



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:33 PM UTC

PDB ID : 3II6 / pdb_00003ii6
Title : Structure of human Xrcc4 in complex with the tandem BRCT domains of DNA LigaseIV.
Authors : Meesala, S.; Junop, M.
Deposited on : 2009-07-31
Resolution : 2.40 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:

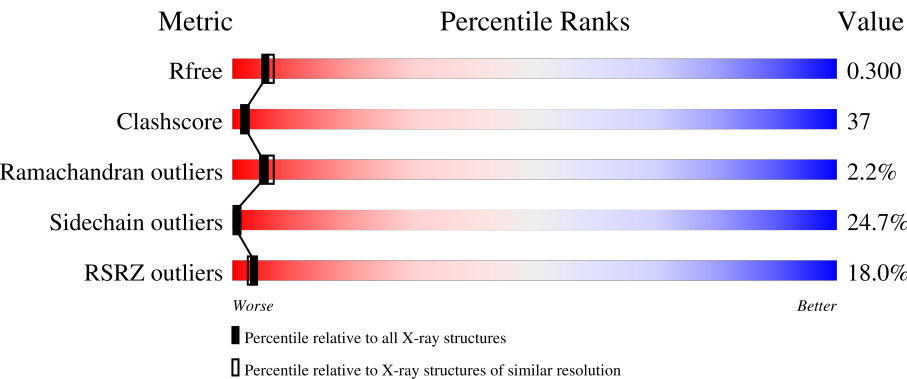
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	203	20% 32%44%16%7%.
1	B	203	33% 21%48%20%7%.
1	C	203	20% 35%36%22%5%.
1	D	203	35% 23%44%19%9%.
2	X	263	3% 21%33%28%15%.

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Mol	Chain	Length	Quality of chain
2	Y	263	3% 23% 41% 24% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10925 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 DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1631	1031	278	315	7			
1	B	196	Total	C	N	O	S	0	0	0
			1606	1016	273	310	7			
1	C	201	Total	C	N	O	S	0	0	0
			1631	1031	278	315	7			
1	D	195	Total	C	N	O	S	0	0	0
			1598	1012	272	307	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLU	ALA	engineered mutation	UNP Q13426
A	134	THR	ILE	engineered mutation	UNP Q13426
B	60	GLU	ALA	engineered mutation	UNP Q13426
B	134	THR	ILE	engineered mutation	UNP Q13426
C	60	GLU	ALA	engineered mutation	UNP Q13426
C	134	THR	ILE	engineered mutation	UNP Q13426
D	60	GLU	ALA	engineered mutation	UNP Q13426
D	134	THR	ILE	engineered mutation	UNP Q13426

- Molecule 2 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	256	Total	C	N	O	S	0	0	0
			2081	1326	351	391	13			
2	Y	258	Total	C	N	O	S	0	0	0
			2095	1333	353	396	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	649	GLY	-	expression tag	UNP P49917
X	650	ALA	-	expression tag	UNP P49917
X	651	MET	-	expression tag	UNP P49917
X	652	GLY	-	expression tag	UNP P49917
X	653	SER	-	expression tag	UNP P49917
Y	649	GLY	-	expression tag	UNP P49917
Y	650	ALA	-	expression tag	UNP P49917
Y	651	MET	-	expression tag	UNP P49917
Y	652	GLY	-	expression tag	UNP P49917
Y	653	SER	-	expression tag	UNP P49917

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Y	2	Total Cl 2 2	0	0

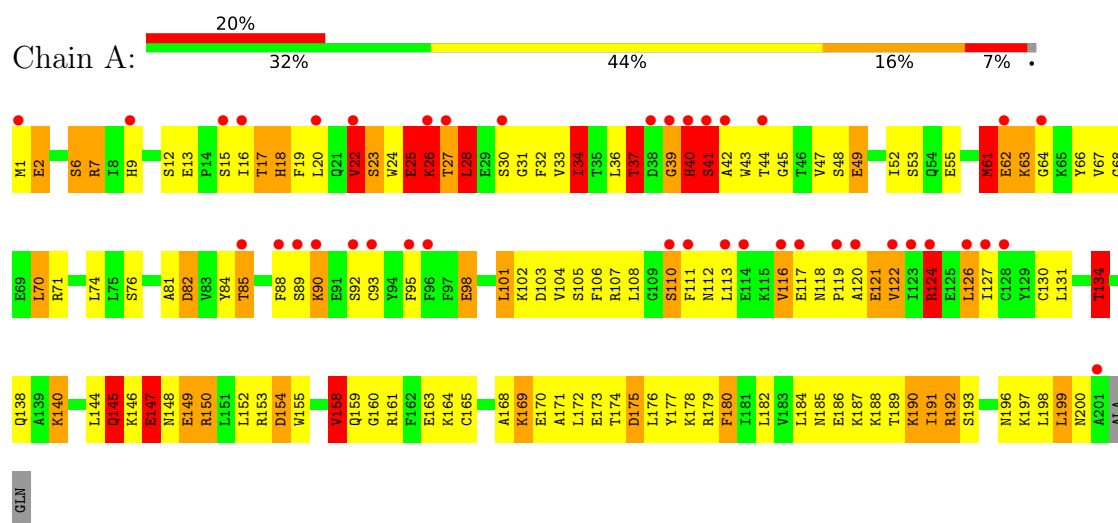
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	0	0
4	B	25	Total O 25 25	0	0
4	C	41	Total O 41 41	0	0
4	D	29	Total O 29 29	0	0
4	X	83	Total O 83 83	0	0
4	Y	59	Total O 59 59	0	0

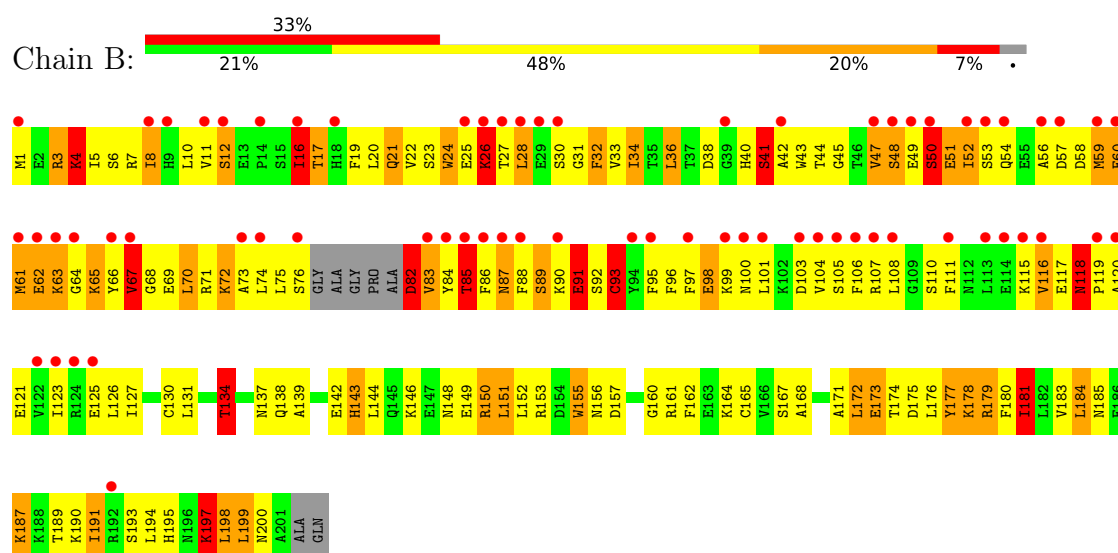
3 Residue-property plots [i](#)

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: DNA repair protein XRCC4

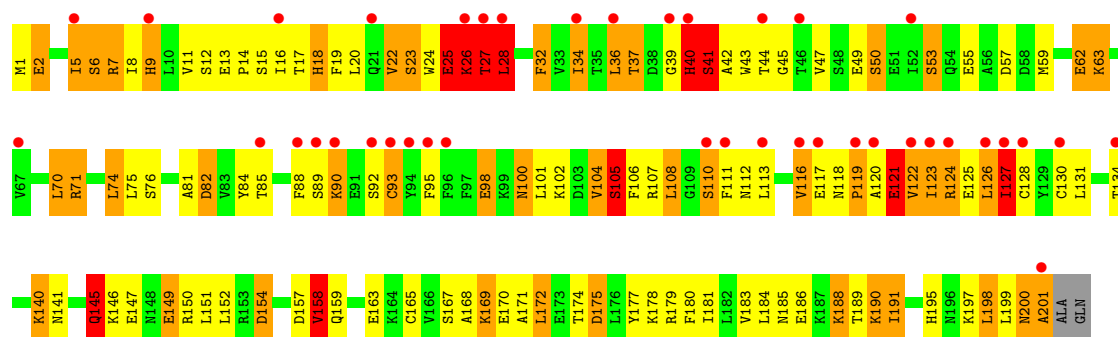


• Molecule 1: DNA repair protein XRCC4

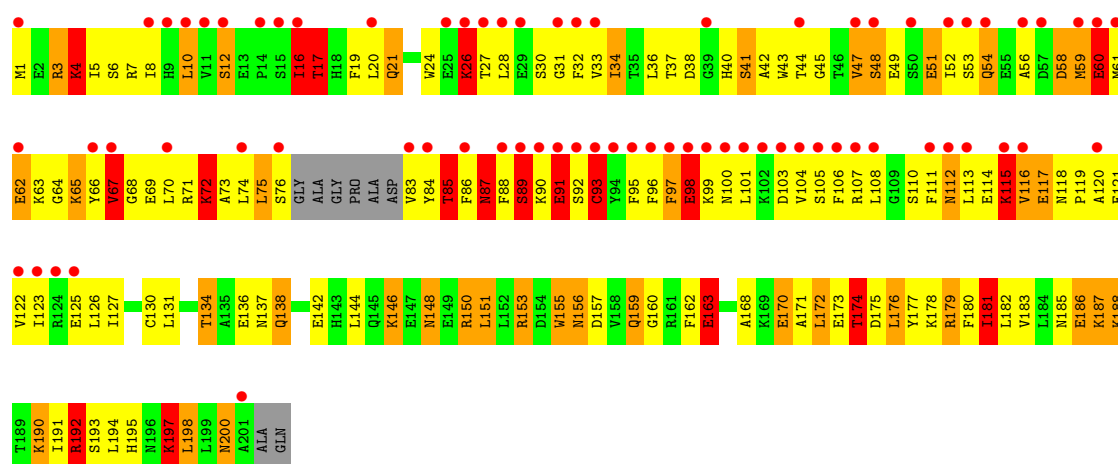


• Molecule 1: DNA repair protein XRCC4

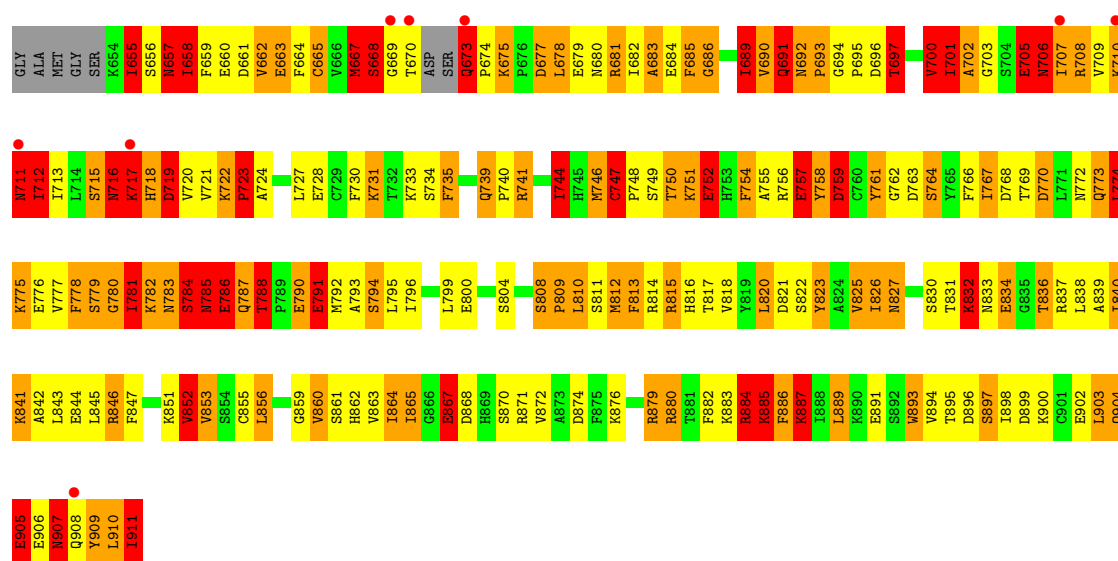
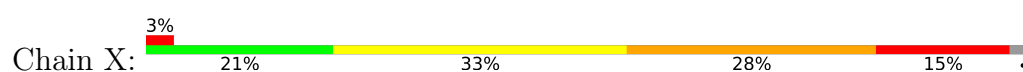




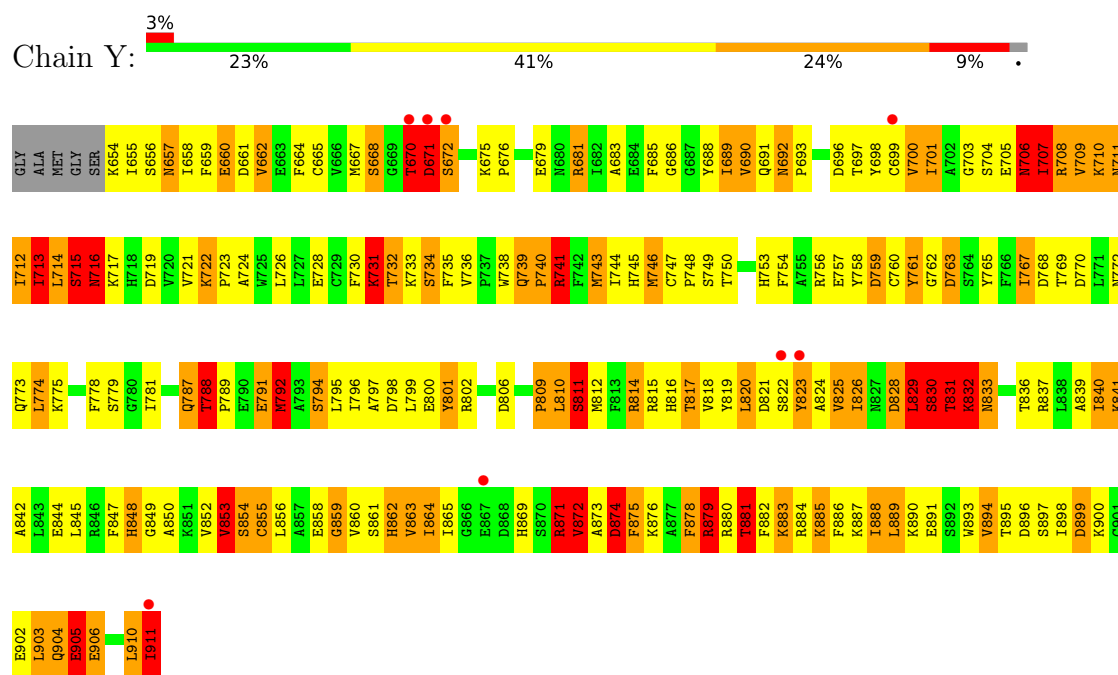
• Molecule 1: DNA repair protein XRCC4



• Molecule 2: DNA ligase 4



• Molecule 2: DNA ligase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.24Å 85.98Å 111.61Å 67.34° 82.86° 74.52°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.9 (20.00-2.40) 96.4 (20.00-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.280 0.254 , 0.300	Depositor DCC
R_{free} test set	3599 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10925	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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:
CL

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	2.24	72/1660 (4.3%)	1.91	56/2232 (2.5%)
1	B	2.00	51/1633 (3.1%)	1.75	41/2193 (1.9%)
1	C	2.17	68/1660 (4.1%)	1.86	46/2232 (2.1%)
1	D	2.00	43/1625 (2.6%)	1.92	58/2182 (2.7%)
2	X	2.69	160/2129 (7.5%)	2.37	135/2873 (4.7%)
2	Y	2.47	122/2144 (5.7%)	2.22	87/2895 (3.0%)
All	All	2.30	516/10851 (4.8%)	2.04	423/14607 (2.9%)

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	3
1	B	0	2
1	C	0	3
1	D	0	1
2	X	1	14
2	Y	0	12
All	All	1	35

