Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 07:28 PM EDT

PDB ID	:	3G8L
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 following versions of software and data (see references ⓘ) were used in the production of this report:

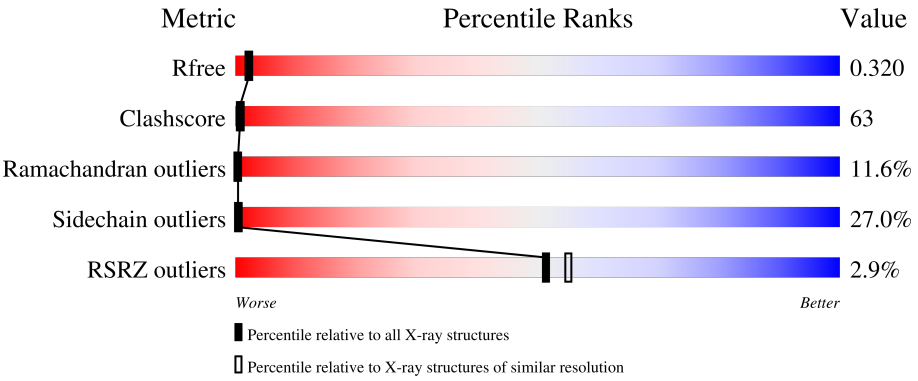
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	.% 13% 29% 28% 12% 17%
1	B	190	4% 17% 37% 21% 9% 15%
1	C	190	3% 14% 31% 26% 11% 19%
1	D	190	2% 16% 29% 19% 16% 20%

2 Entry composition (i)

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.

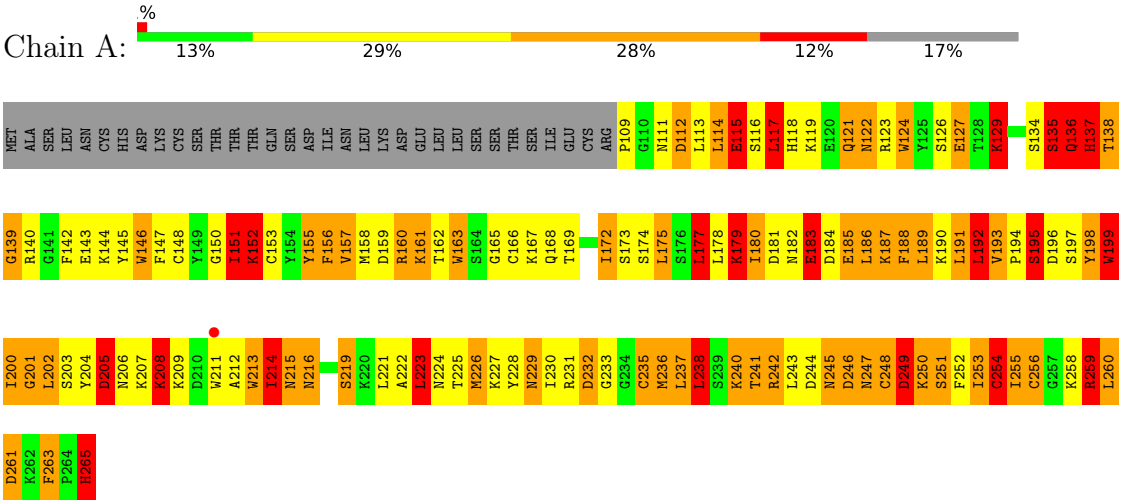
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	6	Total O 6 6	0	0
2	C	2	Total O 2 2	0	0
2	D	2	Total O 2 2	0	0

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.

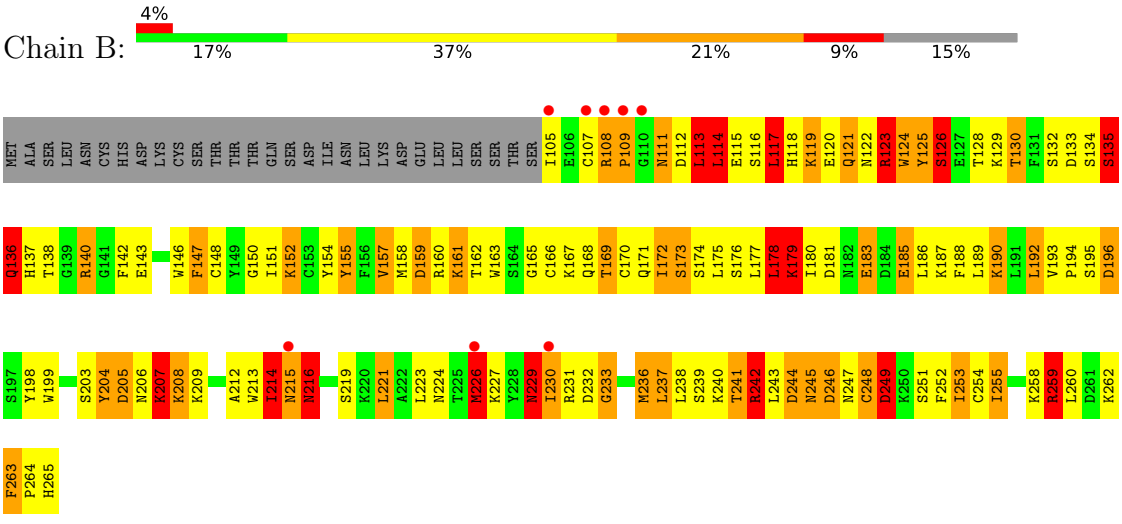
• Molecule 1: Lectin-related NK cell receptor LY49L1

