



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:57 PM UTC

PDB ID : 1QAF / pdb_00001qaf
Title : THE ACTIVE SITE BASE CONTROLS COFACTOR REACTIVITY IN ES-
CHERICHIA COLI AMINE OXIDASE : X-RAY CRYSTALLOGRAPHIC
STUDIES WITH MUTATIONAL VARIANTS
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S.E.; McPherson, M.J.
Deposited on : 1999-03-11
Resolution : 2.20 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

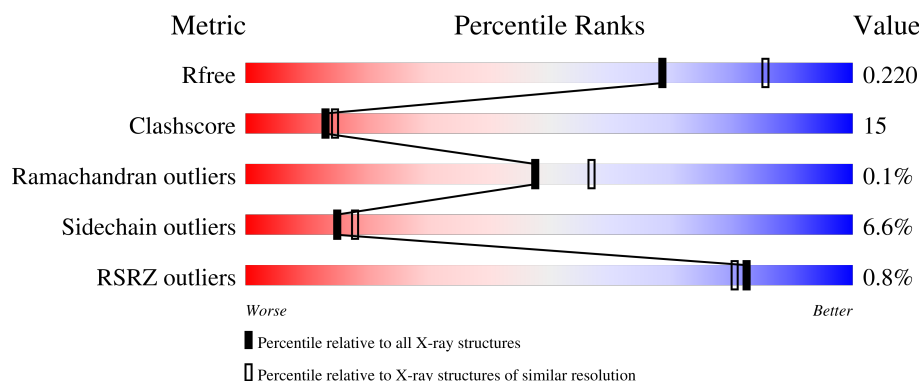
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	721	 52% 34% 13% .
1	B	721	 49% 38% 12% .

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
4	GOL	B	1450	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12775 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 PROTEIN (COPPER AMINE OXIDASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	0	1
			5666	3603	965	1076	22			
1	B	721	Total	C	N	O	S	0	0	0
			5690	3618	970	1080	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	GLU	ASP	engineered mutation	UNP P46883
A	466	TPQ	TYR	modified residue	UNP P46883
B	383	GLU	ASP	engineered mutation	UNP P46883
B	466	TPQ	TYR	modified residue	UNP P46883

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

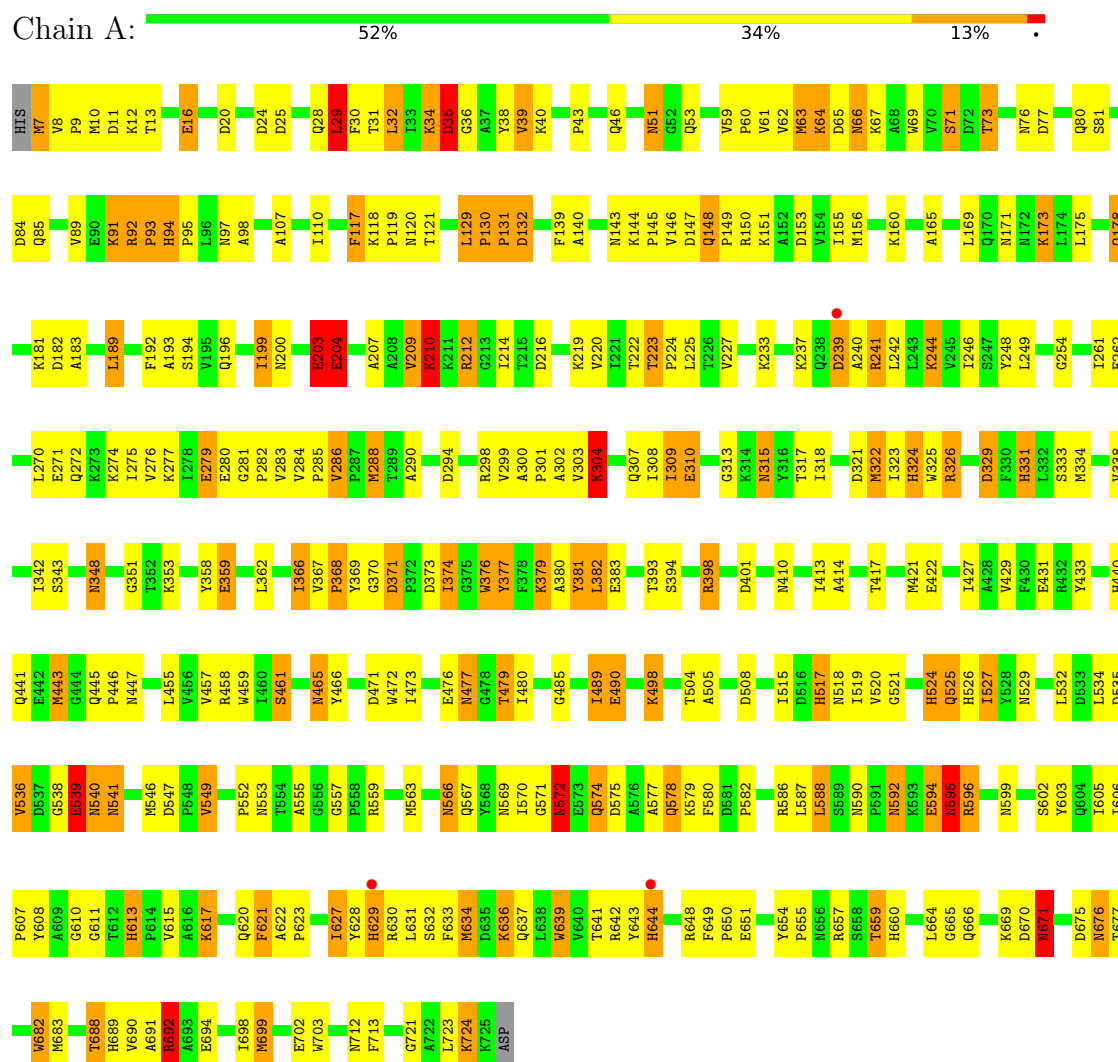
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	767	Total	O	0	0
			767	767		
5	B	640	Total	O	0	0
			640	640		

3 Residue-property plots

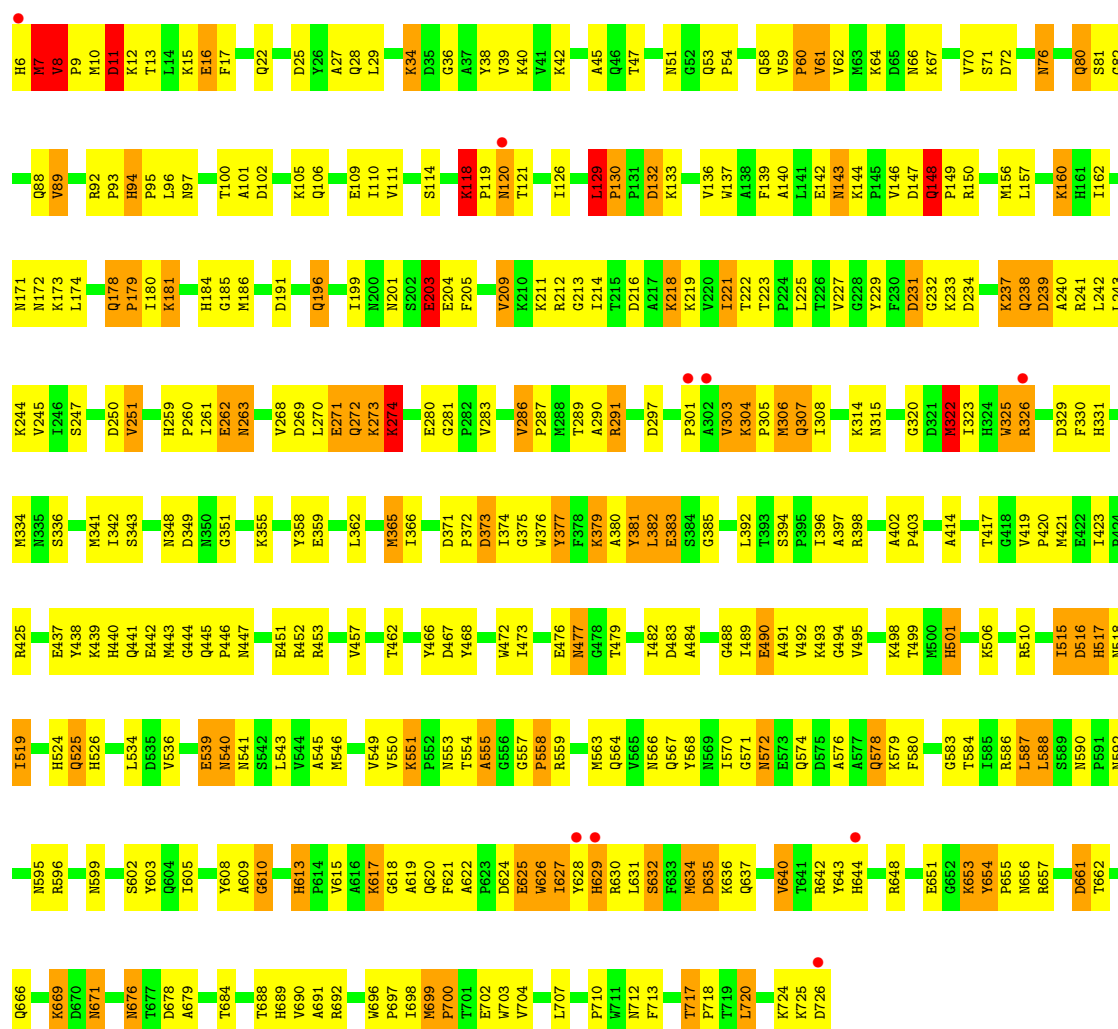
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PROTEIN (COPPER AMINE OXIDASE)



• Molecule 1: PROTEIN (COPPER AMINE OXIDASE)





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.20Å 167.00Å 79.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.6 (20.00-2.20) 88.7 (20.00-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 2.19Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.176 , 0.244 0.158 , 0.220	Depositor DCC
R_{free} test set	2854 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12775	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: CA, GOL, TPQ, CU

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	0.85	3/5795 (0.1%)	2.47	374/7889 (4.7%)
1	B	0.81	2/5820 (0.0%)	2.43	378/7920 (4.8%)
All	All	0.83	5/11615 (0.0%)	2.45	752/15809 (4.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	LYS	C-N	21.45	1.57	1.32
1	B	326	ARG	C-N	-14.71	1.11	1.33
1	B	325	TRP	C-N	-10.03	1.19	1.33
1	A	724	LYS	C-N	-7.10	1.23	1.33
1	A	35	ASP	C-N	-6.67	1.22	1.33