All (516) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	52	ILE	C-O	15.91	1.44	1.24
2	X	781	ILE	CA-C	15.76	1.72	1.52
2	X	781	ILE	CA-CB	13.89	1.73	1.54
1	A	9	HIS	CE1-NE2	13.43	1.46	1.32
2	Y	818	VAL	CA-CB	13.20	1.72	1.54
1	A	179	ARG	CZ-NH1	-12.45	1.15	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	713	ILE	C-O	-12.16	1.09	1.24
1	C	9	HIS	CE1-NE2	11.88	1.44	1.32
1	D	91	GLU	CD-OE1	11.75	1.47	1.25
2	X	777	VAL	CA-CB	10.77	1.66	1.54
2	X	840	ILE	CG1-CD1	-10.47	1.10	1.51
2	Y	715	SER	C-O	10.24	1.36	1.24
1	A	155	TRP	CA-C	10.12	1.65	1.52
2	X	707	ILE	CA-CB	9.99	1.66	1.54
2	X	733	LYS	C-O	-9.91	1.11	1.24
2	X	705	GLU	N-CA	9.89	1.58	1.46
1	B	60	GLU	C-O	9.76	1.39	1.24
1	A	180	PHE	C-O	-9.73	1.12	1.24
2	Y	662	VAL	CA-CB	9.69	1.66	1.54
2	Y	721	VAL	CA-CB	9.63	1.68	1.54
2	Y	862	HIS	CA-C	-9.58	1.40	1.52
2	X	842	ALA	N-CA	9.46	1.57	1.46
1	C	191	ILE	N-CA	9.44	1.57	1.46
2	X	721	VAL	C-O	9.43	1.33	1.24
2	X	817	THR	N-CA	9.43	1.57	1.46
1	B	191	ILE	C-O	-9.29	1.12	1.24
1	C	63	LYS	C-O	-9.26	1.12	1.24
1	D	183	VAL	CA-CB	-9.22	1.43	1.54
2	X	860	VAL	CA-CB	9.22	1.63	1.54
2	Y	731	LYS	C-O	-9.16	1.13	1.24
2	X	693	PRO	C-O	-9.01	1.12	1.23
2	Y	769	THR	CA-CB	8.96	1.66	1.53
1	B	184	LEU	N-CA	8.90	1.56	1.46
2	X	693	PRO	CA-C	-8.89	1.42	1.52
2	Y	716	ASN	N-CA	-8.88	1.34	1.46
1	B	91	GLU	CD-OE1	8.86	1.42	1.25
1	C	178	LYS	C-O	-8.83	1.13	1.24
2	Y	847	PHE	CA-C	8.80	1.64	1.52
2	X	663	GLU	CA-C	-8.77	1.42	1.52
2	Y	905	GLU	CA-C	-8.71	1.42	1.52
1	A	63	LYS	C-O	-8.64	1.14	1.24
1	C	179	ARG	CZ-NH1	-8.61	1.20	1.32
2	X	800	GLU	N-CA	8.55	1.56	1.46
2	Y	861	SER	C-O	-8.53	1.13	1.23
2	X	733	LYS	CA-C	-8.50	1.41	1.52
1	A	155	TRP	C-O	-8.45	1.14	1.24
1	A	189	THR	N-CA	8.43	1.56	1.46
2	X	775	LYS	N-CA	-8.42	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	773	GLN	CD-NE2	8.40	1.50	1.33
2	Y	767	ILE	CA-CB	8.39	1.64	1.54
1	D	116	VAL	CA-CB	8.36	1.65	1.54
1	C	150	ARG	CA-C	-8.34	1.42	1.52
2	Y	894	VAL	CA-CB	8.34	1.65	1.54
1	A	9	HIS	CG-ND1	8.30	1.47	1.38
1	A	9	HIS	CG-CD2	8.29	1.45	1.35
2	X	794	SER	CA-C	-8.26	1.42	1.52
2	X	730	PHE	C-O	-8.24	1.14	1.24
2	X	662	VAL	CA-CB	8.24	1.65	1.54
1	C	197	LYS	N-CA	8.23	1.56	1.46
1	C	154	ASP	CG-OD1	-8.22	1.09	1.25
1	C	195	HIS	C-O	-8.22	1.14	1.24
2	Y	762	GLY	N-CA	8.19	1.57	1.45
2	X	779	SER	C-O	-8.19	1.13	1.24
2	X	898	ILE	C-O	-8.18	1.14	1.24
1	B	165	CYS	N-CA	8.17	1.56	1.46
1	A	182	LEU	N-CA	8.13	1.56	1.46
2	Y	662	VAL	CA-C	8.13	1.62	1.52
2	X	818	VAL	CA-CB	8.04	1.64	1.54
2	Y	898	ILE	C-O	-8.01	1.16	1.24
2	X	667	MET	C-O	-7.98	1.13	1.24
2	X	731	LYS	C-O	-7.98	1.14	1.24
2	X	852	VAL	CA-CB	7.96	1.64	1.54
1	D	98	GLU	CD-OE1	7.96	1.40	1.25
1	C	157	ASP	N-CA	-7.95	1.37	1.46
2	X	864	ILE	N-CA	-7.90	1.35	1.46
2	X	784	SER	C-O	7.89	1.33	1.24
1	B	162	PHE	CD1-CE1	7.86	1.62	1.38
1	B	153	ARG	N-CA	-7.85	1.37	1.46
2	X	785	ASN	CA-C	-7.85	1.41	1.52
1	A	40	HIS	CE1-NE2	7.84	1.40	1.32
2	X	780	GLY	C-O	-7.83	1.13	1.23
2	X	718	HIS	CA-C	-7.74	1.43	1.52
1	D	117	GLU	CB-CG	-7.72	1.29	1.52
1	A	37	THR	CA-CB	7.71	1.67	1.53
1	D	33	VAL	CA-CB	7.71	1.64	1.54
2	Y	791	GLU	CA-C	-7.69	1.42	1.52
2	X	719	ASP	N-CA	-7.68	1.36	1.46
2	X	897	SER	C-O	7.67	1.32	1.24
2	Y	683	ALA	CA-C	7.66	1.62	1.52
2	Y	747	CYS	N-CA	-7.63	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	706	ASN	N-CA	7.62	1.55	1.46
1	B	144	LEU	CA-C	-7.60	1.42	1.52
2	X	846	ARG	CG-CD	7.58	1.75	1.52
2	X	767	ILE	CA-CB	7.58	1.63	1.54
2	Y	853	VAL	CA-CB	-7.57	1.45	1.54
2	X	820	LEU	N-CA	-7.57	1.35	1.46
2	Y	860	VAL	CA-CB	-7.53	1.44	1.54
2	X	758	TYR	CA-C	-7.53	1.43	1.52
2	X	700	VAL	CA-C	-7.53	1.43	1.52
1	D	8	ILE	CB-CG1	7.52	1.68	1.53
2	X	697	THR	N-CA	-7.51	1.36	1.46
2	Y	760	CYS	C-O	-7.47	1.14	1.24
1	A	158	VAL	C-O	-7.43	1.15	1.24
2	Y	741	ARG	C-O	7.42	1.33	1.24
2	X	853	VAL	C-O	7.40	1.31	1.24
1	C	37	THR	CA-CB	7.38	1.66	1.53
1	A	191	ILE	N-CA	7.38	1.55	1.46
1	C	15	SER	CB-OG	7.37	1.56	1.42
2	X	767	ILE	CA-C	7.35	1.61	1.52
1	D	54	GLN	CD-NE2	7.33	1.48	1.33
2	X	904	GLN	CA-C	-7.33	1.43	1.53
1	B	176	LEU	CA-CB	-7.32	1.41	1.53
2	Y	859	GLY	N-CA	7.30	1.55	1.45
2	Y	763	ASP	CA-CB	7.26	1.63	1.53
1	B	160	GLY	C-O	-7.24	1.15	1.24
1	D	190	LYS	C-O	-7.24	1.15	1.24
2	Y	864	ILE	N-CA	-7.24	1.37	1.46
2	X	859	GLY	C-O	-7.21	1.14	1.24
2	X	889	LEU	CA-C	-7.21	1.44	1.52
2	Y	811	SER	CA-C	7.21	1.61	1.53
1	D	195	HIS	C-O	-7.20	1.15	1.24
2	X	855	CYS	C-O	-7.17	1.16	1.24
2	X	784	SER	N-CA	-7.17	1.36	1.46
1	D	181	ILE	CA-CB	7.15	1.62	1.54
1	A	22	VAL	CB-CG2	-7.13	1.29	1.52
2	X	741	ARG	CZ-NH1	7.10	1.42	1.32
1	C	183	VAL	CA-CB	7.10	1.62	1.54
2	X	909	TYR	CD1-CE1	7.09	1.59	1.38
2	Y	890	LYS	CA-C	7.07	1.62	1.52
2	X	894	VAL	CA-CB	7.07	1.62	1.54
2	Y	872	VAL	CA-C	-7.06	1.42	1.52
1	C	200	ASN	C-O	-7.04	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	770	ASP	CA-CB	6.98	1.63	1.53
1	A	199	LEU	CG-CD1	-6.97	1.29	1.52
1	A	199	LEU	CG-CD2	-6.94	1.29	1.52
1	A	169	LYS	CB-CG	-6.93	1.31	1.52
2	Y	708	ARG	C-O	-6.92	1.16	1.24
2	Y	788	THR	CA-CB	-6.92	1.43	1.53
1	C	174	THR	N-CA	6.92	1.55	1.46
1	A	164	LYS	C-O	-6.91	1.15	1.24
1	A	153	ARG	C-O	-6.88	1.15	1.24
2	X	896	ASP	N-CA	6.88	1.54	1.46
1	A	171	ALA	N-CA	6.88	1.55	1.46
2	X	799	LEU	C-O	-6.87	1.16	1.24
1	D	91	GLU	CD-OE2	6.86	1.38	1.25
1	A	200	ASN	C-O	-6.86	1.15	1.24
2	X	817	THR	CA-CB	-6.86	1.43	1.53
2	Y	812	MET	N-CA	6.82	1.55	1.46
2	Y	885	LYS	N-CA	-6.81	1.37	1.46
1	A	101	LEU	C-O	-6.79	1.15	1.24
2	Y	859	GLY	CA-C	6.79	1.61	1.51
1	C	9	HIS	CG-ND1	6.79	1.45	1.38
1	C	15	SER	CA-C	6.79	1.62	1.52
2	Y	774	LEU	C-O	6.79	1.32	1.24
1	A	134	THR	C-O	6.78	1.32	1.24
2	X	786	GLU	N-CA	-6.76	1.37	1.46
1	B	89	SER	CB-OG	6.76	1.55	1.42
1	C	9	HIS	CG-CD2	6.72	1.43	1.35
1	A	199	LEU	CA-C	-6.71	1.44	1.52
2	X	861	SER	N-CA	-6.71	1.37	1.46
2	Y	904	GLN	CA-C	-6.70	1.44	1.52
1	C	189	THR	N-CA	6.68	1.54	1.46
2	Y	715	SER	CA-CB	-6.66	1.44	1.53
1	B	171	ALA	N-CA	6.66	1.54	1.46
1	A	144	LEU	C-O	-6.62	1.16	1.24
2	X	730	PHE	CB-CG	6.62	1.65	1.50
2	X	837	ARG	CZ-NH1	6.62	1.42	1.32
1	C	158	VAL	CA-CB	-6.60	1.46	1.54
1	B	148	ASN	N-CA	-6.58	1.38	1.46
2	X	810	LEU	N-CA	-6.55	1.37	1.46
1	D	148	ASN	N-CA	-6.55	1.37	1.46
2	X	834	GLU	N-CA	6.54	1.53	1.45
2	X	895	THR	CA-C	-6.54	1.44	1.52
2	Y	800	GLU	C-O	-6.54	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	845	LEU	N-CA	-6.53	1.38	1.46
2	X	870	SER	C-O	-6.53	1.16	1.24
1	A	180	PHE	CE1-CZ	6.52	1.58	1.38
1	A	40	HIS	CG-ND1	6.52	1.45	1.38
1	A	41	SER	N-CA	6.46	1.54	1.46
1	C	22	VAL	CB-CG1	-6.46	1.31	1.52
2	Y	852	VAL	CA-C	6.46	1.60	1.52
1	B	193	SER	CA-C	-6.43	1.44	1.52
1	A	20	LEU	C-O	-6.42	1.16	1.24
1	A	186	GLU	CG-CD	6.42	1.68	1.52
1	A	19	PHE	CA-C	-6.40	1.44	1.52
2	Y	744	ILE	CB-CG2	6.38	1.73	1.52
2	Y	796	ILE	N-CA	6.38	1.53	1.46
1	D	155	TRP	C-O	6.36	1.31	1.24
2	X	811	SER	N-CA	6.36	1.53	1.46
2	X	837	ARG	CA-C	-6.36	1.43	1.52
2	X	690	VAL	N-CA	6.35	1.54	1.46
1	B	189	THR	CA-C	6.34	1.61	1.52
1	B	176	LEU	CA-C	6.34	1.61	1.52
2	X	778	PHE	C-O	6.34	1.31	1.24
2	X	723	PRO	C-O	-6.34	1.15	1.24
2	Y	772	ASN	N-CA	-6.34	1.39	1.46
1	A	20	LEU	CG-CD1	6.33	1.73	1.52
2	Y	797	ALA	C-O	-6.33	1.16	1.24
1	A	179	ARG	CD-NE	-6.32	1.37	1.46
1	B	190	LYS	CG-CD	6.32	1.71	1.52
2	X	865	ILE	CA-C	6.30	1.60	1.52
1	A	180	PHE	CD2-CE2	6.28	1.57	1.38
2	Y	873	ALA	N-CA	6.28	1.54	1.46
2	Y	853	VAL	C-O	6.28	1.32	1.24
2	X	862	HIS	C-O	-6.28	1.16	1.23
2	Y	848	HIS	CA-C	-6.27	1.45	1.53
2	Y	739	GLN	CD-NE2	6.27	1.46	1.33
1	B	194	LEU	C-O	-6.25	1.16	1.24
2	Y	899	ASP	C-O	-6.22	1.16	1.24
1	B	143	HIS	C-O	-6.21	1.17	1.24
1	A	178	LYS	C-O	-6.21	1.16	1.24
2	X	880	ARG	N-CA	6.20	1.54	1.46
1	A	182	LEU	CG-CD2	6.19	1.73	1.52
1	A	160	GLY	N-CA	-6.18	1.38	1.45
2	Y	707	ILE	CA-CB	6.17	1.62	1.54
2	Y	689	ILE	CA-CB	-6.17	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	741	ARG	CZ-NH1	6.17	1.41	1.32
1	A	159	GLN	CA-C	6.16	1.60	1.52
2	X	814	ARG	N-CA	6.16	1.53	1.46
1	B	33	VAL	CA-CB	6.15	1.62	1.54
1	D	174	THR	CB-CG2	-6.15	1.32	1.52
1	C	191	ILE	CA-CB	6.15	1.61	1.54
1	D	59	MET	CA-CB	6.14	1.63	1.53
2	X	899	ASP	CA-C	6.13	1.60	1.52
2	Y	759	ASP	CB-CG	-6.13	1.36	1.52
1	A	15	SER	CB-OG	6.13	1.54	1.42
1	C	147	GLU	CD-OE2	-6.12	1.13	1.25
2	Y	761	TYR	N-CA	6.12	1.53	1.45
1	D	156	ASN	CG-ND2	-6.12	1.20	1.33
2	Y	767	ILE	C-O	6.11	1.30	1.24
1	D	8	ILE	CB-CG2	6.10	1.72	1.52
2	X	814	ARG	C-O	6.10	1.31	1.24
1	C	63	LYS	N-CA	6.10	1.54	1.46
1	B	181	ILE	CA-C	6.10	1.60	1.52
1	C	185	ASN	N-CA	6.10	1.54	1.46
1	C	171	ALA	N-CA	6.09	1.54	1.46
2	X	874	ASP	N-CA	6.09	1.53	1.46
1	A	175	ASP	CB-CG	-6.09	1.36	1.52
1	A	62	GLU	CA-C	6.09	1.60	1.52
2	X	823	TYR	N-CA	6.08	1.53	1.46
2	X	712	ILE	CA-CB	6.08	1.62	1.54
1	A	28	LEU	CG-CD2	-6.06	1.32	1.52
1	C	27	THR	CA-CB	6.06	1.63	1.53
2	Y	747	CYS	CA-C	6.05	1.60	1.52
1	C	168	ALA	N-CA	-6.05	1.39	1.46
2	Y	842	ALA	C-O	-6.03	1.16	1.24
2	X	781	ILE	N-CA	6.02	1.53	1.46
1	D	87	ASN	C-O	6.02	1.30	1.23
1	C	180	PHE	CD1-CE1	6.00	1.56	1.38
2	X	856	LEU	CG-CD1	-6.00	1.32	1.52
1	B	134	THR	N-CA	-6.00	1.39	1.46
1	B	184	LEU	CG-CD1	-6.00	1.32	1.52
1	A	186	GLU	CA-CB	-5.99	1.44	1.53
2	X	879	ARG	CZ-NH2	5.98	1.41	1.33
2	X	657	ASN	CB-CG	-5.98	1.37	1.52
2	Y	881	THR	C-O	5.97	1.31	1.24
1	A	150	ARG	CA-C	-5.96	1.45	1.52
2	Y	775	LYS	C-O	5.96	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	186	GLU	CA-C	5.96	1.60	1.52
2	X	770	ASP	CB-CG	-5.95	1.37	1.52
1	D	148	ASN	CA-CB	5.95	1.64	1.53
2	Y	709	VAL	N-CA	5.94	1.53	1.46
2	Y	758	TYR	CA-C	-5.94	1.45	1.52
2	X	787	GLN	CA-CB	-5.94	1.43	1.53
2	Y	794	SER	CA-C	-5.94	1.44	1.52
1	D	89	SER	CA-C	-5.93	1.45	1.52
2	X	896	ASP	C-N	5.93	1.41	1.33
2	Y	811	SER	C-O	-5.92	1.17	1.24
2	Y	865	ILE	CA-C	5.92	1.60	1.52
1	A	22	VAL	CB-CG1	-5.92	1.33	1.52
2	X	825	VAL	CA-C	-5.92	1.45	1.52
2	Y	746	MET	SD-CE	-5.92	1.64	1.79
1	B	137	ASN	CG-ND2	-5.92	1.20	1.33
2	X	836	THR	CA-C	5.92	1.59	1.52
1	C	105	SER	N-CA	-5.91	1.39	1.46
1	A	186	GLU	CD-OE1	5.89	1.36	1.25
2	Y	757	GLU	N-CA	-5.89	1.38	1.46
2	X	847	PHE	CA-C	5.88	1.60	1.52
2	X	759	ASP	CA-C	-5.88	1.45	1.53
2	X	833	ASN	C-O	5.88	1.31	1.24
2	Y	796	ILE	C-O	5.87	1.30	1.24
1	B	50	SER	CB-OG	5.86	1.53	1.42
1	B	173	GLU	CB-CG	-5.85	1.34	1.52
2	Y	873	ALA	C-O	-5.84	1.17	1.24
1	D	182	LEU	CA-C	5.84	1.60	1.52
1	D	146	LYS	CA-C	-5.83	1.45	1.52
1	D	198	LEU	CG-CD2	-5.83	1.33	1.52
1	A	196	ASN	CG-OD1	-5.83	1.12	1.23
2	Y	735	PHE	N-CA	-5.83	1.39	1.46
2	X	755	ALA	CA-CB	5.83	1.63	1.53
2	Y	769	THR	C-O	-5.83	1.16	1.23
2	X	770	ASP	C-O	5.82	1.30	1.23
2	X	863	VAL	CA-CB	5.82	1.63	1.54
1	C	104	VAL	CB-CG2	-5.80	1.33	1.52
1	C	147	GLU	C-O	-5.80	1.17	1.24
2	Y	848	HIS	C-O	5.80	1.31	1.23
2	X	833	ASN	N-CA	5.80	1.53	1.46
1	C	62	GLU	CA-C	5.80	1.59	1.52
2	Y	700	VAL	CA-CB	-5.80	1.47	1.54
2	Y	889	LEU	C-O	-5.79	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	863	VAL	CA-CB	5.78	1.62	1.54
1	D	117	GLU	CA-CB	-5.78	1.44	1.53
2	X	814	ARG	CB-CG	-5.77	1.35	1.52
1	D	12	SER	CB-OG	5.77	1.53	1.42
2	X	907	ASN	CG-ND2	5.76	1.45	1.33
1	C	181	ILE	N-CA	5.75	1.53	1.46
2	X	808	SER	N-CA	-5.74	1.38	1.45
2	Y	711	ASN	CA-CB	5.73	1.63	1.53
1	B	177	TYR	CB-CG	5.73	1.64	1.51
1	D	144	LEU	C-O	-5.73	1.17	1.24
1	C	141	ASN	CG-OD1	-5.73	1.12	1.23
1	A	176	LEU	CA-C	5.72	1.60	1.52
2	X	657	ASN	CA-C	-5.71	1.44	1.52
2	Y	762	GLY	C-O	-5.71	1.16	1.23
1	C	177	TYR	CA-C	-5.71	1.44	1.52
2	X	872	VAL	CA-CB	5.70	1.61	1.54
2	X	814	ARG	CA-C	-5.70	1.45	1.52
2	Y	659	PHE	CA-CB	-5.70	1.45	1.53
2	Y	735	PHE	C-O	-5.69	1.17	1.23
1	A	101	LEU	CA-C	5.69	1.60	1.52
1	A	155	TRP	N-CA	-5.69	1.39	1.46
1	C	50	SER	CA-C	5.68	1.60	1.52
2	Y	741	ARG	CB-CG	-5.68	1.35	1.52
1	B	174	THR	CA-CB	-5.68	1.44	1.53
1	C	186	GLU	CD-OE1	5.67	1.36	1.25
1	A	173	GLU	CD-OE2	-5.67	1.14	1.25
2	Y	703	GLY	C-O	-5.66	1.16	1.23
2	X	719	ASP	CB-CG	-5.65	1.38	1.52
1	A	193	SER	N-CA	5.64	1.53	1.46
2	X	893	TRP	C-O	5.64	1.30	1.24
1	B	181	ILE	C-O	5.64	1.30	1.24
2	X	884	ARG	C-O	5.64	1.31	1.24
2	Y	815	ARG	CZ-NH1	5.63	1.40	1.32
1	D	148	ASN	CB-CG	-5.63	1.38	1.52
1	A	170	GLU	CA-C	-5.63	1.45	1.52
1	D	173	GLU	CB-CG	-5.61	1.35	1.52
2	Y	706	ASN	CA-C	-5.61	1.46	1.52
2	X	842	ALA	CA-C	-5.60	1.45	1.52
2	Y	691	GLN	N-CA	5.60	1.53	1.46
1	B	150	ARG	CA-CB	-5.59	1.44	1.53
2	Y	810	LEU	CG-CD2	5.59	1.71	1.52
1	B	150	ARG	CZ-NH1	5.59	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	GLU	CG-CD	5.59	1.66	1.52
1	B	150	ARG	N-CA	-5.58	1.39	1.46
1	C	175	ASP	CB-CG	-5.57	1.38	1.52
2	X	831	THR	CA-CB	-5.56	1.45	1.53
2	X	785	ASN	N-CA	-5.56	1.38	1.46
1	B	178	LYS	N-CA	5.55	1.53	1.46
2	X	715	SER	N-CA	5.55	1.52	1.45
1	C	36	LEU	C-O	-5.54	1.16	1.23
2	X	695	PRO	CA-C	5.53	1.62	1.52
2	Y	841	LYS	CA-C	-5.53	1.45	1.52
1	D	153	ARG	N-CA	-5.52	1.39	1.46
1	A	23	SER	N-CA	5.51	1.52	1.46
1	A	182	LEU	C-O	-5.51	1.17	1.24
2	X	757	GLU	CG-CD	5.50	1.65	1.52
2	X	749	SER	C-O	5.50	1.30	1.24
1	D	181	ILE	CA-C	5.49	1.59	1.52
1	B	67	VAL	CA-CB	5.49	1.61	1.54
1	B	199	LEU	C-O	-5.49	1.17	1.24
2	Y	767	ILE	CG1-CD1	-5.49	1.30	1.51
2	Y	714	LEU	CG-CD1	5.49	1.70	1.52
2	X	815	ARG	C-O	5.48	1.31	1.24
2	Y	864	ILE	CG1-CD1	5.48	1.73	1.51
2	Y	704	SER	CA-C	5.48	1.59	1.52
1	C	20	LEU	CG-CD1	5.47	1.70	1.52
1	D	150	ARG	CA-CB	-5.47	1.44	1.53
1	B	172	LEU	CG-CD2	-5.47	1.34	1.52
2	X	894	VAL	N-CA	-5.47	1.40	1.46
2	X	691	GLN	C-O	5.47	1.31	1.24
2	X	785	ASN	CB-CG	-5.46	1.38	1.52
1	C	179	ARG	C-O	-5.46	1.17	1.24
2	Y	831	THR	CA-CB	-5.44	1.43	1.53
2	Y	905	GLU	C-O	-5.44	1.17	1.23
1	B	168	ALA	CA-CB	-5.44	1.44	1.53
2	X	868	ASP	N-CA	5.44	1.53	1.46
2	Y	809	PRO	N-CA	-5.43	1.40	1.47
2	X	812	MET	N-CA	5.43	1.52	1.46
2	X	717	LYS	CB-CG	5.43	1.68	1.52
1	A	185	ASN	N-CA	5.42	1.53	1.46
1	D	103	ASP	CA-C	5.42	1.60	1.52
1	C	180	PHE	CA-CB	5.41	1.61	1.53
1	C	169	LYS	N-CA	5.41	1.53	1.46
1	C	181	ILE	CA-CB	5.41	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	LYS	CE-NZ	5.40	1.65	1.49
2	X	867	GLU	CA-C	-5.40	1.45	1.52
1	D	172	LEU	CG-CD2	-5.39	1.34	1.52
1	A	184	LEU	C-O	5.39	1.30	1.24
1	B	150	ARG	CZ-NH2	5.39	1.40	1.33
1	D	171	ALA	N-CA	5.39	1.52	1.46
2	Y	825	VAL	CA-CB	5.39	1.61	1.54
2	Y	662	VAL	C-O	5.39	1.29	1.24
1	C	188	LYS	C-O	-5.38	1.17	1.24
2	Y	897	SER	CA-CB	-5.38	1.45	1.53
2	Y	741	ARG	CA-C	5.38	1.59	1.52
2	X	825	VAL	C-O	-5.38	1.18	1.24
1	B	149	GLU	N-CA	5.38	1.52	1.46
2	X	903	LEU	CA-C	5.37	1.60	1.52
2	Y	715	SER	N-CA	5.37	1.52	1.46
2	X	692	ASN	CA-CB	5.37	1.61	1.54
1	C	5	ILE	CG1-CD1	5.36	1.72	1.51
2	X	800	GLU	CB-CG	5.36	1.68	1.52
1	C	169	LYS	CG-CD	-5.36	1.36	1.52
1	C	134	THR	C-O	5.36	1.30	1.24
2	X	794	SER	C-O	5.35	1.30	1.24
1	C	20	LEU	C-O	-5.35	1.17	1.24
2	X	826	ILE	C-O	5.35	1.29	1.24
1	C	41	SER	N-CA	5.34	1.53	1.46
1	A	52	ILE	CA-CB	5.34	1.60	1.54
1	A	196	ASN	CG-ND2	-5.33	1.22	1.33
1	A	148	ASN	CA-C	5.33	1.59	1.52
2	X	717	LYS	CG-CD	5.33	1.68	1.52
2	Y	860	VAL	N-CA	-5.32	1.40	1.46
1	D	188	LYS	CG-CD	-5.31	1.36	1.52
2	X	813	PHE	N-CA	5.31	1.52	1.46
1	A	174	THR	CB-CG2	-5.30	1.35	1.52
2	Y	854	SER	CA-C	5.30	1.60	1.52
1	B	8	ILE	CB-CG1	5.30	1.64	1.53
1	C	179	ARG	CG-CD	-5.29	1.36	1.52
2	Y	880	ARG	N-CA	5.29	1.53	1.46
2	X	911	ILE	CG1-CD1	5.29	1.72	1.51
1	B	47	VAL	CA-CB	5.28	1.59	1.53
2	X	834	GLU	C-O	5.28	1.29	1.23
2	X	841	LYS	CG-CD	-5.27	1.36	1.52
2	Y	741	ARG	N-CA	5.27	1.52	1.46
2	Y	701	ILE	N-CA	-5.27	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	198	LEU	CG-CD2	5.26	1.70	1.52
2	Y	862	HIS	C-O	-5.26	1.17	1.23
2	Y	698	TYR	CA-C	5.26	1.59	1.52
2	X	691	GLN	CB-CG	5.25	1.68	1.52
2	X	724	ALA	CA-C	5.25	1.59	1.52
1	A	148	ASN	N-CA	-5.25	1.40	1.46
1	D	191	ILE	C-O	-5.25	1.18	1.24
2	X	764	SER	CA-C	-5.25	1.45	1.52
2	X	821	ASP	N-CA	-5.25	1.40	1.46
1	B	179	ARG	CB-CG	-5.24	1.36	1.52
2	Y	883	LYS	CA-C	5.24	1.59	1.52
2	X	735	PHE	N-CA	-5.24	1.40	1.46
2	Y	837	ARG	C-O	5.23	1.30	1.24
2	Y	847	PHE	N-CA	-5.23	1.40	1.46
1	A	145	GLN	CG-CD	-5.23	1.39	1.52
1	A	192	ARG	C-O	5.23	1.30	1.24
1	C	141	ASN	CA-C	-5.23	1.46	1.52
1	A	186	GLU	N-CA	5.22	1.52	1.46
2	Y	696	ASP	N-CA	-5.21	1.38	1.45
1	C	92	SER	CB-OG	5.20	1.52	1.42
2	X	707	ILE	C-O	5.20	1.29	1.24
2	Y	875	PHE	CA-C	-5.20	1.45	1.52
1	C	6	SER	C-O	-5.18	1.18	1.24
1	B	150	ARG	CA-C	5.18	1.59	1.52
1	C	170	GLU	CB-CG	5.18	1.68	1.52
1	D	137	ASN	CA-C	-5.18	1.45	1.52
1	C	19	PHE	CA-C	-5.17	1.46	1.52
2	X	658	ILE	CA-C	5.17	1.59	1.52
2	X	844	GLU	CA-C	-5.17	1.46	1.52
2	X	865	ILE	CA-CB	-5.17	1.48	1.54
1	B	19	PHE	CA-CB	5.17	1.62	1.53
1	A	177	TYR	CA-C	-5.16	1.45	1.52
2	Y	840	ILE	CA-CB	-5.16	1.48	1.54
1	B	167	SER	CA-CB	-5.15	1.45	1.53
1	A	92	SER	CB-OG	5.15	1.52	1.42
2	X	780	GLY	C-N	5.15	1.40	1.33
1	C	168	ALA	CA-C	-5.14	1.46	1.52
1	A	15	SER	CA-C	5.14	1.59	1.52
1	C	201	ALA	N-CA	5.14	1.56	1.46
2	X	684	GLU	CB-CG	-5.14	1.37	1.52
1	B	172	LEU	C-O	-5.13	1.18	1.24
2	Y	864	ILE	C-O	-5.13	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	683	ALA	C-O	-5.13	1.17	1.24
1	C	123	ILE	CA-C	5.13	1.59	1.52
1	D	117	GLU	CD-OE1	5.13	1.35	1.25
2	Y	750	THR	C-N	-5.13	1.27	1.33
2	X	707	ILE	CG1-CD1	5.12	1.71	1.51
2	Y	895	THR	C-O	-5.12	1.18	1.24
1	B	152	LEU	C-O	-5.12	1.18	1.24
1	D	151	LEU	N-CA	5.12	1.52	1.46
1	C	100	ASN	CA-C	5.11	1.58	1.52
2	X	886	PHE	N-CA	-5.11	1.39	1.46
2	X	662	VAL	C-O	5.10	1.29	1.24
1	B	181	ILE	CA-CB	5.10	1.60	1.54
2	X	839	ALA	CA-C	-5.09	1.46	1.52
2	Y	773	GLN	CD-NE2	5.09	1.44	1.33
2	X	717	LYS	CD-CE	5.09	1.67	1.52
1	C	172	LEU	N-CA	5.08	1.52	1.46
1	C	134	THR	CA-CB	5.08	1.61	1.53
2	X	685	PHE	CA-C	-5.08	1.45	1.52
1	A	101	LEU	C-N	-5.07	1.27	1.33
2	Y	656	SER	CA-C	-5.07	1.46	1.52
2	X	677	ASP	C-O	5.07	1.29	1.24
2	Y	825	VAL	CB-CG2	5.07	1.69	1.52
2	X	701	ILE	CA-C	5.06	1.58	1.52
1	D	168	ALA	CA-CB	-5.06	1.45	1.53
2	X	759	ASP	CB-CG	-5.06	1.39	1.52
2	Y	814	ARG	C-O	5.06	1.30	1.24
2	Y	823	TYR	CA-C	-5.06	1.46	1.52
2	Y	719	ASP	C-O	-5.06	1.17	1.23
2	Y	837	ARG	CZ-NH2	5.06	1.40	1.33
2	Y	830	SER	C-O	5.05	1.30	1.24
2	X	791	GLU	CA-C	-5.05	1.47	1.53
1	B	156	ASN	CG-ND2	-5.05	1.22	1.33
2	X	830	SER	C-O	5.04	1.30	1.23
1	A	64	GLY	C-O	5.03	1.30	1.23
1	C	184	LEU	CB-CG	5.03	1.63	1.53
1	C	184	LEU	CA-C	-5.03	1.46	1.52
2	X	762	GLY	N-CA	-5.03	1.38	1.45
2	X	773	GLN	CG-CD	5.03	1.64	1.52
2	X	837	ARG	N-CA	-5.03	1.40	1.46
2	X	851	LYS	C-O	-5.03	1.17	1.24
2	X	774	LEU	N-CA	5.02	1.52	1.46
2	X	727	LEU	CG-CD1	5.02	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	ALA	C-O	5.02	1.29	1.24
2	X	899	ASP	C-O	-5.02	1.18	1.24
1	A	173	GLU	N-CA	5.02	1.52	1.46
2	X	812	MET	CG-SD	-5.02	1.68	1.80
2	X	887	LYS	CA-C	-5.02	1.46	1.52
1	C	32	PHE	CA-C	-5.01	1.46	1.52

