



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:01 PM UTC

PDB ID : 3G8L / pdb_00003g8l
Title : Crystal structure of murine natural killer cell receptor, Ly49L4
Authors : Cho, S.
Deposited on : 2009-02-12
Resolution : 2.50 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

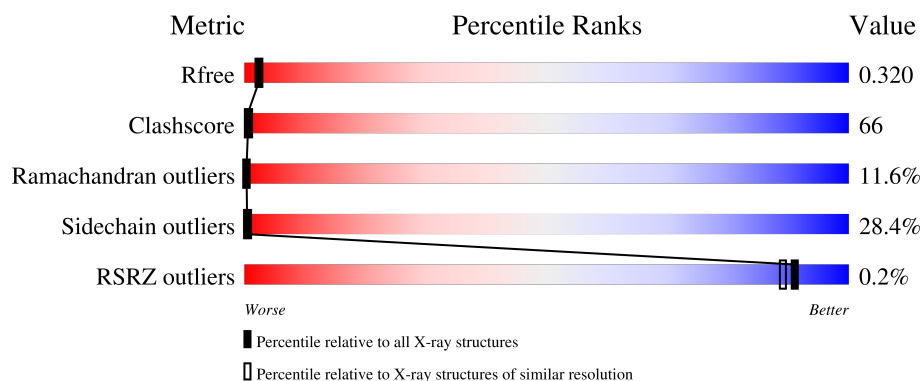
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	190	
1	B	190	
1	C	190	
1	D	190	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5162 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 Lectin-related NK cell receptor LY49L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1293	823	219	240	11			
1	B	161	Total	C	N	O	S	0	0	0
			1327	843	226	246	12			
1	C	154	Total	C	N	O	S	0	0	0
			1267	808	213	235	11			
1	D	152	Total	C	N	O	S	0	0	0
			1258	804	211	231	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	expression tag	UNP Q9JIP9
A	77	ALA	-	expression tag	UNP Q9JIP9
A	78	SER	-	expression tag	UNP Q9JIP9
A	198	TYR	CYS	engineered mutation	UNP Q9JIP9
B	76	MET	-	expression tag	UNP Q9JIP9
B	77	ALA	-	expression tag	UNP Q9JIP9
B	78	SER	-	expression tag	UNP Q9JIP9
B	198	TYR	CYS	engineered mutation	UNP Q9JIP9
C	76	MET	-	expression tag	UNP Q9JIP9
C	77	ALA	-	expression tag	UNP Q9JIP9
C	78	SER	-	expression tag	UNP Q9JIP9
C	198	TYR	CYS	engineered mutation	UNP Q9JIP9
D	76	MET	-	expression tag	UNP Q9JIP9
D	77	ALA	-	expression tag	UNP Q9JIP9
D	78	SER	-	expression tag	UNP Q9JIP9
D	198	TYR	CYS	engineered mutation	UNP Q9JIP9

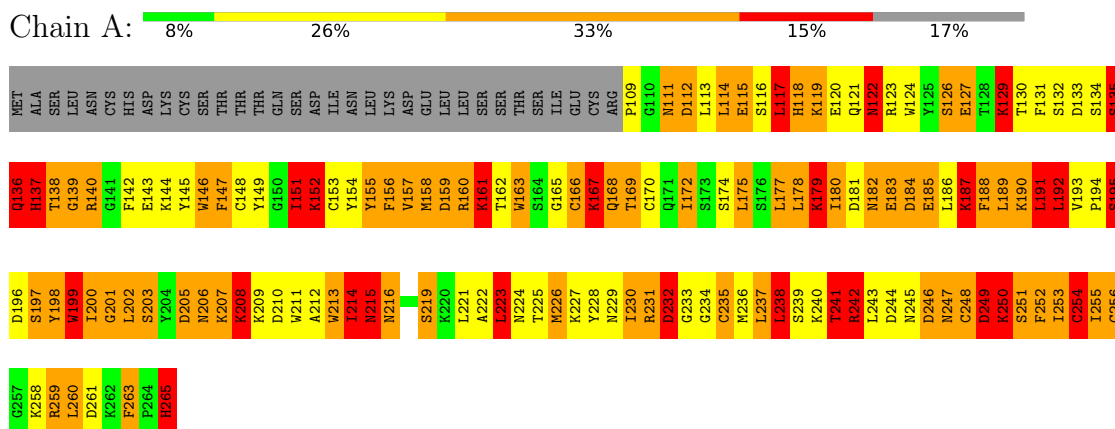
- Molecule 2 is water.

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

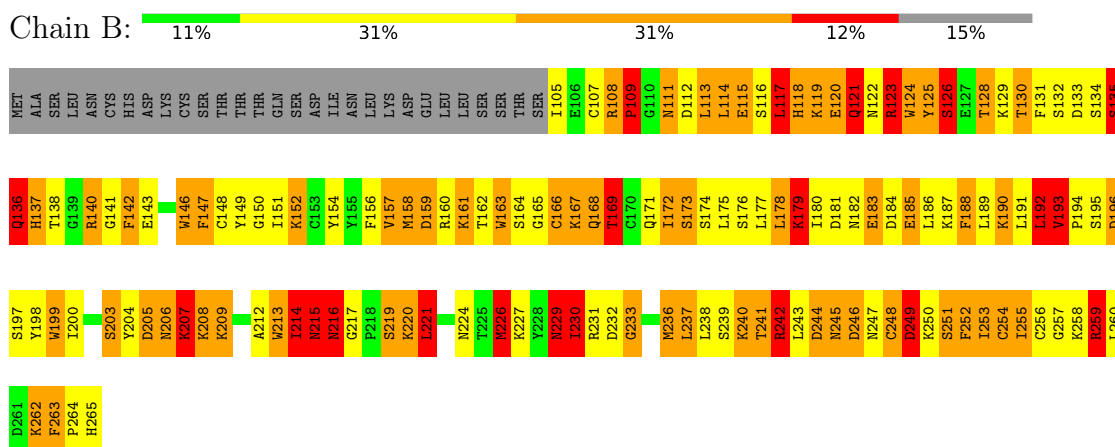
3 Residue-property plots

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

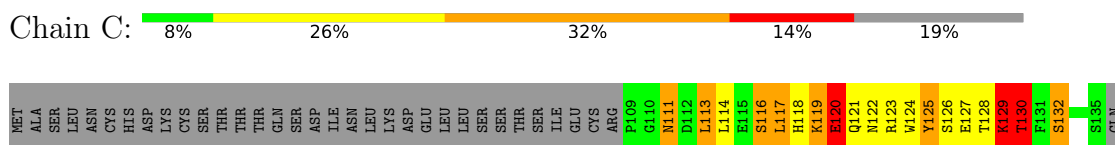
- Molecule 1: Lectin-related NK cell receptor LY49L1

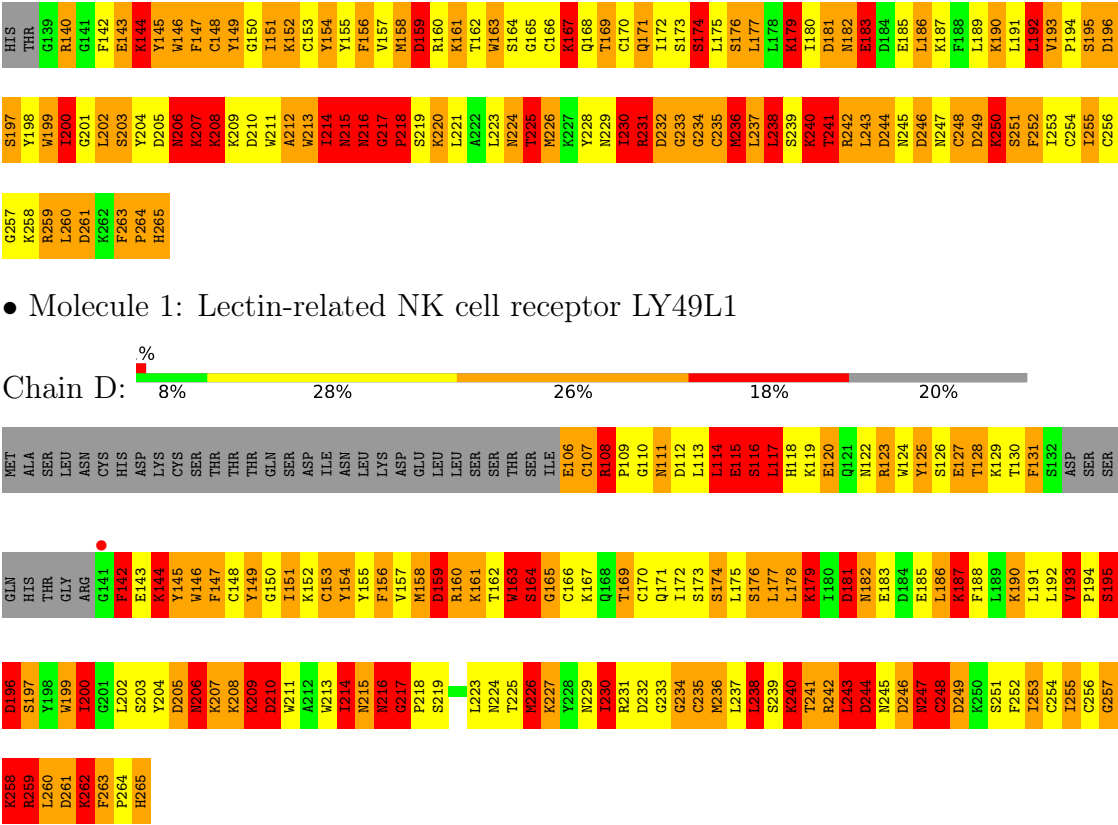


- Molecule 1: Lectin-related NK cell receptor LY49L1



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● Molecule 1: Lectin-related NK cell receptor LY49L1

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	78.05Å 78.05Å 216.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.1 (30.00-2.50) 90.1 (30.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.287 0.221 , 0.320	Depositor DCC
R_{free} test set	1229 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.487 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5162	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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

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	2.57	69/1326 (5.2%)	2.27	65/1781 (3.6%)
1	B	2.49	77/1360 (5.7%)	2.24	83/1827 (4.5%)
1	C	2.49	66/1298 (5.1%)	2.33	80/1741 (4.6%)
1	D	2.42	66/1289 (5.1%)	2.27	75/1730 (4.3%)
All	All	2.49	278/5273 (5.3%)	2.28	303/7079 (4.3%)

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	5
1	B	0	2
1	C	0	4
1	D	0	9
All	All	0	20