All (752) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	ASN	OD1-CG-ND2	26.42	149.02	122.60
1	A	130	PRO	O-C-N	22.80	131.87	121.15
1	B	648	ARG	CD-NE-CZ	18.69	150.57	124.40
1	A	129	LEU	CA-C-O	16.21	132.84	119.71
1	B	8	VAL	N-CA-CB	-15.12	101.40	111.83
1	B	326	ARG	O-C-N	-14.00	103.97	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	ARG	NE-CZ-NH2	13.77	131.59	119.20
1	B	494	GLY	CA-C-O	-12.85	109.82	121.64
1	A	304	LYS	CA-CB-CG	12.79	139.68	114.10
1	B	642	ARG	NE-CZ-NH1	-12.62	108.88	121.50
1	B	143	ASN	OD1-CG-ND2	12.54	135.14	122.60
1	B	66	ASN	OD1-CG-ND2	12.36	134.96	122.60
1	B	148	GLN	CB-CA-C	12.13	127.31	108.63
1	B	692	ARG	NE-CZ-NH2	-12.12	108.30	119.20
1	A	129	LEU	CB-CA-C	11.82	121.08	110.44
1	B	642	ARG	NH1-CZ-NH2	11.81	134.65	119.30
1	B	89	VAL	N-CA-CB	11.50	123.06	110.53
1	A	129	LEU	CA-C-N	11.47	127.92	119.66
1	A	129	LEU	C-N-CA	11.47	127.92	119.66
1	A	566	ASN	CA-CB-CG	-11.37	101.23	112.60
1	A	130	PRO	CB-CA-C	-11.04	100.79	111.17
1	B	539	GLU	CB-CG-CD	10.72	130.82	112.60
1	A	119	PRO	CA-C-N	-10.59	105.36	123.25
1	A	119	PRO	C-N-CA	-10.59	105.36	123.25
1	B	666	GLN	OE1-CD-NE2	-10.49	112.11	122.60
1	B	371	ASP	CA-C-O	10.39	128.18	119.66
1	A	130	PRO	N-CA-CB	10.36	108.61	103.22
1	A	539	GLU	CG-CD-OE2	10.30	142.09	118.40
1	A	76	ASN	OD1-CG-ND2	9.99	132.59	122.60
1	B	22	GLN	OE1-CD-NE2	-9.83	112.77	122.60
1	A	676	ASN	OD1-CG-ND2	-9.80	112.80	122.60
1	A	569	ASN	CB-CG-ND2	9.78	131.07	116.40
1	B	381	TYR	N-CA-C	9.70	124.42	109.96
1	A	526	HIS	CE1-NE2-CD2	9.66	118.67	109.00
1	A	566	ASN	CB-CG-OD1	-9.42	101.96	120.80
1	A	317	THR	OG1-CB-CG2	-9.34	90.63	109.30
1	A	649	PHE	O-C-N	9.32	129.68	121.39
1	A	46	GLN	OE1-CD-NE2	-9.26	113.34	122.60
1	B	699	MET	CA-C-O	9.15	127.16	119.66
1	A	381	TYR	N-CA-C	9.12	123.54	109.96
1	B	25	ASP	CA-CB-CG	-9.08	103.52	112.60
1	B	88	GLN	OE1-CD-NE2	9.01	131.61	122.60
1	A	410	ASN	CA-CB-CG	-8.93	103.67	112.60
1	B	578	GLN	N-CA-C	8.83	120.92	108.74
1	B	39	VAL	N-CA-C	8.80	121.28	108.53
1	A	572	ASN	OD1-CG-ND2	-8.77	113.83	122.60
1	B	351	GLY	CA-C-N	-8.76	110.91	123.00
1	B	351	GLY	C-N-CA	-8.76	110.91	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	692	ARG	CA-CB-CG	8.74	131.58	114.10
1	B	58	GLN	OE1-CD-NE2	8.68	131.28	122.60
1	A	586	ARG	NE-CZ-NH2	8.64	126.97	119.20
1	B	566	ASN	OD1-CG-ND2	8.58	131.18	122.60
1	A	518	ASN	CA-CB-CG	-8.57	104.03	112.60
1	A	721	GLY	CA-C-O	8.55	128.61	122.45
1	A	313	GLY	CA-C-O	-8.54	113.77	122.56
1	B	150	ARG	CD-NE-CZ	-8.49	112.51	124.40
1	B	358	TYR	CA-C-O	8.48	129.44	120.70
1	A	629	HIS	CA-CB-CG	-8.45	105.35	113.80
1	A	713	PHE	N-CA-C	-8.45	102.15	111.36
1	A	571	GLY	N-CA-C	8.45	125.13	114.66
1	B	609	ALA	CA-C-N	-8.44	111.32	122.63
1	B	609	ALA	C-N-CA	-8.44	111.32	122.63
1	A	595	ASN	OD1-CG-ND2	-8.43	114.17	122.60
1	A	194	SER	N-CA-CB	8.39	122.17	110.01
1	A	373	ASP	CA-C-N	8.39	131.42	120.60
1	A	373	ASP	C-N-CA	8.39	131.42	120.60
1	B	81	SER	CA-C-N	-8.37	113.71	123.08
1	B	81	SER	C-N-CA	-8.37	113.71	123.08
1	B	676	ASN	OD1-CG-ND2	-8.35	114.25	122.60
1	B	578	GLN	CG-CD-NE2	8.30	128.85	116.40
1	A	644	HIS	CA-C-O	8.29	127.67	119.22
1	B	263	ASN	OD1-CG-ND2	-8.28	114.32	122.60
1	A	578	GLN	OE1-CD-NE2	-8.27	114.33	122.60
1	A	525	GLN	OE1-CD-NE2	8.24	130.84	122.60
1	A	290	ALA	CA-C-N	-8.23	113.80	122.85
1	A	290	ALA	C-N-CA	-8.23	113.80	122.85
1	B	578	GLN	OE1-CD-NE2	-8.22	114.38	122.60
1	A	642	ARG	NE-CZ-NH2	-8.16	111.86	119.20
1	B	6	HIS	N-CA-CB	8.14	124.34	110.50
1	A	539	GLU	OE1-CD-OE2	-8.05	103.57	122.90
1	B	82	GLY	N-CA-C	-8.05	104.90	114.48
1	B	657	ARG	NE-CZ-NH1	-8.05	113.45	121.50
1	B	524	HIS	CE1-NE2-CD2	8.05	117.05	109.00
1	A	594	GLU	CA-C-O	-8.04	112.31	121.40
1	B	58	GLN	N-CA-CB	8.03	122.16	110.20
1	B	322	MET	CG-SD-CE	7.99	118.49	100.90
1	A	13	THR	CA-CB-CG2	7.99	124.08	110.50
1	B	290	ALA	CA-C-O	-7.98	111.82	120.92
1	B	62	VAL	CA-C-O	7.97	128.76	120.39
1	B	484	ALA	CA-C-N	7.96	130.53	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	ALA	C-N-CA	7.96	130.53	122.80
1	B	398	ARG	NE-CZ-NH2	-7.96	112.04	119.20
1	B	136	VAL	CA-C-O	-7.93	112.70	120.95
1	A	143	ASN	OD1-CG-ND2	-7.93	114.67	122.60
1	B	396	ILE	O-C-N	-7.87	114.64	122.67
1	A	288	MET	N-CA-C	7.87	123.17	113.50
1	B	281	GLY	O-C-N	7.83	129.60	121.77
1	A	338	VAL	N-CA-C	7.78	120.54	112.83
1	A	534	LEU	CA-C-O	-7.78	112.45	121.16
1	B	691	ALA	N-CA-C	7.77	119.96	110.41
1	A	89	VAL	N-CA-CB	7.76	122.24	110.13
1	B	704	VAL	N-CA-CB	7.74	124.86	111.39
1	B	233	LYS	N-CA-CB	7.73	123.45	110.32
1	B	7	MET	N-CA-CB	-7.72	98.69	111.20
1	A	131	PRO	N-CA-C	-7.72	100.42	111.22
1	A	194	SER	CB-CA-C	-7.70	98.79	110.88
1	B	624	ASP	CA-CB-CG	-7.70	104.90	112.60
1	A	130	PRO	CA-C-O	-7.69	114.65	120.73
1	B	586	ARG	NE-CZ-NH1	7.68	129.18	121.50
1	A	526	HIS	ND1-CE1-NE2	-7.67	100.72	108.40
1	A	677	THR	N-CA-CB	-7.67	98.51	111.31
1	B	111	VAL	N-CA-CB	7.66	120.95	110.54
1	B	251	VAL	N-CA-CB	-7.65	102.21	112.16
1	B	501	HIS	CA-C-N	7.64	131.72	120.87
1	B	501	HIS	C-N-CA	7.64	131.72	120.87
1	A	712	ASN	OD1-CG-ND2	-7.64	114.96	122.60
1	B	534	LEU	CA-C-O	-7.64	112.34	121.05
1	B	710	PRO	CA-C-O	-7.62	112.34	121.03
1	B	143	ASN	CA-CB-CG	-7.62	104.98	112.60
1	B	555	ALA	N-CA-CB	-7.60	99.47	110.80
1	B	420	PRO	CA-C-O	7.60	130.00	121.34
1	A	93	PRO	N-CA-CB	7.58	110.09	103.27
1	B	358	TYR	O-C-N	-7.52	113.97	122.09
1	B	13	THR	CA-CB-OG1	-7.51	98.34	109.60
1	B	76	ASN	CA-C-O	-7.49	110.96	119.79
1	A	146	VAL	N-CA-C	-7.46	99.26	109.55
1	B	567	GLN	OE1-CD-NE2	-7.46	115.14	122.60
1	A	36	GLY	O-C-N	-7.45	112.49	122.48
1	A	666	GLN	OE1-CD-NE2	-7.43	115.17	122.60
1	A	53	GLN	OE1-CD-NE2	-7.43	115.17	122.60
1	B	398	ARG	NH1-CZ-NH2	7.42	128.95	119.30
1	B	438	TYR	O-C-N	-7.41	115.49	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	LEU	CA-C-O	-7.40	112.48	121.06
1	B	143	ASN	CB-CG-ND2	-7.40	105.30	116.40
1	A	594	GLU	O-C-N	7.38	132.10	123.17
1	B	362	LEU	N-CA-C	-7.38	100.09	110.50
1	A	171	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	A	526	HIS	CG-CD2-NE2	-7.36	99.84	107.20
1	B	111	VAL	CA-C-O	-7.36	113.30	120.95
1	B	571	GLY	N-CA-C	7.35	123.77	114.66
1	B	365	MET	CA-C-O	-7.34	113.40	121.33
1	A	540	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	B	421	MET	N-CA-CB	-7.33	98.50	110.81
1	B	717	THR	CA-C-N	7.33	127.34	119.28
1	B	717	THR	C-N-CA	7.33	127.34	119.28
1	A	379	LYS	CG-CD-CE	-7.30	94.51	111.30
1	B	610	GLY	CA-C-O	-7.29	117.05	122.37
1	A	414	ALA	CA-C-O	-7.27	112.73	120.80
1	A	20	ASP	O-C-N	-7.25	114.75	123.16
1	A	310	GLU	CA-C-N	7.24	126.95	119.56
1	A	310	GLU	C-N-CA	7.24	126.95	119.56
1	A	630	ARG	NE-CZ-NH1	-7.22	114.28	121.50
1	B	223	THR	CA-C-O	-7.22	112.23	120.03
1	B	234	ASP	CA-CB-CG	7.20	119.80	112.60
1	A	476	GLU	O-C-N	7.18	129.73	122.12
1	B	707	LEU	N-CA-CB	-7.18	98.18	111.53
1	B	280	GLU	O-C-N	7.14	131.98	123.27
1	A	200	ASN	OD1-CG-ND2	-7.13	115.47	122.60
1	A	524	HIS	CE1-NE2-CD2	7.13	116.13	109.00
1	A	95	PRO	N-CA-CB	7.11	110.10	103.41
1	B	698	ILE	O-C-N	-7.10	115.50	123.10
1	B	689	HIS	N-CA-C	7.08	120.46	107.99
1	B	359	GLU	CA-C-O	7.07	128.77	120.43
1	B	482	ILE	CA-C-O	-7.07	113.38	120.31
1	A	129	LEU	N-CA-C	-7.05	94.77	108.59
1	B	398	ARG	CB-CA-C	7.03	119.48	109.71
1	A	654	TYR	CA-C-N	7.02	127.17	119.87
1	A	654	TYR	C-N-CA	7.02	127.17	119.87
1	A	699	MET	N-CA-C	7.02	119.81	109.42
1	B	579	LYS	N-CA-C	-7.00	101.10	110.55
1	B	343	SER	N-CA-C	7.00	120.05	109.41
1	A	343	SER	O-C-N	6.99	131.76	122.96
1	A	34	LYS	CA-C-N	-6.98	106.47	121.76
1	A	34	LYS	C-N-CA	-6.98	106.47	121.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	GLU	N-CA-C	6.97	120.59	110.28
1	B	334	MET	N-CA-CB	-6.95	99.50	110.69
1	A	636	LYS	N-CA-CB	6.94	122.47	110.81
1	A	440	HIS	CA-CB-CG	-6.94	106.86	113.80
1	B	656	ASN	OD1-CG-ND2	-6.93	115.67	122.60
1	A	94	HIS	CA-C-N	6.92	127.07	119.87
1	A	94	HIS	C-N-CA	6.92	127.07	119.87
1	A	572	ASN	CB-CG-ND2	6.92	126.77	116.40
1	A	649	PHE	CA-C-O	-6.90	112.66	119.69
1	A	145	PRO	N-CA-CB	6.88	109.44	103.31
1	B	551	LYS	CA-C-N	6.88	126.85	119.76