All (423) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	722	LYS	CA-C-N	14.65	136.47	119.47
2	Y	722	LYS	C-N-CA	14.65	136.47	119.47
2	X	782	LYS	N-CA-C	13.23	129.73	110.42
2	X	785	ASN	N-CA-C	-13.15	94.65	114.64
2	X	904	GLN	N-CA-C	-12.78	94.69	110.41
2	X	761	TYR	N-CA-C	-12.39	96.90	114.12
2	Y	761	TYR	N-CA-C	-11.82	93.02	110.52
1	A	179	ARG	NE-CZ-NH2	11.21	129.28	119.20
2	X	814	ARG	CB-CA-C	-10.65	93.11	110.79
2	X	787	GLN	N-CA-C	10.60	126.05	107.61
2	Y	759	ASP	N-CA-C	-10.54	95.31	110.59
1	D	148	ASN	CB-CA-C	10.21	127.42	109.65
2	X	719	ASP	CB-CA-C	10.21	128.17	109.70
2	X	719	ASP	N-CA-CB	-10.02	93.46	110.80
1	D	117	GLU	N-CA-CB	-9.99	94.85	110.44
2	Y	747	CYS	CA-C-N	9.85	132.15	119.84
2	Y	747	CYS	C-N-CA	9.85	132.15	119.84
1	D	26	LYS	CB-CA-C	-9.83	90.85	110.42
1	C	62	GLU	CB-CA-C	9.74	123.26	109.71
2	X	784	SER	CA-C-N	-9.68	103.69	121.41
2	X	784	SER	C-N-CA	-9.68	103.69	121.41
1	D	180	PHE	N-CA-C	9.66	122.81	111.02
2	X	764	SER	CA-CB-OG	-9.58	91.95	111.10
2	Y	806	ASP	N-CA-C	9.56	124.48	113.01
2	X	911	ILE	CB-CG1-CD1	-9.42	94.02	113.80
1	D	179	ARG	NE-CZ-NH1	-9.38	112.12	121.50
2	Y	896	ASP	CA-C-O	-9.21	111.14	120.82
2	Y	736	VAL	CA-C-N	9.17	129.20	119.76
2	Y	736	VAL	C-N-CA	9.17	129.20	119.76
2	X	784	SER	CB-CA-C	9.07	128.48	110.42
1	B	180	PHE	N-CA-C	9.07	126.24	111.37
2	X	861	SER	N-CA-C	-9.06	102.35	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	692	ASN	CA-C-N	9.05	129.60	119.92
2	X	692	ASN	C-N-CA	9.05	129.60	119.92
1	D	174	THR	OG1-CB-CG2	-9.01	91.28	109.30
1	B	48	SER	N-CA-C	8.97	122.99	109.63
1	C	63	LYS	O-C-N	-8.91	110.74	122.59
2	Y	731	LYS	N-CA-C	8.81	120.65	111.14
2	X	814	ARG	N-CA-CB	8.80	123.06	110.12
2	Y	904	GLN	CA-C-N	-8.79	108.80	122.59
2	Y	904	GLN	C-N-CA	-8.79	108.80	122.59
1	D	48	SER	N-CA-C	8.72	122.63	109.63
2	X	655	ILE	N-CA-C	8.66	123.81	112.98
2	X	905	GLU	N-CA-C	8.64	119.66	108.34
2	Y	853	VAL	N-CA-CB	-8.53	97.21	110.86
2	X	759	ASP	CB-CA-C	-8.51	91.63	110.19
2	X	904	GLN	CA-C-N	-8.35	108.69	122.39
2	X	904	GLN	C-N-CA	-8.35	108.69	122.39
1	C	16	ILE	N-CA-C	8.28	119.21	108.12
2	X	787	GLN	CA-C-N	8.27	131.90	120.65
2	X	787	GLN	C-N-CA	8.27	131.90	120.65
2	Y	714	LEU	CA-C-N	-8.26	111.43	122.42
2	Y	714	LEU	C-N-CA	-8.26	111.43	122.42
2	X	879	ARG	NE-CZ-NH2	8.21	126.59	119.20
2	X	759	ASP	N-CA-C	-8.19	100.33	110.41
1	A	175	ASP	N-CA-C	8.15	120.89	111.11
1	A	39	GLY	CA-C-N	8.11	135.63	121.52
1	A	39	GLY	C-N-CA	8.11	135.63	121.52
2	Y	903	LEU	CA-C-N	8.07	132.93	120.75
2	Y	903	LEU	C-N-CA	8.07	132.93	120.75
2	Y	716	ASN	N-CA-CB	-8.06	96.87	110.49
1	C	13	GLU	CA-C-N	8.05	129.90	119.84
1	C	13	GLU	C-N-CA	8.05	129.90	119.84
1	B	26	LYS	CB-CA-C	-8.01	94.47	110.42
2	X	755	ALA	N-CA-C	-7.96	102.63	113.30
2	X	785	ASN	O-C-N	7.95	130.35	121.93
1	A	28	LEU	CD1-CG-CD2	-7.90	93.42	110.80
2	X	706	ASN	N-CA-C	7.89	120.43	107.73
1	A	199	LEU	CD1-CG-CD2	-7.88	93.46	110.80
1	C	179	ARG	NE-CZ-NH2	7.87	126.29	119.20
2	X	747	CYS	CA-C-N	7.87	127.79	119.05
2	X	747	CYS	C-N-CA	7.87	127.79	119.05
1	C	174	THR	OG1-CB-CG2	-7.84	93.62	109.30
1	B	197	LYS	N-CA-C	-7.83	102.36	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	696	ASP	CA-C-N	-7.83	110.23	121.42
2	X	696	ASP	C-N-CA	-7.83	110.23	121.42
2	X	657	ASN	N-CA-C	7.80	120.36	110.61
1	D	54	GLN	OE1-CD-NE2	-7.80	114.80	122.60
2	X	719	ASP	N-CA-C	-7.78	95.61	108.76
2	X	911	ILE	CA-CB-CG1	7.78	123.62	110.40
1	D	148	ASN	CB-CG-ND2	7.73	128.00	116.40
1	B	193	SER	CB-CA-C	-7.73	98.63	110.92
2	Y	861	SER	N-CA-C	-7.71	104.10	113.97
2	Y	741	ARG	CG-CD-NE	7.70	128.93	112.00
2	Y	905	GLU	N-CA-C	7.66	121.39	109.52
2	X	658	ILE	CB-CA-C	-7.65	98.74	111.29
1	A	101	LEU	O-C-N	-7.61	112.47	122.59
2	X	853	VAL	CA-CB-CG1	7.55	123.23	110.40
2	X	891	GLU	N-CA-C	-7.54	102.20	111.33
2	X	911	ILE	CB-CA-C	7.54	126.68	111.60
2	X	812	MET	CG-SD-CE	-7.54	84.31	100.90
1	C	200	ASN	CA-C-N	-7.54	108.13	121.70
1	C	200	ASN	C-N-CA	-7.54	108.13	121.70
2	Y	739	GLN	CA-C-N	7.44	129.15	119.84
2	Y	739	GLN	C-N-CA	7.44	129.15	119.84
1	D	8	ILE	CB-CG1-CD1	-7.36	98.34	113.80
1	C	22	VAL	CG1-CB-CG2	-7.34	94.64	110.80
1	A	62	GLU	CA-CB-CG	7.33	128.77	114.10
2	X	744	ILE	CB-CA-C	7.33	122.06	112.24
1	A	63	LYS	N-CA-C	7.33	120.20	111.33
2	Y	726	LEU	N-CA-C	-7.30	103.40	111.36
1	A	13	GLU	CA-C-N	7.29	128.96	119.84
1	A	13	GLU	C-N-CA	7.29	128.96	119.84
1	D	159	GLN	N-CA-C	-7.29	103.27	111.07
2	X	711	ASN	N-CA-C	7.29	119.30	111.36
1	C	82	ASP	N-CA-C	7.27	121.40	110.64
2	Y	759	ASP	N-CA-CB	-7.25	99.40	110.42
2	Y	792	MET	CA-CB-CG	-7.23	99.64	114.10
2	Y	724	ALA	N-CA-C	-7.22	103.45	111.82
1	A	168	ALA	N-CA-C	-7.21	103.51	111.36
2	X	752	GLU	N-CA-C	-7.20	105.02	113.88
1	A	189	THR	CA-C-O	7.20	128.41	120.63
1	D	175	ASP	N-CA-C	7.16	119.76	111.02
2	X	758	TYR	CA-C-N	7.15	134.50	121.06
2	X	758	TYR	C-N-CA	7.15	134.50	121.06
2	X	894	VAL	N-CA-C	-7.14	103.71	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	891	GLU	CA-CB-CG	7.11	128.32	114.10
1	C	158	VAL	CA-CB-CG2	-7.10	98.33	110.40
2	Y	758	TYR	CA-C-N	7.04	136.17	122.03
2	Y	758	TYR	C-N-CA	7.04	136.17	122.03
2	X	754	PHE	N-CA-C	7.01	121.49	113.15
2	Y	761	TYR	CA-C-N	-6.97	107.74	121.41
2	Y	761	TYR	C-N-CA	-6.97	107.74	121.41
1	B	85	THR	CB-CA-C	6.95	120.07	110.34
2	Y	791	GLU	N-CA-C	-6.95	103.78	111.36
1	B	16	ILE	N-CA-C	6.95	117.00	108.53
2	Y	711	ASN	CB-CA-C	6.94	123.64	109.55
1	A	175	ASP	N-CA-CB	-6.94	99.60	109.94
1	D	72	LYS	N-CA-C	-6.93	103.33	111.03
2	X	808	SER	CA-CB-OG	-6.93	97.24	111.10
2	Y	801	TYR	N-CA-C	-6.92	102.07	112.04
1	B	118	ASN	CB-CA-C	-6.92	103.27	110.33
2	Y	891	GLU	CA-CB-CG	6.92	127.93	114.10
2	Y	714	LEU	N-CA-C	-6.91	96.09	110.80
2	Y	895	THR	CB-CA-C	-6.90	99.95	110.92
1	D	190	LYS	N-CA-C	-6.90	103.69	111.14
2	Y	741	ARG	CD-NE-CZ	-6.90	114.75	124.40
1	A	126	LEU	CD1-CG-CD2	-6.89	95.63	110.80
1	C	145	GLN	CB-CG-CD	-6.87	100.92	112.60
2	Y	759	ASP	CB-CA-C	-6.83	97.59	110.51
2	X	722	LYS	N-CA-C	6.80	118.36	109.93
2	X	782	LYS	CA-C-O	6.77	127.72	120.95
2	Y	817	THR	N-CA-C	-6.75	97.97	109.24
1	A	179	ARG	NH1-CZ-NH2	-6.74	110.53	119.30
2	X	722	LYS	CB-CA-C	6.73	119.15	109.26
1	B	200	ASN	N-CA-C	6.71	119.95	111.69
1	C	62	GLU	CA-CB-CG	6.68	127.46	114.10
1	B	185	ASN	N-CA-C	6.67	120.28	111.75
2	Y	902	GLU	N-CA-CB	-6.66	99.20	110.99
2	Y	792	MET	CG-SD-CE	6.66	115.54	100.90
1	C	28	LEU	CD1-CG-CD2	-6.65	96.17	110.80
1	D	162	PHE	N-CA-C	-6.63	104.14	111.36
2	X	808	SER	CA-C-N	6.63	126.13	119.24
2	X	808	SER	C-N-CA	6.63	126.13	119.24
1	D	138	GLN	N-CA-C	6.62	119.34	111.33
2	X	814	ARG	CA-CB-CG	6.62	127.34	114.10
1	B	47	VAL	N-CA-C	6.61	115.85	106.53
1	D	136	GLU	CB-CA-C	-6.58	99.87	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	893	TRP	N-CA-C	6.58	119.00	111.11
1	C	147	GLU	OE1-CD-OE2	-6.56	107.15	122.90
1	D	148	ASN	CB-CG-OD1	-6.56	107.67	120.80
2	X	778	PHE	CA-C-O	6.55	127.49	120.55
1	D	185	ASN	N-CA-C	6.55	118.42	111.28
2	Y	897	SER	CA-C-N	-6.54	112.90	120.88
2	Y	897	SER	C-N-CA	-6.54	112.90	120.88
1	D	16	ILE	N-CA-C	6.54	116.51	108.53
2	X	668	SER	N-CA-C	6.54	118.89	109.14
1	D	117	GLU	CB-CG-CD	-6.53	101.49	112.60
2	X	773	GLN	CB-CA-C	6.53	121.78	110.68
2	Y	712	ILE	N-CA-C	-6.52	102.94	111.09
2	Y	749	SER	N-CA-C	6.50	121.41	112.90
2	X	853	VAL	CB-CA-C	6.49	120.49	110.50
2	X	667	MET	CG-SD-CE	-6.49	86.63	100.90
2	X	781	ILE	CB-CA-C	6.49	121.93	111.29
2	X	898	ILE	N-CA-C	-6.49	104.17	110.72
1	B	32	PHE	N-CA-C	6.46	118.37	108.42
1	C	200	ASN	O-C-N	-6.43	114.03	122.59
1	A	190	LYS	N-CA-CB	-6.42	100.62	110.13
1	D	170	GLU	N-CA-C	6.42	119.10	111.33
2	X	702	ALA	CB-CA-C	-6.42	102.65	111.95
2	X	842	ALA	N-CA-C	-6.41	104.29	111.28
1	B	156	ASN	N-CA-C	-6.39	103.83	111.69
1	C	179	ARG	NH1-CZ-NH2	-6.38	111.00	119.30
2	X	864	ILE	CA-C-N	6.35	131.78	121.62
2	X	864	ILE	C-N-CA	6.35	131.78	121.62
1	C	70	LEU	N-CA-C	6.35	118.20	111.28
1	C	191	ILE	CB-CG1-CD1	6.34	127.11	113.80
2	Y	730	PHE	N-CA-C	-6.33	103.68	111.40
1	D	85	THR	CB-CA-C	6.32	120.55	109.80
2	X	761	TYR	CA-C-N	-6.32	111.89	122.25
2	X	761	TYR	C-N-CA	-6.32	111.89	122.25
2	X	843	LEU	N-CA-C	6.31	118.15	111.28
2	X	764	SER	CB-CA-C	-6.30	100.07	109.90
1	D	173	GLU	N-CA-C	6.29	117.80	111.07
2	X	770	ASP	CB-CA-C	-6.29	98.83	111.17
1	A	70	LEU	N-CA-C	6.29	118.66	111.11
1	D	157	ASP	N-CA-C	6.29	117.93	111.14
2	Y	707	ILE	CB-CG1-CD1	-6.29	100.60	113.80
2	X	842	ALA	CA-C-N	-6.28	111.87	120.28
2	X	842	ALA	C-N-CA	-6.28	111.87	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	GLY	N-CA-C	-6.28	105.74	112.08
2	X	715	SER	CA-C-N	-6.28	111.27	123.13
2	X	715	SER	C-N-CA	-6.28	111.27	123.13
1	A	22	VAL	N-CA-CB	6.27	119.49	112.34
1	A	150	ARG	NE-CZ-NH2	6.25	124.82	119.20
1	A	171	ALA	N-CA-C	-6.23	104.95	113.30
2	Y	689	ILE	CB-CA-C	6.22	119.89	110.62
2	Y	874	ASP	N-CA-C	6.21	117.74	110.97
1	B	161	ARG	CB-CG-CD	-6.20	97.04	111.30
2	Y	848	HIS	O-C-N	6.20	130.13	122.20
2	X	840	ILE	CA-CB-CG1	-6.17	99.91	110.40
2	Y	696	ASP	CB-CA-C	-6.16	99.15	109.75
1	A	190	LYS	N-CA-C	-6.12	103.93	111.40
1	A	165	CYS	N-CA-C	6.12	118.03	111.36
1	D	172	LEU	CD1-CG-CD2	-6.11	97.36	110.80
2	X	884	ARG	CA-C-N	-6.10	113.72	122.68
2	X	884	ARG	C-N-CA	-6.10	113.72	122.68
2	X	867	GLU	N-CA-C	6.09	118.00	111.36
2	X	843	LEU	N-CA-CB	6.09	119.07	110.12
1	B	90	LYS	CA-C-N	6.08	128.70	120.44
1	B	90	LYS	C-N-CA	6.08	128.70	120.44
1	A	63	LYS	O-C-N	-6.07	115.69	122.12
1	A	193	SER	N-CA-C	-6.07	104.00	111.40
2	X	812	MET	N-CA-CB	-6.07	101.21	110.01
2	X	837	ARG	NE-CZ-NH2	-6.04	113.77	119.20
1	B	152	LEU	N-CA-C	6.03	117.86	111.28
1	B	179	ARG	NE-CZ-NH1	-6.03	115.47	121.50
2	X	784	SER	N-CA-C	-6.03	97.96	110.80
1	B	178	LYS	N-CA-C	-6.02	104.80	111.36
1	A	147	GLU	CB-CA-C	-6.01	100.63	110.85
2	X	840	ILE	N-CA-C	6.00	118.55	111.05
2	X	731	LYS	N-CA-C	5.99	117.81	111.28
1	D	32	PHE	N-CA-C	5.98	117.63	108.42
1	B	189	THR	N-CA-CB	-5.98	101.04	109.94
2	X	839	ALA	N-CA-C	-5.97	104.68	111.07
1	D	6	SER	N-CA-C	5.94	118.18	108.55
1	B	173	GLU	N-CA-CB	5.94	118.63	110.01
1	A	148	ASN	CA-C-N	5.93	128.55	120.54
1	A	148	ASN	C-N-CA	5.93	128.55	120.54
1	D	190	LYS	CD-CE-NZ	5.93	130.88	111.90
1	D	176	LEU	N-CA-C	5.93	117.41	111.07
2	Y	741	ARG	CB-CA-C	-5.93	98.63	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	657	ASN	N-CA-C	-5.92	103.78	111.71
1	D	26	LYS	N-CA-C	5.88	123.33	110.80
1	C	175	ASP	CB-CA-C	-5.84	101.46	110.81
1	B	180	PHE	CB-CA-C	-5.84	101.14	110.84
2	X	775	LYS	N-CA-C	-5.84	104.83	111.14
2	X	658	ILE	CB-CG1-CD1	-5.82	101.57	113.80
1	D	136	GLU	CA-CB-CG	5.82	125.74	114.10
2	X	689	ILE	CB-CA-C	5.82	119.53	111.38
2	Y	691	GLN	N-CA-CB	5.82	119.26	110.30
1	D	179	ARG	CG-CD-NE	-5.80	99.24	112.00
1	C	157	ASP	N-CA-CB	-5.77	101.61	109.98
2	X	686	GLY	CA-C-N	-5.76	117.01	122.66
2	X	686	GLY	C-N-CA	-5.76	117.01	122.66
2	Y	871	ARG	CA-C-N	-5.76	111.08	120.64
2	Y	871	ARG	C-N-CA	-5.76	111.08	120.64
2	X	818	VAL	N-CA-C	5.75	116.16	108.11
1	D	24	TRP	N-CA-C	5.75	117.52	108.96
1	A	197	LYS	N-CA-C	-5.74	105.16	111.82
1	B	118	ASN	N-CA-CB	5.74	119.36	110.12
1	B	173	GLU	CB-CA-C	-5.74	101.87	110.88
1	D	163	GLU	CG-CD-OE2	5.74	131.60	118.40
2	X	841	LYS	CD-CE-NZ	-5.73	93.56	111.90
1	D	8	ILE	N-CA-C	5.73	116.95	108.65
2	X	781	ILE	O-C-N	-5.73	115.41	122.57
1	C	189	THR	N-CA-C	5.72	117.19	111.07
2	Y	715	SER	CA-C-O	5.72	126.70	120.58
1	A	145	GLN	CB-CG-CD	-5.72	102.88	112.60
2	Y	874	ASP	N-CA-CB	-5.72	101.56	109.91
1	B	160	GLY	N-CA-C	-5.71	105.30	113.86
2	Y	660	GLU	N-CA-C	-5.70	102.05	110.48
2	Y	708	ARG	N-CA-C	-5.70	105.07	111.28
1	D	90	LYS	CA-C-N	5.70	128.38	120.29
1	D	90	LYS	C-N-CA	5.70	128.38	120.29
1	B	21	GLN	CA-C-N	-5.69	115.73	123.12
1	B	21	GLN	C-N-CA	-5.69	115.73	123.12
2	Y	697	THR	N-CA-C	-5.63	101.52	109.96
1	C	121	GLU	N-CA-C	5.62	120.13	112.04
1	D	173	GLU	CB-CA-C	-5.62	102.06	110.88
1	C	74	LEU	N-CA-C	5.61	120.13	113.28
2	X	813	PHE	N-CA-C	5.58	118.88	112.97
2	X	781	ILE	CA-CB-CG2	5.57	119.97	110.50
2	X	781	ILE	N-CA-C	5.57	120.92	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	880	ARG	N-CA-CB	5.56	118.78	110.22
1	A	22	VAL	CG1-CB-CG2	-5.55	98.59	110.80
1	C	145	GLN	N-CA-C	-5.55	105.14	111.14
2	Y	839	ALA	N-CA-C	-5.55	105.13	111.07
1	A	16	ILE	N-CA-C	5.55	120.88	109.34
1	C	28	LEU	N-CA-C	-5.55	105.24	112.23
1	D	179	ARG	NE-CZ-NH2	5.55	124.19	119.20
2	Y	891	GLU	CB-CA-C	-5.54	99.39	110.42
1	A	179	ARG	N-CA-C	-5.54	104.65	111.40
1	D	47	VAL	N-CA-C	5.54	114.33	106.53
2	X	788	THR	N-CA-C	5.53	117.44	109.48
1	D	197	LYS	N-CA-C	-5.52	105.42	111.82
1	A	174	THR	OG1-CB-CG2	-5.52	98.26	109.30
2	X	827	ASN	N-CA-C	-5.52	105.89	113.56
1	C	165	CYS	N-CA-C	5.51	117.37	111.36
1	D	17	THR	N-CA-C	5.51	117.94	109.07
2	X	784	SER	CA-C-O	5.51	128.39	120.51
1	D	192	ARG	CB-CG-CD	5.50	123.96	111.30
1	C	15	SER	CB-CA-C	5.50	120.50	110.11
2	X	814	ARG	CG-CD-NE	-5.50	99.91	112.00
1	A	17	THR	N-CA-C	5.50	117.82	110.35
2	X	836	THR	N-CA-C	-5.49	99.36	108.75
1	B	195	HIS	N-CA-C	-5.48	104.71	111.40
1	A	163	GLU	N-CA-C	5.48	117.96	111.33
2	X	662	VAL	N-CA-C	-5.48	100.23	108.12
2	Y	791	GLU	O-C-N	5.47	128.39	122.15
1	B	172	LEU	CD1-CG-CD2	-5.47	98.76	110.80
1	C	125	GLU	N-CA-C	-5.47	105.23	111.14
1	C	149	GLU	N-CA-C	5.45	117.22	111.28
1	D	179	ARG	N-CA-C	5.44	117.29	111.36
2	X	665	CYS	N-CA-C	5.43	117.60	108.96
1	A	163	GLU	OE1-CD-OE2	-5.43	109.86	122.90
1	C	53	SER	CA-C-N	5.42	129.66	120.88
1	C	53	SER	C-N-CA	5.42	129.66	120.88
2	X	804	SER	CB-CA-C	-5.42	104.03	111.73
2	Y	743	MET	CG-SD-CE	-5.42	88.98	100.90
1	B	134	THR	OG1-CB-CG2	-5.41	98.47	109.30
1	C	18	HIS	N-CA-C	-5.40	100.86	109.07
1	B	41	SER	N-CA-C	5.39	118.36	109.85
1	C	186	GLU	CB-CA-C	-5.39	101.69	110.85
1	C	126	LEU	CD1-CG-CD2	-5.38	98.95	110.80
2	X	885	LYS	CA-C-N	5.38	128.74	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	885	LYS	C-N-CA	5.38	128.74	120.82
1	D	138	GLN	CA-CB-CG	-5.38	103.34	114.10
2	X	891	GLU	CB-CA-C	-5.38	101.53	110.68
1	C	175	ASP	N-CA-C	5.38	117.56	111.11
2	X	717	LYS	CB-CG-CD	5.37	123.66	111.30
1	A	200	ASN	O-C-N	-5.36	115.42	122.39
2	X	794	SER	CB-CA-C	-5.36	101.74	110.85
2	Y	769	THR	N-CA-C	5.34	117.72	110.35
1	A	154	ASP	OD1-CG-OD2	-5.34	110.08	122.90
2	X	707	ILE	CB-CA-C	5.34	119.01	112.02
2	Y	798	ASP	N-CA-C	5.34	117.10	111.28
2	Y	765	TYR	N-CA-C	5.33	117.09	111.28
1	A	31	GLY	CA-C-O	-5.32	118.49	122.37
1	D	134	THR	OG1-CB-CG2	-5.32	98.66	109.30
1	D	159	GLN	CA-CB-CG	5.31	124.73	114.10
1	C	145	GLN	N-CA-CB	-5.31	102.37	110.07
2	Y	874	ASP	CA-CB-CG	-5.30	107.30	112.60
2	Y	709	VAL	N-CA-C	-5.29	105.56	110.53
2	X	782	LYS	N-CA-CB	5.28	117.42	109.34
1	A	145	GLN	N-CA-CB	-5.27	102.36	110.16
1	A	200	ASN	CB-CA-C	5.27	121.44	110.32
1	A	188	LYS	N-CA-C	-5.26	105.60	112.23
1	A	169	LYS	CD-CE-NZ	5.26	128.73	111.90
1	D	4	LYS	CD-CE-NZ	-5.26	95.07	111.90
1	B	24	TRP	N-CA-C	5.26	116.79	108.96
2	X	754	PHE	CB-CA-C	-5.26	100.64	110.36
2	X	713	ILE	N-CA-C	5.25	115.98	110.62
1	B	151	LEU	CD1-CG-CD2	-5.25	99.25	110.80
2	X	655	ILE	CB-CG1-CD1	-5.25	102.78	113.80
2	X	772	ASN	CA-C-N	5.25	127.57	120.38
2	X	772	ASN	C-N-CA	5.25	127.57	120.38
2	X	678	LEU	N-CA-C	-5.25	105.64	111.36
2	Y	671	ASP	N-CA-CB	-5.24	101.63	110.49
1	C	17	THR	N-CA-C	5.24	117.47	110.35
2	X	684	GLU	N-CA-C	5.24	119.42	113.19
2	Y	829	LEU	CA-CB-CG	-5.22	98.02	116.30
2	Y	885	LYS	N-CA-CB	-5.22	101.92	110.43
1	B	193	SER	CA-C-O	-5.22	115.33	121.07
1	B	89	SER	N-CA-C	5.21	117.56	108.76
1	D	59	MET	CG-SD-CE	5.21	112.36	100.90
2	Y	881	THR	CA-C-N	5.20	130.03	121.39
2	Y	881	THR	C-N-CA	5.20	130.03	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	VAL	N-CA-C	-5.20	101.58	108.96
2	Y	711	ASN	N-CA-C	5.20	119.67	113.23
2	X	860	VAL	CB-CA-C	5.19	119.79	111.32
2	X	716	ASN	N-CA-C	-5.19	104.23	110.88
2	Y	681	ARG	CA-C-N	-5.19	114.02	120.56
2	Y	681	ARG	C-N-CA	-5.19	114.02	120.56
1	C	63	LYS	CA-C-N	-5.19	111.24	121.41
1	C	63	LYS	C-N-CA	-5.19	111.24	121.41
2	X	707	ILE	N-CA-C	5.18	115.40	110.53
2	X	796	ILE	CA-CB-CG1	-5.18	101.59	110.40
1	A	149	GLU	N-CA-C	5.18	117.32	111.11
2	Y	911	ILE	N-CA-C	5.17	125.49	111.00
1	A	186	GLU	CB-CA-C	-5.17	102.22	110.79
1	C	170	GLU	N-CA-C	-5.16	106.49	112.89
1	A	61	MET	CG-SD-CE	5.16	112.25	100.90
2	Y	744	ILE	N-CA-C	5.16	115.93	110.72
1	B	155	TRP	N-CA-C	-5.15	105.85	111.82
2	Y	879	ARG	N-CA-C	5.15	117.29	111.11
2	X	884	ARG	CB-CA-C	5.15	119.49	110.64
2	X	787	GLN	CA-CB-CG	-5.14	103.81	114.10
1	D	156	ASN	N-CA-C	-5.14	105.75	112.23
2	X	808	SER	CB-CA-C	-5.13	101.41	109.52
1	A	6	SER	N-CA-C	-5.13	99.61	108.69
1	B	184	LEU	CB-CA-C	-5.13	102.83	110.88
2	X	832	LYS	CA-C-O	-5.13	115.08	120.92
2	Y	884	ARG	CA-C-O	5.12	125.89	120.36
1	A	40	HIS	N-CA-C	-5.12	108.30	114.75
2	Y	794	SER	CA-CB-OG	-5.12	100.86	111.10
2	X	768	ASP	N-CA-C	-5.11	102.82	110.23
1	C	167	SER	CB-CA-C	-5.10	102.87	110.88
1	A	173	GLU	CG-CD-OE1	5.10	130.14	118.40
2	Y	656	SER	N-CA-C	-5.10	100.38	108.14
1	D	192	ARG	CA-CB-CG	5.10	124.29	114.10
1	D	37	THR	N-CA-C	5.08	116.79	109.07
1	A	124	ARG	CD-NE-CZ	5.08	131.51	124.40
1	B	103	ASP	N-CA-C	5.08	121.61	110.80
1	A	154	ASP	CB-CG-OD1	5.08	130.07	118.40
1	D	91	GLU	N-CA-C	5.07	116.89	111.36
1	D	192	ARG	N-CA-CB	-5.07	102.66	110.16
1	B	4	LYS	N-CA-C	5.06	116.62	108.32
1	D	194	LEU	CA-C-N	5.06	127.37	120.54
1	D	194	LEU	C-N-CA	5.06	127.37	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	750	THR	N-CA-C	-5.05	105.66	111.07
2	X	775	LYS	N-CA-CB	-5.05	102.74	110.07
1	D	103	ASP	N-CA-C	5.05	121.56	110.80
1	A	82	ASP	N-CA-C	5.04	121.54	110.80
1	C	174	THR	N-CA-C	5.03	117.66	111.82
1	B	89	SER	CA-C-N	5.03	127.53	120.28
1	B	89	SER	C-N-CA	5.03	127.53	120.28
1	C	154	ASP	CB-CG-OD2	5.03	129.97	118.40
2	X	895	THR	CB-CA-C	-5.03	102.99	110.88
2	X	770	ASP	N-CA-C	-5.01	101.28	108.60
1	C	9	HIS	N-CA-C	-5.01	99.83	108.69
2	X	871	ARG	N-CA-C	5.01	119.37	113.16
1	A	124	ARG	CG-CD-NE	5.01	123.02	112.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	X	911	ILE	CA