All (278) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	254	CYS	CA-C	14.54	1.71	1.52
1	A	180	ILE	CA-CB	-13.19	1.38	1.54
1	B	180	ILE	CA-CB	-13.02	1.37	1.54
1	C	255	ILE	C-O	12.15	1.38	1.24
1	A	253	ILE	CA-CB	-11.86	1.42	1.54
1	A	136	GLN	CA-C	11.74	1.66	1.52
1	C	252	PHE	N-CA	11.36	1.60	1.46
1	B	253	ILE	CA-CB	-10.88	1.41	1.54
1	A	247	ASN	CA-C	-10.69	1.39	1.52
1	C	145	TYR	C-O	10.50	1.36	1.23
1	A	249	ASP	CA-C	-10.38	1.38	1.52
1	B	157	VAL	CA-CB	-10.25	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	ILE	CG1-CD1	9.94	1.90	1.51
1	D	248	CYS	C-O	9.84	1.36	1.24
1	D	244	ASP	CA-C	9.68	1.65	1.52
1	A	163	TRP	CA-C	-9.42	1.39	1.52
1	C	204	TYR	N-CA	9.28	1.57	1.46
1	D	178	LEU	N-CA	-9.16	1.34	1.46
1	D	145	TYR	C-O	9.15	1.33	1.24
1	B	226	MET	CA-C	9.13	1.65	1.52
1	D	256	CYS	CA-C	9.09	1.64	1.52
1	D	195	SER	N-CA	9.04	1.57	1.46
1	C	118	HIS	CA-C	-8.82	1.41	1.52
1	A	160	ARG	N-CA	8.81	1.57	1.46
1	A	255	ILE	N-CA	-8.70	1.35	1.46
1	A	146	TRP	C-O	8.63	1.33	1.23
1	A	249	ASP	C-O	-8.46	1.13	1.24
1	D	194	PRO	CA-C	8.32	1.60	1.52
1	D	200	ILE	CA-CB	-8.28	1.43	1.54
1	B	249	ASP	CA-C	-8.25	1.41	1.52
1	D	202	LEU	CA-C	8.25	1.62	1.52
1	B	248	CYS	C-O	8.22	1.34	1.24
1	B	185	GLU	N-CA	8.18	1.56	1.46
1	C	151	ILE	CA-C	8.15	1.63	1.52
1	D	257	GLY	CA-C	8.10	1.58	1.52
1	B	160	ARG	C-O	-8.10	1.13	1.23
1	D	156	PHE	C-O	8.04	1.33	1.24
1	A	237	LEU	C-O	8.02	1.34	1.23
1	B	161	LYS	C-O	7.91	1.34	1.23
1	B	141	GLY	CA-C	7.91	1.59	1.52
1	A	156	PHE	C-O	7.91	1.33	1.24
1	B	137	HIS	CA-C	7.85	1.63	1.53
1	A	248	CYS	CA-C	-7.84	1.42	1.52
1	B	216	ASN	CA-C	7.83	1.63	1.52
1	C	230	ILE	CA-CB	-7.56	1.43	1.54
1	A	152	LYS	CE-NZ	7.55	1.72	1.49
1	A	246	ASP	C-O	7.36	1.31	1.24
1	C	225	THR	CA-CB	7.34	1.65	1.53
1	D	114	LEU	CA-C	-7.33	1.43	1.52
1	D	199	TRP	N-CA	-7.27	1.37	1.46
1	A	175	LEU	CA-C	-7.25	1.43	1.52
1	B	229	ASN	CG-OD1	7.25	1.37	1.23
1	B	149	TYR	N-CA	-7.23	1.36	1.46
1	A	242	ARG	CA-C	-7.21	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	LYS	CB-CG	7.19	1.74	1.52
1	D	239	SER	N-CA	7.19	1.54	1.45
1	C	146	TRP	CE3-CZ3	7.17	1.60	1.38
1	D	235	CYS	CA-C	-7.16	1.44	1.52
1	A	248	CYS	C-O	7.12	1.32	1.24
1	C	253	ILE	CA-C	-7.09	1.44	1.52
1	A	182	ASN	CA-C	-7.08	1.44	1.52
1	B	158	MET	C-O	-7.06	1.15	1.24
1	D	194	PRO	N-CA	-7.05	1.39	1.47
1	C	251	SER	CA-CB	-7.05	1.43	1.53
1	D	258	LYS	CD-CE	7.01	1.73	1.52
1	D	117	LEU	CA-CB	-7.01	1.42	1.53
1	D	146	TRP	C-O	6.99	1.31	1.23
1	A	252	PHE	C-O	-6.98	1.15	1.23
1	C	155	TYR	CA-C	6.95	1.61	1.52
1	B	142	PHE	CA-C	6.94	1.60	1.52
1	A	250	LYS	CA-C	6.93	1.62	1.53
1	D	230	ILE	CA-CB	-6.86	1.44	1.54
1	B	156	PHE	C-O	6.83	1.32	1.24
1	D	245	ASN	N-CA	6.83	1.54	1.45
1	C	208	LYS	N-CA	6.82	1.54	1.46
1	C	212	ALA	CA-C	6.77	1.61	1.52
1	B	132	SER	N-CA	-6.76	1.37	1.45
1	A	255	ILE	CA-C	-6.76	1.44	1.52
1	C	214	ILE	N-CA	-6.74	1.38	1.46
1	B	246	ASP	N-CA	6.74	1.55	1.46
1	C	235	CYS	CA-C	-6.70	1.44	1.52
1	A	255	ILE	CB-CG2	6.69	1.74	1.52
1	B	146	TRP	C-O	6.69	1.31	1.23
1	C	183	GLU	C-O	6.67	1.31	1.24
1	C	179	LYS	CG-CD	6.65	1.72	1.52
1	B	123	ARG	CA-C	-6.62	1.43	1.52
1	B	198	TYR	CA-CB	6.61	1.65	1.53
1	C	187	LYS	N-CA	6.60	1.54	1.46
1	B	253	ILE	CA-C	-6.59	1.44	1.52
1	C	261	ASP	C-O	6.56	1.32	1.24
1	C	193	VAL	C-N	-6.56	1.25	1.33
1	D	188	PHE	CA-C	-6.53	1.44	1.52
1	D	160	ARG	CA-C	6.53	1.61	1.52
1	C	215	ASN	N-CA	6.51	1.54	1.46
1	B	255	ILE	C-O	6.48	1.31	1.24
1	A	152	LYS	CG-CD	6.45	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	213	TRP	CA-C	-6.43	1.45	1.52
1	B	164	SER	C-O	-6.40	1.15	1.24
1	D	125	TYR	CA-CB	6.40	1.63	1.53
1	B	182	ASN	C-O	6.39	1.32	1.24
1	C	199	TRP	C-O	-6.38	1.16	1.24
1	C	117	LEU	CA-CB	-6.29	1.42	1.53
1	B	143	GLU	C-O	6.28	1.31	1.23
1	C	169	THR	CA-C	6.25	1.60	1.52
1	B	259	ARG	N-CA	-6.25	1.38	1.46
1	A	197	SER	N-CA	6.23	1.53	1.45
1	C	147	PHE	CA-C	-6.22	1.45	1.52
1	D	187	LYS	CG-CD	6.22	1.71	1.52
1	C	187	LYS	CB-CG	6.19	1.71	1.52
1	B	163	TRP	N-CA	-6.18	1.38	1.46
1	D	251	SER	C-O	6.16	1.30	1.24
1	C	130	THR	CA-CB	6.16	1.62	1.54
1	D	190	LYS	CA-C	-6.15	1.44	1.52
1	C	193	VAL	CA-CB	-6.15	1.46	1.54
1	B	200	ILE	CA-CB	-6.13	1.46	1.54
1	A	133	ASP	N-CA	6.13	1.53	1.45
1	A	126	SER	CA-C	-6.10	1.44	1.52
1	D	254	CYS	CA-C	6.09	1.60	1.52
1	D	209	LYS	C-O	6.09	1.31	1.23
1	A	198	TYR	CD2-CE2	6.08	1.56	1.38
1	C	122	ASN	CA-CB	6.06	1.63	1.53
1	C	154	TYR	CA-CB	-6.06	1.44	1.53
1	A	241	THR	CA-CB	6.06	1.63	1.53
1	D	155	TYR	CA-CB	-6.04	1.44	1.53
1	A	238	LEU	CA-CB	-6.04	1.44	1.53
1	D	255	ILE	C-O	6.04	1.31	1.23
1	D	155	TYR	CA-C	6.03	1.59	1.52
1	C	238	LEU	CA-C	-6.02	1.45	1.52
1	D	259	ARG	C-O	6.02	1.31	1.24
1	C	151	ILE	CG1-CD1	6.01	1.75	1.51
1	D	169	THR	CA-C	6.00	1.61	1.52
1	D	193	VAL	C-N	-5.99	1.27	1.33
1	B	206	ASN	CA-C	5.99	1.60	1.52
1	B	257	GLY	CA-C	-5.97	1.47	1.52
1	B	187	LYS	CA-C	5.96	1.61	1.52
1	D	142	PHE	N-CA	5.95	1.53	1.46
1	A	182	ASN	CA-CB	5.95	1.63	1.53
1	A	155	TYR	CE2-CZ	5.94	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	246	ASP	CG-OD2	5.94	1.36	1.25
1	A	140	ARG	C-O	-5.93	1.17	1.24
1	B	187	LYS	CG-CD	5.92	1.70	1.52
1	B	252	PHE	C-O	-5.92	1.16	1.23
1	C	236	MET	CA-CB	-5.92	1.43	1.53
1	B	262	LYS	C-O	-5.91	1.16	1.23
1	A	178	LEU	C-O	5.91	1.31	1.24
1	B	148	CYS	CA-C	-5.89	1.45	1.52
1	A	253	ILE	CG1-CD1	5.87	1.74	1.51
1	A	137	HIS	N-CA	5.84	1.53	1.46
1	C	253	ILE	C-O	5.83	1.30	1.24
1	C	202	LEU	CA-C	5.82	1.59	1.52
1	D	193	VAL	N-CA	-5.82	1.41	1.47
1	C	161	LYS	CA-C	5.82	1.59	1.52
1	B	131	PHE	CA-C	-5.82	1.45	1.52
1	A	129	LYS	CD-CE	5.81	1.69	1.52
1	C	203	SER	CA-CB	-5.80	1.45	1.54
1	A	199	TRP	N-CA	-5.79	1.38	1.46
1	B	126	SER	CA-C	-5.77	1.45	1.52
1	B	226	MET	CG-SD	5.76	1.95	1.80
1	C	254	CYS	CB-SG	5.76	2.00	1.81
1	D	148	CYS	CA-C	-5.76	1.45	1.52
1	D	181	ASP	C-O	-5.76	1.16	1.24
1	B	221	LEU	CA-C	5.76	1.60	1.52
1	D	230	ILE	N-CA	-5.75	1.39	1.46
1	D	265	HIS	CA-CB	5.74	1.65	1.53
1	B	169	THR	CA-C	5.74	1.60	1.52
1	D	258	LYS	CG-CD	5.73	1.69	1.52
1	B	152	LYS	CE-NZ	5.73	1.66	1.49
1	C	119	LYS	N-CA	5.70	1.53	1.46
1	D	175	LEU	N-CA	5.70	1.53	1.45
1	C	231	ARG	NE-CZ	5.69	1.39	1.33
1	B	252	PHE	N-CA	5.69	1.53	1.45
1	C	224	ASN	CA-C	5.68	1.60	1.52
1	A	161	LYS	C-O	5.68	1.30	1.23
1	B	179	LYS	CG-CD	5.68	1.69	1.52
1	A	203	SER	N-CA	5.67	1.52	1.46
1	A	232	ASP	CA-C	5.66	1.60	1.52
1	B	168	GLN	N-CA	5.65	1.53	1.46
1	D	120	GLU	CA-C	5.65	1.60	1.52
1	B	199	TRP	CA-CB	5.64	1.60	1.53
1	B	252	PHE	CA-C	5.63	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	206	ASN	CA-C	5.63	1.60	1.52
1	D	116	SER	C-O	5.63	1.30	1.24
1	D	256	CYS	N-CA	5.63	1.53	1.46
1	A	184	ASP	C-O	5.63	1.30	1.24
1	D	247	ASN	CA-CB	5.62	1.61	1.53
1	B	251	SER	C-O	5.62	1.30	1.24
1	A	136	GLN	N-CA	5.62	1.53	1.46
1	B	185	GLU	CD-OE1	5.59	1.35	1.25
1	D	151	ILE	CA-CB	-5.59	1.46	1.54
1	C	148	CYS	CA-C	-5.58	1.45	1.52
1	A	198	TYR	CA-CB	5.57	1.63	1.53
1	A	166	CYS	CA-CB	-5.56	1.44	1.53
1	B	120	GLU	N-CA	-5.56	1.39	1.46
1	C	248	CYS	C-O	5.56	1.30	1.24
1	B	197	SER	N-CA	5.55	1.52	1.45
1	C	154	TYR	CA-C	-5.55	1.46	1.52
1	C	214	ILE	CA-C	5.54	1.59	1.52
1	B	249	ASP	C-O	-5.54	1.17	1.24
1	D	176	SER	CA-C	5.54	1.58	1.52
1	B	118	HIS	CA-C	-5.52	1.46	1.52
1	B	179	LYS	CD-CE	5.51	1.69	1.52
1	A	167	LYS	C-O	-5.51	1.17	1.24
1	B	109	PRO	CA-C	5.51	1.60	1.52
1	C	175	LEU	N-CA	5.50	1.54	1.45
1	B	250	LYS	N-CA	-5.50	1.39	1.46
1	B	203	SER	C-O	5.49	1.30	1.23
1	B	166	CYS	C-O	5.49	1.30	1.24
1	B	118	HIS	N-CA	-5.48	1.39	1.46
1	A	187	LYS	CD-CE	5.47	1.68	1.52
1	A	239	SER	CA-C	5.47	1.60	1.53
1	C	144	LYS	CG-CD	5.47	1.68	1.52
1	A	131	PHE	CA-C	-5.46	1.46	1.52
1	A	258	LYS	N-CA	5.46	1.52	1.46
1	B	213	TRP	CA-CB	5.46	1.62	1.53
1	C	233	GLY	N-CA	5.45	1.51	1.45
1	C	233	GLY	C-O	-5.45	1.19	1.23
1	A	169	THR	N-CA	-5.45	1.39	1.46
1	B	143	GLU	CD-OE1	5.42	1.35	1.25
1	B	164	SER	N-CA	5.42	1.53	1.46
1	D	262	LYS	N-CA	-5.42	1.39	1.46
1	C	260	LEU	CA-C	-5.42	1.46	1.52
1	A	185	GLU	CB-CG	-5.40	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	GLU	N-CA	5.40	1.53	1.46
1	A	169	THR	CA-C	5.40	1.60	1.52
1	D	234	GLY	CA-C	5.39	1.59	1.51
1	D	128	THR	N-CA	-5.39	1.39	1.46
1	D	154	TYR	C-O	-5.37	1.17	1.23
1	B	143	GLU	CG-CD	5.36	1.65	1.52
1	A	151	ILE	CB-CG1	5.36	1.64	1.53
1	B	151	ILE	CG1-CD1	5.35	1.72	1.51
1	D	259	ARG	CA-CB	-5.34	1.45	1.53
1	B	213	TRP	CA-C	-5.33	1.46	1.52
1	B	169	THR	N-CA	-5.33	1.39	1.46
1	A	149	TYR	C-O	5.33	1.29	1.23
1	D	261	ASP	N-CA	5.32	1.53	1.46
1	B	151	ILE	CA-CB	5.32	1.61	1.54
1	B	171	GLN	CB-CG	5.32	1.68	1.52
1	A	213	TRP	CA-CB	5.30	1.61	1.53
1	D	253	ILE	N-CA	-5.30	1.39	1.46
1	B	200	ILE	CA-C	-5.29	1.46	1.52
1	A	188	PHE	C-O	5.28	1.30	1.24
1	B	217	GLY	N-CA	5.27	1.51	1.44
1	C	167	LYS	CG-CD	5.25	1.68	1.52
1	C	241	THR	CA-CB	5.25	1.62	1.53
1	D	160	ARG	CB-CG	5.25	1.68	1.52
1	A	191	LEU	N-CA	5.21	1.52	1.46
1	C	245	ASN	C-O	-5.21	1.17	1.23
1	D	239	SER	CA-C	5.21	1.60	1.53
1	C	183	GLU	CA-C	5.18	1.59	1.52
1	D	186	LEU	N-CA	-5.18	1.39	1.46
1	A	132	SER	C-O	-5.17	1.17	1.24
1	A	246	ASP	N-CA	5.16	1.53	1.46
1	D	245	ASN	C-O	-5.16	1.17	1.23
1	A	152	LYS	C-O	5.16	1.30	1.24
1	C	231	ARG	CB-CG	5.15	1.67	1.52
1	A	166	CYS	CA-C	5.15	1.60	1.52
1	B	148	CYS	C-O	-5.14	1.17	1.23
1	B	172	ILE	C-O	-5.14	1.18	1.24
1	D	187	LYS	C-O	5.14	1.30	1.24
1	B	248	CYS	CA-C	-5.13	1.45	1.52
1	C	199	TRP	CB-CG	5.13	1.66	1.50
1	C	224	ASN	N-CA	5.13	1.52	1.46
1	C	254	CYS	CA-CB	5.12	1.61	1.53
1	A	234	GLY	CA-C	5.12	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	144	LYS	CG-CD	5.12	1.67	1.52
1	A	202	LEU	CA-C	5.12	1.59	1.52
1	A	154	TYR	C-O	-5.10	1.18	1.24
1	B	130	THR	CB-CG2	5.09	1.69	1.52
1	B	231	ARG	CZ-NH2	5.06	1.40	1.33
1	D	263	PHE	C-O	-5.06	1.17	1.24
1	C	161	LYS	C-O	5.03	1.29	1.23
1	C	236	MET	CA-C	-5.02	1.46	1.52
1	C	152	LYS	C-O	-5.02	1.18	1.23
1	D	248	CYS	N-CA	-5.02	1.39	1.46
1	A	214	ILE	C-O	5.01	1.30	1.24
1	B	136	GLN	CB-CG	5.01	1.67	1.52
1	D	115	GLU	N-CA	-5.01	1.40	1.46
1	C	146	TRP	CD2-CE2	5.00	1.49	1.41