1	B	551	LYS	C-N-CA	6.88	126.85	119.76
1	B	570	ILE	N-CA-C	-6.87	97.09	106.85
1	A	7	MET	N-CA-CB	6.87	122.18	110.50
1	A	535	ASP	CA-CB-CG	6.86	119.46	112.60
1	B	34	LYS	CA-CB-CG	-6.86	100.37	114.10
1	B	60	PRO	N-CA-CB	6.85	109.31	103.35
1	B	692	ARG	NH1-CZ-NH2	6.84	128.20	119.30
1	A	61	VAL	CA-C-O	-6.83	113.25	121.04
1	B	526	HIS	CE1-NE2-CD2	6.82	115.82	109.00
1	B	414	ALA	CB-CA-C	-6.82	98.50	109.75
1	A	690	VAL	N-CA-C	-6.80	98.06	107.99
1	A	129	LEU	O-C-N	-6.80	113.98	120.85
1	A	659	THR	CA-C-O	6.80	126.90	119.15
1	A	578	GLN	N-CA-C	6.79	119.08	108.96
1	B	713	PHE	N-CA-C	-6.78	103.97	111.36
1	B	203	GLU	CB-CG-CD	6.77	124.11	112.60
1	A	650	PRO	O-C-N	6.76	130.94	122.22
1	B	397	ALA	CA-C-O	6.75	127.81	120.58
1	A	472	TRP	N-CA-C	-6.74	96.05	107.99
1	B	635	ASP	N-CA-C	6.74	121.50	113.28
1	B	437	GLU	N-CA-C	-6.72	104.03	111.36
1	A	524	HIS	CG-CD2-NE2	-6.71	100.49	107.20
1	B	467	ASP	CA-CB-CG	6.70	119.30	112.60
1	A	35	ASP	O-C-N	-6.69	108.00	121.92
1	B	587	LEU	CA-C-O	6.69	128.67	121.11
1	B	495	VAL	CA-C-O	-6.68	115.02	121.63
1	A	666	GLN	CA-C-O	-6.68	113.34	120.42
1	A	566	ASN	CB-CA-C	-6.67	100.11	110.78
1	A	118	LYS	CA-C-N	6.66	128.17	119.84
1	A	118	LYS	C-N-CA	6.66	128.17	119.84
1	B	22	GLN	CG-CD-NE2	6.64	126.36	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	518	ASN	CA-CB-CG	-6.64	105.96	112.60
1	B	540	ASN	N-CA-C	6.64	118.96	108.67
1	B	629	HIS	CA-C-O	-6.63	112.02	120.31
1	B	417	THR	N-CA-CB	6.63	120.30	110.49
1	B	524	HIS	CG-CD2-NE2	-6.62	100.58	107.20
1	A	617	LYS	CA-C-O	6.62	127.52	119.38
1	A	476	GLU	CB-CA-C	-6.61	99.81	110.79
1	A	261	ILE	N-CA-C	-6.61	97.21	106.53
1	A	590	ASN	OD1-CG-ND2	6.61	129.21	122.60
1	A	536	VAL	CA-C-O	-6.60	112.53	120.78
1	A	657	ARG	NE-CZ-NH2	-6.60	113.26	119.20
1	B	690	VAL	N-CA-C	-6.59	98.36	107.99
1	A	117	PHE	CA-CB-CG	-6.59	107.21	113.80
1	B	81	SER	N-CA-C	6.59	119.30	111.33
1	B	119	PRO	N-CA-C	6.59	126.04	112.47
1	B	178	GLN	CB-CG-CD	6.58	123.79	112.60
1	B	204	GLU	CA-C-N	-6.58	111.47	120.28
1	B	204	GLU	C-N-CA	-6.58	111.47	120.28
1	A	148	GLN	OE1-CD-NE2	-6.57	116.03	122.60
1	A	203	GLU	CB-CG-CD	6.57	123.76	112.60
1	A	525	GLN	CG-CD-OE1	-6.56	107.68	120.80
1	A	689	HIS	N-CA-C	6.56	119.42	108.20
1	A	595	ASN	CA-CB-CG	6.55	119.15	112.60
1	A	212	ARG	NE-CZ-NH2	-6.55	113.31	119.20
1	B	473	ILE	N-CA-C	6.54	117.06	107.37
1	B	644	HIS	CA-C-N	6.53	127.04	119.47
1	B	644	HIS	C-N-CA	6.53	127.04	119.47
1	B	297	ASP	N-CA-CB	-6.53	101.03	110.56
1	B	304	LYS	N-CA-CB	-6.51	101.25	110.04
1	B	590	ASN	OD1-CG-ND2	6.50	129.10	122.60
1	A	110	ILE	O-C-N	-6.49	115.57	121.87
1	A	480	ILE	CA-C-O	-6.49	113.48	120.36
1	B	92	ARG	CA-C-O	6.49	126.59	119.32
1	B	440	HIS	N-CA-CB	6.49	120.63	110.71
1	B	661	ASP	CB-CG-OD2	6.48	133.31	118.40
1	A	648	ARG	N-CA-CB	-6.48	102.43	110.98
1	A	536	VAL	O-C-N	6.47	130.66	122.57
1	B	525	GLN	OE1-CD-NE2	6.47	129.07	122.60
1	A	657	ARG	NH1-CZ-NH2	6.46	127.70	119.30
1	B	281	GLY	CA-C-O	-6.45	112.29	121.52
1	A	698	ILE	O-C-N	-6.44	116.21	123.10
1	A	723	LEU	O-C-N	6.44	130.61	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ALA	O-C-N	6.44	131.74	123.11
1	A	275	ILE	N-CA-C	-6.44	100.39	108.89
1	B	148	GLN	OE1-CD-NE2	6.44	129.04	122.60
1	B	213	GLY	CA-C-O	-6.42	112.24	119.04
1	A	567	GLN	OE1-CD-NE2	-6.42	116.18	122.60
1	A	262	GLU	N-CA-C	6.41	119.07	110.35
1	B	307	GLN	CA-C-O	-6.41	113.29	120.66
1	B	323	ILE	CA-C-O	-6.40	113.69	120.48
1	A	457	VAL	O-C-N	6.39	129.83	122.99
1	A	146	VAL	CA-C-N	-6.39	109.34	121.54
1	A	146	VAL	C-N-CA	-6.39	109.34	121.54
1	A	505	ALA	N-CA-CB	6.39	119.64	110.06
1	A	210	LYS	CA-C-O	6.38	127.31	120.55
1	B	283	VAL	O-C-N	6.38	129.89	122.81
1	B	8	VAL	CA-C-N	6.37	128.07	120.23
1	B	8	VAL	C-N-CA	6.37	128.07	120.23
1	A	300	ALA	N-CA-CB	-6.37	100.81	110.11
1	A	309	ILE	N-CA-CB	-6.37	101.77	112.47
1	B	684	THR	CA-CB-OG1	-6.36	100.06	109.60
1	A	422	GLU	CA-C-N	-6.36	118.01	122.59
1	A	422	GLU	C-N-CA	-6.36	118.01	122.59
1	A	92	ARG	CD-NE-CZ	-6.35	115.51	124.40
1	A	35	ASP	CA-C-O	-6.35	111.75	120.83
1	B	232	GLY	CA-C-O	-6.34	112.19	119.10
1	A	691	ALA	N-CA-C	6.32	118.19	110.41
1	A	300	ALA	CA-C-N	6.32	126.08	119.76
1	A	300	ALA	C-N-CA	6.32	126.08	119.76
1	A	300	ALA	O-C-N	-6.31	114.58	121.53
1	A	51	ASN	O-C-N	-6.31	114.72	122.55
1	B	586	ARG	NE-CZ-NH2	-6.31	113.52	119.20
1	A	617	LYS	CA-C-N	6.30	128.20	120.51
1	A	617	LYS	C-N-CA	6.30	128.20	120.51
1	B	359	GLU	CB-CA-C	6.30	121.20	109.86
1	A	577	ALA	CA-C-N	-6.29	111.56	121.87
1	A	577	ALA	C-N-CA	-6.29	111.56	121.87
1	A	476	GLU	N-CA-CB	6.29	119.36	110.12
1	B	305	PRO	CB-CA-C	-6.29	103.18	111.23
1	B	359	GLU	CA-CB-CG	6.28	126.66	114.10
1	A	622	ALA	N-CA-C	-6.28	101.42	110.08
1	B	308	ILE	N-CA-C	-6.27	98.70	107.80
1	B	330	PHE	CA-CB-CG	6.24	120.03	113.80
1	A	574	GLN	O-C-N	6.23	128.49	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	349	ASP	CA-C-O	6.23	127.12	120.46
1	B	625	GLU	CA-C-O	-6.21	113.91	121.36
1	A	89	VAL	CA-CB-CG2	6.21	120.95	110.40
1	B	126	ILE	CA-C-O	-6.20	114.00	120.51
1	A	321	ASP	CA-CB-CG	-6.20	106.40	112.60
1	A	324	HIS	CA-CB-CG	-6.20	107.60	113.80
1	B	272	GLN	CG-CD-NE2	6.19	125.69	116.40
1	B	76	ASN	O-C-N	6.19	130.63	122.33
1	B	260	PRO	CA-C-O	-6.18	114.14	121.67
1	B	130	PRO	N-CA-C	6.17	118.23	110.70
1	A	529	ASN	O-C-N	-6.17	116.09	123.31
1	B	129	LEU	N-CA-C	-6.17	102.01	109.72
1	B	102	ASP	CB-CG-OD1	6.17	132.58	118.40
1	B	373	ASP	N-CA-C	6.17	118.28	110.33
1	A	570	ILE	N-CA-C	-6.15	98.11	106.85
1	A	588	LEU	N-CA-C	-6.15	95.50	107.62
1	A	632	SER	CA-C-O	-6.15	113.15	120.10
1	A	398	ARG	NE-CZ-NH1	6.15	127.65	121.50
1	A	220	VAL	CA-C-O	-6.13	113.50	120.74
1	A	302	ALA	CB-CA-C	6.13	120.81	109.54
1	A	611	GLY	CA-C-O	-6.12	115.61	121.49
1	A	353	LYS	N-CA-CB	6.11	119.12	109.71
1	B	59	VAL	CA-C-N	6.11	126.08	119.78
1	B	59	VAL	C-N-CA	6.11	126.08	119.78
1	B	118	LYS	CA-C-N	6.11	127.48	119.84
1	B	118	LYS	C-N-CA	6.11	127.48	119.84
1	B	524	HIS	CA-CB-CG	-6.10	107.70	113.80
1	A	587	LEU	O-C-N	6.10	131.12	123.19
1	A	271	GLU	CG-CD-OE1	6.08	132.39	118.40
1	A	588	LEU	CB-CA-C	6.08	121.67	111.22
1	B	599	ASN	CA-C-N	6.08	126.39	119.83
1	B	599	ASN	C-N-CA	6.08	126.39	119.83
1	B	34	LYS	CG-CD-CE	-6.06	97.35	111.30
1	A	643	TYR	CA-C-O	-6.06	114.53	121.19
1	A	569	ASN	CB-CG-OD1	-6.05	108.69	120.80
1	B	322	MET	CA-C-N	-6.05	115.69	123.19
1	B	322	MET	C-N-CA	-6.05	115.69	123.19
1	A	541	ASN	CA-CB-CG	6.05	118.65	112.60
1	B	66	ASN	CA-CB-CG	-6.05	106.55	112.60
1	A	443	MET	CA-C-O	-6.04	114.38	120.96
1	B	241	ARG	NE-CZ-NH1	6.03	127.53	121.50
1	A	588	LEU	O-C-N	-6.03	115.17	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	LEU	N-CA-C	6.03	119.37	109.85
1	A	271	GLU	CG-CD-OE2	-6.03	104.54	118.40
1	A	149	PRO	O-C-N	-6.02	115.65	123.00
1	A	595	ASN	CA-C-N	6.02	128.63	120.38
1	A	595	ASN	C-N-CA	6.02	128.63	120.38
1	B	105	LYS	CA-C-O	6.02	126.93	120.55
1	B	557	GLY	O-C-N	6.02	127.79	121.77
1	B	689	HIS	ND1-CE1-NE2	-6.01	102.39	108.40
1	B	329	ASP	N-CA-CB	5.99	120.88	110.81
1	A	401	ASP	N-CA-C	-5.99	105.23	112.54
1	A	160	LYS	N-CA-C	-5.99	104.43	113.89
1	B	348	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	B	280	GLU	CA-C-O	-5.98	113.78	120.66
1	A	473	ILE	N-CA-C	5.98	116.22	107.37
1	B	120	ASN	N-CA-C	-5.98	105.57	112.92
1	B	572	ASN	CA-CB-CG	-5.98	106.62	112.60
1	B	602	SER	N-CA-CB	-5.98	102.12	111.56
1	A	489	ILE	CA-C-O	-5.97	114.12	120.39
1	B	271	GLU	CA-C-O	5.97	126.59	119.60
1	A	331	HIS	O-C-N	-5.97	116.19	123.30
1	A	566	ASN	N-CA-CB	-5.97	100.52	110.37
1	A	34	LYS	N-CA-CB	5.97	119.08	110.37
1	B	702	GLU	CA-C-O	-5.96	114.39	120.71
1	A	329	ASP	N-CA-CB	5.96	120.83	110.81
1	B	186	MET	CA-C-O	-5.96	115.75	122.01
1	B	130	PRO	CB-CA-C	-5.95	103.66	110.92
1	B	261	ILE	N-CA-C	-5.95	96.96	109.34
1	A	178	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	B	348	ASN	CA-C-O	-5.91	113.92	120.60
1	B	425	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	B	493	LYS	CA-C-N	-5.91	114.04	120.71
1	B	493	LYS	C-N-CA	-5.91	114.04	120.71
1	A	307	GLN	CA-C-O	5.91	128.02	121.11