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	GLU	Peptide
1	A	26	LYS	Peptide
1	A	39	GLY	Peptide
1	B	82	ASP	Peptide
1	B	83	VAL	Peptide
1	C	127	ILE	Peptide
1	C	25	GLU	Peptide
1	C	26	LYS	Peptide
1	D	60	GLU	Peptide
2	X	668	SER	Peptide
2	X	669	GLY	Peptide
2	X	673	GLN	Peptide
2	X	701	ILE	Peptide
2	X	746	MET	Peptide
2	X	759	ASP	Mainchain
2	X	781	ILE	Peptide
2	X	783	ASN	Peptide
2	X	784	SER	Peptide
2	X	785	ASN	Peptide
2	X	813	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	X	884	ARG	Peptide
2	X	905	GLU	Peptide
2	X	910	LEU	Peptide
2	Y	668	SER	Peptide
2	Y	670	THR	Peptide
2	Y	671	ASP	Peptide
2	Y	713	ILE	Peptide
2	Y	714	LEU	Peptide
2	Y	817	THR	Peptide
2	Y	830	SER	Peptide
2	Y	833	ASN	Peptide
2	Y	859	GLY	Peptide
2	Y	881	THR	Peptide
2	Y	903	LEU	Peptide
2	Y	905	GLU	Peptide

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	1631	0	1617	90	0
1	B	1606	0	1593	151	0
1	C	1631	0	1617	98	0
1	D	1598	0	1589	144	0
2	X	2081	0	2036	198	0
2	Y	2095	0	2046	151	0
3	Y	2	0	0	0	0
4	A	44	0	0	2	0
4	B	25	0	0	2	0
4	C	41	0	0	4	0
4	D	29	0	0	5	0
4	X	83	0	0	3	0
4	Y	59	0	0	3	0
All	All	10925	0	10498	780	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 37.