All (303) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	VAL	CA-C-N	-16.24	103.95	120.03
1	C	193	VAL	C-N-CA	-16.24	103.95	120.03
1	C	217	GLY	CA-C-N	-14.50	101.71	119.84
1	C	217	GLY	C-N-CA	-14.50	101.71	119.84
1	A	181	ASP	N-CA-C	13.47	127.44	111.82
1	D	240	LYS	N-CA-C	-12.89	96.86	112.59
1	B	141	GLY	N-CA-C	11.64	125.32	111.93
1	B	120	GLU	N-CA-C	-11.33	98.62	110.97
1	C	125	TYR	N-CA-C	-10.27	98.79	111.11
1	C	251	SER	CB-CA-C	-10.21	93.54	110.29
1	A	260	LEU	CA-C-N	-10.10	106.38	122.23
1	A	260	LEU	C-N-CA	-10.10	106.38	122.23
1	D	194	PRO	CB-CA-C	-9.95	100.72	111.56
1	D	244	ASP	N-CA-C	9.94	123.47	108.46
1	B	172	ILE	CB-CA-C	-9.91	99.19	111.88
1	D	210	ASP	N-CA-C	9.84	123.31	108.46
1	C	208	LYS	N-CA-C	9.81	131.69	110.80
1	D	116	SER	N-CA-C	9.79	121.71	111.14
1	D	251	SER	N-CA-C	9.70	124.25	108.34
1	B	233	GLY	N-CA-C	-9.61	98.31	111.09
1	A	157	VAL	CB-CA-C	-9.59	100.56	112.45
1	A	163	TRP	CA-C-N	-9.50	104.94	121.66
1	A	163	TRP	C-N-CA	-9.50	104.94	121.66
1	B	184	ASP	N-CA-C	-9.38	99.95	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	TRP	N-CA-C	-9.31	97.68	110.35
1	B	263	PHE	CA-C-N	9.27	131.43	119.84
1	B	263	PHE	C-N-CA	9.27	131.43	119.84
1	A	163	TRP	N-CA-C	-9.22	101.29	112.54
1	D	170	CYS	N-CA-C	-9.21	100.17	111.40
1	A	263	PHE	N-CA-C	-9.03	95.31	109.04
1	A	238	LEU	N-CA-C	8.95	125.00	109.96
1	C	165	GLY	N-CA-C	-8.89	103.67	115.32
1	A	237	LEU	CB-CA-C	-8.85	93.79	109.71
1	B	213	TRP	CA-C-O	-8.76	112.27	121.55
1	C	250	LYS	N-CA-C	-8.74	97.34	110.28
1	B	137	HIS	N-CA-C	8.74	123.53	111.74
1	D	251	SER	CA-CB-OG	-8.58	93.94	111.10
1	A	120	GLU	N-CA-C	-8.55	102.11	112.54
1	D	206	ASN	N-CA-C	-8.54	92.60	110.80
1	C	149	TYR	CA-C-N	-8.45	113.37	121.31
1	C	149	TYR	C-N-CA	-8.45	113.37	121.31
1	D	118	HIS	N-CA-C	8.38	120.04	111.07
1	D	241	THR	N-CA-C	-8.37	92.97	110.80
1	D	165	GLY	N-CA-C	-8.36	103.30	113.99
1	B	124	TRP	N-CA-C	-8.35	102.14	111.07
1	C	236	MET	CA-CB-CG	-8.22	97.66	114.10
1	D	193	VAL	N-CA-CB	-8.15	101.60	109.99
1	D	241	THR	CB-CA-C	8.14	126.61	110.42
1	A	213	TRP	N-CA-C	-8.11	96.33	109.96
1	B	216	ASN	N-CA-C	7.96	127.76	110.80
1	B	138	THR	CB-CA-C	-7.84	96.00	109.65
1	D	190	LYS	N-CA-C	-7.84	102.82	111.36
1	D	196	ASP	CA-C-N	-7.83	111.19	122.94
1	D	196	ASP	C-N-CA	-7.83	111.19	122.94
1	C	156	PHE	CA-C-N	-7.80	113.04	123.10
1	C	156	PHE	C-N-CA	-7.80	113.04	123.10
1	C	212	ALA	N-CA-C	7.66	120.37	108.96
1	C	193	VAL	N-CA-C	7.60	117.31	108.96
1	C	216	ASN	N-CA-C	-7.58	94.65	110.80
1	C	164	SER	N-CA-C	-7.58	103.50	112.89
1	C	220	LYS	N-CA-C	-7.57	103.94	113.02
1	D	179	LYS	N-CA-C	-7.55	99.31	110.48
1	D	145	TYR	N-CA-C	-7.53	97.26	107.88
1	A	215	ASN	N-CA-C	7.50	122.50	112.30
1	B	220	LYS	N-CA-C	-7.39	105.13	112.97
1	A	238	LEU	CB-CA-C	-7.38	97.35	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	161	LYS	N-CA-C	7.32	120.33	108.76
1	A	168	GLN	N-CA-C	7.24	120.60	111.69
1	A	175	LEU	N-CA-C	-7.15	95.57	110.80
1	A	248	CYS	CA-CB-SG	-7.11	98.06	114.40
1	A	132	SER	CA-C-O	-7.05	113.58	121.40
1	C	203	SER	N-CA-C	7.05	117.79	108.07
1	A	207	LYS	CA-C-N	-7.04	109.60	120.31
1	A	207	LYS	C-N-CA	-7.04	109.60	120.31
1	D	182	ASN	N-CA-C	6.98	118.97	107.73
1	C	118	HIS	CA-C-O	-6.98	112.49	120.24
1	A	179	LYS	CB-CA-C	-6.91	99.24	110.77
1	D	244	ASP	N-CA-CB	-6.88	99.34	110.77
1	B	217	GLY	CA-C-N	-6.88	112.88	119.76
1	B	217	GLY	C-N-CA	-6.88	112.88	119.76
1	A	214	ILE	CA-C-N	-6.86	110.69	122.14
1	A	214	ILE	C-N-CA	-6.86	110.69	122.14
1	D	123	ARG	N-CA-C	-6.82	103.78	111.07
1	C	232	ASP	N-CA-C	6.80	121.17	113.01
1	D	149	TYR	CB-CA-C	6.80	119.64	110.94
1	C	259	ARG	CA-C-N	-6.80	112.52	122.65
1	C	259	ARG	C-N-CA	-6.80	112.52	122.65
1	A	147	PHE	CA-C-O	-6.79	113.52	121.06
1	A	206	ASN	CA-C-N	-6.77	111.23	120.44
1	A	206	ASN	C-N-CA	-6.77	111.23	120.44
1	B	205	ASP	N-CA-C	6.72	121.25	109.96
1	B	254	CYS	CA-C-N	6.70	134.04	121.97
1	B	254	CYS	C-N-CA	6.70	134.04	121.97
1	D	117	LEU	CB-CG-CD1	-6.67	90.69	110.70
1	B	128	THR	N-CA-C	-6.66	106.10	114.56
1	A	247	ASN	N-CA-C	-6.65	97.89	108.73
1	B	253	ILE	CB-CA-C	-6.64	100.77	111.59
1	D	122	ASN	N-CA-C	6.64	118.17	111.07
1	C	220	LYS	CA-C-N	-6.61	112.15	121.99
1	C	220	LYS	C-N-CA	-6.61	112.15	121.99
1	A	247	ASN	O-C-N	6.57	130.71	123.22
1	D	218	PRO	N-CA-C	6.56	120.97	110.21
1	D	195	SER	CA-CB-OG	-6.54	98.02	111.10
1	A	254	CYS	CB-CA-C	-6.53	98.47	109.50
1	C	204	TYR	N-CA-C	6.52	119.33	108.96
1	C	111	ASN	N-CA-C	6.50	124.66	110.80
1	D	114	LEU	CB-CA-C	-6.50	100.67	110.88
1	C	156	PHE	N-CA-C	-6.48	98.67	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ASP	N-CA-C	-6.44	98.69	108.67
1	D	195	SER	CB-CA-C	-6.42	97.63	110.42
1	A	191	LEU	N-CA-C	6.40	117.92	111.07
1	C	251	SER	CA-C-O	-6.37	113.11	120.49
1	D	117	LEU	CB-CA-C	-6.36	100.63	110.81
1	C	213	TRP	N-CA-C	-6.31	98.44	108.73
1	C	200	ILE	CB-CA-C	6.30	120.32	111.63
1	B	197	SER	CA-C-O	-6.27	114.56	121.33
1	D	131	PHE	O-C-N	6.26	126.60	122.03
1	B	188	PHE	CA-C-N	-6.25	111.91	120.28
1	B	188	PHE	C-N-CA	-6.25	111.91	120.28
1	C	234	GLY	O-C-N	-6.25	114.58	122.70
1	B	179	LYS	CA-C-N	-6.25	113.04	121.66
1	B	179	LYS	C-N-CA	-6.25	113.04	121.66
1	B	242	ARG	N-CA-C	-6.24	99.62	108.23
1	B	157	VAL	CB-CA-C	-6.24	103.27	111.81
1	B	175	LEU	N-CA-C	-6.23	100.08	108.86
1	B	205	ASP	CB-CA-C	-6.23	99.25	109.53
1	C	207	LYS	CA-C-N	6.23	133.43	121.54
1	C	207	LYS	C-N-CA	6.23	133.43	121.54
1	D	200	ILE	N-CA-C	6.22	122.28	109.34
1	C	231	ARG	CG-CD-NE	6.22	125.67	112.00
1	C	234	GLY	CA-C-N	-6.21	113.20	122.39
1	C	234	GLY	C-N-CA	-6.21	113.20	122.39
1	B	167	LYS	N-CA-CB	6.20	119.17	109.94
1	A	253	ILE	CB-CG1-CD1	-6.18	100.83	113.80
1	D	244	ASP	CB-CA-C	6.17	119.66	109.72
1	B	253	ILE	N-CA-C	-6.17	101.04	109.37
1	A	140	ARG	N-CA-C	6.16	118.02	109.15
1	D	261	ASP	N-CA-CB	6.14	119.38	110.47
1	B	209	LYS	CB-CA-C	-6.10	100.83	110.04
1	A	255	ILE	CB-CA-C	-6.07	102.10	110.96
1	A	258	LYS	CA-CB-CG	6.06	126.21	114.10
1	C	120	GLU	O-C-N	-6.05	115.80	122.09
1	D	142	PHE	CA-C-N	-6.02	114.21	122.16
1	D	142	PHE	C-N-CA	-6.02	114.21	122.16
1	A	192	LEU	N-CA-C	6.00	120.22	113.02
1	C	196	ASP	CA-C-N	-5.99	112.27	122.33
1	C	196	ASP	C-N-CA	-5.99	112.27	122.33
1	B	214	ILE	N-CA-CB	5.98	121.10	111.23
1	B	250	LYS	N-CA-C	-5.97	101.44	110.28
1	D	243	LEU	CA-C-N	-5.96	108.94	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	243	LEU	C-N-CA	-5.96	108.94	121.81
1	B	237	LEU	CB-CA-C	-5.95	99.41	109.83
1	D	261	ASP	CA-C-N	-5.94	110.19	121.54
1	D	261	ASP	C-N-CA	-5.94	110.19	121.54
1	B	164	SER	N-CA-C	-5.92	104.77	112.23
1	B	240	LYS	N-CA-C	5.92	119.33	111.75
1	C	182	ASN	CA-C-N	-5.92	112.55	120.54
1	C	182	ASN	C-N-CA	-5.92	112.55	120.54
1	D	187	LYS	CA-C-N	-5.92	111.88	120.29
1	D	187	LYS	C-N-CA	-5.92	111.88	120.29
1	A	122	ASN	N-CA-C	-5.92	104.91	111.71
1	A	182	ASN	N-CA-C	-5.91	99.16	108.14
1	D	119	LYS	N-CA-C	-5.89	104.94	111.36
1	D	243	LEU	CB-CA-C	-5.88	101.54	109.71
1	C	123	ARG	CB-CA-C	-5.83	101.69	110.90
1	C	233	GLY	CA-C-O	-5.83	116.53	121.66
1	A	160	ARG	N-CA-C	-5.82	102.03	110.24
1	A	253	ILE	N-CA-CB	-5.81	100.78	110.14
1	D	196	ASP	O-C-N	-5.81	114.86	122.59
1	D	188	PHE	CA-C-N	-5.81	111.31	120.60
1	D	188	PHE	C-N-CA	-5.81	111.31	120.60
1	B	120	GLU	CA-C-N	-5.80	111.32	120.60
1	B	120	GLU	C-N-CA	-5.80	111.32	120.60
1	B	190	LYS	CB-CA-C	-5.80	98.34	110.17
1	A	265	HIS	CB-CA-C	5.79	121.11	110.10
1	B	256	CYS	CA-C-N	-5.78	116.96	121.82
1	B	256	CYS	C-N-CA	-5.78	116.96	121.82
1	C	161	LYS	N-CA-C	5.78	116.92	108.14
1	A	235	CYS	CA-CB-SG	-5.77	101.12	114.40
1	C	195	SER	CA-C-O	5.76	127.65	121.02
1	B	193	VAL	N-CA-CB	-5.75	104.08	110.23
1	B	230	ILE	CB-CA-C	-5.74	101.88	111.29
1	C	163	TRP	N-CA-C	-5.72	104.25	111.11
1	D	238	LEU	CA-CB-CG	5.71	136.30	116.30
1	B	159	ASP	N-CA-C	-5.69	97.16	107.75
1	C	256	CYS	CA-C-N	-5.68	117.42	122.47
1	C	256	CYS	C-N-CA	-5.68	117.42	122.47
1	C	148	CYS	N-CA-C	5.68	118.50	109.81
1	B	158	MET	O-C-N	-5.67	115.04	122.59
1	D	196	ASP	N-CA-C	-5.67	98.72	110.80
1	D	249	ASP	N-CA-C	-5.67	105.31	114.09
1	C	249	ASP	CA-C-N	-5.65	112.84	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ASP	C-N-CA	-5.65	112.84	120.87
1	A	136	GLN	N-CA-C	5.62	117.52	107.80
1	B	192	LEU	CA-C-N	5.62	128.98	121.23
1	B	192	LEU	C-N-CA	5.62	128.98	121.23
1	A	195	SER	N-CA-C	-5.61	99.38	108.41
1	B	131	PHE	CA-C-N	-5.61	113.79	122.59
1	B	131	PHE	C-N-CA	-5.61	113.79	122.59
1	C	241	THR	N-CA-C	-5.60	98.86	110.80
1	D	196	ASP	CB-CA-C	5.60	121.56	110.42
1	D	179	LYS	N-CA-CB	5.59	118.78	110.29
1	C	162	THR	N-CA-C	-5.58	103.12	110.43
1	C	151	ILE	N-CA-CB	-5.57	102.05	111.23
1	C	214	ILE	N-CA-CB	-5.57	102.05	111.23
1	D	257	GLY	N-CA-C	5.56	120.60	110.71
1	C	122	ASN	N-CA-C	5.55	118.10	111.71
1	B	135	SER	N-CA-CB	-5.55	101.93	109.98
1	D	147	PHE	N-CA-C	-5.53	99.73	108.14
1	C	200	ILE	N-CA-CB	-5.53	100.81	110.49
1	B	142	PHE	CA-C-N	5.52	128.54	120.71
1	B	142	PHE	C-N-CA	5.52	128.54	120.71
1	D	236	MET	CA-CB-CG	-5.51	103.08	114.10
1	A	156	PHE	CA-C-N	5.50	128.64	122.59
1	A	156	PHE	C-N-CA	5.50	128.64	122.59
1	A	118	HIS	CA-CB-CG	-5.48	108.32	113.80
1	A	230	ILE	CB-CA-C	-5.47	102.32	111.29
1	A	203	SER	CB-CA-C	-5.47	100.65	111.91
1	B	168	GLN	CA-C-N	-5.46	110.94	121.58
1	B	168	GLN	C-N-CA	-5.46	110.94	121.58
1	B	219	SER	N-CA-C	-5.44	99.81	109.06
1	D	246	ASP	N-CA-CB	-5.44	101.30	110.49
1	D	153	CYS	N-CA-C	5.43	118.12	109.81
1	A	131	PHE	CB-CA-C	-5.42	101.95	110.79
1	D	114	LEU	CA-C-O	5.40	126.49	120.82
1	B	250	LYS	CG-CD-CE	-5.39	98.89	111.30
1	B	252	PHE	N-CA-C	5.39	117.38	109.24
1	C	238	LEU	N-CA-C	-5.38	99.96	108.73
1	D	253	ILE	N-CA-C	-5.38	100.69	108.71
1	B	231	ARG	N-CA-C	-5.37	106.68	113.18
1	D	260	LEU	CA-C-N	-5.36	113.33	122.56
1	D	260	LEU	C-N-CA	-5.36	113.33	122.56
1	B	252	PHE	CA-C-N	5.36	127.76	120.63
1	B	252	PHE	C-N-CA	5.36	127.76	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	HIS	N-CA-CB	5.35	119.54	110.49
1	C	117	LEU	CA-CB-CG	-5.34	97.60	116.30
1	B	180	ILE	N-CA-C	5.33	115.93	108.89
1	D	127	GLU	N-CA-C	5.33	120.73	113.37
1	D	156	PHE	CA-C-N	-5.33	116.19	123.12
1	D	156	PHE	C-N-CA	-5.33	116.19	123.12
1	B	157	VAL	N-CA-CB	-5.31	105.23	111.60
1	D	265	HIS	CB-CA-C	5.31	120.19	110.10
1	C	111	ASN	CA-C-N	5.30	127.92	120.28
1	C	111	ASN	C-N-CA	5.30	127.92	120.28
1	C	203	SER	CA-CB-OG	-5.30	100.49	111.10
1	C	159	ASP	CB-CA-C	5.29	118.71	110.67
1	A	180	ILE	CB-CA-C	-5.27	104.91	111.08
1	C	206	ASN	N-CA-C	-5.25	99.61	110.80
1	A	210	ASP	N-CA-C	-5.25	100.93	108.60
1	C	257	GLY	N-CA-C	5.25	120.70	111.57
1	C	193	VAL	CA-C-O	5.24	124.37	119.76
1	D	178	LEU	CA-C-N	-5.23	112.71	121.39
1	D	178	LEU	C-N-CA	-5.23	112.71	121.39
1	B	230	ILE	N-CA-C	5.22	120.20	109.34
1	A	133	ASP	CA-C-N	-5.22	115.80	123.00
1	A	133	ASP	C-N-CA	-5.22	115.80	123.00
1	A	170	CYS	N-CA-C	-5.20	105.69	111.36
1	B	126	SER	CB-CA-C	-5.20	100.06	110.42
1	D	123	ARG	CA-C-N	-5.20	113.31	120.28
1	D	123	ARG	C-N-CA	-5.20	113.31	120.28
1	C	181	ASP	CA-C-N	-5.19	111.63	121.54
1	C	181	ASP	C-N-CA	-5.19	111.63	121.54
1	D	111	ASN	CB-CA-C	5.19	121.26	110.32
1	B	169	THR	CA-C-N	5.18	129.44	120.58
1	B	169	THR	C-N-CA	5.18	129.44	120.58
1	C	246	ASP	CB-CG-OD1	-5.17	106.51	118.40
1	C	215	ASN	N-CA-C	5.16	121.80	110.80
1	C	192	LEU	N-CA-C	-5.16	104.59	111.24
1	A	208	LYS	CB-CA-C	5.15	120.56	110.67
1	D	200	ILE	CA-C-N	-5.15	111.32	121.41
1	D	200	ILE	C-N-CA	-5.15	111.32	121.41
1	B	236	MET	N-CA-C	5.14	117.14	108.96
1	A	180	ILE	N-CA-C	5.14	116.15	108.54
1	B	132	SER	CA-CB-OG	-5.14	100.83	111.10
1	A	111	ASN	CA-C-O	5.13	125.00	119.15
1	B	154	TYR	N-CA-C	-5.13	99.61	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	CYS	CA-C-N	-5.13	111.75	121.54
1	B	248	CYS	C-N-CA	-5.13	111.75	121.54
1	A	131	PHE	N-CA-C	-5.13	98.92	107.99
1	B	121	GLN	CA-C-N	-5.12	112.90	120.28
1	B	121	GLN	C-N-CA	-5.12	112.90	120.28
1	B	242	ARG	CG-CD-NE	-5.12	100.73	112.00
1	B	191	LEU	CA-C-N	-5.11	112.66	121.66
1	B	191	LEU	C-N-CA	-5.11	112.66	121.66
1	B	259	ARG	CB-CG-CD	5.10	123.03	111.30
1	C	217	GLY	C-N-CD	5.09	145.89	125.00
1	C	263	PHE	CA-C-N	-5.09	113.48	119.84
1	C	263	PHE	C-N-CA	-5.09	113.48	119.84
1	D	122	ASN	N-CA-CB	5.08	117.37	110.01
1	C	132	SER	N-CA-C	-5.07	100.01	110.80
1	C	175	LEU	N-CA-CB	5.06	115.19	108.96
1	A	135	SER	CA-C-N	5.05	129.77	122.44
1	A	135	SER	C-N-CA	5.05	129.77	122.44
1	D	163	TRP	CB-CA-C	-5.05	100.36	110.42
1	A	190	LYS	CG-CD-CE	5.04	122.90	111.30
1	A	131	PHE	CA-C-O	-5.03	115.07	120.46
1	B	168	GLN	N-CA-C	5.02	116.83	111.36
1	B	179	LYS	CB-CG-CD	5.02	122.84	111.30
1	C	248	CYS	CA-CB-SG	-5.02	102.86	114.40
1	B	158	MET	CA-C-N	-5.01	115.88	122.85
1	B	158	MET	C-N-CA	-5.01	115.88	122.85
1	A	203	SER	N-CA-C	5.01	115.14	108.38
1	C	224	ASN	N-CA-C	5.00	121.46	110.80