1	A	410	ASN	CA-C-O	-5.91	114.31	121.28
1	B	303	VAL	CA-C-O	5.91	127.22	120.90
1	B	703	TRP	CA-C-O	-5.90	114.44	121.11
1	A	51	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	A	665	GLY	N-CA-C	-5.88	105.68	112.50
1	B	554	THR	CA-CB-CG2	5.88	120.50	110.50
1	A	461	SER	CA-C-O	-5.88	113.80	120.32
1	B	493	LYS	CA-C-O	-5.88	114.03	120.43
1	A	120	ASN	CA-CB-CG	-5.88	106.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	PRO	N-CA-CB	5.87	108.80	103.34
1	B	205	PHE	CA-C-O	5.87	126.78	120.55
1	A	382	LEU	N-CA-CB	5.87	119.18	110.49
1	A	586	ARG	NH1-CZ-NH2	-5.87	111.67	119.30
1	A	682	TRP	CA-C-O	-5.87	114.03	120.36
1	B	635	ASP	CA-CB-CG	-5.87	106.73	112.60
1	B	301	PRO	CA-C-O	5.86	130.75	122.31
1	B	376	TRP	O-C-N	5.86	128.85	121.64
1	A	383	GLU	N-CA-C	5.86	120.98	111.37
1	A	29	LEU	CD1-CG-CD2	-5.85	97.92	110.80
1	B	28	GLN	CG-CD-NE2	5.85	125.18	116.40
1	A	712	ASN	N-CA-C	-5.85	105.73	112.86
1	B	517	HIS	CA-CB-CG	-5.85	107.95	113.80
1	A	118	LYS	CG-CD-CE	5.84	124.73	111.30
1	A	526	HIS	N-CA-CB	5.84	119.72	110.84
1	A	212	ARG	NH1-CZ-NH2	5.84	126.89	119.30
1	A	394	SER	CA-C-N	5.84	126.18	119.93
1	A	394	SER	C-N-CA	5.84	126.18	119.93
1	B	307	GLN	O-C-N	5.84	130.39	123.27
1	B	653	LYS	N-CA-C	5.84	117.72	111.36
1	A	641	THR	CA-C-O	-5.83	114.61	121.44
1	B	699	MET	N-CA-C	5.83	117.01	109.72
1	A	563	MET	O-C-N	5.82	130.14	123.27
1	A	203	GLU	N-CA-C	-5.82	105.02	111.36
1	B	28	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	B	273	LYS	CG-CD-CE	5.82	124.68	111.30
1	A	377	TYR	N-CA-C	5.82	119.20	111.75
1	A	421	MET	N-CA-CB	5.81	120.25	110.77
1	A	473	ILE	N-CA-CB	-5.81	104.35	111.67
1	A	457	VAL	CA-C-O	-5.80	114.09	120.48
1	A	144	LYS	CA-C-N	5.80	125.74	119.76
1	A	144	LYS	C-N-CA	5.80	125.74	119.76
1	A	698	ILE	CA-C-O	5.80	127.17	120.67
1	A	315	ASN	N-CA-C	-5.80	106.21	113.28
1	A	429	VAL	CA-C-N	-5.80	110.50	121.63
1	A	429	VAL	C-N-CA	-5.80	110.50	121.63
1	B	603	TYR	O-C-N	-5.79	116.40	123.30
1	B	140	ALA	N-CA-C	5.79	117.67	111.36
1	B	201	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	B	287	PRO	N-CA-C	-5.79	101.57	110.95
1	B	703	TRP	N-CA-C	5.79	118.98	109.72
1	B	223	THR	OG1-CB-CG2	-5.78	97.73	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ARG	CA-C-O	5.78	126.67	120.08
1	A	140	ALA	O-C-N	5.78	128.74	122.15
1	A	31	THR	N-CA-CB	5.77	119.61	110.55
1	B	451	GLU	CA-C-O	5.77	128.53	121.72
1	A	286	VAL	CB-CA-C	-5.77	104.66	110.89
1	A	362	LEU	N-CA-C	-5.77	101.74	110.28
1	B	291	ARG	CA-C-O	5.76	127.62	121.28
1	A	178	GLN	CB-CA-C	-5.76	100.99	110.55
1	A	623	PRO	N-CA-CB	5.76	108.99	103.52
1	B	147	ASP	CA-CB-CG	-5.76	106.84	112.60
1	B	377	TYR	N-CA-C	5.76	119.12	111.75
1	B	519	ILE	N-CA-C	5.75	116.41	108.12
1	B	626	TRP	O-C-N	-5.75	115.59	122.15
1	B	274	LYS	CA-CB-CG	5.75	125.60	114.10
1	B	306	MET	CA-C-O	-5.75	113.19	120.20
1	B	414	ALA	CA-C-O	-5.75	114.17	120.43
1	A	688	THR	N-CA-C	-5.74	97.83	107.99
1	A	31	THR	CA-C-O	-5.73	114.02	120.32
1	B	419	VAL	N-CA-CB	-5.73	103.93	111.21
1	B	590	ASN	CA-C-N	5.73	125.83	119.87
1	B	590	ASN	C-N-CA	5.73	125.83	119.87
1	B	472	TRP	N-CA-C	-5.72	98.41	108.20
1	B	462	THR	CA-C-O	5.72	126.61	120.38
1	B	710	PRO	N-CA-CB	5.71	108.39	103.36
1	B	72	ASP	CB-CG-OD1	5.71	131.52	118.40
1	B	587	LEU	N-CA-C	5.71	118.85	109.72
1	A	10	MET	N-CA-C	5.71	117.30	111.14
1	B	640	VAL	N-CA-CB	5.70	120.43	111.99
1	B	379	LYS	N-CA-C	5.70	117.35	109.15
1	B	603	TYR	N-CA-CB	5.70	120.25	110.68
1	B	490	GLU	OE1-CD-OE2	5.69	136.55	122.90
1	B	499	THR	CA-C-O	-5.69	114.97	121.40
1	B	342	ILE	CA-C-O	-5.69	114.39	120.59
1	B	576	ALA	N-CA-C	-5.68	105.84	112.89
1	B	720	LEU	CA-C-N	-5.68	110.28	121.41
1	B	720	LEU	C-N-CA	-5.68	110.28	121.41
1	B	643	TYR	CA-C-O	-5.67	114.95	121.19
1	A	596	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	B	678	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	371	ASP	CB-CA-C	5.66	116.27	109.31
1	A	692	ARG	CG-CD-NE	-5.66	99.55	112.00
1	B	383	GLU	N-CA-C	5.66	117.92	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	GLN	CA-C-N	5.66	125.42	119.76
1	A	53	GLN	C-N-CA	5.66	125.42	119.76
1	A	671	ASN	CB-CA-C	-5.65	103.39	112.09
1	A	153	ASP	N-CA-C	-5.64	100.04	109.24
1	B	58	GLN	O-C-N	5.64	129.57	122.23
1	B	622	ALA	CA-C-N	5.64	125.31	119.56
1	B	622	ALA	C-N-CA	5.64	125.31	119.56
1	A	596	ARG	CD-NE-CZ	5.63	132.29	124.40
1	B	286	VAL	N-CA-CB	5.63	115.32	110.08
1	B	698	ILE	CA-C-O	5.63	126.98	120.67
1	B	180	ILE	CA-C-O	5.62	126.67	120.48
1	A	322	MET	CA-C-O	5.62	126.72	120.43
1	B	492	VAL	O-C-N	-5.62	116.92	122.76
1	A	359	GLU	CB-CA-C	-5.61	99.76	109.86
1	A	505	ALA	O-C-N	5.61	128.07	122.12
1	A	588	LEU	CA-C-O	5.61	127.10	120.70
1	B	671	ASN	N-CA-C	5.61	118.93	111.30
1	A	150	ARG	N-CA-C	-5.60	101.55	109.96
1	A	343	SER	N-CA-C	5.59	117.47	109.14
1	B	171	ASN	CA-CB-CG	-5.59	107.01	112.60
1	B	692	ARG	CB-CA-C	5.59	122.47	110.45
1	A	621	PHE	CA-CB-CG	-5.59	108.21	113.80
1	A	703	TRP	O-C-N	5.58	130.59	123.11
1	B	144	LYS	CA-C-N	5.58	125.53	119.78
1	B	144	LYS	C-N-CA	5.58	125.53	119.78
1	A	578	GLN	N-CA-CB	-5.57	102.76	111.56
1	A	61	VAL	CA-C-N	-5.57	115.92	123.10
1	A	61	VAL	C-N-CA	-5.57	115.92	123.10
1	A	592	ASN	OD1-CG-ND2	5.57	128.16	122.60
1	A	622	ALA	CA-C-N	5.56	125.27	119.82
1	A	622	ALA	C-N-CA	5.56	125.27	119.82
1	A	353	LYS	CA-C-O	-5.56	114.13	120.58
1	A	440	HIS	N-CA-CB	5.56	119.21	110.71
1	B	10	MET	N-CA-C	5.56	117.80	111.02
1	A	93	PRO	CB-CA-C	-5.55	104.64	111.64
1	B	398	ARG	CG-CD-NE	5.55	124.22	112.00
1	B	160	LYS	CG-CD-CE	-5.55	98.53	111.30
1	A	623	PRO	CA-C-N	-5.55	113.94	122.60
1	A	623	PRO	C-N-CA	-5.55	113.94	122.60
1	A	343	SER	CA-C-O	-5.54	115.31	121.51
1	B	172	ASN	N-CA-C	5.54	119.03	111.39
1	B	239	ASP	CB-CA-C	-5.54	98.42	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ALA	N-CA-CB	-5.53	101.70	110.06
1	B	490	GLU	CA-CB-CG	-5.53	103.03	114.10
1	B	184	HIS	CA-CB-CG	-5.53	108.27	113.80
1	A	193	ALA	CA-C-N	-5.53	113.25	120.44
1	A	193	ALA	C-N-CA	-5.53	113.25	120.44
1	A	207	ALA	N-CA-CB	-5.53	102.05	110.07
1	A	699	MET	CB-CA-C	-5.52	100.67	109.51
1	A	85	GLN	N-CA-CB	-5.52	102.46	110.47
1	B	417	THR	CA-C-O	-5.52	112.89	119.35
1	B	374	ILE	N-CA-C	5.52	116.91	110.62
1	B	304	LYS	CA-C-N	5.51	125.46	119.78
1	B	304	LYS	C-N-CA	5.51	125.46	119.78
1	A	433	TYR	O-C-N	-5.50	116.61	123.04
1	A	476	GLU	CA-C-O	-5.50	114.72	120.55
1	B	377	TYR	N-CA-CB	-5.50	101.45	110.14
1	A	579	LYS	O-C-N	-5.50	116.37	122.86
1	B	654	TYR	CA-C-N	5.50	125.59	119.87
1	B	654	TYR	C-N-CA	5.50	125.59	119.87
1	A	607	PRO	CA-C-N	-5.49	115.04	122.95
1	A	607	PRO	C-N-CA	-5.49	115.04	122.95
1	B	526	HIS	N-CA-CB	5.49	119.33	110.65
1	B	385	GLY	CA-C-O	-5.49	115.07	121.00
1	A	303	VAL	N-CA-CB	-5.49	101.66	111.92
1	B	359	GLU	N-CA-CB	-5.49	101.28	110.99
1	B	61	VAL	N-CA-C	-5.48	102.51	109.58
1	B	568	TYR	O-C-N	-5.48	117.13	123.33
1	A	527	ILE	CA-C-O	-5.47	114.46	120.48
1	B	492	VAL	CA-C-N	5.47	130.27	122.72
1	B	492	VAL	C-N-CA	5.47	130.27	122.72
1	A	25	ASP	CB-CG-OD1	5.45	130.94	118.40
1	A	539	GLU	N-CA-CB	-5.45	102.09	110.16
1	B	94	HIS	CB-CA-C	5.45	118.66	109.67
1	B	700	PRO	N-CD-CG	-5.45	95.03	103.20
1	B	280	GLU	OE1-CD-OE2	5.44	135.96	122.90
1	A	308	ILE	CA-C-N	-5.44	113.60	122.57
1	A	308	ILE	C-N-CA	-5.44	113.60	122.57
1	A	241	ARG	CA-C-O	-5.44	115.11	120.98
1	B	336	SER	N-CA-C	5.44	119.01	112.38
1	B	191	ASP	N-CA-CB	5.43	118.11	110.12
1	B	654	TYR	O-C-N	-5.43	116.50	121.34
1	A	283	VAL	CB-CA-C	-5.43	104.18	110.91
1	B	545	ALA	O-C-N	5.42	129.69	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	A	189	LEU	O-C-N	5.41	127.72	122.09
1	A	642	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	A	194	SER	CA-C-O	-5.41	115.14	120.82
1	B	662	THR	N-CA-C	-5.41	105.99	112.59
1	A	563	MET	CA-C-N	-5.40	113.39	123.01
1	A	563	MET	C-N-CA	-5.40	113.39	123.01
1	A	557	GLY	CA-C-N	5.40	125.22	119.28
1	A	557	GLY	C-N-CA	5.40	125.22	119.28
1	B	130	PRO	O-C-N	5.40	127.83	121.46
1	A	519	ILE	N-CA-C	5.40	115.76	107.77
1	B	610	GLY	N-CA-C	5.40	117.53	112.08