All (780) 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:X:846:ARG:CD	2:X:846:ARG:CG	1.75	1.61
1:B:82:ASP:N	1:B:83:VAL:HG23	1.09	1.36
1:A:127:ILE:HD11	1:B:127:ILE:CD1	1.65	1.27
1:B:82:ASP:N	1:B:83:VAL:CG2	1.95	1.26
1:C:40:HIS:CD2	1:D:120:ALA:HB2	1.73	1.22
1:B:119:PRO:O	1:B:123:ILE:HD12	1.37	1.22
1:D:49:GLU:O	1:D:49:GLU:HG3	1.39	1.18
1:A:127:ILE:CD1	1:B:127:ILE:HD11	1.76	1.15
2:X:673:GLN:N	2:X:674:PRO:HD3	1.47	1.13
2:X:717:LYS:HG2	2:X:718:HIS:CE1	1.84	1.12
1:C:44:THR:HG22	1:C:45:GLY:H	0.96	1.12
2:X:719:ASP:HB2	2:X:747:CYS:HB3	1.30	1.12
2:Y:671:ASP:HB2	2:Y:672:SER:HB2	1.30	1.12
1:D:192:ARG:HB2	1:D:192:ARG:HH11	1.12	1.12
2:X:673:GLN:O	2:X:673:GLN:HG2	1.52	1.10
1:C:40:HIS:HD2	1:D:120:ALA:HB2	0.96	1.09
1:A:44:THR:HG22	1:A:45:GLY:H	0.95	1.08
1:C:140:LYS:HE2	4:C:209:HOH:O	1.49	1.08
1:B:65:LYS:O	1:B:65:LYS:HG2	1.51	1.07
1:D:119:PRO:O	1:D:123:ILE:HD12	1.54	1.06
1:A:104:VAL:HG23	1:A:106:PHE:CE1	1.92	1.04
1:B:86:PHE:C	1:B:87:ASN:HD22	1.64	1.04
2:X:711:ASN:C	2:X:711:ASN:HD22	1.65	1.04
1:A:44:THR:CG2	1:A:45:GLY:H	1.69	1.03
1:C:123:ILE:O	1:C:127:ILE:HG23	1.56	1.03
2:X:663:GLU:OE1	2:X:697:THR:HG22	1.58	1.03
1:C:40:HIS:HD2	1:D:120:ALA:CB	1.72	1.02
2:Y:878:PHE:CE1	2:Y:882:PHE:HE2	1.78	1.02
2:X:719:ASP:OD1	2:X:750:THR:HG21	1.58	1.02
1:A:127:ILE:HG12	1:B:127:ILE:HG12	1.41	1.02
1:D:192:ARG:HH11	1:D:192:ARG:CB	1.73	1.02
2:Y:905:GLU:HB3	4:Y:117:HOH:O	1.57	1.02
2:Y:732:THR:CG2	2:Y:734:SER:HB3	1.90	1.01
2:Y:732:THR:HG22	2:Y:734:SER:HB3	1.41	1.01
1:D:197:LYS:HE3	4:D:269:HOH:O	1.60	1.01
1:C:44:THR:HG22	1:C:45:GLY:N	1.75	1.01
1:C:44:THR:CG2	1:C:45:GLY:H	1.73	1.00
1:D:107:ARG:HD3	1:D:108:LEU:H	1.26	1.00
2:X:785:ASN:C	2:X:787:GLN:H	1.64	1.00
2:X:702:ALA:HB3	2:X:744:ILE:HD11	1.44	1.00
1:D:92:SER:O	1:D:93:CYS:HB2	1.61	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:PHE:C	1:D:87:ASN:HD22	1.72	0.98
2:X:836:THR:HG22	2:X:838:LEU:H	1.28	0.98
1:A:44:THR:HG22	1:A:45:GLY:N	1.71	0.97
2:Y:660:GLU:HA	2:Y:686:GLY:O	1.65	0.97
2:X:812:MET:HE1	2:X:897:SER:C	1.90	0.96
2:X:910:LEU:C	2:X:911:ILE:HG23	1.90	0.95
2:X:679:GLU:HB3	2:X:689:ILE:HD13	1.48	0.95
2:X:759:ASP:HB3	2:X:761:TYR:H	1.32	0.95
2:X:673:GLN:N	2:X:674:PRO:CD	2.30	0.94
2:X:792:MET:HE2	2:X:792:MET:HA	1.50	0.94
2:Y:759:ASP:HB3	2:Y:761:TYR:O	1.67	0.94
1:B:130:CYS:O	1:B:134:THR:HG22	1.68	0.93
2:X:667:MET:HE3	2:X:709:VAL:HG22	1.49	0.93
2:X:812:MET:CE	2:X:897:SER:HB3	1.98	0.93
1:B:83:VAL:HG11	1:B:100:ASN:O	1.67	0.92
1:B:107:ARG:HD3	1:B:108:LEU:H	1.35	0.92
2:X:739:GLN:HE22	2:X:741:ARG:HH21	1.07	0.91
2:X:660:GLU:HA	2:X:686:GLY:O	1.69	0.91
1:D:59:MET:O	1:D:60:GLU:HB2	1.69	0.90
1:C:120:ALA:HB2	1:D:40:HIS:HB2	1.54	0.90
2:X:711:ASN:C	2:X:711:ASN:ND2	2.28	0.90
1:B:20:LEU:HD11	1:B:34:ILE:HD11	1.54	0.89
1:B:83:VAL:CG1	1:B:100:ASN:O	2.21	0.89
2:X:658:ILE:CG2	2:X:735:PHE:HB2	2.04	0.88
1:B:16:ILE:CG2	1:B:17:THR:N	2.37	0.87
2:X:910:LEU:C	2:X:911:ILE:CG2	2.47	0.86
1:B:16:ILE:HG23	1:B:17:THR:H	1.40	0.86
1:D:20:LEU:HD11	1:D:34:ILE:HD11	1.57	0.86
2:Y:878:PHE:CE1	2:Y:882:PHE:CE2	2.64	0.85
1:D:88:PHE:HB2	1:D:95:PHE:HD2	1.40	0.85
2:Y:728:GLU:O	2:Y:732:THR:HB	1.77	0.85
2:Y:732:THR:CG2	2:Y:734:SER:CB	2.55	0.85
2:Y:654:LYS:HG3	2:Y:655:ILE:H	1.40	0.85
1:D:16:ILE:HG23	1:D:17:THR:N	1.92	0.85
2:Y:878:PHE:HE1	2:Y:882:PHE:HE2	1.21	0.84
1:C:124:ARG:HG3	1:C:124:ARG:HH11	1.41	0.84
2:Y:819:TYR:O	2:Y:863:VAL:HA	1.77	0.84
1:C:131:LEU:HD21	1:D:5:ILE:HG22	1.57	0.84
1:A:24:TRP:CD1	1:A:27:THR:O	2.31	0.84
2:Y:732:THR:HG22	2:Y:734:SER:CB	2.06	0.83
1:A:118:ASN:O	1:A:118:ASN:ND2	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:904:GLN:O	2:Y:905:GLU:HG3	1.79	0.83
1:D:192:ARG:HB2	1:D:192:ARG:NH1	1.93	0.83
2:X:739:GLN:NE2	2:X:741:ARG:HH21	1.75	0.83
1:C:118:ASN:O	1:C:118:ASN:ND2	2.10	0.83
2:X:846:ARG:HG3	2:X:852:VAL:HG13	1.60	0.83
2:X:670:THR:HA	2:X:675:LYS:H	1.44	0.82
1:B:92:SER:O	1:B:93:CYS:HB2	1.78	0.82
1:D:63:LYS:O	1:D:67:VAL:HB	1.80	0.82
1:B:89:SER:HB3	1:B:91:GLU:OE1	1.78	0.82
2:X:706:ASN:ND2	2:X:709:VAL:HG23	1.95	0.82
2:Y:820:LEU:HD13	2:Y:864:ILE:HB	1.61	0.82
1:A:22:VAL:HG12	1:A:34:ILE:HG12	1.62	0.81
1:A:24:TRP:HD1	1:A:27:THR:O	1.63	0.81
1:D:170:GLU:O	1:D:174:THR:HG22	1.80	0.81
1:D:49:GLU:O	1:D:49:GLU:CG	2.24	0.81
2:X:722:LYS:HE2	2:X:741:ARG:O	1.80	0.81
2:X:780:GLY:O	2:X:781:ILE:CG1	2.29	0.81
1:D:65:LYS:O	1:D:69:GLU:CG	2.29	0.80
1:D:116:VAL:HG12	1:D:117:GLU:H	1.44	0.80
1:C:104:VAL:HG23	1:C:106:PHE:CE1	2.16	0.80
2:X:910:LEU:HB3	2:X:911:ILE:HG23	1.61	0.80
2:Y:889:LEU:HD21	2:Y:906:GLU:HB2	1.63	0.80
1:A:88:PHE:CE1	1:A:113:LEU:HD12	2.17	0.80
1:B:116:VAL:HG12	1:B:117:GLU:H	1.47	0.79
1:B:61:MET:HE3	1:B:62:GLU:HG2	1.64	0.79
1:C:120:ALA:CB	1:D:40:HIS:HB2	2.12	0.79
1:D:186:GLU:HG3	2:Y:759:ASP:OD2	1.81	0.79
2:X:706:ASN:C	2:X:706:ASN:HD22	1.90	0.79
1:C:26:LYS:HG2	1:C:26:LYS:O	1.81	0.79
1:C:128:CYS:SG	1:D:19:PHE:HZ	2.05	0.79
1:C:28:LEU:HD13	1:C:75:LEU:HD11	1.65	0.79
2:X:910:LEU:HB3	2:X:911:ILE:CG2	2.12	0.79
2:Y:706:ASN:O	2:Y:710:LYS:HD3	1.83	0.78
2:Y:710:LYS:HD2	2:Y:710:LYS:N	1.99	0.78
2:X:786:GLU:O	2:X:787:GLN:HG3	1.84	0.78
1:B:83:VAL:O	1:B:83:VAL:HG12	1.82	0.78
2:X:660:GLU:O	2:X:661:ASP:HB2	1.82	0.78
2:X:846:ARG:HG3	2:X:852:VAL:CG1	2.14	0.77
1:B:83:VAL:HG13	1:B:100:ASN:HB2	1.66	0.77
2:Y:787:GLN:HB3	2:Y:792:MET:HG3	1.66	0.77
1:C:128:CYS:HG	1:D:19:PHE:HZ	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:878:PHE:HE1	2:Y:882:PHE:CE2	1.99	0.77
1:B:4:LYS:HD2	1:B:75:LEU:HB3	1.67	0.77
1:B:59:MET:HE3	1:B:59:MET:HA	1.66	0.77
1:B:86:PHE:C	1:B:87:ASN:ND2	2.43	0.76
2:X:785:ASN:C	2:X:787:GLN:N	2.30	0.76
1:C:127:ILE:CG1	1:C:127:ILE:O	2.30	0.76
1:D:89:SER:HB3	1:D:91:GLU:OE1	1.86	0.76
2:X:846:ARG:CD	2:X:846:ARG:CB	2.63	0.76
2:Y:705:GLU:HG3	2:Y:710:LYS:HE2	1.68	0.76
1:B:88:PHE:HB2	1:B:95:PHE:HD2	1.50	0.76
2:Y:706:ASN:ND2	2:Y:709:VAL:HG23	2.01	0.76
1:A:44:THR:O	1:A:113:LEU:HA	1.86	0.75
1:D:16:ILE:CG2	1:D:17:THR:N	2.49	0.75
1:B:16:ILE:CG2	1:B:17:THR:H	1.97	0.75
1:A:104:VAL:HG23	1:A:106:PHE:CZ	2.22	0.75
2:X:667:MET:CE	2:X:709:VAL:HG22	2.16	0.75
2:X:823:TYR:CE2	2:X:832:LYS:HG2	2.22	0.75
1:A:34:ILE:CG2	1:A:34:ILE:O	2.34	0.75
2:X:658:ILE:HG22	2:X:735:PHE:HB2	1.66	0.74
2:Y:654:LYS:HG3	2:Y:655:ILE:N	2.02	0.74
2:Y:862:HIS:HD2	2:Y:889:LEU:CD1	2.00	0.74
1:D:65:LYS:O	1:D:69:GLU:HB2	1.88	0.74
2:X:782:LYS:HG3	2:X:783:ASN:H	1.52	0.74
1:C:44:THR:O	1:C:113:LEU:HA	1.88	0.73
1:D:107:ARG:HD3	1:D:108:LEU:N	2.02	0.73
1:D:87:ASN:HB2	1:D:96:PHE:CZ	2.23	0.73
2:X:673:GLN:O	2:X:673:GLN:CG	2.30	0.73
2:Y:823:TYR:OH	2:Y:832:LYS:NZ	2.22	0.73
1:B:53:SER:HB3	1:B:63:LYS:NZ	2.04	0.73
2:Y:887:LYS:HE2	2:Y:906:GLU:HG3	1.70	0.73
1:A:198:LEU:HD21	1:B:197:LYS:HG2	1.71	0.72
1:D:3:ARG:HG2	1:D:4:LYS:N	2.04	0.72
1:B:87:ASN:HB2	1:B:96:PHE:CZ	2.24	0.72
1:A:131:LEU:HD21	1:B:5:ILE:HG22	1.71	0.72
1:B:16:ILE:HG22	1:B:17:THR:N	2.03	0.72
1:A:127:ILE:CG1	1:B:127:ILE:HG12	2.18	0.72
2:X:780:GLY:O	2:X:781:ILE:HG12	1.87	0.72
1:B:138:GLN:O	1:B:142:GLU:HG3	1.90	0.72
2:Y:671:ASP:HB2	2:Y:672:SER:CB	2.14	0.72
2:Y:862:HIS:HD2	2:Y:889:LEU:HD12	1.54	0.71
2:Y:876:LYS:NZ	2:Y:911:ILE:HG12	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:SER:O	1:A:111:PHE:CD2	2.43	0.71
1:A:147:GLU:OE1	1:A:150:ARG:NH2	2.23	0.71
1:B:52:ILE:CG2	1:B:53:SER:N	2.54	0.71
1:A:127:ILE:HD11	1:B:127:ILE:HD11	0.80	0.71
2:X:706:ASN:ND2	2:X:709:VAL:H	1.88	0.71
1:A:127:ILE:O	1:A:127:ILE:HG22	1.89	0.71
1:B:69:GLU:OE2	1:B:72:LYS:NZ	2.25	0.70
1:D:65:LYS:O	1:D:69:GLU:CB	2.39	0.70
2:Y:823:TYR:CE1	2:Y:832:LYS:NZ	2.59	0.70
2:Y:887:LYS:HD3	2:Y:910:LEU:HD21	1.73	0.70
2:X:792:MET:CE	2:X:795:LEU:HD12	2.22	0.70
2:X:879:ARG:HB2	2:X:886:PHE:CZ	2.27	0.70
2:Y:828:ASP:O	2:Y:830:SER:N	2.25	0.70
1:C:124:ARG:NH1	1:D:38:ASP:O	2.25	0.69
2:Y:716:ASN:OD1	2:Y:745:HIS:HE1	1.75	0.69
2:Y:706:ASN:O	2:Y:710:LYS:CD	2.40	0.69
1:D:16:ILE:HG23	1:D:17:THR:H	1.55	0.69
1:B:8:ILE:HD13	1:B:20:LEU:HB2	1.75	0.69
1:D:192:ARG:NH2	4:D:212:HOH:O	2.24	0.69
1:C:131:LEU:HD21	1:D:5:ILE:CG2	2.22	0.69
1:A:18:HIS:HD2	1:A:36:LEU:HD11	1.57	0.69
1:B:134:THR:O	1:B:138:GLN:HG3	1.93	0.69
1:B:3:ARG:HG2	1:B:4:LYS:N	2.08	0.69
2:X:904:GLN:O	2:X:905:GLU:HG3	1.92	0.68
2:Y:819:TYR:HH	2:Y:823:TYR:HD2	1.41	0.68
1:B:131:LEU:HA	1:B:134:THR:CG2	2.23	0.68
1:A:127:ILE:CD1	1:B:127:ILE:CG1	2.71	0.68
1:D:68:GLY:HA2	1:D:71:ARG:HG2	1.74	0.68
2:X:702:ALA:CB	2:X:744:ILE:HD11	2.22	0.68
2:Y:713:ILE:O	2:Y:713:ILE:CG2	2.41	0.68
1:D:177:TYR:O	1:D:181:ILE:HG12	1.93	0.68
1:B:177:TYR:O	1:B:181:ILE:HG13	1.93	0.68
1:A:34:ILE:O	1:A:34:ILE:HG22	1.94	0.68
1:C:89:SER:O	1:C:93:CYS:HA	1.93	0.68
1:C:128:CYS:SG	1:D:19:PHE:CZ	2.85	0.67
2:X:706:ASN:ND2	2:X:706:ASN:C	2.51	0.67
1:B:63:LYS:O	1:B:67:VAL:HB	1.95	0.67
2:X:812:MET:HE2	2:X:897:SER:HB3	1.74	0.67
1:D:85:THR:HB	1:D:100:ASN:HD21	1.59	0.67
1:D:181:ILE:HD13	2:Y:799:LEU:HD11	1.76	0.67
2:X:657:ASN:HB2	2:X:660:GLU:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ILE:HG23	1:C:34:ILE:O	1.95	0.67
2:X:667:MET:HE3	2:X:709:VAL:CG2	2.25	0.67
1:A:127:ILE:CD1	1:B:127:ILE:CD1	2.53	0.67
1:D:10:LEU:HA	1:D:86:PHE:O	1.95	0.67
1:B:107:ARG:HD3	1:B:108:LEU:N	2.08	0.66
1:D:51:GLU:HA	1:D:54:GLN:HB3	1.77	0.66
1:D:86:PHE:C	1:D:87:ASN:ND2	2.48	0.66
1:A:124:ARG:HG3	1:A:124:ARG:HH11	1.59	0.66
1:D:62:GLU:C	1:D:64:GLY:H	2.01	0.66
2:X:711:ASN:ND2	2:X:711:ASN:O	2.27	0.66
1:A:18:HIS:CD2	1:A:36:LEU:HD11	2.30	0.66
1:A:104:VAL:CG2	1:A:106:PHE:CZ	2.79	0.66
2:Y:707:ILE:HA	2:Y:710:LYS:HG2	1.78	0.66
1:B:48:SER:O	1:B:52:ILE:HB	1.95	0.66
2:Y:671:ASP:CB	2:Y:672:SER:HB2	2.18	0.66
2:X:739:GLN:HE21	2:X:741:ARG:HE	1.43	0.66
2:X:657:ASN:HA	2:X:685:PHE:O	1.95	0.66
1:B:51:GLU:HA	1:B:54:GLN:HB3	1.77	0.65
1:C:127:ILE:O	1:C:127:ILE:HG12	1.95	0.65
1:B:62:GLU:C	1:B:64:GLY:H	2.05	0.65
1:D:73:ALA:HA	1:D:84:TYR:CD2	2.32	0.65
1:D:36:LEU:O	1:D:43:TRP:HE3	1.78	0.65
2:X:722:LYS:HB3	2:X:744:ILE:HD13	1.79	0.65
2:X:739:GLN:HE22	2:X:741:ARG:NH2	1.89	0.65
1:B:41:SER:HA	1:B:119:PRO:HB3	1.78	0.65
1:B:49:GLU:O	1:B:50:SER:HB2	1.96	0.65
2:X:905:GLU:HG2	2:X:906:GLU:HG3	1.79	0.65
2:X:783:ASN:HA	2:X:784:SER:OG	1.95	0.65
2:Y:657:ASN:ND2	4:Y:92:HOH:O	2.30	0.65
2:Y:661:ASP:H	2:Y:688:TYR:HE1	1.44	0.65
1:A:127:ILE:HD11	1:B:127:ILE:CG1	2.27	0.65
1:B:52:ILE:HG23	1:B:53:SER:N	2.12	0.65
1:B:30:SER:O	1:B:49:GLU:HB2	1.96	0.65
1:B:31:GLY:HA3	1:B:48:SER:HA	1.79	0.65
1:A:34:ILE:HD12	1:A:111:PHE:CE1	2.33	0.64
1:A:1:MET:HA	1:A:25:GLU:HG3	1.80	0.64
1:D:56:ALA:O	1:D:61:MET:N	2.31	0.64
1:D:192:ARG:CB	1:D:192:ARG:NH1	2.54	0.64
2:Y:732:THR:HG21	2:Y:734:SER:OG	1.97	0.64
1:A:42:ALA:O	1:A:116:VAL:HB	1.98	0.64
2:Y:878:PHE:CD1	2:Y:882:PHE:HE2	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:PHE:HB2	1:D:95:PHE:CD2	2.29	0.64
2:X:719:ASP:HB2	2:X:747:CYS:CB	2.19	0.64
1:C:18:HIS:HD2	1:C:36:LEU:HD11	1.63	0.64
1:C:59:MET:HE1	1:C:108:LEU:HA	1.79	0.63
1:D:65:LYS:O	1:D:69:GLU:HG2	1.97	0.63
2:X:790:GLU:CD	2:X:790:GLU:H	2.05	0.63
2:Y:904:GLN:O	2:Y:905:GLU:CG	2.47	0.63
1:D:159:GLN:O	1:D:163:GLU:HG2	1.98	0.63
1:D:92:SER:O	1:D:93:CYS:CB	2.42	0.63
1:C:18:HIS:CD2	1:C:36:LEU:HD11	2.33	0.63
2:X:887:LYS:NZ	2:X:906:GLU:OE1	2.24	0.63
1:D:41:SER:HA	1:D:119:PRO:HB3	1.81	0.62
1:C:119:PRO:O	1:C:123:ILE:HG13	1.97	0.62
2:Y:876:LYS:HZ2	2:Y:911:ILE:HG12	1.64	0.62
2:Y:874:ASP:O	2:Y:875:PHE:C	2.37	0.62
1:C:200:ASN:O	1:C:201:ALA:HB3	1.99	0.62