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	SER	Peptide
1	A	136	GLN	Peptide
1	A	205	ASP	Peptide
1	A	215	ASN	Peptide
1	A	256	CYS	Peptide
1	B	136	GLN	Peptide
1	B	264	PRO	Peptide
1	C	196	ASP	Mainchain,Peptide
1	C	240	LYS	Peptide
1	C	242	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	D	164	SER	Peptide
1	D	177	LEU	Peptide
1	D	200	ILE	Peptide
1	D	205	ASP	Peptide
1	D	210	ASP	Peptide
1	D	217	GLY	Peptide
1	D	224	ASN	Peptide
1	D	238	LEU	Peptide
1	D	240	LYS	Peptide

5.2 Too-close contacts [i](#)

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	1293	0	1252	195	0
1	B	1327	0	1285	149	0
1	C	1267	0	1229	173	0
1	D	1258	0	1221	176	0
2	A	7	0	0	2	0
2	B	6	0	0	1	0
2	C	2	0	0	2	0
2	D	2	0	0	1	0
All	All	5162	0	4987	665	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 66.

All (665) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ILE:CD1	1:A:253:ILE:CG1	1.74	1.61
1:A:255:ILE:CB	1:A:255:ILE:CG2	1.74	1.60
1:C:151:ILE:CG1	1:C:151:ILE:CD1	1.75	1.59
1:A:152:LYS:CE	1:A:152:LYS:NZ	1.72	1.51
1:A:151:ILE:CD1	1:A:151:ILE:CG1	1.90	1.50
1:B:188:PHE:O	1:B:192:LEU:HD22	1.32	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PRO:HA	1:A:112:ASP:OD1	1.30	1.23
1:C:217:GLY:O	1:C:218:PRO:C	1.81	1.22
1:D:205:ASP:HA	1:D:206:ASN:HB2	1.24	1.18
1:B:214:ILE:HG12	1:B:215:ASN:H	1.05	1.14
1:A:214:ILE:HD13	1:A:214:ILE:O	1.46	1.13
1:A:222:ALA:O	1:A:223:LEU:HD12	1.48	1.13
1:B:161:LYS:CE	1:B:169:THR:HG21	1.79	1.12
1:D:108:ARG:H	1:D:109:PRO:CD	1.60	1.12
1:B:195:SER:O	1:B:196:ASP:HB2	1.41	1.10
1:D:108:ARG:N	1:D:109:PRO:HD2	1.68	1.08
1:B:242:ARG:HG3	1:B:243:LEU:H	1.10	1.07
1:A:111:ASN:O	1:A:115:GLU:HG3	1.54	1.07
1:C:113:LEU:HD23	1:C:114:LEU:N	1.70	1.07
1:A:179:LYS:H	1:A:179:LYS:HD2	1.19	1.06
1:B:229:ASN:HB3	1:B:232:ASP:OD2	1.55	1.06
1:C:143:GLU:HG2	1:C:144:LYS:H	1.10	1.05
1:D:160:ARG:HA	1:D:252:PHE:O	1.55	1.05
1:C:243:LEU:H	1:C:243:LEU:HD22	1.15	1.04
1:D:214:ILE:O	1:D:214:ILE:HG13	1.29	1.04
1:A:229:ASN:O	1:A:232:ASP:HB2	1.57	1.03
1:D:205:ASP:HA	1:D:206:ASN:CB	1.87	1.03
1:C:113:LEU:HD23	1:C:113:LEU:C	1.87	1.00
1:D:162:THR:HB	1:D:165:GLY:H	1.25	0.99
1:D:108:ARG:H	1:D:109:PRO:HD2	0.84	0.99
1:A:214:ILE:O	1:A:214:ILE:CD1	2.11	0.98
1:C:177:LEU:HD22	1:C:201:GLY:CA	1.92	0.98
1:D:129:LYS:HE2	1:D:131:PHE:CB	1.93	0.97
1:A:151:ILE:CD1	1:A:151:ILE:H	1.77	0.96
1:D:143:GLU:O	1:D:158:MET:HB2	1.66	0.96
1:C:233:GLY:HA3	1:C:246:ASP:O	1.66	0.95
1:D:162:THR:C	1:D:164:SER:H	1.74	0.95
1:D:162:THR:O	1:D:164:SER:N	1.99	0.95
1:B:161:LYS:HE3	1:B:169:THR:HG21	1.44	0.95
1:B:121:GLN:HG2	1:B:192:LEU:O	1.66	0.94
1:D:214:ILE:O	1:D:214:ILE:CG1	2.15	0.94
1:B:214:ILE:HG12	1:B:215:ASN:N	1.83	0.94
1:C:237:LEU:HD12	1:C:237:LEU:C	1.91	0.93
1:C:236:MET:HG3	1:C:237:LEU:N	1.80	0.93
1:A:232:ASP:HB3	1:A:245:ASN:HD21	1.31	0.93
1:D:144:LYS:HE3	1:D:144:LYS:H	1.31	0.93
1:D:129:LYS:HE2	1:D:131:PHE:HB3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:LYS:O	1:D:240:LYS:HE2	1.69	0.93
1:A:151:ILE:HD11	2:C:7:HOH:O	1.66	0.92
1:D:203:SER:O	1:D:211:TRP:HA	1.69	0.92
1:B:213:TRP:O	1:B:214:ILE:O	1.88	0.92
1:B:214:ILE:CG1	1:B:215:ASN:H	1.82	0.92
1:C:143:GLU:HG2	1:C:144:LYS:N	1.83	0.92
1:D:108:ARG:HB3	1:D:108:ARG:NH1	1.85	0.91
1:A:230:ILE:O	1:A:232:ASP:N	2.04	0.90
1:A:253:ILE:CD1	1:A:253:ILE:CB	2.49	0.90
1:C:230:ILE:HD12	1:C:230:ILE:N	1.87	0.90
1:A:161:LYS:HD3	1:A:165:GLY:HA3	1.53	0.90
1:D:243:LEU:O	1:D:244:ASP:HB2	1.69	0.90
1:A:219:SER:OG	1:A:221:LEU:HB3	1.73	0.89
1:D:108:ARG:HB3	1:D:108:ARG:CZ	2.02	0.89
1:A:138:THR:HG23	1:A:139:GLY:H	1.34	0.88
1:D:230:ILE:HD12	1:D:230:ILE:H	1.35	0.88
1:D:195:SER:H	1:D:240:LYS:HD2	1.36	0.87
1:D:230:ILE:H	1:D:230:ILE:CD1	1.80	0.86
1:D:243:LEU:O	1:D:244:ASP:CB	2.19	0.86
1:A:109:PRO:CA	1:A:112:ASP:OD1	2.20	0.86
1:D:181:ASP:N	1:D:181:ASP:OD1	2.09	0.86
1:A:115:GLU:O	1:A:119:LYS:HG3	1.76	0.85
1:D:179:LYS:HD3	1:D:179:LYS:H	1.38	0.85
1:B:161:LYS:HE2	1:B:169:THR:HG21	1.58	0.85
1:C:163:TRP:CZ2	1:C:203:SER:HB3	2.11	0.85
1:C:160:ARG:HA	1:C:252:PHE:O	1.77	0.84
1:D:229:ASN:O	1:D:232:ASP:HB2	1.77	0.84
1:C:237:LEU:HD11	1:C:239:SER:HB2	1.59	0.84
1:C:247:ASN:O	1:C:249:ASP:N	2.10	0.84
1:C:143:GLU:CG	1:C:144:LYS:H	1.88	0.84
1:C:240:LYS:C	1:C:241:THR:O	2.17	0.84
1:A:255:ILE:HG22	1:A:256:CYS:O	1.76	0.84
1:A:188:PHE:O	1:A:192:LEU:HD22	1.78	0.84
1:B:188:PHE:O	1:B:192:LEU:CD2	2.24	0.84
1:C:236:MET:HG3	1:C:237:LEU:H	1.41	0.84
1:C:237:LEU:CD1	1:C:239:SER:HB2	2.09	0.83
1:A:214:ILE:HD13	1:A:214:ILE:C	2.03	0.83
1:C:230:ILE:HD12	1:C:230:ILE:H	1.43	0.82
1:C:237:LEU:C	1:C:237:LEU:CD1	2.52	0.82
1:C:243:LEU:H	1:C:243:LEU:CD2	1.92	0.82
1:A:230:ILE:C	1:A:232:ASP:H	1.87	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:O	1:A:187:LYS:HD3	1.80	0.82
1:C:181:ASP:O	1:C:182:ASN:HB3	1.79	0.82
1:D:143:GLU:OE2	1:D:144:LYS:HE2	1.80	0.81
1:A:127:GLU:OE1	1:C:151:ILE:HD13	1.80	0.81
1:B:242:ARG:HG3	1:B:243:LEU:N	1.86	0.81
1:A:213:TRP:O	1:A:215:ASN:N	2.13	0.81
1:C:217:GLY:O	1:C:219:SER:N	2.13	0.80
1:A:196:ASP:OD1	1:A:197:SER:N	2.14	0.80
1:A:253:ILE:HG21	1:A:253:ILE:HD13	1.63	0.80
1:A:246:ASP:OD1	1:A:250:LYS:HD3	1.81	0.80
1:D:260:LEU:N	1:D:260:LEU:HD22	1.97	0.79
1:C:228:TYR:CE1	1:C:236:MET:HE1	2.17	0.79
1:D:230:ILE:HD12	1:D:230:ILE:N	1.97	0.79
1:D:163:TRP:O	1:D:163:TRP:CE3	2.35	0.79
1:D:129:LYS:HE2	1:D:131:PHE:HB2	1.64	0.79
1:C:237:LEU:HD12	1:C:237:LEU:O	1.81	0.79
1:D:214:ILE:O	1:D:215:ASN:HB2	1.83	0.78
1:B:189:LEU:HA	1:B:192:LEU:CD2	2.13	0.78
1:D:163:TRP:O	1:D:163:TRP:CD2	2.38	0.77
1:A:265:HIS:CD2	1:C:258:LYS:HE2	2.20	0.76
1:B:214:ILE:O	1:B:215:ASN:C	2.28	0.76
1:C:193:VAL:HG12	1:C:194:PRO:O	1.86	0.76
1:A:162:THR:HA	1:A:199:TRP:HE1	1.51	0.76
1:D:114:LEU:N	1:D:114:LEU:HD22	2.01	0.76
1:A:179:LYS:H	1:A:179:LYS:CD	1.98	0.75
1:A:214:ILE:O	1:A:214:ILE:CG1	2.33	0.75
1:C:143:GLU:O	1:C:158:MET:HB2	1.85	0.75
1:C:228:TYR:CZ	1:C:236:MET:HE1	2.22	0.75
1:A:207:LYS:O	1:A:209:LYS:HG3	1.85	0.75
1:B:230:ILE:HG22	1:B:230:ILE:O	1.87	0.75
1:C:214:ILE:C	1:C:215:ASN:HD22	1.95	0.75
1:C:263:PHE:O	1:C:265:HIS:N	2.19	0.75
1:A:151:ILE:H	1:A:151:ILE:HD12	1.52	0.74
1:B:199:TRP:CZ3	1:B:237:LEU:HD21	2.21	0.74
1:A:137:HIS:O	1:A:138:THR:O	2.06	0.74
1:A:255:ILE:CG2	1:A:255:ILE:CA	2.65	0.74
1:B:147:PHE:CD1	1:B:147:PHE:C	2.65	0.74
1:C:144:LYS:CG	1:C:157:VAL:HG13	2.18	0.74
1:C:160:ARG:O	1:C:161:LYS:HG3	1.88	0.74
1:C:230:ILE:H	1:C:230:ILE:CD1	2.00	0.73
1:A:138:THR:HG23	1:A:139:GLY:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ASP:OD2	1:D:206:ASN:HB3	1.88	0.73
1:A:232:ASP:HB3	1:A:245:ASN:ND2	2.02	0.73
1:A:247:ASN:C	1:A:249:ASP:H	1.97	0.73
1:C:247:ASN:O	1:C:250:LYS:N	2.21	0.72
1:B:245:ASN:HD22	1:B:245:ASN:H	1.37	0.72
1:A:197:SER:HA	1:A:238:LEU:O	1.90	0.72
1:C:177:LEU:HD22	1:C:201:GLY:N	2.04	0.71
1:A:179:LYS:HD2	1:A:179:LYS:N	2.02	0.71
1:A:179:LYS:O	1:A:179:LYS:HG2	1.91	0.71
1:C:151:ILE:CD1	1:C:151:ILE:HG21	2.20	0.71
1:C:243:LEU:HD22	1:C:243:LEU:N	1.99	0.71
1:A:152:LYS:NZ	1:A:185:GLU:OE2	2.23	0.71
1:B:179:LYS:HA	1:B:213:TRP:CE3	2.25	0.71
1:B:161:LYS:HE3	1:B:169:THR:CG2	2.19	0.70
1:A:187:LYS:O	1:A:191:LEU:HD23	1.92	0.70
1:B:263:PHE:CZ	1:D:153:CYS:HB2	2.27	0.70
1:A:183:GLU:O	1:A:187:LYS:CD	2.39	0.70
1:A:265:HIS:NE2	1:C:258:LYS:HE2	2.07	0.70
1:B:163:TRP:CZ2	1:B:203:SER:HB3	2.27	0.70
1:D:144:LYS:HE3	1:D:144:LYS:N	2.06	0.70
1:B:204:TYR:C	1:B:204:TYR:CD2	2.69	0.70
1:C:234:GLY:O	1:C:235:CYS:SG	2.49	0.70
1:B:165:GLY:O	1:B:169:THR:HG23	1.92	0.69
1:D:127:GLU:C	1:D:128:THR:HG23	2.16	0.69
1:C:171:GLN:HA	1:C:171:GLN:NE2	2.06	0.69
1:D:234:GLY:O	1:D:235:CYS:SG	2.50	0.69
1:A:201:GLY:HA3	1:A:214:ILE:HG22	1.73	0.69
1:D:205:ASP:CA	1:D:206:ASN:CB	2.66	0.69
1:A:195:SER:O	1:A:196:ASP:HB2	1.93	0.69
1:B:152:LYS:NZ	1:B:181:ASP:OD1	2.24	0.68
1:C:205:ASP:OD1	1:C:208:LYS:HB3	1.92	0.68
1:D:110:GLY:HA2	1:D:113:LEU:CB	2.23	0.68
1:A:183:GLU:HG3	1:A:187:LYS:HD3	1.74	0.68
1:C:237:LEU:HG	1:C:244:ASP:O	1.92	0.68
1:B:108:ARG:HB3	1:B:109:PRO:CD	2.23	0.68
1:A:151:ILE:CD1	2:C:7:HOH:O	2.34	0.68
1:A:222:ALA:O	1:A:223:LEU:CD1	2.34	0.68
1:B:195:SER:O	1:B:196:ASP:CB	2.24	0.68
1:C:151:ILE:HD13	1:C:151:ILE:HG21	1.76	0.68
1:A:168:GLN:O	1:A:172:ILE:HG23	1.92	0.68
1:B:111:ASN:HD22	1:B:111:ASN:H	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ARG:HH21	1:C:160:ARG:HG3	1.58	0.68
1:D:156:PHE:CE2	1:D:255:ILE:HG12	2.29	0.68
1:D:187:LYS:O	1:D:191:LEU:CD2	2.42	0.67
1:B:199:TRP:CE3	1:B:237:LEU:CD2	2.77	0.67
1:B:241:THR:HG21	2:B:6:HOH:O	1.93	0.67
1:A:219:SER:HG	1:A:221:LEU:HB3	1.59	0.67
1:C:160:ARG:O	1:C:161:LYS:CG	2.42	0.67
1:D:240:LYS:O	1:D:240:LYS:HG3	1.94	0.67
1:A:174:SER:O	1:A:175:LEU:HD23	1.95	0.67
1:B:129:LYS:O	1:B:130:THR:CG2	2.43	0.67
1:A:203:SER:HA	1:A:211:TRP:CE3	2.30	0.67
1:A:192:LEU:HD22	1:A:192:LEU:H	1.60	0.67
1:C:195:SER:HB2	1:C:240:LYS:HE2	1.77	0.67
1:D:261:ASP:O	1:D:262:LYS:HB3	1.94	0.67
1:A:179:LYS:O	1:A:179:LYS:CG	2.41	0.66
1:B:258:LYS:HE2	1:D:264:PRO:O	1.95	0.66
1:A:190:LYS:O	1:A:240:LYS:NZ	2.28	0.66
1:A:179:LYS:HA	1:A:213:TRP:CE3	2.29	0.66
1:A:146:TRP:O	1:A:147:PHE:HB3	1.95	0.66
1:A:230:ILE:C	1:A:232:ASP:N	2.48	0.66
1:B:245:ASN:HD22	1:B:245:ASN:N	1.93	0.66
1:B:262:LYS:O	1:B:263:PHE:C	2.36	0.66
1:A:255:ILE:CG2	1:A:255:ILE:CG1	2.71	0.66
1:B:142:PHE:HB2	1:B:159:ASP:HB2	1.78	0.65
1:C:160:ARG:C	1:C:161:LYS:HG3	2.21	0.65
1:A:121:GLN:HG3	1:A:192:LEU:O	1.96	0.65
1:A:193:VAL:O	1:A:240:LYS:HE2	1.96	0.65
1:A:136:GLN:HB2	1:A:172:ILE:HD12	1.79	0.65
1:A:161:LYS:HD3	1:A:165:GLY:CA	2.26	0.65
1:B:120:GLU:O	1:B:121:GLN:C	2.37	0.65
1:B:214:ILE:O	1:B:216:ASN:N	2.30	0.65
1:D:110:GLY:HA2	1:D:113:LEU:HB2	1.79	0.65
1:B:124:TRP:CE2	1:D:150:GLY:CA	2.80	0.64
1:B:128:THR:O	1:B:130:THR:HG23	1.96	0.64
1:B:157:VAL:HG12	1:B:159:ASP:H	1.62	0.64
1:C:177:LEU:HD22	1:C:201:GLY:HA2	1.78	0.64
1:A:200:ILE:CG2	1:A:238:LEU:CD1	2.76	0.64
1:B:219:SER:OG	1:B:221:LEU:HB2	1.98	0.64
1:A:253:ILE:CD1	1:A:253:ILE:CG2	2.75	0.64
1:B:199:TRP:CE3	1:B:237:LEU:HD21	2.33	0.64