1	A	175	LEU	CA-C-O	-5.39	113.31	119.41
1	A	634	MET	N-CA-C	5.39	119.12	112.54
1	B	586	ARG	N-CA-CB	5.39	119.06	110.65
1	A	633	PHE	N-CA-C	5.39	117.91	111.71
1	B	263	ASN	CB-CG-ND2	5.39	124.48	116.40
1	A	220	VAL	O-C-N	5.38	128.86	122.83
1	B	526	HIS	ND1-CE1-NE2	-5.38	103.02	108.40
1	A	298	ARG	N-CA-C	5.38	117.59	109.41
1	B	101	ALA	N-CA-C	-5.38	105.41	111.28
1	B	419	VAL	CA-C-N	5.38	125.30	119.76
1	B	419	VAL	C-N-CA	5.38	125.30	119.76
1	B	588	LEU	N-CA-CB	5.38	119.26	110.39
1	A	207	ALA	CA-C-O	5.38	126.24	120.70
1	B	457	VAL	N-CA-C	-5.38	100.01	107.80
1	B	382	LEU	N-CA-C	-5.37	99.21	108.56
1	B	515	ILE	O-C-N	-5.37	116.83	122.20
1	B	588	LEU	N-CA-C	-5.37	97.76	107.75
1	A	254	GLY	N-CA-C	-5.37	106.63	114.90
1	B	516	ASP	OD1-CG-OD2	-5.37	110.02	122.90
1	A	498	LYS	N-CA-C	-5.37	106.86	113.41
1	A	36	GLY	CA-C-O	5.37	127.73	119.15
1	B	144	LYS	CA-C-O	5.36	124.53	119.76
1	B	617	LYS	CG-CD-CE	-5.36	98.96	111.30
1	A	455	LEU	CA-C-N	-5.36	114.64	122.68
1	A	455	LEU	C-N-CA	-5.36	114.64	122.68
1	B	66	ASN	O-C-N	5.36	128.72	121.97
1	A	139	PHE	O-C-N	-5.35	116.31	122.09
1	A	155	ILE	O-C-N	5.35	130.04	122.97
1	B	439	LYS	CD-CE-NZ	5.35	129.02	111.90
1	B	653	LYS	CA-C-O	-5.34	114.75	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	703	TRP	O-C-N	5.34	130.14	123.19
1	B	262	GLU	O-C-N	5.34	129.40	122.89
1	A	301	PRO	N-CA-CB	5.34	108.30	103.34
1	B	143	ASN	CB-CA-C	-5.33	102.35	111.26
1	B	491	ALA	N-CA-C	-5.32	99.84	108.41
1	B	440	HIS	CA-CB-CG	-5.32	108.48	113.80
1	A	16	GLU	N-CA-C	-5.32	105.56	111.36
1	A	517	HIS	CA-C-O	-5.32	114.85	120.92
1	A	613	HIS	CA-CB-CG	5.32	119.12	113.80
1	B	238	GLN	N-CA-C	5.32	118.55	111.75
1	A	67	LYS	N-CA-C	-5.31	101.22	109.72
1	A	376	TRP	N-CA-CB	-5.31	103.39	111.15
1	A	644	HIS	O-C-N	-5.31	115.90	122.16
1	B	618	GLY	N-CA-C	-5.30	103.35	110.56
1	A	76	ASN	CA-CB-CG	-5.30	107.30	112.60
1	B	179	PRO	O-C-N	-5.29	116.63	123.03
1	B	626	TRP	CA-C-O	5.28	126.02	120.42
1	A	490	GLU	N-CA-C	5.28	117.95	110.50
1	A	639	TRP	CA-C-O	-5.28	114.27	120.60
1	B	174	LEU	CA-C-O	-5.28	114.37	120.49
1	A	173	LYS	O-C-N	5.27	129.38	123.27
1	A	130	PRO	CA-CB-CG	-5.26	94.50	104.50
1	B	231	ASP	O-C-N	-5.26	115.59	122.59
1	B	671	ASN	CA-C-N	5.26	130.55	120.97
1	B	671	ASN	C-N-CA	5.26	130.55	120.97
1	B	72	ASP	OD1-CG-OD2	-5.26	110.28	122.90
1	B	201	ASN	CB-CG-ND2	5.26	124.29	116.40
1	A	524	HIS	CA-CB-CG	-5.25	108.55	113.80
1	B	212	ARG	O-C-N	5.25	129.04	122.22
1	A	677	THR	O-C-N	-5.25	115.81	122.78
1	B	247	SER	N-CA-C	5.25	118.14	109.85
1	A	84	ASP	N-CA-C	-5.24	99.97	108.41
1	B	16	GLU	CA-CB-CG	5.24	124.58	114.10
1	B	11	ASP	N-CA-C	5.24	117.41	111.02
1	B	320	GLY	N-CA-C	-5.24	100.77	113.18
1	A	284	VAL	CA-C-O	5.23	124.48	119.98
1	B	420	PRO	O-C-N	-5.23	116.70	123.03
1	A	98	ALA	CA-C-N	-5.23	113.29	120.71
1	A	98	ALA	C-N-CA	-5.23	113.29	120.71
1	A	538	GLY	N-CA-C	-5.23	104.74	110.96
1	B	688	THR	N-CA-C	-5.22	98.75	107.99
1	A	622	ALA	CB-CA-C	5.22	117.67	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	THR	OG1-CB-CG2	-5.22	98.86	109.30
1	A	606	ILE	CA-C-N	5.22	124.88	119.56
1	A	606	ILE	C-N-CA	5.22	124.88	119.56
1	B	132	ASP	CA-C-O	5.22	126.81	120.81
1	A	39	VAL	N-CA-C	5.22	116.09	108.53
1	A	132	ASP	CA-C-N	5.22	127.58	120.54
1	A	132	ASP	C-N-CA	5.22	127.58	120.54
1	A	394	SER	CB-CA-C	-5.22	103.90	109.85
1	B	628	TYR	O-C-N	5.22	129.66	122.46
1	B	617	LYS	CA-C-N	5.21	128.96	121.56
1	B	617	LYS	C-N-CA	5.21	128.96	121.56
1	A	689	HIS	ND1-CG-CD2	-5.21	100.89	106.10
1	B	136	VAL	O-C-N	5.21	126.92	121.87
1	B	376	TRP	CB-CA-C	-5.21	102.44	109.16
1	B	381	TYR	O-C-N	-5.21	116.08	123.01
1	A	413	ILE	CB-CA-C	-5.21	103.31	110.91
1	B	629	HIS	O-C-N	5.21	129.33	122.30
1	B	489	ILE	O-C-N	-5.21	117.72	123.18
1	B	109	GLU	CB-CG-CD	5.20	121.44	112.60
1	B	110	ILE	N-CA-CB	5.20	116.28	110.51
1	B	129	LEU	CB-CA-C	5.20	116.82	109.08
1	B	510	ARG	NE-CZ-NH1	-5.20	116.30	121.50
1	B	564	GLN	CA-C-N	-5.20	115.22	122.71
1	B	564	GLN	C-N-CA	-5.20	115.22	122.71
1	A	657	ARG	CA-CB-CG	-5.20	103.71	114.10
1	B	251	VAL	CG1-CB-CG2	5.20	122.23	110.80
1	A	148	GLN	CA-C-O	5.20	126.59	120.41
1	A	244	LYS	N-CA-C	-5.19	101.81	110.17
1	A	515	ILE	O-C-N	5.19	128.14	122.12
1	A	615	VAL	CB-CA-C	-5.18	104.11	111.21
1	B	494	GLY	O-C-N	5.18	128.25	122.96
1	A	596	ARG	NH1-CZ-NH2	-5.17	112.57	119.30
1	B	526	HIS	N-CA-C	-5.17	98.97	108.02
1	A	374	ILE	CA-CB-CG2	5.17	119.28	110.50
1	A	63	MET	CA-C-O	5.17	126.11	120.58
1	B	550	VAL	N-CA-CB	-5.16	105.17	111.21
1	B	583	GLY	N-CA-C	-5.16	108.26	114.66
1	A	374	ILE	CA-C-O	-5.16	115.90	121.27
1	A	521	GLY	O-C-N	-5.16	116.00	122.70
1	A	294	ASP	O-C-N	-5.16	115.74	122.39
1	B	558	PRO	N-CA-C	5.16	120.61	113.65
1	A	144	LYS	CA-C-O	5.15	124.34	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	ARG	CA-C-O	5.15	126.04	120.43
1	B	697	PRO	N-CA-C	5.15	125.49	112.10
1	B	27	ALA	O-C-N	5.15	129.72	122.41
1	B	584	THR	OG1-CB-CG2	5.15	119.60	109.30
1	A	602	SER	N-CA-CB	-5.15	102.61	111.21
1	A	675	ASP	CA-CB-CG	-5.15	107.45	112.60
1	A	446	PRO	N-CA-CB	5.14	107.89	103.31
1	B	602	SER	N-CA-C	5.14	116.62	108.96
1	A	417	THR	N-CA-CB	5.14	118.10	110.49
1	B	442	GLU	N-CA-C	-5.14	102.67	110.28
1	A	526	HIS	CA-C-O	-5.14	114.78	120.33
1	B	613	HIS	ND1-CE1-NE2	-5.13	103.27	108.40
1	B	245	VAL	O-C-N	5.13	128.52	123.18
1	B	306	MET	CB-CA-C	-5.13	102.24	110.14
1	A	11	ASP	O-C-N	5.12	127.35	122.07
1	A	603	TYR	CA-C-O	5.12	126.01	120.32
1	A	526	HIS	CA-C-N	-5.12	116.27	123.13
1	A	526	HIS	C-N-CA	-5.12	116.27	123.13
1	A	445	GLN	CB-CA-C	-5.12	101.44	109.22
1	A	427	ILE	CA-C-N	-5.11	115.52	122.93
1	A	427	ILE	C-N-CA	-5.11	115.52	122.93
1	A	549	VAL	CB-CA-C	-5.11	101.66	110.30
1	A	309	ILE	CA-C-N	5.11	128.16	122.74
1	A	309	ILE	C-N-CA	5.11	128.16	122.74
1	A	204	GLU	CB-CG-CD	5.11	121.29	112.60
1	A	458	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	A	285	PRO	N-CA-CB	5.11	107.86	103.31
1	B	423	ILE	CB-CA-C	-5.10	105.25	110.71
1	A	165	ALA	CB-CA-C	-5.10	99.77	109.66
1	A	279	GLU	OE1-CD-OE2	-5.10	110.67	122.90
1	A	547	ASP	CA-C-O	5.09	123.64	119.36
1	B	17	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	661	ASP	OD1-CG-OD2	-5.09	110.67	122.90
1	B	599	ASN	CB-CG-ND2	-5.09	108.76	116.40
1	B	157	LEU	CA-C-O	-5.09	115.06	120.40
1	B	526	HIS	CG-CD2-NE2	-5.09	102.11	107.20
1	B	100	THR	CA-C-N	5.08	127.09	120.28
1	B	100	THR	C-N-CA	5.08	127.09	120.28
1	A	199	ILE	CA-CB-CG2	5.08	119.14	110.50
1	B	712	ASN	N-CA-C	-5.08	106.66	112.86
1	A	171	ASN	CB-CG-ND2	5.08	124.02	116.40
1	A	615	VAL	N-CA-C	5.08	116.59	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	PHE	N-CA-CB	5.07	117.37	110.01
1	B	132	ASP	CA-CB-CG	-5.07	107.53	112.60
1	B	613	HIS	N-CA-C	-5.07	101.30	109.82
1	B	307	GLN	CA-C-N	-5.07	116.53	123.12
1	B	307	GLN	C-N-CA	-5.07	116.53	123.12
1	A	471	ASP	O-C-N	-5.07	117.27	123.30
1	B	718	PRO	N-CD-CG	-5.07	95.59	103.20
1	A	183	ALA	N-CA-C	5.07	117.56	109.96
1	A	91	LYS	CG-CD-CE	5.06	122.95	111.30
1	B	524	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	B	451	GLU	O-C-N	-5.06	117.27	122.94
1	A	248	TYR	CA-C-N	-5.06	115.74	122.72
1	A	248	TYR	C-N-CA	-5.06	115.74	122.72
1	B	590	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	479	THR	CA-CB-OG1	-5.05	102.03	109.60
1	A	233	LYS	CA-C-N	-5.05	114.21	122.54
1	A	233	LYS	C-N-CA	-5.05	114.21	122.54
1	A	194	SER	O-C-N	5.04	127.26	122.07
1	B	268	VAL	CA-CB-CG2	5.04	118.97	110.40
1	A	193	ALA	CA-C-O	-5.04	114.65	120.24
1	B	16	GLU	N-CA-CB	5.04	117.32	110.01
1	B	270	LEU	O-C-N	-5.04	115.68	122.43
1	A	199	ILE	O-C-N	5.03	127.13	121.90
1	A	299	VAL	CA-C-O	5.02	124.69	120.22
1	B	453	ARG	CA-C-O	-5.02	115.28	120.70
1	B	394	SER	CA-CB-OG	-5.02	101.06	111.10
1	A	676	ASN	CB-CG-ND2	5.02	123.92	116.40
1	B	106	GLN	OE1-CD-NE2	5.01	127.61	122.60
1	B	382	LEU	CB-CA-C	5.01	119.84	112.03
1	B	483	ASP	OD1-CG-OD2	-5.00	110.89	122.90
1	A	644	HIS	CB-CA-C	5.00	116.16	109.65
1	B	549	VAL	CA-C-O	-5.00	116.68	121.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	ASP	Mainchain