2:X:832:LYS:HD2	2:X:834:GLU:HG3	1.81	0.62
2:Y:889:LEU:HD21	2:Y:906:GLU:CB	2.29	0.62
2:Y:706:ASN:ND2	2:Y:709:VAL:H	1.98	0.62
1:D:58:ASP:OD1	1:D:58:ASP:O	2.18	0.62
2:Y:823:TYR:CZ	2:Y:832:LYS:NZ	2.68	0.62
1:D:87:ASN:HD22	1:D:87:ASN:N	1.96	0.62
2:X:679:GLU:CB	2:X:689:ILE:HD13	2.26	0.62
1:B:98:GLU:HB2	1:B:106:PHE:O	1.98	0.62
2:X:782:LYS:CG	2:X:783:ASN:N	2.62	0.62
2:X:681:ARG:HG2	2:X:681:ARG:HH11	1.65	0.61
2:X:792:MET:HE2	2:X:792:MET:CA	2.27	0.61
2:X:792:MET:HE1	2:X:795:LEU:HD12	1.82	0.61
2:X:846:ARG:CG	2:X:852:VAL:HG13	2.30	0.61
2:X:900:LYS:O	2:X:902:GLU:N	2.33	0.61
2:Y:706:ASN:C	2:Y:706:ASN:HD22	2.07	0.61
1:A:98:GLU:HB3	1:A:107:ARG:HA	1.82	0.61
1:D:73:ALA:HB2	1:D:84:TYR:CE1	2.36	0.61
2:Y:713:ILE:O	2:Y:713:ILE:HG22	1.99	0.61
1:D:71:ARG:HB2	1:D:75:LEU:HD12	1.82	0.61
2:X:665:CYS:SG	2:X:693:PRO:HD3	2.40	0.61
2:X:780:GLY:O	2:X:781:ILE:HG13	2.00	0.61
2:Y:690:VAL:HG13	2:Y:692:ASN:O	2.00	0.61
1:D:30:SER:O	1:D:49:GLU:HB2	2.00	0.61
1:A:127:ILE:HG12	1:B:127:ILE:CG1	2.23	0.61
1:C:40:HIS:NE2	1:D:119:PRO:HD2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:905:GLU:HB3	4:X:88:HOH:O	2.01	0.61
1:D:138:GLN:O	1:D:142:GLU:HG3	2.01	0.61
1:C:42:ALA:O	1:C:116:VAL:HB	2.02	0.60
2:X:711:ASN:HD22	2:X:712:ILE:N	1.99	0.60
1:A:130:CYS:O	1:A:134:THR:HG22	2.00	0.60
2:Y:738:TRP:HB3	2:Y:743:MET:HE3	1.83	0.60
1:D:59:MET:O	1:D:60:GLU:CB	2.48	0.60
2:X:659:PHE:O	2:X:662:VAL:HB	2.01	0.60
1:B:61:MET:HE3	1:B:62:GLU:CG	2.31	0.60
2:X:717:LYS:CG	2:X:718:HIS:CE1	2.74	0.60
2:Y:670:THR:HB	2:Y:671:ASP:CB	2.31	0.60
1:C:172:LEU:O	1:C:175:ASP:HB2	2.02	0.59
2:Y:716:ASN:OD1	2:Y:745:HIS:CE1	2.55	0.59
1:D:62:GLU:C	1:D:64:GLY:N	2.56	0.59
1:D:153:ARG:HD2	4:D:204:HOH:O	2.02	0.59
1:D:200:ASN:N	1:D:200:ASN:HD22	2.00	0.59
1:B:70:LEU:CD2	1:B:97:PHE:HE2	2.15	0.59
2:X:846:ARG:CG	2:X:846:ARG:NE	2.64	0.59
2:X:706:ASN:O	2:X:710:LYS:CG	2.51	0.59
1:B:40:HIS:O	1:B:119:PRO:HB2	2.01	0.59
1:D:73:ALA:HB2	1:D:84:TYR:CZ	2.38	0.59
1:C:50:SER:HB3	4:C:261:HOH:O	2.02	0.59
1:B:42:ALA:O	1:B:115:LYS:HB2	2.02	0.58
1:D:118:ASN:HB3	1:D:121:GLU:HB3	1.85	0.58
2:X:663:GLU:OE1	2:X:697:THR:CG2	2.41	0.58
1:A:120:ALA:HB2	1:B:40:HIS:HB2	1.86	0.58
1:B:59:MET:HA	1:B:59:MET:CE	2.32	0.58
1:B:62:GLU:C	1:B:64:GLY:N	2.57	0.58
2:X:706:ASN:HD22	2:X:709:VAL:H	1.48	0.58
2:Y:829:LEU:O	2:Y:830:SER:CB	2.47	0.58
1:A:120:ALA:CB	1:B:40:HIS:HB2	2.33	0.58
1:B:150:ARG:HG3	4:B:211:HOH:O	2.03	0.58
1:D:53:SER:HB3	1:D:63:LYS:NZ	2.19	0.58
2:X:746:MET:SD	2:X:754:PHE:HD1	2.26	0.58
2:Y:844:GLU:O	2:Y:848:HIS:HD2	1.86	0.58
1:D:131:LEU:HA	1:D:134:THR:CG2	2.34	0.58
2:X:719:ASP:OD1	2:X:750:THR:CG2	2.42	0.58
1:B:4:LYS:HG3	1:B:5:ILE:N	2.15	0.58
2:Y:705:GLU:CG	2:Y:710:LYS:HE2	2.34	0.58
1:A:88:PHE:CZ	1:A:113:LEU:HD12	2.38	0.58
1:A:145:GLN:O	1:A:149:GLU:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:LEU:HD22	1:D:97:PHE:HE2	1.69	0.58
2:X:693:PRO:HA	2:X:697:THR:HG21	1.86	0.58
2:X:782:LYS:HG3	2:X:783:ASN:N	2.18	0.58
1:B:73:ALA:HB2	1:B:84:TYR:CE1	2.39	0.57
1:B:86:PHE:O	1:B:87:ASN:ND2	2.37	0.57
1:B:31:GLY:HA2	1:B:52:ILE:HD13	1.85	0.57
1:C:104:VAL:HG23	1:C:106:PHE:CZ	2.38	0.57
1:A:7:ARG:O	1:A:7:ARG:HG3	2.05	0.57
2:X:825:VAL:O	2:X:826:ILE:C	2.47	0.57
2:Y:872:VAL:O	2:Y:876:LYS:HG3	2.03	0.57
1:C:70:LEU:HD22	1:C:74:LEU:HD12	1.86	0.57
1:D:181:ILE:HD13	2:Y:799:LEU:CD1	2.35	0.57
1:C:34:ILE:O	1:C:34:ILE:CG2	2.52	0.57
2:Y:819:TYR:OH	2:Y:823:TYR:HD2	1.88	0.57
1:C:36:LEU:HG	1:C:37:THR:N	2.19	0.57
1:B:68:GLY:HA2	1:B:71:ARG:HG2	1.87	0.57
1:C:7:ARG:HG3	1:C:7:ARG:O	2.05	0.57
1:B:179:ARG:NH1	2:X:781:ILE:HB	2.20	0.56
1:C:88:PHE:CE1	1:C:113:LEU:HD12	2.40	0.56
2:X:780:GLY:C	2:X:781:ILE:HG13	2.30	0.56
2:Y:732:THR:CG2	2:Y:734:SER:OG	2.54	0.56
2:Y:816:HIS:CD2	2:Y:893:TRP:HH2	2.23	0.56
2:X:675:LYS:O	2:X:679:GLU:HG3	2.05	0.56
2:X:910:LEU:CB	2:X:911:ILE:HG23	2.33	0.56
1:A:127:ILE:O	1:A:127:ILE:CG2	2.54	0.56
1:B:85:THR:HB	1:B:100:ASN:HD21	1.71	0.56
1:B:87:ASN:HD22	1:B:87:ASN:N	2.01	0.56
1:D:70:LEU:CD2	1:D:97:PHE:HE2	2.18	0.56
2:Y:828:ASP:OD2	2:Y:828:ASP:C	2.48	0.56
1:A:101:LEU:O	1:A:103:ASP:N	2.38	0.56
1:C:151:LEU:CD1	1:D:148:ASN:HB2	2.35	0.56
1:D:190:LYS:NZ	4:D:237:HOH:O	2.32	0.56
2:X:717:LYS:HG2	2:X:718:HIS:NE2	2.18	0.56
1:D:131:LEU:HA	1:D:134:THR:HG22	1.88	0.56
1:D:187:LYS:NZ	2:Y:759:ASP:OD1	2.34	0.56
2:X:908:GLN:HB2	2:X:909:TYR:CD1	2.40	0.56
2:Y:825:VAL:O	2:Y:826:ILE:C	2.49	0.56
2:Y:670:THR:HB	2:Y:671:ASP:HB2	1.88	0.55
1:D:31:GLY:HA3	1:D:48:SER:HA	1.87	0.55
2:X:812:MET:CE	2:X:897:SER:CB	2.78	0.55
1:B:118:ASN:H	1:B:118:ASN:HD22	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LEU:HD22	1:C:74:LEU:CD1	2.36	0.55
2:Y:657:ASN:OD1	2:Y:657:ASN:N	2.36	0.55
1:C:1:MET:HG3	1:C:24:TRP:O	2.07	0.55
1:C:24:TRP:HD1	1:C:27:THR:O	1.89	0.55
1:A:70:LEU:HD22	1:A:74:LEU:HD12	1.89	0.55
1:B:36:LEU:O	1:B:43:TRP:HE3	1.90	0.55
1:B:53:SER:HB3	1:B:63:LYS:HZ3	1.69	0.55
1:C:127:ILE:O	1:C:127:ILE:HG13	2.05	0.55
2:X:783:ASN:CA	2:X:784:SER:OG	2.54	0.55
2:Y:821:ASP:OD1	2:Y:871:ARG:NH1	2.38	0.55
1:B:91:GLU:CD	1:B:91:GLU:H	2.15	0.55
1:D:98:GLU:HB2	1:D:106:PHE:O	2.06	0.55
1:D:179:ARG:NH1	2:Y:781:ILE:O	2.35	0.55
1:A:172:LEU:O	1:A:175:ASP:HB3	2.07	0.55
1:B:25:GLU:O	1:B:26:LYS:HB2	2.06	0.55
1:D:4:LYS:HG2	1:D:75:LEU:HB3	1.89	0.55
2:X:716:ASN:HD22	2:X:748:PRO:HD3	1.72	0.55
1:A:70:LEU:HD22	1:A:74:LEU:CD1	2.37	0.54
1:B:71:ARG:HB2	1:B:75:LEU:HD12	1.90	0.54
1:B:119:PRO:O	1:B:123:ILE:CD1	2.32	0.54
2:Y:675:LYS:N	2:Y:676:PRO:CD	2.70	0.54
1:B:56:ALA:CB	1:B:63:LYS:HG3	2.37	0.54
1:C:32:PHE:CE1	1:C:34:ILE:HD12	2.42	0.54
1:C:100:ASN:OD1	1:C:105:SER:HB2	2.08	0.54
1:A:131:LEU:HD21	1:B:5:ILE:CG2	2.38	0.54
2:X:681:ARG:HH11	2:X:681:ARG:CG	2.20	0.54
2:X:694:GLY:H	2:X:697:THR:HG23	1.71	0.54
1:B:85:THR:HB	1:B:100:ASN:ND2	2.23	0.54
1:B:95:PHE:O	1:B:110:SER:HA	2.08	0.54
1:C:34:ILE:HD13	1:C:111:PHE:CE1	2.43	0.54
2:Y:710:LYS:HD2	2:Y:710:LYS:H	1.69	0.54
1:A:36:LEU:HG	1:A:37:THR:N	2.23	0.54
2:X:823:TYR:CD2	2:X:832:LYS:HA	2.42	0.54
1:C:154:ASP:O	1:C:158:VAL:HG23	2.08	0.54
1:C:39:GLY:O	1:D:120:ALA:HA	2.08	0.54
2:X:705:GLU:HG3	2:X:710:LYS:NZ	2.22	0.54
2:X:884:ARG:O	2:X:885:LYS:C	2.50	0.54
1:C:44:THR:CG2	1:C:45:GLY:N	2.44	0.53
2:X:668:SER:C	2:X:703:GLY:H	2.15	0.53
2:X:706:ASN:ND2	2:X:707:ILE:N	2.56	0.53
2:X:706:ASN:H	2:X:710:LYS:HG2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:PHE:HB2	1:B:95:PHE:CD2	2.39	0.53
1:C:2:GLU:OE2	1:C:26:LYS:HB2	2.08	0.53
1:C:190:LYS:NZ	4:C:219:HOH:O	2.41	0.53
1:D:69:GLU:OE1	1:D:99:LYS:HD2	2.06	0.53
2:X:665:CYS:O	2:X:700:VAL:HA	2.07	0.53
1:D:69:GLU:OE2	1:D:72:LYS:NZ	2.40	0.53
1:D:172:LEU:HD11	1:D:176:LEU:HD11	1.91	0.53
2:Y:658:ILE:HD11	2:Y:685:PHE:HD2	1.73	0.53
1:D:85:THR:O	1:D:97:PHE:HA	2.08	0.53
2:X:752:GLU:O	2:X:756:ARG:HG3	2.09	0.53
2:X:903:LEU:C	2:X:904:GLN:O	2.41	0.53
1:B:53:SER:HB3	1:B:63:LYS:HZ2	1.70	0.53
1:C:121:GLU:O	1:C:124:ARG:HB2	2.08	0.53
1:D:70:LEU:O	1:D:74:LEU:N	2.42	0.53
1:D:192:ARG:HH11	1:D:192:ARG:CG	2.20	0.53
2:X:680:ASN:O	2:X:683:ALA:HB3	2.09	0.53
2:X:876:LYS:HE2	2:X:911:ILE:CD1	2.38	0.53
2:X:658:ILE:HG21	2:X:735:PHE:HB2	1.90	0.53
2:X:792:MET:HE2	2:X:795:LEU:HD12	1.90	0.53
1:A:117:GLU:HG3	1:A:118:ASN:N	2.22	0.53
1:B:56:ALA:HB3	1:B:63:LYS:HG3	1.91	0.53
1:B:187:LYS:NZ	2:X:759:ASP:OD1	2.42	0.53
2:X:710:LYS:HA	2:X:710:LYS:CE	2.39	0.53
2:X:780:GLY:C	2:X:781:ILE:CG1	2.82	0.53
1:B:21:GLN:OE1	1:B:126:LEU:HD12	2.09	0.52
1:B:70:LEU:O	1:B:74:LEU:N	2.42	0.52
1:B:177:TYR:O	1:B:181:ILE:CG1	2.57	0.52
2:X:691:GLN:NE2	2:X:691:GLN:HA	2.24	0.52
1:A:127:ILE:CG1	1:B:127:ILE:CG1	2.85	0.52
1:C:59:MET:CE	1:C:108:LEU:HA	2.38	0.52
1:A:118:ASN:ND2	1:A:122:VAL:HG22	2.24	0.52
1:D:130:CYS:O	1:D:134:THR:HG22	2.09	0.52
1:C:117:GLU:HG3	1:C:118:ASN:N	2.24	0.52
2:X:706:ASN:O	2:X:710:LYS:HB2	2.10	0.52
2:X:786:GLU:C	2:X:787:GLN:HG3	2.34	0.52
2:X:906:GLU:O	2:X:909:TYR:N	2.40	0.52
2:Y:710:LYS:N	2:Y:710:LYS:CD	2.72	0.52
2:Y:825:VAL:HG23	2:Y:831:THR:HG21	1.90	0.52
1:D:85:THR:HB	1:D:100:ASN:ND2	2.23	0.52
1:D:97:PHE:CD1	1:D:97:PHE:N	2.76	0.52
1:B:40:HIS:O	1:B:119:PRO:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LEU:HA	1:B:134:THR:HG22	1.91	0.52
1:C:32:PHE:HE1	1:C:34:ILE:HD12	1.74	0.52
1:D:56:ALA:HB1	1:D:61:MET:O	2.10	0.52
1:D:159:GLN:HG2	2:Y:840:ILE:HD11	1.90	0.52
2:X:693:PRO:HB2	2:X:718:HIS:CE1	2.45	0.52
2:Y:710:LYS:CD	2:Y:710:LYS:H	2.23	0.52
1:B:179:ARG:O	1:B:183:VAL:HG23	2.10	0.51
1:D:155:TRP:CZ3	1:D:159:GLN:HG3	2.46	0.51
2:X:681:ARG:O	2:X:682:ILE:C	2.51	0.51
1:B:31:GLY:HA2	1:B:52:ILE:CD1	2.40	0.51
1:A:53:SER:HA	1:A:63:LYS:HE3	1.91	0.51
1:A:154:ASP:O	1:A:158:VAL:HG23	2.10	0.51
1:C:104:VAL:CG2	1:C:106:PHE:CZ	2.93	0.51
2:X:907:ASN:HA	2:X:910:LEU:HG	1.92	0.51
1:B:178:LYS:NZ	2:X:784:SER:O	2.29	0.51
2:X:790:GLU:CD	2:X:790:GLU:N	2.69	0.51
2:Y:829:LEU:HD21	2:Y:854:SER:HB2	1.91	0.51
1:A:121:GLU:O	1:A:124:ARG:HB2	2.11	0.51
1:C:47:VAL:HG21	1:C:111:PHE:CE2	2.45	0.51
1:B:73:ALA:HA	1:B:84:TYR:CD2	2.45	0.51
1:C:28:LEU:CD1	1:C:75:LEU:HD11	2.38	0.51
2:Y:824:ALA:N	2:Y:833:ASN:OD1	2.43	0.51
1:C:1:MET:HA	1:C:25:GLU:HG3	1.92	0.51
2:X:667:MET:HG2	2:X:708:ARG:HD3	1.92	0.51
2:X:691:GLN:HE21	2:X:691:GLN:CA	2.23	0.51
2:Y:862:HIS:HD2	2:Y:889:LEU:HD11	1.75	0.51
1:C:26:LYS:O	1:C:26:LYS:CG	2.52	0.51
1:D:42:ALA:O	1:D:115:LYS:HB2	2.11	0.51
1:D:116:VAL:CG1	1:D:117:GLU:H	2.18	0.51
2:Y:879:ARG:HG3	2:Y:886:PHE:CZ	2.46	0.51
1:B:117:GLU:HB3	1:D:117:GLU:OE2	2.10	0.50
1:A:104:VAL:HG23	1:A:106:PHE:HE1	1.64	0.50
1:B:87:ASN:CB	1:B:96:PHE:CZ	2.92	0.50
1:B:118:ASN:N	1:B:118:ASN:ND2	2.57	0.50
1:A:180:PHE:N	1:A:180:PHE:CD2	2.79	0.50
2:X:826:ILE:O	2:X:827:ASN:HB2	2.11	0.50
2:Y:670:THR:HB	2:Y:671:ASP:CG	2.37	0.50
2:X:770:ASP:O	2:X:774:LEU:HB2	2.12	0.50
1:B:74:LEU:C	1:B:76:SER:H	2.18	0.50
2:X:785:ASN:O	2:X:787:GLN:N	2.45	0.50
2:X:739:GLN:NE2	2:X:741:ARG:NH2	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:910:LEU:CB	2:X:911:ILE:CG2	2.87	0.50
2:Y:823:TYR:HE1	2:Y:832:LYS:HZ2	1.50	0.50
2:Y:828:ASP:O	2:Y:828:ASP:OD2	2.30	0.50
2:Y:878:PHE:CD1	2:Y:882:PHE:CE2	2.97	0.50
1:A:82:ASP:HB3	1:A:84:TYR:CE1	2.47	0.50
2:X:784:SER:HB2	2:X:786:GLU:OE1	2.11	0.49
1:B:56:ALA:O	1:B:61:MET:N	2.44	0.49
2:Y:732:THR:HG23	2:Y:734:SER:HB3	1.89	0.49
2:X:784:SER:HB2	2:X:786:GLU:CD	2.36	0.49
1:A:28:LEU:HD23	1:A:32:PHE:CD2	2.48	0.49
1:A:118:ASN:O	1:A:122:VAL:HG22	2.11	0.49
1:A:124:ARG:NH1	1:B:38:ASP:O	2.45	0.49
1:B:89:SER:HA	4:B:206:HOH:O	2.12	0.49
1:C:118:ASN:O	1:C:122:VAL:HG22	2.12	0.49
2:Y:675:LYS:N	2:Y:676:PRO:HD3	2.28	0.49
2:Y:821:ASP:CG	2:Y:871:ARG:HH11	2.20	0.49
1:B:30:SER:O	1:B:49:GLU:CB	2.61	0.49
1:B:118:ASN:HD22	1:B:118:ASN:N	2.11	0.49
1:C:1:MET:CE	1:C:23:SER:HB3	2.42	0.49
1:D:112:ASN:ND2	1:D:112:ASN:H	2.11	0.49
1:B:65:LYS:O	1:B:69:GLU:CG	2.61	0.49
2:Y:826:ILE:HD11	2:Y:871:ARG:HB3	1.95	0.49
1:A:44:THR:CG2	1:A:45:GLY:N	2.39	0.49
2:Y:664:PHE:HD1	2:Y:699:CYS:SG	2.36	0.49
2:Y:876:LYS:HZ1	2:Y:911:ILE:HG12	1.75	0.49
1:A:1:MET:CA	1:A:25:GLU:HG3	2.42	0.49
2:X:706:ASN:O	2:X:710:LYS:CB	2.61	0.49
1:C:151:LEU:HD12	1:D:148:ASN:HB2	1.93	0.48
2:Y:882:PHE:O	2:Y:885:LYS:NZ	2.46	0.48
1:B:52:ILE:HG22	1:B:53:SER:H	1.77	0.48
2:X:876:LYS:HE2	2:X:911:ILE:HD11	1.94	0.48
2:Y:706:ASN:HD22	2:Y:709:VAL:H	1.59	0.48
1:B:69:GLU:OE1	1:B:99:LYS:HD2	2.13	0.48
1:D:61:MET:O	1:D:62:GLU:C	2.56	0.48