1:B:227:LYS:HG3	1:B:227:LYS:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ASP:C	1:A:249:ASP:OD1	2.41	0.64
1:D:110:GLY:HA2	1:D:113:LEU:H	1.62	0.64
1:A:152:LYS:NZ	1:A:185:GLU:CD	2.56	0.63
1:C:151:ILE:CD1	1:C:151:ILE:CG2	2.75	0.63
1:A:151:ILE:HG13	1:C:127:GLU:OE2	1.98	0.63
1:D:160:ARG:O	1:D:161:LYS:HG3	1.98	0.63
1:D:144:LYS:HA	1:D:156:PHE:O	1.99	0.63
1:D:260:LEU:H	1:D:260:LEU:CD2	2.12	0.63
1:A:225:THR:O	1:A:227:LYS:N	2.32	0.62
1:B:129:LYS:O	1:B:130:THR:HG22	2.00	0.62
1:D:163:TRP:O	1:D:163:TRP:CG	2.48	0.62
1:D:178:LEU:HB2	1:D:255:ILE:O	1.98	0.62
1:A:214:ILE:CD1	1:A:214:ILE:C	2.67	0.62
1:A:229:ASN:O	1:A:232:ASP:CB	2.40	0.62
1:C:190:LYS:NZ	1:C:242:ARG:HD2	2.15	0.62
1:A:192:LEU:H	1:A:192:LEU:CD2	2.12	0.62
1:B:120:GLU:HG3	1:D:149:TYR:OH	1.99	0.62
1:D:108:ARG:HG2	1:D:111:ASN:HB2	1.81	0.62
1:D:181:ASP:O	1:D:182:ASN:HB3	1.98	0.62
1:A:166:CYS:SG	1:A:199:TRP:HD1	2.23	0.62
1:D:114:LEU:O	1:D:115:GLU:C	2.43	0.62
1:C:183:GLU:O	1:C:186:LEU:HB3	2.00	0.62
1:B:114:LEU:O	1:B:116:SER:N	2.33	0.62
1:B:124:TRP:CE2	1:D:150:GLY:HA3	2.35	0.61
1:C:182:ASN:O	1:C:183:GLU:C	2.44	0.61
1:D:260:LEU:N	1:D:260:LEU:CD2	2.62	0.61
1:D:106:GLU:OE1	1:D:108:ARG:HB2	1.99	0.61
1:D:237:LEU:O	1:D:244:ASP:N	2.28	0.61
1:A:114:LEU:O	1:A:116:SER:N	2.34	0.61
1:B:207:LYS:O	1:B:209:LYS:HG3	2.00	0.61
1:B:233:GLY:HA3	1:B:246:ASP:O	2.00	0.61
1:C:151:ILE:CD1	1:C:151:ILE:CB	2.75	0.61
1:A:129:LYS:HD2	1:A:143:GLU:OE1	2.01	0.61
1:D:182:ASN:O	1:D:183:GLU:C	2.42	0.61
1:A:134:SER:OG	1:A:172:ILE:HD11	2.01	0.61
1:A:265:HIS:CE1	1:C:258:LYS:HD3	2.36	0.61
1:C:186:LEU:O	1:C:190:LYS:HB2	2.00	0.61
1:A:161:LYS:HE2	1:A:169:THR:OG1	1.99	0.61
1:D:151:ILE:C	1:D:260:LEU:HD23	2.25	0.61
1:D:214:ILE:O	1:D:215:ASN:CB	2.49	0.61
1:A:178:LEU:HB3	1:A:200:ILE:HB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ASP:HA	1:D:115:GLU:HB3	1.82	0.61
1:D:179:LYS:HD3	1:D:179:LYS:N	2.14	0.60
1:C:203:SER:C	1:C:211:TRP:CE3	2.79	0.60
1:D:126:SER:O	1:D:129:LYS:NZ	2.35	0.60
1:D:179:LYS:HA	1:D:213:TRP:CE3	2.37	0.60
1:A:162:THR:CA	1:A:199:TRP:HE1	2.15	0.60
1:A:250:LYS:HB2	1:A:250:LYS:NZ	2.17	0.60
1:C:179:LYS:H	1:C:179:LYS:HD2	1.66	0.60
1:D:258:LYS:HG3	1:D:259:ARG:O	2.01	0.60
1:A:180:ILE:HG22	1:A:221:LEU:HD22	1.83	0.60
1:A:114:LEU:O	1:A:115:GLU:C	2.44	0.60
1:C:129:LYS:HA	1:C:144:LYS:O	2.02	0.60
1:C:236:MET:CG	1:C:237:LEU:N	2.60	0.60
1:A:247:ASN:C	1:A:249:ASP:N	2.58	0.59
1:B:253:ILE:HG22	1:B:254:CYS:O	2.01	0.59
1:C:200:ILE:HD13	1:C:200:ILE:N	2.17	0.59
1:B:247:ASN:O	1:B:249:ASP:N	2.33	0.59
1:A:202:LEU:HD12	1:A:212:ALA:O	2.02	0.59
1:A:236:MET:SD	1:A:244:ASP:O	2.60	0.59
1:D:187:LYS:O	1:D:191:LEU:HD23	2.02	0.59
1:D:229:ASN:HA	1:D:230:ILE:HD12	1.84	0.59
1:C:185:GLU:O	1:C:189:LEU:HG	2.03	0.59
1:D:183:GLU:O	1:D:186:LEU:HB3	2.02	0.59
1:D:163:TRP:CZ2	1:D:203:SER:HB3	2.38	0.59
1:D:205:ASP:CG	1:D:206:ASN:HB3	2.26	0.59
1:A:233:GLY:HA3	1:A:246:ASP:C	2.27	0.59
1:D:162:THR:C	1:D:164:SER:N	2.37	0.59
1:C:160:ARG:HG3	1:C:160:ARG:NH2	2.17	0.59
1:C:214:ILE:O	1:C:215:ASN:HB2	2.01	0.59
1:A:157:VAL:HG12	1:A:157:VAL:O	2.02	0.58
1:C:237:LEU:HD13	1:C:239:SER:HB2	1.85	0.58
1:C:219:SER:OG	1:C:221:LEU:N	2.32	0.58
1:C:203:SER:O	1:C:212:ALA:N	2.34	0.58
1:D:187:LYS:O	1:D:191:LEU:HD22	2.04	0.58
1:A:188:PHE:O	1:A:192:LEU:CD2	2.48	0.58
1:B:224:ASN:O	1:B:224:ASN:ND2	2.36	0.58
1:B:236:MET:SD	1:B:244:ASP:C	2.87	0.58
1:A:138:THR:O	1:A:140:ARG:N	2.36	0.58
1:B:111:ASN:HA	1:B:114:LEU:HD23	1.84	0.58
1:A:225:THR:C	1:A:227:LYS:H	2.10	0.58
1:A:253:ILE:HD13	1:A:253:ILE:CG2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:TRP:CE3	1:B:237:LEU:HD23	2.39	0.58
1:C:171:GLN:C	1:C:173:SER:H	2.10	0.58
1:C:240:LYS:O	1:C:241:THR:O	2.21	0.58
1:C:247:ASN:C	1:C:249:ASP:H	2.10	0.58
1:D:110:GLY:CA	1:D:113:LEU:H	2.16	0.58
1:B:120:GLU:O	1:B:123:ARG:N	2.30	0.57
1:C:177:LEU:HD22	1:C:201:GLY:HA3	1.84	0.57
1:C:148:CYS:O	1:C:149:TYR:HB2	2.04	0.57
1:D:260:LEU:HD22	1:D:260:LEU:H	1.64	0.57
1:C:177:LEU:HD21	1:C:199:TRP:O	2.03	0.57
1:A:137:HIS:O	1:A:138:THR:C	2.47	0.57
1:C:171:GLN:HA	1:C:171:GLN:HE21	1.68	0.57
1:C:200:ILE:HG12	1:C:238:LEU:HB2	1.84	0.57
1:D:216:ASN:O	1:D:217:GLY:O	2.23	0.57
1:D:110:GLY:C	1:D:113:LEU:H	2.13	0.57
1:C:166:CYS:O	1:C:167:LYS:C	2.47	0.57
1:D:127:GLU:C	1:D:128:THR:CG2	2.77	0.57
1:D:196:ASP:OD2	1:D:197:SER:N	2.37	0.57
1:A:253:ILE:CD1	1:A:253:ILE:HG21	2.31	0.57
1:B:147:PHE:C	1:B:147:PHE:HD1	2.11	0.57
1:D:195:SER:O	1:D:196:ASP:HB2	2.05	0.57
1:A:111:ASN:C	1:A:115:GLU:HG3	2.28	0.56
1:C:179:LYS:HA	1:C:213:TRP:CZ3	2.39	0.56
1:B:214:ILE:CG1	1:B:215:ASN:N	2.50	0.56
1:D:203:SER:HB2	1:D:234:GLY:O	2.05	0.56
1:A:147:PHE:CD1	1:A:147:PHE:C	2.82	0.56
1:C:198:TYR:O	1:C:237:LEU:HB2	2.04	0.56
1:D:230:ILE:CD1	1:D:230:ILE:N	2.54	0.56
1:A:200:ILE:HG23	1:A:238:LEU:HD12	1.88	0.56
1:C:180:ILE:HG22	1:C:182:ASN:H	1.70	0.56
1:D:163:TRP:CD1	1:D:235:CYS:HB3	2.40	0.56
1:A:119:LYS:HA	1:A:122:ASN:HD22	1.70	0.56
1:C:233:GLY:CA	1:C:246:ASP:O	2.50	0.56
1:D:114:LEU:N	1:D:114:LEU:CD2	2.69	0.56
1:B:113:LEU:HD12	1:D:113:LEU:HD23	1.87	0.56
1:A:263:PHE:CZ	1:C:153:CYS:HB2	2.41	0.56
1:B:204:TYR:CD2	1:B:205:ASP:N	2.74	0.56
1:B:230:ILE:O	1:B:230:ILE:CG2	2.53	0.56
1:C:203:SER:C	1:C:211:TRP:HE3	2.12	0.56
1:C:200:ILE:HD11	1:C:255:ILE:HD12	1.88	0.56
1:C:247:ASN:C	1:C:249:ASP:N	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:SER:C	1:A:136:GLN:H	2.15	0.55
1:A:212:ALA:HB1	1:A:216:ASN:HD22	1.71	0.55
1:C:250:LYS:HE2	1:C:250:LYS:HA	1.86	0.55
1:B:124:TRP:NE1	1:D:150:GLY:HA3	2.20	0.55
1:B:165:GLY:O	1:B:169:THR:CG2	2.53	0.55
1:C:213:TRP:O	1:C:215:ASN:N	2.39	0.55
1:D:166:CYS:HB2	1:D:177:LEU:HD11	1.89	0.55
1:A:178:LEU:O	1:A:200:ILE:HB	2.06	0.55
1:A:223:LEU:HD12	1:A:224:ASN:H	1.71	0.55
1:A:197:SER:HB3	1:A:237:LEU:HD22	1.87	0.55
1:A:142:PHE:HB2	1:A:159:ASP:HB2	1.89	0.55
1:D:193:VAL:O	1:D:240:LYS:HE3	2.07	0.55
1:A:111:ASN:O	1:A:115:GLU:CG	2.43	0.55
1:A:224:ASN:C	1:A:224:ASN:ND2	2.61	0.55
1:A:247:ASN:O	1:A:249:ASP:N	2.26	0.55
1:B:232:ASP:HB2	1:B:245:ASN:OD1	2.06	0.55
1:C:214:ILE:O	1:C:215:ASN:CB	2.54	0.55
1:B:189:LEU:HA	1:B:192:LEU:HD21	1.87	0.55
1:B:194:PRO:O	1:B:195:SER:C	2.50	0.55
1:D:129:LYS:CE	1:D:131:PHE:HB2	2.36	0.55
1:A:152:LYS:NZ	1:A:185:GLU:OE1	2.39	0.55
1:A:212:ALA:HB1	1:A:216:ASN:ND2	2.21	0.55
1:B:229:ASN:CB	1:B:232:ASP:OD2	2.44	0.55
1:B:242:ARG:NH1	1:B:242:ARG:HG2	2.21	0.55
1:D:185:GLU:HG2	1:D:185:GLU:O	2.04	0.54
1:A:135:SER:O	1:A:136:GLN:HG2	2.06	0.54
1:A:177:LEU:HD22	1:A:199:TRP:O	2.06	0.54
1:D:185:GLU:O	1:D:185:GLU:CG	2.54	0.54
1:D:233:GLY:HA3	1:D:246:ASP:O	2.07	0.54
1:B:118:HIS:O	1:B:119:LYS:C	2.49	0.54
1:A:151:ILE:CD1	1:A:151:ILE:N	2.60	0.54
1:A:250:LYS:HB2	1:A:250:LYS:HZ3	1.73	0.54
1:C:144:LYS:HG2	1:C:157:VAL:HG13	1.88	0.54
1:A:250:LYS:NZ	1:A:250:LYS:CB	2.70	0.54
1:B:233:GLY:HA3	1:B:246:ASP:C	2.33	0.54
1:D:125:TYR:O	1:D:126:SER:C	2.49	0.54
1:D:178:LEU:HD22	1:D:255:ILE:CG2	2.37	0.54
1:C:124:TRP:O	1:C:125:TYR:C	2.51	0.53
1:D:242:ARG:HG2	1:D:243:LEU:O	2.08	0.53
1:B:119:LYS:O	1:B:120:GLU:C	2.50	0.53
1:C:214:ILE:C	1:C:215:ASN:ND2	2.65	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:TRP:O	1:B:147:PHE:HB3	2.08	0.53
1:A:202:LEU:HB3	1:A:236:MET:HB2	1.91	0.53
1:B:114:LEU:HD12	1:B:118:HIS:HE1	1.74	0.53
1:C:189:LEU:O	1:C:190:LYS:C	2.50	0.53
1:D:117:LEU:HG	1:D:192:LEU:HD12	1.90	0.53
1:D:226:MET:O	1:D:227:LYS:HG2	2.09	0.53
1:A:208:LYS:HE3	2:A:17:HOH:O	2.08	0.53
1:B:124:TRP:CE2	1:D:150:GLY:HA2	2.44	0.53
1:D:236:MET:HG3	1:D:237:LEU:N	2.23	0.53
1:B:108:ARG:HB3	1:B:109:PRO:HD3	1.90	0.53
1:C:200:ILE:N	1:C:200:ILE:CD1	2.69	0.53
1:D:114:LEU:HD22	1:D:114:LEU:H	1.74	0.53
1:B:168:GLN:O	1:B:172:ILE:HG13	2.09	0.52
1:C:179:LYS:HD2	1:C:179:LYS:O	2.09	0.52
1:C:181:ASP:O	1:C:182:ASN:CB	2.45	0.52
1:A:200:ILE:HG23	1:A:238:LEU:CD1	2.39	0.52
1:C:160:ARG:C	1:C:161:LYS:CG	2.82	0.52
1:A:229:ASN:HB3	1:A:232:ASP:OD1	2.09	0.52
1:B:108:ARG:O	1:B:112:ASP:HB3	2.09	0.52
1:B:166:CYS:SG	1:B:199:TRP:HD1	2.32	0.52
1:A:119:LYS:C	1:A:121:GLN:N	2.64	0.52
1:B:229:ASN:O	1:B:232:ASP:HB2	2.09	0.52
1:A:211:TRP:CD1	1:A:211:TRP:N	2.78	0.52
1:B:212:ALA:HB1	1:B:216:ASN:ND2	2.24	0.52
1:A:114:LEU:C	1:A:116:SER:N	2.67	0.52
1:A:144:LYS:NZ	1:A:155:TYR:OH	2.31	0.52
1:D:211:TRP:CD1	1:D:225:THR:HG1	2.28	0.52
1:A:200:ILE:HG21	1:A:238:LEU:HD11	1.91	0.52
1:A:117:LEU:O	1:A:118:HIS:C	2.51	0.51
1:A:214:ILE:O	1:A:214:ILE:HG12	2.09	0.51
1:A:230:ILE:O	1:A:231:ARG:C	2.51	0.51
1:B:213:TRP:C	1:B:214:ILE:O	2.53	0.51
1:D:123:ARG:O	1:D:124:TRP:C	2.49	0.51
1:A:211:TRP:CD1	1:A:211:TRP:H	2.28	0.51
1:A:233:GLY:HA3	1:A:246:ASP:O	2.10	0.51
1:A:236:MET:CE	1:A:244:ASP:O	2.58	0.51
1:C:203:SER:HA	1:C:211:TRP:CZ3	2.46	0.51
1:C:264:PRO:O	1:C:265:HIS:OXT	2.29	0.51
1:D:166:CYS:CB	1:D:177:LEU:HD11	2.40	0.51
1:B:199:TRP:CZ3	1:B:237:LEU:CD2	2.91	0.51
1:D:234:GLY:C	1:D:235:CYS:SG	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LYS:CD	1:A:179:LYS:N	2.68	0.51
1:B:126:SER:HA	1:B:129:LYS:HE3	1.92	0.51
1:D:161:LYS:O	1:D:199:TRP:CD1	2.64	0.51
1:D:213:TRP:O	1:D:214:ILE:C	2.53	0.51
1:A:123:ARG:NH1	1:C:220:LYS:NZ	2.59	0.51
1:C:152:LYS:HA	1:C:258:LYS:O	2.11	0.51
1:D:181:ASP:O	1:D:182:ASN:CB	2.56	0.51
1:B:142:PHE:CB	1:B:159:ASP:HB2	2.40	0.51
1:A:119:LYS:HA	1:A:122:ASN:ND2	2.27	0.50
1:C:199:TRP:C	1:C:200:ILE:HD13	2.36	0.50
1:C:215:ASN:O	1:C:216:ASN:HB2	2.10	0.50
1:D:225:THR:O	1:D:227:LYS:N	2.40	0.50
1:A:161:LYS:O	1:A:251:SER:HA	2.10	0.50
1:A:250:LYS:HZ3	1:A:250:LYS:CB	2.24	0.50
1:B:121:GLN:C	1:B:121:GLN:CD	2.79	0.50
1:C:147:PHE:CD1	1:C:147:PHE:C	2.90	0.50
1:C:229:ASN:O	1:C:232:ASP:HB2	2.11	0.50
1:A:205:ASP:CG	1:A:206:ASN:H	2.19	0.50
1:B:108:ARG:O	1:B:109:PRO:C	2.55	0.50
1:B:152:LYS:NZ	1:B:185:GLU:OE1	2.44	0.50
1:C:130:THR:HB	1:C:143:GLU:HG3	1.94	0.50
1:C:190:LYS:HZ1	1:C:242:ARG:HD2	1.75	0.50
1:C:146:TRP:CB	1:C:154:TYR:O	2.60	0.50
1:C:160:ARG:HB3	1:C:252:PHE:HA	1.92	0.50
1:A:203:SER:HA	1:A:211:TRP:HE3	1.75	0.50
1:B:188:PHE:C	1:B:192:LEU:HD22	2.26	0.50