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	5666	0	5542	181	0
1	B	5690	0	5563	169	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	B	6	0	7	6	0
5	A	767	0	0	21	0
5	B	640	0	0	14	0
All	All	12775	0	11112	334	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 15.

All (334) 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)
1:B:322:MET:HG3	5:B:1792:HOH:O	1.60	1.00
1:B:326:ARG:HH11	1:B:476:GLU:CD	1.74	0.95
1:B:203:GLU:CD	1:B:203:GLU:H	1.74	0.94
1:B:572:ASN:HD22	1:B:671:ASN:HD21	1.14	0.93
1:B:366:ILE:HD11	1:B:627:ILE:HD11	1.50	0.93
1:A:382:LEU:HD13	1:A:655:PRO:HB2	1.50	0.93
1:A:304:LYS:H	1:B:315:ASN:HD21	1.19	0.90
1:A:35:ASP:OD1	1:A:398:ARG:NH1	2.06	0.88
1:B:120:ASN:HA	5:B:1818:HOH:O	1.73	0.87
1:A:223:THR:HG23	1:A:225:LEU:HD21	1.56	0.86
1:A:527:ILE:CD1	1:A:634:MET:HE2	2.06	0.85
1:B:580:PHE:H	1:B:637:GLN:HE21	1.21	0.84
1:A:465:ASN:HD22	1:A:465:ASN:H	1.25	0.84
1:B:382:LEU:HD23	1:B:651:GLU:HG3	1.58	0.84
1:B:572:ASN:ND2	1:B:671:ASN:HD21	1.77	0.83
1:A:7:MET:HE1	1:A:59:VAL:HG11	1.62	0.81
1:A:527:ILE:HD12	1:A:634:MET:HE2	1.61	0.81
1:A:227:VAL:HG12	1:A:244:LYS:HG3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.62	0.81
1:B:237:LYS:HD3	1:B:240:ALA:HB2	1.63	0.81
1:A:210:LYS:HE2	1:A:210:LYS:HA	1.63	0.80
1:B:94:HIS:HD2	1:B:96:LEU:H	1.25	0.80
4:B:1450:GOL:O1	5:B:1465:HOH:O	1.99	0.79
1:A:572:ASN:ND2	1:A:575:ASP:H	1.80	0.78
1:A:227:VAL:CG1	1:A:244:LYS:HG3	2.13	0.77
1:A:574:GLN:H	1:A:671:ASN:ND2	1.82	0.77
1:A:71:SER:OG	1:A:73:THR:HG22	1.85	0.77
1:A:28:GLN:HG3	5:A:1176:HOH:O	1.84	0.76
1:A:288:MET:HE2	1:A:288:MET:HA	1.66	0.76
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.66	0.76
1:A:539:GLU:CD	5:A:1201:HOH:O	2.29	0.74
1:A:203:GLU:CD	1:A:203:GLU:H	1.93	0.74
1:B:209:VAL:HG13	1:B:214:ILE:HB	1.69	0.74
1:B:61:VAL:HG22	1:B:70:VAL:HG12	1.69	0.74
1:B:326:ARG:NH1	1:B:476:GLU:CD	2.46	0.73
1:A:8:VAL:HG22	1:A:9:PRO:HD2	1.68	0.73
1:B:221:ILE:CD1	1:B:250:ASP:HB2	2.19	0.73
1:B:574:GLN:H	1:B:671:ASN:ND2	1.84	0.73
1:A:272:GLN:HE21	1:A:274:LYS:HD3	1.53	0.73
1:B:38:TYR:H	1:B:51:ASN:ND2	1.86	0.73
1:B:578:GLN:HA	1:B:636:LYS:HD2	1.71	0.72
1:A:580:PHE:H	1:A:637:GLN:HE21	1.37	0.72
1:A:132:ASP:HB3	5:A:1534:HOH:O	1.88	0.72
1:B:38:TYR:H	1:B:51:ASN:HD21	1.37	0.71
1:A:498:LYS:O	1:A:517:HIS:HD2	1.73	0.71
1:A:315:ASN:HD21	1:B:304:LYS:H	1.37	0.71
1:A:527:ILE:HD12	1:A:634:MET:CE	2.20	0.71
1:B:218:LYS:H	1:B:218:LYS:HD2	1.56	0.71
1:A:553:ASN:ND2	1:A:555:ALA:H	1.89	0.71
1:B:203:GLU:CD	1:B:203:GLU:N	2.49	0.71
1:B:227:VAL:HG12	1:B:244:LYS:HG3	1.72	0.71
1:A:35:ASP:OD2	5:A:1084:HOH:O	2.09	0.70
1:A:73:THR:HG23	1:A:77:ASP:OD2	1.92	0.69
1:A:286:VAL:HG12	1:A:288:MET:HE3	1.73	0.69
1:A:366:ILE:HG21	1:A:634:MET:HE3	1.75	0.69
1:B:382:LEU:HD22	1:B:655:PRO:HB2	1.75	0.69
1:B:536:VAL:H	1:B:541:ASN:HD21	1.40	0.68
1:A:670:ASP:HB2	5:A:1547:HOH:O	1.94	0.67
1:A:219:LYS:HD3	5:A:1183:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:HIS:CE1	1:B:596:ARG:HH11	2.12	0.67
1:A:536:VAL:H	1:A:541:ASN:HD21	1.42	0.67
4:B:1450:GOL:C1	5:B:1465:HOH:O	2.42	0.67
1:B:580:PHE:H	1:B:637:GLN:NE2	1.90	0.67
1:A:286:VAL:CG1	1:A:288:MET:HE3	2.25	0.67
1:A:368:PRO:HG3	1:A:634:MET:HE1	1.77	0.67
1:B:632:SER:OG	1:B:661:ASP:OD2	2.13	0.66
1:B:225:LEU:HD23	4:B:1450:GOL:H31	1.76	0.66
1:A:465:ASN:H	1:A:465:ASN:ND2	1.88	0.66
1:B:553:ASN:HD21	1:B:555:ALA:HB3	1.59	0.66
1:B:8:VAL:CG2	1:B:9:PRO:HD2	2.26	0.66
1:A:358:TYR:CD2	1:A:359:GLU:HG3	2.32	0.65
1:B:525:GLN:HE22	1:B:620:GLN:H	1.42	0.65
1:A:203:GLU:OE2	1:A:204:GLU:HG3	1.96	0.65
1:B:381:TYR:CE1	4:B:1450:GOL:H11	2.32	0.65
1:A:38:TYR:H	1:A:51:ASN:ND2	1.94	0.65
1:B:231:ASP:HB2	1:B:626:TRP:CZ2	2.32	0.64
1:A:692:ARG:HG3	1:A:694:GLU:OE1	1.97	0.64
1:B:366:ILE:CD1	1:B:627:ILE:HD11	2.26	0.64
1:B:525:GLN:NE2	1:B:620:GLN:H	1.95	0.64
1:A:379:LYS:HG2	1:A:381:TYR:CZ	2.33	0.64
1:A:366:ILE:HD11	1:A:627:ILE:HD11	1.79	0.63
1:A:644:HIS:HB3	5:A:1278:HOH:O	1.98	0.63
1:A:322:MET:HE1	5:A:1147:HOH:O	1.99	0.63
1:A:431:GLU:HB3	1:B:306:MET:HE1	1.81	0.63
1:B:498:LYS:O	1:B:517:HIS:HD2	1.82	0.63
1:A:241:ARG:HG2	1:A:270:LEU:HD12	1.80	0.63
1:B:12:LYS:O	1:B:16:GLU:HG2	1.98	0.62
1:A:574:GLN:HG2	1:A:671:ASN:ND2	2.15	0.62
1:B:574:GLN:HB2	1:B:671:ASN:ND2	2.15	0.62
1:A:572:ASN:HD22	1:A:575:ASP:H	1.45	0.62
1:A:43:PRO:HB3	1:A:63:MET:HG2	1.82	0.62
1:A:38:TYR:H	1:A:51:ASN:HD21	1.48	0.61
1:B:216:ASP:HB3	1:B:219:LYS:HD2	1.83	0.61
1:A:210:LYS:HE2	1:A:210:LYS:CA	2.27	0.61
1:A:249:LEU:HD23	1:A:288:MET:HE1	1.83	0.61
1:A:279:GLU:OE1	1:A:374:ILE:HD11	2.01	0.61
1:B:540:ASN:HB3	1:B:676:ASN:ND2	2.15	0.61
1:B:381:TYR:CD1	4:B:1450:GOL:H11	2.37	0.60
1:B:326:ARG:NH1	1:B:476:GLU:OE1	2.33	0.60
1:A:574:GLN:H	1:A:671:ASN:HD22	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:HH12	1:B:303:VAL:HG22	1.66	0.59
1:B:214:ILE:HD11	1:B:286:VAL:HG21	1.83	0.59
1:B:620:GLN:HG3	5:B:1637:HOH:O	2.02	0.59
1:B:592:ASN:HD21	1:B:676:ASN:HD21	1.51	0.59
1:A:366:ILE:CD1	1:A:627:ILE:HD11	2.32	0.59
1:A:629:HIS:HB2	5:A:1184:HOH:O	2.01	0.59
1:A:286:VAL:HG12	1:A:288:MET:CE	2.33	0.58
1:A:443:MET:HE1	1:B:392:LEU:HD22	1.84	0.58
1:A:223:THR:HG21	5:A:858:HOH:O	2.03	0.58
1:B:366:ILE:HG21	1:B:634:MET:HE3	1.85	0.58
1:A:366:ILE:CG2	1:A:634:MET:HE3	2.33	0.58
1:B:218:LYS:HD2	1:B:218:LYS:N	2.19	0.57
1:A:525:GLN:HE22	1:A:620:GLN:H	1.50	0.57
1:B:490:GLU:HG3	1:B:699:MET:SD	2.44	0.57
1:A:594:GLU:OE1	1:B:501:HIS:HE1	1.87	0.57
1:B:441:GLN:OE1	1:B:447:ASN:HB2	2.04	0.57
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.51	0.57
1:A:34:LYS:O	1:A:35:ASP:C	2.48	0.57
1:A:29:LEU:HD13	1:A:30:PHE:N	2.20	0.57
1:B:291:ARG:NH1	1:B:516:ASP:OD2	2.38	0.57
1:A:7:MET:HE2	1:A:71:SER:HA	1.86	0.56
1:A:639:TRP:HB2	1:A:682:TRP:HB2	1.88	0.56
1:B:380:ALA:CB	1:B:627:ILE:HD12	2.36	0.56
1:B:216:ASP:OD1	1:B:216:ASP:C	2.49	0.56
1:A:286:VAL:CG1	1:A:288:MET:CE	2.83	0.56
1:A:540:ASN:HB3	1:A:676:ASN:ND2	2.21	0.56
1:B:366:ILE:HD12	1:B:631:LEU:HD13	1.88	0.56
1:B:445:GLN:HB3	1:B:446:PRO:HD2	1.88	0.56
1:A:525:GLN:NE2	1:A:620:GLN:H	2.04	0.56
1:A:532:LEU:HD11	1:A:683:MET:HE2	1.86	0.55
1:B:29:LEU:HD21	1:B:40:LYS:HD2	1.88	0.55
1:A:578:GLN:HA	1:A:636:LYS:HD2	1.88	0.55
1:A:366:ILE:HG13	1:A:367:VAL:N	2.20	0.55
1:B:45:ALA:O	1:B:60:PRO:HB3	2.07	0.55
1:B:160:LYS:HD3	1:B:271:GLU:OE1	2.07	0.55
1:B:717:THR:HB	1:B:720:LEU:HG	1.89	0.55
1:A:224:PRO:O	1:A:224:PRO:HG2	2.06	0.54
1:A:477:ASN:C	1:A:477:ASN:HD22	2.15	0.54
1:A:574:GLN:HG2	1:A:671:ASN:CG	2.32	0.54
1:A:443:MET:HE1	1:B:392:LEU:CD2	2.37	0.54
1:A:196:GLN:HE22	1:A:222:THR:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:TYR:CE1	1:B:558:PRO:HG2	2.43	0.53
1:B:53:GLN:OE1	5:B:2011:HOH:O	2.19	0.53
1:B:262:GLU:O	1:B:263:ASN:HB2	2.08	0.53
1:A:29:LEU:HD13	1:A:30:PHE:O	2.09	0.53
1:B:120:ASN:CA	5:B:1818:HOH:O	2.40	0.53
1:B:546:MET:HE3	1:B:587:LEU:CD1	2.39	0.53
1:A:552:PRO:HD2	5:A:1352:HOH:O	2.08	0.52
1:A:325:TRP:O	1:A:326:ARG:HB2	2.09	0.52
1:A:489:ILE:C	1:A:699:MET:HE2	2.34	0.52
1:A:580:PHE:H	1:A:637:GLN:NE2	2.06	0.52
1:A:379:LYS:HG2	1:A:381:TYR:OH	2.10	0.51
1:B:95:PRO:HB3	1:B:146:VAL:HG21	1.93	0.51
1:A:370:GLY:HA2	1:B:559:ARG:HH22	1.76	0.51
1:A:366:ILE:HD13	1:A:631:LEU:CD1	2.41	0.50
1:B:227:VAL:CG1	1:B:244:LYS:HG3	2.40	0.50
1:A:203:GLU:CD	1:A:203:GLU:N	2.66	0.50
1:A:596:ARG:NH1	5:A:1541:HOH:O	2.30	0.50
1:B:574:GLN:HB2	1:B:671:ASN:CG	2.36	0.50
1:A:572:ASN:CG	1:A:671:ASN:HD21	2.20	0.50
1:A:117:PHE:CZ	1:A:121:THR:HB	2.47	0.49
1:A:559:ARG:HD2	1:B:625:GLU:OE1	2.12	0.49
1:A:608:TYR:HE2	1:B:608:TYR:HE2	1.60	0.49
1:B:580:PHE:N	1:B:637:GLN:HE21	1.99	0.49
1:B:129:LEU:CD1	1:B:130:PRO:HD2	2.42	0.49
1:B:488:GLY:O	1:B:699:MET:HG3	2.13	0.49
1:B:619:ALA:HB2	1:B:634:MET:HB2	1.94	0.49
1:B:621:PHE:CZ	1:B:627:ILE:HG21	2.48	0.49
1:A:77:ASP:O	1:A:81:SER:HB3	2.12	0.49
1:A:223:THR:HG22	1:A:246:ILE:HB	1.95	0.49
1:A:527:ILE:HD13	1:A:634:MET:HE2	1.93	0.49
1:B:40:LYS:HE2	5:B:1864:HOH:O	2.13	0.49
1:B:307:GLN:HB3	5:B:1730:HOH:O	2.12	0.49
1:B:380:ALA:HB1	1:B:627:ILE:HD12	1.94	0.49
1:A:237:LYS:HG2	1:A:239:ASP:H	1.78	0.48
1:B:477:ASN:HD22	1:B:477:ASN:C	2.20	0.48
1:A:441:GLN:OE1	1:A:447:ASN:HB2	2.13	0.48
1:B:578:GLN:CA	1:B:636:LYS:HD2	2.42	0.48
1:A:65:ASP:O	1:A:66:ASN:HB2	2.14	0.48
1:A:549:VAL:HA	5:A:1306:HOH:O	2.13	0.48
1:A:227:VAL:HG11	1:A:244:LYS:HG3	1.91	0.48
1:B:380:ALA:HB1	1:B:627:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:LEU:HD21	1:A:682:TRP:CD2	2.48	0.48
1:B:148:GLN:HA	1:B:149:PRO:HD3	1.75	0.48
1:A:131:PRO:HB3	1:A:148:GLN:NE2	2.29	0.48
1:A:574:GLN:CG	1:A:671:ASN:CG	2.87	0.48
1:A:588:LEU:HB2	1:A:605:ILE:HD11	1.95	0.48
1:A:32:LEU:HB2	1:A:39:VAL:HB	1.96	0.47
1:B:574:GLN:H	1:B:671:ASN:HD22	1.59	0.47
1:B:272:GLN:HE21	1:B:274:LYS:CD	2.27	0.47
1:A:272:GLN:NE2	1:A:274:LYS:HD3	2.26	0.47
1:B:61:VAL:HG22	1:B:70:VAL:CG1	2.42	0.47
1:B:546:MET:HE3	1:B:587:LEU:HD11	1.96	0.47
1:A:147:ASP:HB2	5:A:1171:HOH:O	2.14	0.47
1:B:214:ILE:HD12	1:B:214:ILE:N	2.30	0.47
1:A:12:LYS:O	1:A:16:GLU:HG3	2.14	0.47
1:A:181:LYS:HG2	1:A:182:ASP:OD2	2.15	0.47
1:B:7:MET:HE3	1:B:7:MET:HB3	1.74	0.47
1:B:553:ASN:ND2	1:B:555:ALA:H	2.13	0.47
1:A:28:GLN:CD	5:A:1176:HOH:O	2.57	0.47
1:A:281:GLY:O	1:A:282:PRO:C	2.58	0.47
1:A:324:HIS:HD2	1:A:329:ASP:OD1	1.97	0.47
1:A:574:GLN:HB3	5:A:1562:HOH:O	2.15	0.47
1:B:93:PRO:HG2	5:B:1921:HOH:O	2.15	0.47
1:B:725:LYS:O	1:B:726:ASP:CB	2.63	0.47
1:A:43:PRO:HD2	5:A:1236:HOH:O	2.13	0.47
1:A:209:VAL:HG13	1:A:214:ILE:HB	1.96	0.47
1:A:214:ILE:HD12	1:A:214:ILE:H	1.80	0.47
1:A:310:GLU:CD	1:B:306:MET:HE2	2.40	0.47
1:A:331:HIS:HE1	1:A:333:SER:HB3	1.79	0.47
1:A:465:ASN:ND2	1:A:465:ASN:N	2.60	0.47
1:B:669:LYS:HA	1:B:669:LYS:CE	2.45	0.46
1:B:382:LEU:CD2	1:B:655:PRO:HB2	2.45	0.46
1:A:498:LYS:NZ	1:A:498:LYS:HB3	2.31	0.46
1:A:223:THR:HG23	1:A:225:LEU:CD2	2.39	0.46
1:B:445:GLN:HB3	1:B:446:PRO:CD	2.44	0.46
1:A:8:VAL:CG2	1:A:9:PRO:HD2	2.41	0.46
1:A:381:TYR:HE1	5:A:1546:HOH:O	1.98	0.46
1:B:51:ASN:N	1:B:51:ASN:HD22	2.14	0.46
1:B:181:LYS:HE2	5:B:1989:HOH:O	2.16	0.46
1:B:525:GLN:HE22	1:B:619:ALA:HA	1.80	0.46
1:A:331:HIS:CE1	1:A:333:SER:HB3	2.50	0.46
1:A:366:ILE:HD11	1:A:380:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:HD12	1:A:214:ILE:N	2.30	0.46
1:A:227:VAL:HG12	1:A:244:LYS:CG	2.41	0.46
1:A:595:ASN:ND2	1:A:599:ASN:H	2.14	0.46
1:A:28:GLN:CG	5:A:1176:HOH:O	2.54	0.45
1:A:156:MET:HE3	1:A:156:MET:HB2	1.82	0.45
1:A:348:ASN:HD22	1:A:348:ASN:C	2.24	0.45
1:B:118:LYS:HE2	1:B:118:LYS:HB3	1.84	0.45
1:B:699:MET:HA	1:B:700:PRO:HD3	1.70	0.45
1:A:517:HIS:CE1	1:B:596:ARG:NH1	2.83	0.45
1:B:129:LEU:HD12	1:B:130:PRO:HD2	1.97	0.45
1:B:196:GLN:HE22	1:B:222:THR:H	1.63	0.45
1:A:38:TYR:N	1:A:51:ASN:HD21	2.11	0.45
1:A:224:PRO:O	1:A:224:PRO:CG	2.65	0.45
1:A:366:ILE:HD13	1:A:631:LEU:HD12	1.98	0.45
1:B:38:TYR:N	1:B:51:ASN:HD21	2.11	0.45
1:B:97:ASN:ND2	1:B:331:HIS:NE2	2.64	0.45
1:A:477:ASN:HD22	1:A:479:THR:H	1.65	0.45
1:A:485:GLY:HA2	1:A:702:GLU:O	2.16	0.45
1:B:272:GLN:HE21	1:B:274:LYS:HG2	1.81	0.45
1:A:348:ASN:HD21	1:A:351:GLY:CA	2.30	0.45
1:B:626:TRP:O	1:B:627:ILE:C	2.56	0.45
1:A:574:GLN:CG	1:A:671:ASN:ND2	2.80	0.45
1:B:626:TRP:O	1:B:629:HIS:N	2.48	0.45
1:A:382:LEU:HD22	1:A:651:GLU:HG3	1.98	0.45
1:B:209:VAL:CG1	1:B:214:ILE:HB	2.44	0.45
1:A:369:TYR:CD2	1:A:524:HIS:HB3	2.52	0.44
1:B:181:LYS:CD	1:B:181:LYS:H	2.29	0.44
1:A:371:ASP:OD1	1:A:371:ASP:C	2.59	0.44
1:B:259:HIS:HE1	1:B:289:THR:O	2.01	0.44
1:B:402:ALA:HB1	1:B:403:PRO:HD2	2.00	0.44
1:B:516:ASP:HB3	1:B:519:ILE:HB	1.98	0.44
1:A:64:LYS:O	1:A:66:ASN:N	2.44	0.44
1:A:620:GLN:HB2	1:B:563:MET:HE2	1.99	0.44
1:B:229:TYR:HB3	1:B:630:ARG:HD2	1.98	0.44
1:B:619:ALA:HB2	1:B:634:MET:HE2	1.99	0.44
1:B:11:ASP:O	1:B:15:LYS:HD3	2.18	0.44
1:B:653:LYS:HE2	1:B:654:TYR:OH	2.18	0.44
1:A:465:ASN:HD22	1:A:465:ASN:N	2.04	0.43
1:B:238:GLN:HE21	1:B:238:GLN:HA	1.83	0.43
1:B:242:LEU:HD23	1:B:269:ASP:HA	1.99	0.43
1:B:588:LEU:HD12	1:B:588:LEU:HA	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ARG:HH21	1:A:280:GLU:HB3	1.83	0.43
1:B:121:THR:CG2	1:B:156:MET:HB3	2.49	0.43
1:B:365:MET:HE2	1:B:383:GLU:HG3	2.00	0.43
1:B:76:ASN:O	1:B:80:GLN:HB2	2.18	0.43
1:B:325:TRP:O	1:B:326:ARG:C	2.61	0.43
1:A:334:MET:HE1	1:A:393:THR:OG1	2.18	0.43
1:A:24:ASP:OD2	1:B:40:LYS:HE3	2.17	0.43
1:A:212:ARG:NH2	1:A:280:GLU:HB3	2.34	0.43
1:B:221:ILE:HD13	1:B:250:ASP:HB2	1.99	0.43
1:B:129:LEU:HD12	1:B:130:PRO:CD	2.48	0.43
1:B:139:PHE:O	1:B:143:ASN:HA	2.19	0.43
1:B:239:ASP:HB2	5:B:1806:HOH:O	2.18	0.43
1:B:272:GLN:NE2	1:B:274:LYS:HG2	2.33	0.43
1:B:375:GLY:O	1:B:379:LYS:HE3	2.19	0.43
1:A:130:PRO:O	1:A:130:PRO:HG2	2.18	0.42
1:A:368:PRO:HB2	1:A:621:PHE:CZ	2.54	0.42
1:A:582:PRO:C	1:B:615:VAL:HG12	2.43	0.42
1:A:216:ASP:OD1	1:A:216:ASP:C	2.62	0.42
1:B:341:MET:HE2	5:B:1568:HOH:O	2.20	0.42
1:B:679:ALA:HB2	5:B:1803:HOH:O	2.19	0.42
1:B:543:LEU:HD22	1:B:640:VAL:HG21	2.01	0.42
1:A:595:ASN:HD22	1:A:595:ASN:C	2.27	0.42
1:B:132:ASP:O	1:B:133:LYS:C	2.62	0.42
1:B:178:GLN:HA	1:B:179:PRO:HD3	1.76	0.42
1:B:365:MET:HE1	1:B:468:TYR:CE1	2.55	0.42
1:B:379:LYS:HD3	1:B:381:TYR:OH	2.19	0.42
1:B:214:ILE:HD11	1:B:286:VAL:CG2	2.47	0.42
1:B:366:ILE:HD13	1:B:634:MET:HE3	2.02	0.42
1:B:373:ASP:N	1:B:373:ASP:OD1	2.53	0.42
1:B:653:LYS:HG2	1:B:654:TYR:CE2	2.55	0.42
1:B:142:GLU:O	1:B:143:ASN:CB	2.66	0.42
1:B:381:TYR:CD1	4:B:1450:GOL:C1	3.02	0.42
1:B:443:MET:HG3	1:B:444:GLY:N	2.35	0.42
1:A:91:LYS:NZ	5:A:1298:HOH:O	2.52	0.41
1:B:477:ASN:HD22	1:B:479:THR:H	1.67	0.41
1:B:515:ILE:HD12	1:B:696:TRP:HB2	2.02	0.41
1:A:276:VAL:O	1:A:277:LYS:HB2	2.20	0.41
1:A:610:GLY:HA3	1:B:610:GLY:HA3	2.03	0.41
1:A:659:THR:OG1	1:A:660:HIS:HD2	2.02	0.41
1:B:669:LYS:HA	1:B:669:LYS:HE3	2.02	0.41
1:A:376:TRP:O	1:A:379:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ILE:HD12	1:B:631:LEU:CD1	2.50	0.41
1:B:36:GLY:HA2	1:B:314:LYS:HE2	2.03	0.41
1:B:272:GLN:HE21	1:B:274:LYS:HD3	1.84	0.41
1:A:29:LEU:HD13	1:A:29:LEU:C	2.46	0.41
1:A:29:LEU:HD21	1:A:40:LYS:HB3	2.02	0.41
1:A:92:ARG:HH11	1:A:92:ARG:HD2	1.73	0.41
1:A:318:ILE:HG12	1:A:323:ILE:HG12	2.02	0.41
1:A:379:LYS:CG	1:A:381:TYR:OH	2.68	0.41
1:A:107:ALA:HB2	1:A:169:LEU:HD21	2.03	0.41
1:A:309:ILE:HD13	1:A:309:ILE:HG21	1.91	0.41
1:B:229:TYR:CZ	1:B:231:ASP:HA	2.56	0.41
1:A:29:LEU:HD13	1:A:30:PHE:C	2.45	0.41
1:A:286:VAL:CB	1:A:288:MET:HE3	2.51	0.41
1:A:546:MET:CE	5:A:1030:HOH:O	2.69	0.41
1:A:504:THR:O	1:A:508:ASP:HB2	2.21	0.41
1:A:59:VAL:HA	1:A:60:PRO:HD3	1.89	0.41
1:A:628:TYR:CD1	1:A:628:TYR:C	2.99	0.41
1:B:216:ASP:OD1	1:B:218:LYS:N	2.52	0.41
1:A:94:HIS:HB3	1:A:97:ASN:ND2	2.36	0.40
1:B:162:ILE:HD11	1:B:185:GLY:CA	2.51	0.40
1:B:540:ASN:HB3	1:B:676:ASN:HD22	1.84	0.40
1:A:80:GLN:N	1:A:80:GLN:OE1	2.54	0.40
1:B:605:ILE:HG21	1:B:605:ILE:HD13	1.88	0.40
1:A:129:LEU:HA	1:A:130:PRO:HD2	1.77	0.40
1:A:459:TRP:CZ2	1:A:461:SER:HB2	2.56	0.40
1:B:137:TRP:CD2	1:B:355:LYS:HE2	2.55	0.40
1:B:238:GLN:HE21	1:B:238:GLN:CA	2.33	0.40
1:A:62:VAL:HG23	1:A:69:TRP:HB2	2.03	0.40
1:A:92:ARG:HA	1:A:93:PRO:HD2	1.87	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	716/721 (99%)	691 (96%)	24 (3%)	1 (0%)	48	57
1	B	718/721 (100%)	687 (96%)	31 (4%)	0	100	100
All	All	1434/1442 (99%)	1378 (96%)	55 (4%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	ARG