2:Y:787:GLN:HA	2:Y:791:GLU:OE1	2.13	0.48
1:B:44:THR:OG1	1:B:116:VAL:HG23	2.13	0.48
1:D:26:LYS:O	1:D:27:THR:HG23	2.14	0.48
2:X:702:ALA:HB2	2:X:720:VAL:HG12	1.95	0.48
2:Y:788:THR:HG22	2:Y:789:PRO:HD2	1.95	0.48
1:A:30:SER:HA	1:A:49:GLU:OE1	2.13	0.48
2:X:746:MET:HB2	2:X:751:LYS:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:759:ASP:HB2	2:X:763:ASP:H	1.78	0.48
2:Y:862:HIS:CD2	2:Y:889:LEU:HD12	2.42	0.48
1:A:41:SER:HB2	1:A:43:TRP:CH2	2.49	0.48
1:A:61:MET:HG2	1:A:66:TYR:HB2	1.95	0.48
1:B:52:ILE:CG2	1:B:53:SER:H	2.26	0.48
1:B:66:TYR:O	1:B:67:VAL:C	2.57	0.48
2:X:674:PRO:O	2:X:675:LYS:C	2.56	0.48
1:D:131:LEU:C	1:D:134:THR:HG22	2.39	0.48
1:D:160:GLY:HA2	1:D:163:GLU:HG3	1.96	0.48
2:X:910:LEU:C	2:X:911:ILE:HG22	2.37	0.48
2:X:910:LEU:CA	2:X:911:ILE:CG2	2.92	0.48
2:Y:706:ASN:ND2	2:Y:706:ASN:C	2.72	0.48
1:C:24:TRP:CD1	1:C:27:THR:O	2.67	0.48
1:B:23:SER:O	1:B:32:PHE:HB2	2.14	0.48
1:B:73:ALA:HB2	1:B:84:TYR:CZ	2.49	0.48
1:D:179:ARG:NH1	2:Y:778:PHE:O	2.47	0.47
1:D:193:SER:O	1:D:197:LYS:HB2	2.13	0.47
1:C:130:CYS:HB3	1:D:130:CYS:HB3	1.96	0.47
2:Y:746:MET:SD	2:Y:754:PHE:CD1	3.07	0.47
1:C:53:SER:HA	1:C:63:LYS:HE3	1.95	0.47
2:X:757:GLU:O	2:X:757:GLU:HG3	2.06	0.47
1:B:49:GLU:O	1:B:49:GLU:HG3	2.14	0.47
1:B:70:LEU:HD22	1:B:97:PHE:HE2	1.79	0.47
1:B:130:CYS:C	1:B:134:THR:HG22	2.39	0.47
2:Y:662:VAL:HG12	2:Y:664:PHE:CZ	2.49	0.47
2:Y:831:THR:O	2:Y:832:LYS:C	2.56	0.47
1:A:98:GLU:OE2	1:A:105:SER:OG	2.32	0.47
1:B:83:VAL:CG1	1:B:83:VAL:O	2.55	0.47
1:D:40:HIS:O	1:D:119:PRO:HB2	2.14	0.47
1:D:44:THR:HG22	1:D:45:GLY:H	1.80	0.47
1:D:73:ALA:HA	1:D:84:TYR:CE2	2.50	0.47
1:D:89:SER:CB	1:D:91:GLU:OE1	2.61	0.47
2:X:812:MET:HE1	2:X:897:SER:CB	2.45	0.47
1:A:67:VAL:O	1:A:68:GLY:C	2.57	0.47
2:Y:738:TRP:CG	2:Y:743:MET:HE1	2.50	0.47
1:B:187:LYS:O	1:B:191:ILE:HG13	2.15	0.47
1:C:118:ASN:ND2	1:C:122:VAL:HG22	2.30	0.47
1:D:53:SER:HB3	1:D:63:LYS:HZ3	1.79	0.47
2:X:757:GLU:HG2	2:X:758:TYR:CE1	2.50	0.47
2:Y:679:GLU:O	2:Y:689:ILE:CD1	2.63	0.47
1:C:26:LYS:HE2	1:C:26:LYS:HB3	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:691:GLN:NE2	2:X:691:GLN:CA	2.78	0.46
2:X:787:GLN:HG2	2:X:792:MET:HE3	1.96	0.46
1:A:161:ARG:NH2	4:A:220:HOH:O	2.41	0.46
1:C:200:ASN:O	1:C:201:ALA:CB	2.51	0.46
2:X:885:LYS:HE3	4:X:146:HOH:O	2.15	0.46
2:X:908:GLN:O	4:X:137:HOH:O	2.21	0.46
1:B:61:MET:HE3	1:B:62:GLU:H	1.80	0.46
1:B:72:LYS:O	1:B:76:SER:C	2.58	0.46
2:X:706:ASN:O	2:X:710:LYS:HG2	2.15	0.46
2:Y:845:LEU:HB3	2:Y:850:ALA:HB3	1.97	0.46
1:B:121:GLU:OE1	1:D:121:GLU:OE1	2.33	0.46
1:D:95:PHE:O	1:D:110:SER:HA	2.14	0.46
2:X:787:GLN:HB3	2:X:792:MET:HE3	1.97	0.46
2:Y:665:CYS:SG	2:Y:693:PRO:HD3	2.56	0.46
1:B:131:LEU:CA	1:B:134:THR:HG22	2.45	0.46
1:A:40:HIS:HB2	1:B:120:ALA:HB2	1.98	0.46
1:D:113:LEU:O	1:D:114:GLU:HG3	2.16	0.46
2:Y:759:ASP:OD1	2:Y:763:ASP:HB3	2.15	0.46
1:D:30:SER:O	1:D:49:GLU:CB	2.64	0.46
1:A:161:ARG:HA	1:A:161:ARG:HD3	1.70	0.46
1:B:69:GLU:OE2	1:B:99:LYS:NZ	2.49	0.45
1:C:158:VAL:HG23	1:C:158:VAL:H	1.19	0.45
1:C:159:GLN:NE2	1:C:163:GLU:OE1	2.42	0.45
2:X:900:LYS:O	2:X:902:GLU:HG2	2.16	0.45
2:X:677:ASP:O	2:X:680:ASN:HB2	2.17	0.45
2:X:705:GLU:HG3	2:X:710:LYS:HZ2	1.81	0.45
2:Y:712:ILE:O	2:Y:715:SER:O	2.35	0.45
2:Y:809:PRO:HD2	4:Y:228:HOH:O	2.16	0.45
1:A:187:LYS:HD3	1:A:187:LYS:HA	1.77	0.45
1:D:74:LEU:C	1:D:76:SER:H	2.24	0.45
1:D:131:LEU:CA	1:D:134:THR:HG22	2.47	0.45
2:Y:738:TRP:HB3	2:Y:743:MET:CE	2.46	0.45
1:C:98:GLU:HB3	1:C:107:ARG:HA	1.98	0.45
2:X:655:ILE:HG23	2:X:655:ILE:HD13	1.60	0.45
2:Y:675:LYS:O	2:Y:679:GLU:HG3	2.17	0.45
2:Y:862:HIS:CD2	2:Y:889:LEU:CD1	2.90	0.45
1:C:89:SER:O	1:C:93:CYS:CA	2.62	0.45
1:D:43:TRP:HA	1:D:115:LYS:HB2	1.97	0.45
2:Y:731:LYS:HG3	2:Y:732:THR:N	2.31	0.45
1:A:118:ASN:HB2	1:A:121:GLU:OE1	2.17	0.45
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:655:ILE:O	2:X:656:SER:HB2	2.16	0.45
2:Y:829:LEU:O	2:Y:830:SER:HB2	2.17	0.45
1:A:85:THR:HG22	1:A:98:GLU:HG3	1.99	0.45
1:A:140:LYS:O	1:A:140:LYS:HG3	2.17	0.45
1:C:26:LYS:HB3	1:C:26:LYS:NZ	2.28	0.45
2:X:662:VAL:HG12	2:X:664:PHE:CE1	2.52	0.45
1:B:20:LEU:HD12	1:B:36:LEU:HB2	1.97	0.45
2:X:667:MET:HE3	2:X:667:MET:HB3	1.57	0.45
2:Y:658:ILE:HD11	2:Y:685:PHE:CD2	2.51	0.45
2:Y:879:ARG:HH12	2:Y:888:ILE:HG13	1.82	0.45
1:A:1:MET:N	1:A:26:LYS:HE3	2.32	0.44
1:D:66:TYR:O	1:D:67:VAL:C	2.59	0.44
1:D:118:ASN:O	1:D:122:VAL:HG23	2.17	0.44
1:D:131:LEU:O	1:D:134:THR:HG22	2.18	0.44
1:D:51:GLU:H	1:D:51:GLU:HG3	1.74	0.44
2:X:787:GLN:CG	2:X:792:MET:HE3	2.47	0.44
1:C:95:PHE:O	1:C:111:PHE:N	2.39	0.44
2:Y:706:ASN:HD21	2:Y:708:ARG:HB2	1.83	0.44
2:Y:788:THR:OG1	2:Y:791:GLU:CD	2.60	0.44
1:A:34:ILE:O	1:A:34:ILE:HG23	2.14	0.44
1:B:85:THR:O	1:B:97:PHE:HA	2.16	0.44
2:X:816:HIS:CD2	2:X:893:TRP:HH2	2.34	0.44
2:X:865:ILE:H	2:X:865:ILE:HG12	1.48	0.44
1:B:82:ASP:CA	1:B:83:VAL:HG23	2.25	0.44
2:X:910:LEU:CA	2:X:911:ILE:HG22	2.47	0.44
2:Y:753:HIS:O	2:Y:756:ARG:HG2	2.18	0.44
1:A:104:VAL:HG21	1:A:106:PHE:CZ	2.52	0.44
1:D:87:ASN:ND2	1:D:87:ASN:N	2.66	0.44
2:X:717:LYS:CG	2:X:718:HIS:NE2	2.80	0.44
2:X:788:THR:HG22	2:X:791:GLU:H	1.82	0.44
2:Y:679:GLU:HB3	2:Y:689:ILE:HD13	1.99	0.44
2:X:701:ILE:HG22	2:X:723:PRO:HG3	2.00	0.44
2:Y:853:VAL:HG13	2:Y:855:CYS:H	1.83	0.44
1:D:91:GLU:CD	1:D:91:GLU:H	2.26	0.44
2:X:864:ILE:HD13	2:X:889:LEU:HB2	2.00	0.44
2:Y:828:ASP:C	2:Y:830:SER:N	2.75	0.44
2:Y:706:ASN:O	2:Y:710:LYS:HG2	2.17	0.43
1:A:61:MET:HE3	1:A:66:TYR:HA	2.00	0.43
1:A:90:LYS:HB2	1:A:90:LYS:HE3	1.28	0.43
1:B:44:THR:HG22	1:B:45:GLY:H	1.83	0.43
2:X:812:MET:HE1	2:X:897:SER:CA	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:GLU:O	1:B:119:PRO:HD3	2.18	0.43
2:X:702:ALA:HB2	2:X:720:VAL:CG1	2.47	0.43
2:Y:706:ASN:N	2:Y:710:LYS:HD3	2.32	0.43
2:Y:759:ASP:HB2	2:Y:763:ASP:O	2.18	0.43
2:Y:819:TYR:O	2:Y:863:VAL:CA	2.60	0.43
1:C:110:SER:O	1:C:111:PHE:CD2	2.71	0.43
2:X:739:GLN:NE2	2:X:741:ARG:HE	2.11	0.43
2:Y:869:HIS:O	2:Y:872:VAL:HG13	2.19	0.43
1:B:10:LEU:HB3	1:B:12:SER:OG	2.17	0.43
1:C:41:SER:HB2	1:C:43:TRP:CH2	2.53	0.43
1:C:90:LYS:H	1:C:90:LYS:HG3	1.48	0.43
1:D:101:LEU:HB2	1:D:104:VAL:HG23	2.01	0.43
1:D:197:LYS:CE	4:D:269:HOH:O	2.39	0.43
2:X:767:ILE:HD12	2:X:767:ILE:HG23	1.67	0.43
2:Y:665:CYS:O	2:Y:700:VAL:HA	2.18	0.43
1:D:58:ASP:OD1	1:D:58:ASP:C	2.62	0.43
1:D:117:GLU:O	1:D:119:PRO:HD3	2.17	0.43
2:X:744:ILE:HD12	2:X:744:ILE:HG21	1.44	0.43
1:B:116:VAL:HG12	1:B:117:GLU:N	2.25	0.43
1:C:159:GLN:OE1	1:C:159:GLN:HA	2.17	0.43
2:X:783:ASN:HB3	2:X:784:SER:OG	2.18	0.43
2:X:867:GLU:H	2:X:867:GLU:HG3	1.57	0.43
2:Y:799:LEU:HD23	2:Y:799:LEU:HA	1.90	0.43
1:A:48:SER:O	1:A:49:GLU:C	2.60	0.43
1:B:85:THR:CB	1:B:100:ASN:HD21	2.31	0.43
1:C:120:ALA:O	1:C:124:ARG:NH1	2.52	0.43
2:X:904:GLN:O	2:X:905:GLU:CG	2.63	0.43
2:X:655:ILE:HG21	2:X:655:ILE:HD12	1.52	0.43
2:Y:722:LYS:HA	2:Y:723:PRO:HD2	1.15	0.43
2:Y:878:PHE:HD1	2:Y:878:PHE:C	2.27	0.43
1:A:102:LYS:HE2	4:A:211:HOH:O	2.18	0.42
1:B:24:TRP:CD1	1:B:27:THR:C	2.97	0.42
1:B:83:VAL:CG1	1:B:100:ASN:HB2	2.44	0.42
1:D:106:PHE:CD1	1:D:106:PHE:C	2.97	0.42
1:A:192:ARG:HD3	2:X:766:PHE:O	2.19	0.42
1:B:87:ASN:HB2	1:B:96:PHE:CE2	2.53	0.42
2:X:705:GLU:O	2:X:706:ASN:CB	2.68	0.42
1:C:82:ASP:HB3	1:C:84:TYR:CE1	2.54	0.42
2:X:739:GLN:O	2:X:740:PRO:C	2.62	0.42
2:X:790:GLU:O	2:X:793:ALA:HB3	2.19	0.42
1:A:118:ASN:HB2	1:A:121:GLU:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:TRP:HD1	1:B:115:LYS:HB3	1.84	0.42
1:C:8:ILE:HG13	1:C:9:HIS:N	2.34	0.42
1:C:11:VAL:O	1:C:14:PRO:HD3	2.19	0.42
1:B:118:ASN:HB2	1:B:121:GLU:HB3	2.01	0.42
2:X:707:ILE:HD13	2:X:707:ILE:HA	1.95	0.42
2:X:900:LYS:O	2:X:902:GLU:CG	2.67	0.42
2:Y:788:THR:OG1	2:Y:791:GLU:OE1	2.38	0.42
2:Y:878:PHE:CD1	2:Y:878:PHE:C	2.97	0.42
1:B:65:LYS:O	1:B:65:LYS:CG	2.38	0.42
1:B:175:ASP:OD2	1:B:175:ASP:C	2.63	0.42
2:X:659:PHE:HD2	2:X:659:PHE:HA	1.68	0.42
1:A:47:VAL:HG21	1:A:111:PHE:CE2	2.54	0.42
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.82	0.42
1:C:59:MET:HE2	1:C:107:ARG:O	2.19	0.42
1:C:151:LEU:HD13	1:D:148:ASN:HB2	2.00	0.42
1:A:110:SER:O	1:A:111:PHE:HD2	2.01	0.42
1:B:26:LYS:O	1:B:27:THR:HG23	2.20	0.42
1:C:119:PRO:HD2	4:C:229:HOH:O	2.19	0.42
2:Y:706:ASN:O	2:Y:710:LYS:CG	2.68	0.42
1:D:115:LYS:CG	1:D:116:VAL:N	2.83	0.41
2:X:820:LEU:O	2:X:822:SER:N	2.50	0.41
2:Y:706:ASN:H	2:Y:710:LYS:HD3	1.83	0.41
2:Y:801:TYR:O	2:Y:802:ARG:C	2.58	0.41
1:C:5:ILE:HD13	1:C:130:CYS:SG	2.61	0.41
2:X:658:ILE:HG21	2:X:658:ILE:HD13	1.82	0.41
1:C:158:VAL:O	1:C:159:GLN:C	2.63	0.41
1:D:87:ASN:HB2	1:D:96:PHE:CE1	2.54	0.41
2:Y:814:ARG:HA	2:Y:849:GLY:O	2.20	0.41
1:C:188:LYS:HD2	2:Y:768:ASP:HA	2.03	0.41
1:D:21:GLN:OE1	1:D:126:LEU:HD12	2.20	0.41
1:D:68:GLY:HA2	1:D:71:ARG:CG	2.47	0.41
1:A:95:PHE:O	1:A:111:PHE:N	2.49	0.41
2:X:681:ARG:C	2:X:683:ALA:N	2.76	0.41
2:X:808:SER:HA	2:X:809:PRO:HD3	1.83	0.41
2:Y:900:LYS:CB	2:Y:904:GLN:NE2	2.83	0.41
1:B:198:LEU:HD23	1:B:198:LEU:HA	1.86	0.41
2:X:657:ASN:HB3	2:X:686:GLY:HA3	2.03	0.41
2:X:783:ASN:CB	2:X:784:SER:OG	2.69	0.41
2:Y:705:GLU:O	2:Y:706:ASN:HB3	2.20	0.41
1:A:2:GLU:HB2	1:A:24:TRP:CZ2	2.56	0.41
1:B:101:LEU:HB2	1:B:104:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:884:ARG:O	2:X:884:ARG:CD	2.69	0.41
2:Y:701:ILE:HG23	2:Y:701:ILE:HD12	1.71	0.41
1:C:71:ARG:HB3	1:C:75:LEU:HD12	2.01	0.41
2:Y:809:PRO:C	2:Y:811:SER:H	2.29	0.41
2:Y:878:PHE:O	2:Y:881:THR:HB	2.20	0.41
1:B:155:TRP:CZ2	2:X:840:ILE:CD1	3.04	0.41
1:C:101:LEU:O	1:C:102:LYS:C	2.63	0.41
1:C:118:ASN:O	1:C:118:ASN:CG	2.63	0.41
1:C:145:GLN:O	1:C:149:GLU:HG3	2.20	0.41
1:D:123:ILE:HG22	1:D:127:ILE:HD12	2.03	0.41
2:X:678:LEU:O	2:X:682:ILE:HG13	2.20	0.41
2:X:820:LEU:HD23	2:X:838:LEU:HD22	2.02	0.41
2:Y:705:GLU:HG3	2:Y:710:LYS:CE	2.46	0.41
2:Y:792:MET:HA	2:Y:795:LEU:HD12	2.03	0.41
2:Y:879:ARG:HG2	2:Y:886:PHE:CE1	2.56	0.41
1:A:118:ASN:HD22	1:A:122:VAL:HG22	1.86	0.41
1:C:43:TRP:HB3	1:C:113:LEU:HB3	2.03	0.41
1:D:151:LEU:HD23	1:D:151:LEU:HA	1.94	0.41
2:X:812:MET:HE1	2:X:897:SER:HB3	1.93	0.41
1:D:40:HIS:O	1:D:119:PRO:CB	2.68	0.40
1:D:115:LYS:HG3	1:D:116:VAL:N	2.36	0.40
2:X:700:VAL:HG22	2:X:720:VAL:HG13	2.02	0.40
2:X:776:GLU:O	2:X:779:SER:HB3	2.21	0.40
2:Y:660:GLU:O	2:Y:661:ASP:HB2	2.21	0.40
1:A:89:SER:O	1:A:93:CYS:HA	2.21	0.40
1:B:49:GLU:O	1:B:49:GLU:CG	2.69	0.40
1:D:87:ASN:CB	1:D:96:PHE:CZ	3.01	0.40
1:D:107:ARG:CD	1:D:108:LEU:N	2.80	0.40
1:D:186:GLU:CG	2:Y:759:ASP:OD2	2.62	0.40
2:X:679:GLU:HA	2:X:689:ILE:HD11	2.03	0.40
2:X:744:ILE:HD13	2:X:744:ILE:HG23	1.45	0.40
2:X:836:THR:HG22	2:X:838:LEU:N	2.13	0.40
2:Y:715:SER:C	2:Y:717:LYS:N	2.78	0.40
2:Y:739:GLN:HA	2:Y:740:PRO:HD3	1.87	0.40
1:B:28:LEU:HB2	1:B:71:ARG:NH2	2.37	0.40
1:B:87:ASN:HB2	1:B:96:PHE:CE1	2.56	0.40
1:B:139:ALA:O	1:B:143:HIS:ND1	2.55	0.40
1:C:198:LEU:HD21	1:D:197:LYS:HD2	2.03	0.40
2:X:769:THR:OG1	2:X:770:ASP:N	2.48	0.40
2:X:882:PHE:O	2:X:885:LYS:NZ	2.52	0.40
1:B:179:ARG:NH1	2:X:778:PHE:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:THR:O	1:D:178:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	199/203 (98%)	170 (85%)	26 (13%)	3 (2%)	8	12
1	B	192/203 (95%)	168 (88%)	19 (10%)	5 (3%)	4	4
1	C	199/203 (98%)	172 (86%)	22 (11%)	5 (2%)	4	5
1	D	191/203 (94%)	167 (87%)	19 (10%)	5 (3%)	4	4
2	X	252/263 (96%)	217 (86%)	32 (13%)	3 (1%)	10	16
2	Y	256/263 (97%)	221 (86%)	27 (10%)	8 (3%)	3	3
All	All	1289/1338 (96%)	1115 (86%)	145 (11%)	29 (2%)	5	6