1:C:193:VAL:HG12	1:C:194:PRO:N	2.26	0.50
1:A:118:HIS:O	1:A:122:ASN:ND2	2.44	0.50
1:B:113:LEU:CD1	1:D:113:LEU:HD23	2.42	0.50
1:B:114:LEU:HD12	1:B:118:HIS:CE1	2.46	0.50
1:C:128:THR:C	1:C:129:LYS:O	2.53	0.50
1:C:261:ASP:OD2	1:C:261:ASP:N	2.38	0.50
1:B:129:LYS:C	1:B:130:THR:CG2	2.85	0.49
1:A:182:ASN:OD1	1:A:185:GLU:N	2.41	0.49
1:D:195:SER:N	1:D:240:LYS:HD2	2.17	0.49
1:A:200:ILE:HG21	1:A:238:LEU:CD1	2.41	0.49
1:B:224:ASN:O	1:B:224:ASN:CG	2.55	0.49
1:D:160:ARG:O	1:D:161:LYS:CG	2.60	0.49
1:D:164:SER:C	1:D:166:CYS:N	2.68	0.49
1:D:171:GLN:O	1:D:174:SER:N	2.44	0.49
1:D:127:GLU:O	1:D:128:THR:CG2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASN:H	1:B:111:ASN:ND2	2.09	0.49
1:B:189:LEU:O	1:B:193:VAL:HB	2.13	0.49
1:C:114:LEU:HA	1:C:114:LEU:HD12	1.52	0.49
1:D:261:ASP:O	1:D:262:LYS:CB	2.51	0.49
1:D:240:LYS:O	1:D:240:LYS:CG	2.60	0.48
1:A:124:TRP:CE2	1:C:150:GLY:HA2	2.48	0.48
1:A:114:LEU:HG	1:A:118:HIS:HE1	1.78	0.48
1:A:162:THR:C	1:A:199:TRP:NE1	2.71	0.48
1:A:151:ILE:H	1:A:151:ILE:HD13	1.71	0.48
1:A:207:LYS:O	1:A:208:LYS:C	2.52	0.48
1:B:120:GLU:OE1	1:B:123:ARG:HD2	2.14	0.48
1:B:122:ASN:O	1:B:125:TYR:HB3	2.12	0.48
1:C:215:ASN:HD22	1:C:215:ASN:N	2.10	0.48
1:D:234:GLY:C	1:D:248:CYS:SG	2.97	0.48
1:B:113:LEU:CD1	1:D:113:LEU:CD2	2.91	0.48
1:A:225:THR:C	1:A:227:LYS:N	2.68	0.48
1:D:237:LEU:HD13	1:D:252:PHE:CE1	2.49	0.48
1:C:205:ASP:O	1:C:207:LYS:N	2.47	0.48
1:A:198:TYR:HD2	1:A:253:ILE:HG22	1.78	0.48
1:B:237:LEU:HD11	1:B:246:ASP:HB2	1.96	0.48
1:C:113:LEU:C	1:C:113:LEU:CD2	2.64	0.48
1:C:179:LYS:H	1:C:179:LYS:CD	2.26	0.48
1:C:197:SER:HB2	1:C:237:LEU:HD22	1.96	0.48
1:C:160:ARG:HA	1:C:252:PHE:C	2.39	0.47
1:B:205:ASP:OD1	1:B:205:ASP:C	2.54	0.47
1:B:245:ASN:H	1:B:245:ASN:ND2	2.08	0.47
1:C:193:VAL:CG1	1:C:194:PRO:N	2.78	0.47
1:C:208:LYS:O	1:C:208:LYS:HG3	2.14	0.47
1:C:167:LYS:O	1:C:168:GLN:C	2.57	0.47
1:A:213:TRP:C	1:A:215:ASN:N	2.72	0.47
1:C:193:VAL:HG13	1:C:194:PRO:HD2	1.96	0.47
1:C:203:SER:HB2	1:C:234:GLY:O	2.14	0.47
1:D:106:GLU:O	1:D:107:CYS:HB3	2.14	0.47
1:A:153:CYS:SG	1:C:264:PRO:HG2	2.55	0.47
1:A:180:ILE:CG2	1:A:221:LEU:HD22	2.44	0.47
1:D:114:LEU:CD2	1:D:114:LEU:H	2.27	0.47
1:A:236:MET:CE	1:A:243:LEU:HB3	2.45	0.47
1:A:259:ARG:O	1:A:260:LEU:C	2.57	0.46
1:B:147:PHE:CD1	1:B:147:PHE:O	2.68	0.46
1:B:204:TYR:C	1:B:204:TYR:HD2	2.21	0.46
1:B:166:CYS:O	1:B:167:LYS:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:LEU:O	1:D:187:LYS:C	2.59	0.46
1:D:247:ASN:C	1:D:249:ASP:H	2.23	0.46
1:B:212:ALA:HB1	1:B:216:ASN:HD21	1.80	0.46
1:C:209:LYS:O	1:C:210:ASP:HB2	2.16	0.46
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.38	0.46
1:C:203:SER:HA	1:C:211:TRP:CE3	2.50	0.46
1:C:205:ASP:O	1:C:206:ASN:C	2.56	0.46
1:C:171:GLN:C	1:C:173:SER:N	2.74	0.46
1:D:171:GLN:C	1:D:173:SER:N	2.73	0.46
1:C:210:ASP:OD2	1:C:211:TRP:N	2.48	0.46
1:C:237:LEU:HD13	1:C:238:LEU:C	2.40	0.46
1:D:143:GLU:HB3	1:D:144:LYS:HE3	1.97	0.46
1:A:169:THR:HA	1:A:172:ILE:HD13	1.97	0.46
1:B:163:TRP:CZ3	1:B:167:LYS:HE3	2.50	0.46
1:B:219:SER:C	1:B:221:LEU:H	2.23	0.46
1:C:195:SER:HB2	1:C:240:LYS:CE	2.45	0.46
1:C:230:ILE:O	1:C:231:ARG:C	2.59	0.46
1:A:241:THR:C	1:A:242:ARG:HG3	2.40	0.46
1:B:120:GLU:O	1:B:122:ASN:N	2.48	0.46
1:B:129:LYS:C	1:B:130:THR:HG23	2.41	0.46
1:D:144:LYS:HB3	1:D:156:PHE:O	2.16	0.46
1:B:245:ASN:N	1:B:245:ASN:ND2	2.63	0.46
1:C:203:SER:O	1:C:211:TRP:HA	2.16	0.46
1:A:124:TRP:CE2	1:C:150:GLY:CA	2.99	0.45
1:A:202:LEU:HD12	1:A:202:LEU:HA	1.51	0.45
1:A:265:HIS:HE1	1:C:174:SER:O	1.99	0.45
1:C:237:LEU:O	1:C:243:LEU:HA	2.16	0.45
1:B:133:ASP:C	1:B:134:SER:O	2.56	0.45
1:C:149:TYR:HB3	1:C:154:TYR:HE1	1.81	0.45
1:B:135:SER:C	1:B:137:HIS:H	2.24	0.45
1:A:178:LEU:HD21	1:A:189:LEU:HD21	1.99	0.45
1:A:228:TYR:HB3	1:A:245:ASN:OD1	2.17	0.45
1:B:238:LEU:HD12	1:B:239:SER:O	2.17	0.45
1:D:208:LYS:NZ	1:D:208:LYS:HB3	2.31	0.45
1:D:211:TRP:HD1	1:D:225:THR:HG1	1.64	0.45
1:A:144:LYS:HA	1:A:156:PHE:O	2.17	0.45
1:A:177:LEU:HD21	1:A:254:CYS:HB3	1.97	0.45
1:B:111:ASN:ND2	1:B:111:ASN:N	2.64	0.45
1:B:150:GLY:HA2	1:D:124:TRP:CE2	2.52	0.45
1:D:204:TYR:OH	1:D:209:LYS:HA	2.17	0.45
1:D:225:THR:C	1:D:227:LYS:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ASP:CG	1:A:206:ASN:N	2.73	0.45
1:D:178:LEU:HD22	1:D:255:ILE:HG21	1.99	0.45
1:D:236:MET:HE2	1:D:236:MET:HB2	1.79	0.45
1:D:110:GLY:HA2	1:D:113:LEU:N	2.31	0.45
1:D:178:LEU:O	1:D:213:TRP:HZ3	1.99	0.45
1:A:192:LEU:CD2	1:A:192:LEU:N	2.80	0.45
1:B:162:THR:O	1:B:165:GLY:N	2.50	0.45
1:C:228:TYR:CZ	1:C:236:MET:CE	2.97	0.45
1:D:179:LYS:H	1:D:179:LYS:CD	2.20	0.45
1:C:259:ARG:CZ	1:C:259:ARG:HB2	2.47	0.44
1:A:166:CYS:O	1:A:167:LYS:C	2.57	0.44
1:A:227:LYS:O	1:A:227:LYS:HG2	2.17	0.44
1:D:164:SER:N	1:D:166:CYS:H	2.15	0.44
1:C:163:TRP:O	1:C:166:CYS:HB2	2.18	0.44
1:B:152:LYS:CE	1:B:181:ASP:OD1	2.66	0.44
1:B:162:THR:O	1:B:163:TRP:C	2.60	0.44
1:C:143:GLU:CG	1:C:144:LYS:N	2.61	0.44
1:D:129:LYS:HG3	1:D:130:THR:N	2.32	0.44
1:D:178:LEU:O	1:D:213:TRP:CZ3	2.70	0.44
1:B:105:ILE:HG21	1:D:111:ASN:OD1	2.17	0.44
1:B:113:LEU:O	1:B:116:SER:OG	2.24	0.44
1:D:106:GLU:O	1:D:107:CYS:CB	2.66	0.44
1:A:123:ARG:HH11	1:C:220:LYS:NZ	2.15	0.44
1:A:249:ASP:OD1	1:A:250:LYS:N	2.51	0.44
1:B:183:GLU:O	1:B:186:LEU:HB3	2.18	0.44
1:C:120:GLU:OE2	1:C:120:GLU:HA	2.17	0.44
1:C:146:TRP:HB2	1:C:154:TYR:O	2.16	0.44
1:C:240:LYS:HG3	1:C:241:THR:N	2.30	0.44
1:D:114:LEU:C	1:D:116:SER:N	2.75	0.44
1:D:147:PHE:CD1	1:D:147:PHE:C	2.95	0.44
1:C:114:LEU:HD11	1:C:191:LEU:HD13	1.99	0.44
1:C:214:ILE:O	1:C:214:ILE:HG12	2.17	0.44
1:B:178:LEU:HD12	1:B:178:LEU:HA	1.47	0.43
1:B:236:MET:HB2	1:B:236:MET:HE2	1.45	0.43
1:D:157:VAL:O	1:D:253:ILE:HG23	2.18	0.43
1:D:205:ASP:HA	1:D:206:ASN:HB3	1.91	0.43
1:B:226:MET:H	1:B:226:MET:HG3	1.36	0.43
1:D:163:TRP:CG	1:D:235:CYS:SG	3.11	0.43
1:D:181:ASP:OD1	1:D:185:GLU:OE1	2.36	0.43
1:A:138:THR:CG2	1:A:139:GLY:N	2.78	0.43
1:A:237:LEU:HD21	1:A:252:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:GLN:O	1:D:173:SER:N	2.51	0.43
1:B:159:ASP:OD2	1:B:161:LYS:NZ	2.50	0.43
1:C:125:TYR:HA	1:C:145:TYR:CD1	2.54	0.43
1:C:202:LEU:HB2	1:C:213:TRP:CZ3	2.54	0.43
1:C:163:TRP:CH2	1:C:203:SER:HB3	2.53	0.43
1:D:160:ARG:CA	1:D:252:PHE:O	2.47	0.43
1:D:216:ASN:C	1:D:217:GLY:O	2.61	0.43
1:B:113:LEU:HD13	1:D:113:LEU:HD21	2.01	0.43
1:B:114:LEU:O	1:B:115:GLU:C	2.62	0.43
1:B:238:LEU:HD12	1:B:239:SER:N	2.34	0.43
1:C:117:LEU:HD12	1:C:117:LEU:HA	1.38	0.43
1:D:114:LEU:HA	1:D:114:LEU:HD13	1.16	0.43
1:D:205:ASP:CG	1:D:207:LYS:H	2.27	0.43
1:D:226:MET:C	1:D:227:LYS:HG2	2.44	0.43
1:A:213:TRP:C	1:A:215:ASN:H	2.27	0.43
1:A:198:TYR:CD2	1:A:253:ILE:CG2	3.02	0.43
1:B:255:ILE:HD13	1:B:255:ILE:HG21	1.61	0.43
1:C:156:PHE:CE2	1:C:255:ILE:HG12	2.54	0.43
1:D:153:CYS:O	1:D:257:GLY:HA2	2.19	0.43
1:A:124:TRP:CD2	1:C:150:GLY:HA2	2.54	0.43
1:B:114:LEU:C	1:B:116:SER:N	2.77	0.43
1:D:214:ILE:HD12	1:D:215:ASN:OD1	2.19	0.43
1:A:251:SER:HB2	2:A:11:HOH:O	2.18	0.42
1:B:208:LYS:O	1:B:209:LYS:HB2	2.20	0.42
1:C:125:TYR:O	1:C:126:SER:C	2.62	0.42
1:D:199:TRP:CZ3	1:D:235:CYS:HB3	2.54	0.42
1:A:185:GLU:O	1:A:186:LEU:C	2.56	0.42
1:A:200:ILE:HD12	1:A:238:LEU:HD12	2.01	0.42
1:C:190:LYS:HZ2	1:C:242:ARG:HD2	1.84	0.42
1:A:200:ILE:HG13	1:A:213:TRP:HZ3	1.84	0.42
1:C:258:LYS:NZ	1:C:259:ARG:O	2.48	0.42
1:D:142:PHE:HZ	1:D:160:ARG:NH1	2.17	0.42
1:D:205:ASP:OD1	1:D:208:LYS:HB2	2.18	0.42
1:A:193:VAL:CG1	1:A:198:TYR:CE1	3.02	0.42
1:B:190:LYS:HD3	1:B:240:LYS:O	2.20	0.42
1:B:113:LEU:HD13	1:D:113:LEU:CD2	2.49	0.42
1:B:245:ASN:ND2	1:B:245:ASN:O	2.51	0.42
1:D:247:ASN:O	1:D:249:ASP:N	2.51	0.42
1:B:207:LYS:O	1:B:209:LYS:N	2.53	0.42
1:A:193:VAL:HG12	1:A:194:PRO:O	2.19	0.42
1:C:170:CYS:HB3	1:C:176:SER:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:THR:OG1	1:D:145:TYR:HB2	2.20	0.42
1:D:146:TRP:CB	1:D:154:TYR:O	2.67	0.42
1:D:206:ASN:ND2	2:D:5:HOH:O	2.52	0.42
1:A:200:ILE:HD12	1:A:238:LEU:CD1	2.50	0.42
1:C:144:LYS:CD	1:C:157:VAL:HG13	2.49	0.42
1:A:236:MET:HE1	1:A:244:ASP:N	2.35	0.41
1:A:119:LYS:C	1:A:121:GLN:H	2.26	0.41
1:A:160:ARG:HE	1:A:160:ARG:HB2	1.78	0.41
1:B:199:TRP:CZ2	1:B:252:PHE:HD1	2.37	0.41
1:A:163:TRP:CG	1:A:235:CYS:SG	3.13	0.41
1:B:111:ASN:HA	1:B:114:LEU:CD2	2.49	0.41
1:B:147:PHE:CZ	1:B:192:LEU:HG	2.55	0.41
1:B:152:LYS:HA	1:B:258:LYS:O	2.19	0.41
1:C:120:GLU:O	1:C:121:GLN:C	2.60	0.41
1:C:237:LEU:CG	1:C:244:ASP:O	2.64	0.41
1:B:114:LEU:O	1:B:117:LEU:N	2.54	0.41
1:B:173:SER:O	1:B:174:SER:HB2	2.20	0.41
1:C:146:TRP:HA	1:C:154:TYR:O	2.20	0.41
1:C:216:ASN:HD22	1:C:216:ASN:HA	1.72	0.41
1:A:158:MET:HA	1:A:253:ILE:HG12	2.03	0.41
1:B:179:LYS:CE	1:B:259:ARG:HH11	2.33	0.41
1:C:147:PHE:CZ	1:C:192:LEU:HD12	2.56	0.41
1:D:179:LYS:HA	1:D:213:TRP:CZ3	2.55	0.41
1:B:242:ARG:NH1	1:B:242:ARG:CG	2.83	0.41
1:C:159:ASP:HB2	1:C:161:LYS:HE3	2.02	0.41
1:C:224:ASN:O	1:C:226:MET:N	2.54	0.41
1:D:159:ASP:HB3	1:D:161:LYS:HE2	2.02	0.41
1:C:226:MET:O	1:C:226:MET:CG	2.69	0.41
1:D:160:ARG:C	1:D:161:LYS:HG3	2.46	0.41
1:D:142:PHE:CZ	1:D:160:ARG:NH1	2.89	0.40
1:A:184:ASP:OD1	1:C:116:SER:OG	2.40	0.40
1:C:193:VAL:HG13	1:C:194:PRO:CD	2.51	0.40
1:D:166:CYS:O	1:D:167:LYS:C	2.64	0.40
1:A:198:TYR:HD2	1:A:253:ILE:CG2	2.34	0.40
1:C:229:ASN:HD21	1:C:231:ARG:HE	1.69	0.40
1:D:262:LYS:O	1:D:263:PHE:C	2.64	0.40
1:A:165:GLY:O	1:A:166:CYS:C	2.64	0.40
1:B:186:LEU:HD22	1:B:221:LEU:HD11	2.02	0.40
1:B:189:LEU:HD23	1:B:192:LEU:HD21	2.03	0.40
1:A:148:CYS:HA	1:A:153:CYS:HA	2.04	0.40
1:B:105:ILE:C	1:B:107:CYS:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ARG:H	1:B:140:ARG:HG3	1.45	0.40
1:B:179:LYS:HA	1:B:213:TRP:CZ3	2.56	0.40
1:D:211:TRP:HD1	1:D:225:THR:OG1	2.05	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	155/190 (82%)	119 (77%)	22 (14%)	14 (9%)	0	0
1	B	159/190 (84%)	114 (72%)	24 (15%)	21 (13%)	0	0
1	C	150/190 (79%)	108 (72%)	23 (15%)	19 (13%)	0	0
1	D	148/190 (78%)	108 (73%)	23 (16%)	17 (12%)	0	0
All	All	612/760 (80%)	449 (73%)	92 (15%)	71 (12%)	0	0