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	609/612 (100%)	572 (94%)	37 (6%)	17	20
1	B	611/612 (100%)	568 (93%)	43 (7%)	14	16
All	All	1220/1224 (100%)	1140 (93%)	80 (7%)	15	18

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	32	LEU
1	A	64	LYS
1	A	66	ASN
1	A	71	SER
1	A	151	LYS
1	A	173	LYS
1	A	178	GLN
1	A	189	LEU
1	A	199	ILE
1	A	203	GLU
1	A	204	GLU
1	A	209	VAL
1	A	210	LYS
1	A	223	THR

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Mol	Chain	Res	Type
1	A	239	ASP
1	A	304	LYS
1	A	342	ILE
1	A	348	ASN
1	A	366	ILE
1	A	368	PRO
1	A	465	ASN
1	A	477	ASN
1	A	490	GLU
1	A	520	VAL
1	A	539	GLU
1	A	566	ASN
1	A	572	ASN
1	A	595	ASN
1	A	613	HIS
1	A	617	LYS
1	A	627	ILE
1	A	669	LYS
1	A	671	ASN
1	A	688	THR
1	A	692	ARG
1	A	724	LYS
1	B	7	MET
1	B	8	VAL
1	B	11	ASP
1	B	34	LYS
1	B	42	LYS
1	B	47	THR
1	B	64	LYS
1	B	67	LYS
1	B	71	SER
1	B	80	GLN
1	B	89	VAL
1	B	114	SER
1	B	118	LYS
1	B	129	LEU
1	B	148	GLN
1	B	173	LYS
1	B	181	LYS
1	B	199	ILE
1	B	203	GLU
1	B	209	VAL