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	50	SER
2	X	747	CYS
2	X	786	GLU
2	Y	829	LEU
1	A	34	ILE
1	B	67	VAL
1	C	34	ILE
1	D	115	LYS
2	Y	741	ARG
1	B	26	LYS
1	B	63	LYS

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Mol	Chain	Res	Type
1	D	26	LYS
1	D	60	GLU
1	D	67	VAL
2	Y	716	ASN
2	Y	832	LYS
1	A	81	ALA
1	C	40	HIS
1	C	93	CYS
2	Y	899	ASP
1	A	119	PRO
1	B	93	CYS
1	C	119	PRO
1	D	93	CYS
2	Y	858	GLU
1	C	81	ALA
2	X	781	ILE
2	Y	810	LEU
2	Y	826	ILE

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	181/182 (100%)	137 (76%)	44 (24%)	1	1
1	B	180/182 (99%)	130 (72%)	50 (28%)	0	0
1	C	181/182 (100%)	141 (78%)	40 (22%)	1	1
1	D	179/182 (98%)	132 (74%)	47 (26%)	0	0
2	X	232/236 (98%)	170 (73%)	62 (27%)	0	0
2	Y	234/236 (99%)	184 (79%)	50 (21%)	1	1
All	All	1187/1200 (99%)	894 (75%)	293 (25%)	1	1

All (293) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	6	SER
1	A	7	ARG
1	A	12	SER
1	A	17	THR
1	A	18	HIS
1	A	22	VAL
1	A	23	SER
1	A	25	GLU
1	A	26	LYS
1	A	27	THR
1	A	28	LEU
1	A	34	ILE
1	A	37	THR
1	A	40	HIS
1	A	41	SER
1	A	49	GLU
1	A	55	GLU
1	A	61	MET
1	A	62	GLU
1	A	71	ARG
1	A	76	SER
1	A	85	THR
1	A	90	LYS
1	A	98	GLU
1	A	108	LEU
1	A	110	SER
1	A	112	ASN
1	A	116	VAL
1	A	121	GLU
1	A	122	VAL
1	A	124	ARG
1	A	126	LEU
1	A	134	THR
1	A	138	GLN
1	A	140	LYS
1	A	145	GLN
1	A	146	LYS
1	A	147	GLU
1	A	152	LEU
1	A	158	VAL
1	A	169	LYS
1	A	190	LYS

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Mol	Chain	Res	Type
1	A	191	ILE
1	B	1	MET
1	B	3	ARG
1	B	4	LYS
1	B	6	SER
1	B	7	ARG
1	B	11	VAL
1	B	12	SER
1	B	16	ILE
1	B	17	THR
1	B	22	VAL
1	B	26	LYS
1	B	28	LEU
1	B	34	ILE
1	B	36	LEU
1	B	41	SER
1	B	47	VAL
1	B	51	GLU
1	B	52	ILE
1	B	57	ASP
1	B	58	ASP
1	B	59	MET
1	B	60	GLU
1	B	61	MET
1	B	62	GLU
1	B	65	LYS
1	B	67	VAL
1	B	70	LEU
1	B	72	LYS
1	B	82	ASP
1	B	85	THR
1	B	87	ASN
1	B	91	GLU
1	B	93	CYS
1	B	98	GLU
1	B	105	SER
1	B	111	PHE
1	B	116	VAL
1	B	118	ASN
1	B	125	GLU
1	B	134	THR
1	B	146	LYS

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Mol	Chain	Res	Type
1	B	157	ASP
1	B	172	LEU
1	B	173	GLU
1	B	181	ILE
1	B	184	LEU
1	B	187	LYS
1	B	197	LYS
1	B	198	LEU
1	B	199	LEU
1	C	2	GLU
1	C	6	SER
1	C	7	ARG
1	C	12	SER
1	C	22	VAL
1	C	23	SER
1	C	25	GLU
1	C	26	LYS
1	C	27	THR
1	C	28	LEU
1	C	40	HIS
1	C	41	SER
1	C	49	GLU
1	C	55	GLU
1	C	57	ASP
1	C	62	GLU
1	C	71	ARG
1	C	76	SER
1	C	85	THR
1	C	90	LYS
1	C	98	GLU
1	C	105	SER
1	C	108	LEU
1	C	110	SER
1	C	112	ASN
1	C	116	VAL
1	C	121	GLU
1	C	122	VAL
1	C	124	ARG
1	C	126	LEU
1	C	127	ILE
1	C	140	LYS
1	C	145	GLN

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Mol	Chain	Res	Type
1	C	146	LYS
1	C	152	LEU
1	C	158	VAL
1	C	169	LYS
1	C	190	LYS
1	C	191	ILE
1	C	199	LEU
1	D	1	MET
1	D	3	ARG
1	D	4	LYS
1	D	7	ARG
1	D	10	LEU
1	D	12	SER
1	D	16	ILE
1	D	17	THR
1	D	21	GLN
1	D	26	LYS
1	D	28	LEU
1	D	34	ILE
1	D	41	SER
1	D	47	VAL
1	D	51	GLU
1	D	58	ASP
1	D	60	GLU
1	D	62	GLU
1	D	65	LYS
1	D	67	VAL
1	D	72	LYS
1	D	75	LEU
1	D	83	VAL
1	D	85	THR
1	D	87	ASN
1	D	89	SER
1	D	91	GLU
1	D	93	CYS
1	D	97	PHE
1	D	98	GLU
1	D	105	SER
1	D	111	PHE
1	D	112	ASN
1	D	115	LYS
1	D	125	GLU

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Mol	Chain	Res	Type
1	D	146	LYS
1	D	150	ARG
1	D	156	ASN
1	D	163	GLU
1	D	174	THR
1	D	181	ILE
1	D	187	LYS
1	D	188	LYS
1	D	192	ARG
1	D	197	LYS
1	D	198	LEU
1	D	200	ASN
2	X	655	ILE
2	X	657	ASN
2	X	658	ILE
2	X	667	MET
2	X	673	GLN
2	X	675	LYS
2	X	681	ARG
2	X	689	ILE
2	X	690	VAL
2	X	691	GLN
2	X	692	ASN
2	X	697	THR
2	X	700	VAL
2	X	705	GLU
2	X	706	ASN
2	X	708	ARG
2	X	710	LYS
2	X	711	ASN
2	X	712	ILE
2	X	715	SER
2	X	716	ASN
2	X	717	LYS
2	X	719	ASP
2	X	723	PRO
2	X	728	GLU
2	X	731	LYS
2	X	734	SER
2	X	739	GLN
2	X	744	ILE
2	X	747	CYS

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Mol	Chain	Res	Type
2	X	750	THR
2	X	751	LYS
2	X	752	GLU
2	X	757	GLU
2	X	759	ASP
2	X	764	SER
2	X	773	GLN
2	X	774	LEU
2	X	775	LYS
2	X	785	ASN
2	X	786	GLU
2	X	788	THR
2	X	790	GLU
2	X	791	GLU
2	X	794	SER
2	X	809	PRO
2	X	810	LEU
2	X	815	ARG
2	X	832	LYS
2	X	841	LYS
2	X	852	VAL
2	X	853	VAL
2	X	856	LEU
2	X	860	VAL
2	X	867	GLU
2	X	880	ARG
2	X	883	LYS
2	X	884	ARG
2	X	885	LYS
2	X	887	LYS
2	X	907	ASN
2	X	911	ILE
2	Y	667	MET
2	Y	668	SER
2	Y	670	THR
2	Y	672	SER
2	Y	681	ARG
2	Y	690	VAL
2	Y	692	ASN
2	Y	706	ASN
2	Y	707	ILE
2	Y	710	LYS

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Mol	Chain	Res	Type
2	Y	711	ASN
2	Y	713	ILE
2	Y	715	SER
2	Y	731	LYS
2	Y	732	THR
2	Y	733	LYS
2	Y	734	SER
2	Y	740	PRO
2	Y	741	ARG
2	Y	748	PRO
2	Y	767	ILE
2	Y	774	LEU
2	Y	779	SER
2	Y	787	GLN
2	Y	788	THR
2	Y	792	MET
2	Y	794	SER
2	Y	811	SER
2	Y	820	LEU
2	Y	822	SER
2	Y	828	ASP
2	Y	830	SER
2	Y	831	THR
2	Y	832	LYS
2	Y	836	THR
2	Y	841	LYS
2	Y	853	VAL
2	Y	855	CYS
2	Y	856	LEU
2	Y	871	ARG
2	Y	872	VAL
2	Y	874	ASP
2	Y	878	PHE
2	Y	879	ARG
2	Y	883	LYS
2	Y	888	ILE
2	Y	894	VAL
2	Y	906	GLU
2	Y	910	LEU
2	Y	911	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	138	GLN
1	A	195	HIS
1	B	18	HIS
1	B	54	GLN
1	B	87	ASN
1	B	100	ASN
1	B	112	ASN
1	B	118	ASN
1	B	200	ASN
1	C	9	HIS
1	C	40	HIS
1	C	141	ASN
1	D	18	HIS
1	D	87	ASN
1	D	100	ASN
1	D	112	ASN
1	D	137	ASN
1	D	156	ASN
1	D	196	ASN
1	D	200	ASN
2	X	673	GLN
2	X	706	ASN
2	X	711	ASN
2	X	716	ASN
2	X	718	HIS
2	X	739	GLN
2	X	773	GLN
2	X	816	HIS
2	X	848	HIS
2	X	907	ASN
2	Y	706	ASN
2	Y	745	HIS
2	Y	773	GLN
2	Y	787	GLN
2	Y	848	HIS
2	Y	904	GLN
2	Y	907	ASN
2	Y	908	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	201/203 (99%)	0.92	40 (19%)	3	2	35, 71, 104, 125	0
1	B	196/203 (96%)	1.48	67 (34%)	1	1	33, 99, 134, 147	0
1	C	201/203 (99%)	0.99	40 (19%)	3	2	32, 72, 103, 132	0
1	D	195/203 (96%)	1.60	72 (36%)	1	0	29, 94, 134, 148	0
2	X	256/263 (97%)	0.16	8 (3%)	51	47	31, 50, 83, 96	0
2	Y	258/263 (98%)	0.18	8 (3%)	51	47	33, 49, 79, 112	0
All	All	1307/1338 (97%)	0.82	235 (17%)	3	3	29, 63, 125, 148	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	56	ALA	6.9
1	D	59	MET	6.5
1	B	61	MET	5.9
1	D	61	MET	5.9
1	A	39	GLY	5.6
1	A	120	ALA	5.6
1	B	67	VAL	5.4
1	D	66	TYR	5.4
1	D	52	ILE	5.2
1	D	101	LEU	5.2
1	C	116	VAL	5.1
1	B	59	MET	5.0
1	D	84	TYR	5.0
1	A	116	VAL	4.9
1	D	74	LEU	4.8
1	D	106	PHE	4.7
1	D	113	LEU	4.7
1	D	103	ASP	4.7
1	B	66	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	56	ALA	4.6
1	D	47	VAL	4.5
1	D	83	VAL	4.5
1	B	52	ILE	4.4
1	B	27	THR	4.4
1	A	124	ARG	4.4
1	D	116	VAL	4.4
1	D	105	SER	4.4
1	D	9	HIS	4.3
1	C	126	LEU	4.3
1	B	125	GLU	4.3
1	D	60	GLU	4.3
1	D	104	VAL	4.2
1	D	100	ASN	4.2
1	D	53	SER	4.2
1	B	47	VAL	4.2
1	B	88	PHE	4.2
1	D	8	ILE	4.1
1	D	111	PHE	4.1
1	A	128	CYS	4.1
1	B	106	PHE	4.1
1	B	83	VAL	4.0
1	B	111	PHE	4.0
1	B	101	LEU	3.9
1	A	26	LYS	3.9
1	D	125	GLU	3.9
1	B	116	VAL	3.8
1	D	70	LEU	3.8
1	B	50	SER	3.8
1	D	90	LYS	3.7
1	D	26	LYS	3.7
1	B	12	SER	3.7
1	B	60	GLU	3.7
1	B	90	LYS	3.7
1	C	40	HIS	3.7
1	D	88	PHE	3.7
1	A	127	ILE	3.7
1	C	124	ARG	3.7
1	D	201	ALA	3.6
1	A	40	HIS	3.6
1	B	105	SER	3.6
1	D	95	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	94	TYR	3.6
1	C	117	GLU	3.5
1	D	25	GLU	3.5
1	A	113	LEU	3.5
1	B	95	PHE	3.5
1	B	26	LYS	3.5
1	B	113	LEU	3.5
1	C	127	ILE	3.5
1	D	86	PHE	3.5
1	C	128	CYS	3.5
1	C	119	PRO	3.4
1	C	113	LEU	3.4
2	Y	911	ILE	3.4
2	X	669	GLY	3.3
2	X	707	ILE	3.3
1	B	11	VAL	3.3
1	B	86	PHE	3.3
1	D	112	ASN	3.3
1	B	107	ARG	3.3
1	B	64	GLY	3.3
1	A	93	CYS	3.2
1	B	63	LYS	3.2
1	D	67	VAL	3.2
2	X	908	GLN	3.2
1	A	90	LYS	3.2
1	C	39	GLY	3.2
1	D	27	THR	3.2
1	D	96	PHE	3.1
1	C	110	SER	3.1
1	B	42	ALA	3.1
1	B	115	LYS	3.1
1	C	85	THR	3.1
1	D	57	ASP	3.1
1	A	92	SER	3.1
1	A	27	THR	3.0
1	B	120	ALA	3.0
1	B	28	LEU	3.0
1	D	107	ARG	3.0
1	D	48	SER	3.0
1	C	94	TYR	3.0
1	D	94	TYR	3.0
1	C	95	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	90	LYS	3.0
2	X	711	ASN	3.0
1	A	123	ILE	2.9
1	D	11	VAL	2.9
1	D	1	MET	2.9
1	A	126	LEU	2.9
1	B	1	MET	2.9
1	B	49	GLU	2.9
2	Y	867	GLU	2.9
1	B	29	GLU	2.9
1	B	8	ILE	2.8
1	D	108	LEU	2.8
1	B	103	ASP	2.8
1	C	122	VAL	2.8
1	B	54	GLN	2.8
2	Y	671	ASP	2.8
1	C	92	SER	2.8
1	B	104	VAL	2.8
1	C	130	CYS	2.8
1	D	124	ARG	2.8
1	C	111	PHE	2.8
1	B	74	LEU	2.8
1	C	134	THR	2.8
1	B	73	ALA	2.7
1	D	93	CYS	2.7
1	C	16	ILE	2.7
1	C	27	THR	2.7
1	D	115	LYS	2.7
1	A	22	VAL	2.7
1	A	30	SER	2.7
1	A	110	SER	2.7
1	D	28	LEU	2.7
2	Y	672	SER	2.7
1	B	25	GLU	2.7
1	B	39	GLY	2.6
1	D	99	LYS	2.6
1	A	114	GLU	2.6
1	C	9	HIS	2.6
1	D	102	LYS	2.6
2	X	717	LYS	2.6
1	C	5	ILE	2.6
1	B	108	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	53	SER	2.6
1	C	201	ALA	2.6
2	Y	670	THR	2.6
1	B	9	HIS	2.6
1	B	97	PHE	2.6
1	C	88	PHE	2.6
1	C	96	PHE	2.6
1	B	114	GLU	2.6
1	D	16	ILE	2.6
1	B	122	VAL	2.6
1	A	15	SER	2.6
1	A	201	ALA	2.6
1	D	50	SER	2.6
1	C	26	LYS	2.6
1	C	123	ILE	2.5
1	B	100	ASN	2.5
1	B	48	SER	2.5
1	C	89	SER	2.5
1	D	15	SER	2.5
1	B	84	TYR	2.5
1	D	14	PRO	2.5
1	C	36	LEU	2.5
1	A	41	SER	2.5
1	A	16	ILE	2.5
1	A	117	GLU	2.5
1	B	30	SER	2.5
1	D	89	SER	2.5
1	A	62	GLU	2.5
1	D	123	ILE	2.5
1	B	14	PRO	2.4
1	D	20	LEU	2.4
1	D	54	GLN	2.4
1	A	89	SER	2.4
1	B	62	GLU	2.4
1	D	33	VAL	2.4
1	C	21	GLN	2.4
1	D	10	LEU	2.4
1	A	96	PHE	2.4
1	B	99	LYS	2.4
1	D	29	GLU	2.4
1	D	98	GLU	2.4
1	D	39	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	38	ASP	2.3
1	C	93	CYS	2.3
1	C	120	ALA	2.3
1	B	85	THR	2.3
2	Y	699	CYS	2.3
1	C	67	VAL	2.3
1	D	31	GLY	2.3
1	D	12	SER	2.2
1	D	91	GLU	2.2
1	B	192	ARG	2.2
1	D	120	ALA	2.2
1	C	46	THR	2.2
1	B	16	ILE	2.2
2	Y	822	SER	2.2
1	A	95	PHE	2.2
1	C	44	THR	2.2
2	Y	823	TYR	2.2
1	A	64	GLY	2.2
1	D	76	SER	2.2
1	D	32	PHE	2.2
1	A	9	HIS	2.2
1	D	44	THR	2.2
1	D	97	PHE	2.2
1	D	122	VAL	2.1
1	A	85	THR	2.1
1	C	34	ILE	2.1
1	C	52	ILE	2.1
1	B	76	SER	2.1
1	B	124	ARG	2.1
1	A	119	PRO	2.1
1	B	18	HIS	2.1
1	C	28	LEU	2.1
1	D	62	GLU	2.1
1	D	92	SER	2.1
1	B	57	ASP	2.1
1	A	122	VAL	2.0
1	B	123	ILE	2.0
2	X	710	LYS	2.0
1	B	119	PRO	2.0
1	A	1	MET	2.0
2	X	673	GLN	2.0
1	A	88	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	111	PHE	2.0
1	A	20	LEU	2.0
1	A	42	ALA	2.0
1	B	87	ASN	2.0
1	A	44	THR	2.0
2	X	670	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
3	CL	Y	302	1/1	0.92	0.10	65,65,65,65	0
3	CL	Y	301	1/1	0.94	0.10	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.