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLU
1	A	138	THR
1	A	214	ILE
1	A	226	MET
1	A	231	ARG
1	A	248	CYS
1	B	108	ARG
1	B	109	PRO
1	B	114	LEU
1	B	206	ASN
1	B	214	ILE
1	B	216	ASN

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Mol	Chain	Res	Type
1	B	226	MET
1	B	248	CYS
1	C	111	ASN
1	C	207	LYS
1	C	208	LYS
1	C	214	ILE
1	C	215	ASN
1	C	216	ASN
1	C	225	THR
1	C	240	LYS
1	C	241	THR
1	C	248	CYS
1	D	107	CYS
1	D	108	ARG
1	D	163	TRP
1	D	214	ILE
1	D	215	ASN
1	D	216	ASN
1	D	226	MET
1	A	139	GLY
1	B	115	GLU
1	B	117	LEU
1	B	178	LEU
1	B	196	ASP
1	C	218	PRO
1	D	142	PHE
1	D	159	ASP
1	D	206	ASN
1	A	114	LEU
1	A	117	LEU
1	A	137	HIS
1	A	223	LEU
1	B	125	TYR
1	B	158	MET
1	B	215	ASN
1	B	229	ASN
1	B	244	ASP
1	C	129	LYS
1	C	140	ARG
1	C	167	LYS
1	C	174	SER
1	C	264	PRO