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Mol	Chain	Res	Type
1	B	211	LYS
1	B	218	LYS
1	B	221	ILE
1	B	237	LYS
1	B	251	VAL
1	B	273	LYS
1	B	274	LYS
1	B	322	MET
1	B	372	PRO
1	B	377	TYR
1	B	477	ASN
1	B	506	LYS
1	B	539	GLU
1	B	551	LYS
1	B	595	ASN
1	B	613	HIS
1	B	617	LYS
1	B	627	ILE
1	B	632	SER
1	B	634	MET
1	B	635	ASP
1	B	669	LYS
1	B	724	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	51	ASN
1	A	53	GLN
1	A	97	ASN
1	A	143	ASN
1	A	148	GLN
1	A	161	HIS
1	A	170	GLN
1	A	196	GLN
1	A	200	ASN
1	A	201	ASN
1	A	263	ASN
1	A	272	GLN
1	A	315	ASN
1	A	324	HIS

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Mol	Chain	Res	Type
1	A	327	ASN
1	A	348	ASN
1	A	445	GLN
1	A	447	ASN
1	A	465	ASN
1	A	477	ASN
1	A	517	HIS
1	A	525	GLN
1	A	529	ASN
1	A	541	ASN
1	A	553	ASN
1	A	564	GLN
1	A	567	GLN
1	A	572	ASN
1	A	595	ASN
1	A	599	ASN
1	A	637	GLN
1	A	660	HIS
1	A	666	GLN
1	A	671	ASN
1	A	676	ASN
1	B	51	ASN
1	B	80	GLN
1	B	94	HIS
1	B	97	ASN
1	B	143	ASN
1	B	148	GLN
1	B	161	HIS
1	B	172	ASN
1	B	196	GLN
1	B	197	ASN
1	B	200	ASN
1	B	238	GLN
1	B	272	GLN
1	B	315	ASN
1	B	327	ASN
1	B	350	ASN
1	B	447	ASN
1	B	477	ASN
1	B	501	HIS
1	B	517	HIS
1	B	518	ASN

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Mol	Chain	Res	Type
1	B	525	GLN
1	B	541	ASN
1	B	553	ASN
1	B	567	GLN
1	B	572	ASN
1	B	574	GLN
1	B	595	ASN
1	B	599	ASN
1	B	637	GLN
1	B	671	ASN
1	B	676	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
1	TPQ	A	466	1	13,14,15	2.11	4 (30%)	13,19,21	2.02	4 (30%)
1	TPQ	B	466	1	13,14,15	1.97	2 (15%)	13,19,21	1.59	2 (15%)

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
1	TPQ	A	466	1	-	1/5/22/24	0/1/1/1
1	TPQ	B	466	1	-	0/5/22/24	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	TPQ	C1-C2	-4.90	1.42	1.49
1	B	466	TPQ	C1-C2	-4.60	1.42	1.49
1	A	466	TPQ	CB-C1	3.42	1.56	1.50
1	B	466	TPQ	CB-C1	3.14	1.56	1.50
1	A	466	TPQ	C4-C5	-3.12	1.38	1.47
1	A	466	TPQ	C3-C4	2.09	1.39	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	TPQ	C4-C3-C2	-3.93	116.06	120.30
1	A	466	TPQ	O5-C5-C4	-3.30	114.23	119.43
1	B	466	TPQ	O5-C5-C4	-3.23	114.34	119.43
1	B	466	TPQ	O5-C5-C6	2.74	128.07	121.83
1	A	466	TPQ	O2-C2-C3	-2.46	116.23	121.83
1	A	466	TPQ	O5-C5-C6	2.16	126.76	121.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	466	TPQ	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\# Z > 2$
4	GOL	B	1450	-	5,5,5	0.45	0	5,5,5	1.52	2 (40%)

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
4	GOL	B	1450	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	1450	GOL	C3-C2-C1	2.38	120.53	111.80
4	B	1450	GOL	O2-C2-C1	2.12	117.94	109.18

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1450	GOL	O1-C1-C2-C3
4	B	1450	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1450	GOL	6	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	325:TRP	C	326:ARG	N	1.19
1	B	326:ARG	C	327:ASN	N	1.11

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	718/721 (99%)	-0.66	3 (0%) 88 87	16, 28, 51, 71	0
1	B	720/721 (99%)	-0.56	9 (1%) 75 73	17, 29, 55, 84	0
All	All	1438/1442 (99%)	-0.61	12 (0%) 82 80	16, 28, 53, 84	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	HIS	4.0
1	B	726	ASP	3.4
1	B	301	PRO	3.1
1	B	644	HIS	2.4
1	B	326	ARG	2.4
1	A	239	ASP	2.3
1	B	302	ALA	2.3
1	A	629	HIS	2.3
1	B	629	HIS	2.3
1	B	120	ASN	2.2
1	B	628	TYR	2.1
1	A	644	HIS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	TPQ	B	466	14/15	0.96	0.06	22,29,36,38	0
1	TPQ	A	466	14/15	0.97	0.06	22,28,32,33	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($\text{\AA}^2$)	Q<0.9
4	GOL	B	1450	6/6	0.86	0.15	63,67,68,68	0
3	CA	B	803	1/1	0.93	0.10	53,53,53,53	0
3	CA	A	803	1/1	0.95	0.09	53,53,53,53	0
2	CU	A	801	1/1	0.99	0.08	33,33,33,33	0
2	CU	B	801	1/1	0.99	0.06	32,32,32,32	0
3	CA	A	802	1/1	0.99	0.04	25,25,25,25	0
3	CA	B	802	1/1	1.00	0.03	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.