 (83%)	0.49	2 (8%) 18 25	23, 32, 55, 67	0
All	All	278/306 (90%)	0.49	13 (4%) 36 46	21, 35, 65, 94	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	2	VAL	4.1
2	F	20	GLY	4.0
2	L	20	GLY	3.6
2	D	25	TYR	3.5
2	D	23	GLY	2.8
1	I	14	TYR	2.6
2	B	25	TYR	2.5
2	J	2	VAL	2.4
1	G	20	CYS	2.3
2	L	1	PHE	2.2
2	B	27	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	8	THR	2.1
1	A	10	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MEA	B	26	12/13	0.83	0.18	83,90,94,95	0
2	MEA	L	26	12/13	0.83	0.14	58,69,80,82	0
2	MEA	F	26	12/13	0.87	0.12	44,49,53,53	0
2	MEA	D	26	12/13	0.87	0.11	53,65,71,73	0
2	MEA	H	26	12/13	0.91	0.09	36,41,45,46	0
2	MEA	J	26	12/13	0.95	0.07	28,31,37,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IPH	C	1022	7/7	0.92	0.09	27,32,33,34	0
3	IPH	A	1022	7/7	0.93	0.10	29,31,36,36	0
3	IPH	E	1022	7/7	0.93	0.10	32,33,35,35	0
3	IPH	K	1022	7/7	0.93	0.07	28,28,31,32	0
3	IPH	I	1022	7/7	0.95	0.06	25,26,28,30	0
3	IPH	G	1022	7/7	0.96	0.09	25,27,29,32	0
4	CL	B	1028	1/1	0.99	0.03	27,27,27,27	0
4	CL	C	1028	1/1	0.99	0.04	25,25,25,25	0
5	ZN	D	1030	1/1	0.99	0.04	23,23,23,23	0
5	ZN	B	1030	1/1	1.00	0.01	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.