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Mol	Chain	Res	Type
1	D	262	LYS
1	A	135	SER
1	B	126	SER
1	B	207	LYS
1	B	249	ASP
1	D	164	SER
1	D	248	CYS
1	A	129	LYS
1	A	201	GLY
1	C	206	ASN
1	D	195	SER
1	D	227	LYS
1	D	196	ASP
1	B	230	ILE
1	C	217	GLY
1	D	217	GLY
1	C	172	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	145/177 (82%)	102 (70%)	43 (30%)	0	0
1	B	149/177 (84%)	117 (78%)	32 (22%)	1	2
1	C	142/177 (80%)	98 (69%)	44 (31%)	0	0
1	D	141/177 (80%)	96 (68%)	45 (32%)	0	0
All	All	577/708 (82%)	413 (72%)	164 (28%)	0	0

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ASP
1	A	113	LEU
1	A	117	LEU
1	A	119	LYS

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Mol	Chain	Res	Type
1	A	122	ASN
1	A	126	SER
1	A	129	LYS
1	A	130	THR
1	A	137	HIS
1	A	145	TYR
1	A	151	ILE
1	A	152	LYS
1	A	158	MET
1	A	161	LYS
1	A	167	LYS
1	A	172	ILE
1	A	177	LEU
1	A	179	LYS
1	A	183	GLU
1	A	187	LYS
1	A	189	LEU
1	A	191	LEU
1	A	192	LEU
1	A	195	SER
1	A	199	TRP
1	A	200	ILE
1	A	208	LYS
1	A	214	ILE
1	A	216	ASN
1	A	219	SER
1	A	223	LEU
1	A	226	MET
1	A	232	ASP
1	A	238	LEU
1	A	241	THR
1	A	242	ARG
1	A	249	ASP
1	A	250	LYS
1	A	251	SER
1	A	254	CYS
1	A	259	ARG
1	A	261	ASP
1	A	265	HIS
1	B	111	ASN
1	B	113	LEU
1	B	117	LEU

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Mol	Chain	Res	Type
1	B	119	LYS
1	B	121	GLN
1	B	123	ARG
1	B	135	SER
1	B	136	GLN
1	B	140	ARG
1	B	147	PHE
1	B	169	THR
1	B	173	SER
1	B	176	SER
1	B	177	LEU
1	B	179	LYS
1	B	183	GLU
1	B	192	LEU
1	B	193	VAL
1	B	207	LYS
1	B	208	LYS
1	B	214	ILE
1	B	215	ASN
1	B	220	LYS
1	B	221	LEU
1	B	226	MET
1	B	241	THR
1	B	242	ARG
1	B	245	ASN
1	B	251	SER
1	B	259	ARG
1	B	260	LEU
1	B	265	HIS
1	C	113	LEU
1	C	116	SER
1	C	119	LYS
1	C	120	GLU
1	C	129	LYS
1	C	130	THR
1	C	132	SER
1	C	140	ARG
1	C	142	PHE
1	C	143	GLU
1	C	144	LYS
1	C	158	MET
1	C	159	ASP

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Mol	Chain	Res	Type
1	C	169	THR
1	C	171	GLN
1	C	174	SER
1	C	176	SER
1	C	177	LEU
1	C	179	LYS
1	C	183	GLU
1	C	186	LEU
1	C	190	LYS
1	C	192	LEU
1	C	197	SER
1	C	200	ILE
1	C	207	LYS
1	C	208	LYS
1	C	215	ASN
1	C	216	ASN
1	C	218	PRO
1	C	223	LEU
1	C	225	THR
1	C	226	MET
1	C	230	ILE
1	C	231	ARG
1	C	236	MET
1	C	237	LEU
1	C	238	LEU
1	C	243	LEU
1	C	244	ASP
1	C	250	LYS
1	C	251	SER
1	C	260	LEU
1	C	265	HIS
1	D	106	GLU
1	D	108	ARG
1	D	114	LEU
1	D	115	GLU
1	D	116	SER
1	D	117	LEU
1	D	120	GLU
1	D	142	PHE
1	D	144	LYS
1	D	152	LYS
1	D	158	MET

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Mol	Chain	Res	Type
1	D	159	ASP
1	D	164	SER
1	D	169	THR
1	D	172	ILE
1	D	174	SER
1	D	176	SER
1	D	179	LYS
1	D	181	ASP
1	D	187	LYS
1	D	193	VAL
1	D	197	SER
1	D	200	ILE
1	D	207	LYS
1	D	208	LYS
1	D	209	LYS
1	D	210	ASP
1	D	214	ILE
1	D	216	ASN
1	D	219	SER
1	D	223	LEU
1	D	226	MET
1	D	230	ILE
1	D	231	ARG
1	D	238	LEU
1	D	240	LYS
1	D	241	THR
1	D	242	ARG
1	D	243	LEU
1	D	244	ASP
1	D	247	ASN
1	D	258	LYS
1	D	259	ARG
1	D	262	LYS
1	D	265	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	122	ASN
1	A	216	ASN
1	A	229	ASN

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Mol	Chain	Res	Type
1	A	245	ASN
1	A	265	HIS
1	B	111	ASN
1	B	118	HIS
1	B	216	ASN
1	B	224	ASN
1	B	229	ASN
1	B	245	ASN
1	C	111	ASN
1	C	121	GLN
1	C	171	GLN
1	C	215	ASN
1	C	216	ASN
1	C	229	ASN
1	C	265	HIS
1	D	118	HIS
1	D	121	GLN
1	D	224	ASN

5.3.3 RNA [i](#)

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9	
1	A	157/190 (82%)	-1.16	0	100	100	37, 55, 79, 85	0
1	B	161/190 (84%)	-1.14	0	100	100	37, 56, 86, 119	0
1	C	154/190 (81%)	-1.15	0	100	100	36, 58, 88, 99	0
1	D	152/190 (80%)	-1.09	1 (0%)	84	81	36, 56, 89, 116	0
All	All	624/760 (82%)	-1.14	1 (0%)	91	89	36, 56, 86, 119	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	141	GLY	3.9

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.