Chain A:



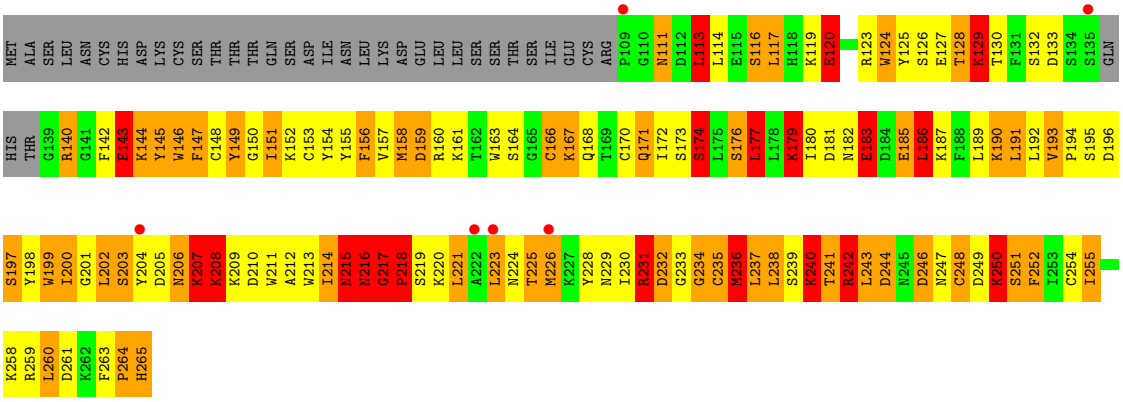
• Molecule 1: Lectin-related NK cell receptor LY49L1

Chain B:

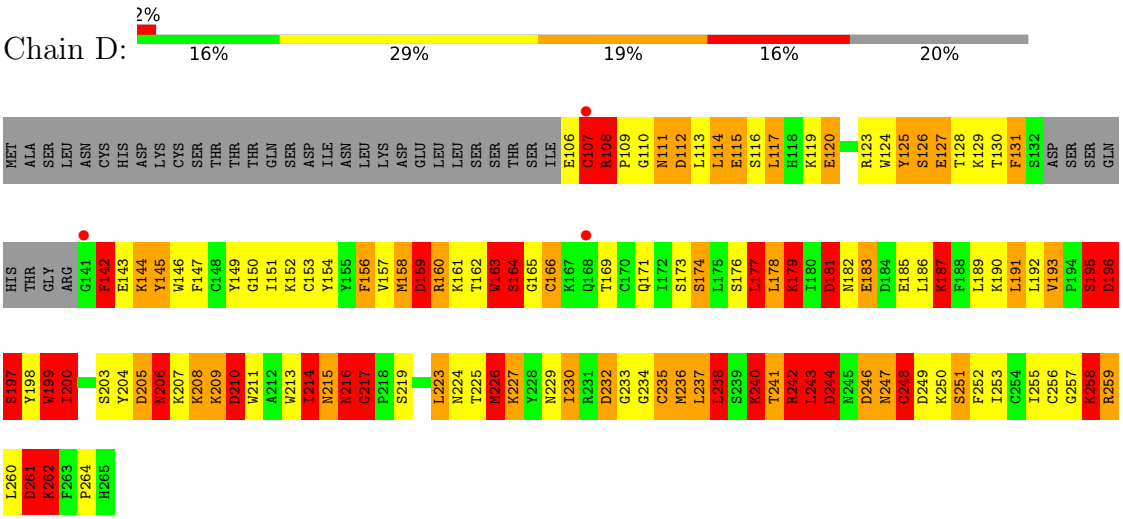


• Molecule 1: Lectin-related NK cell receptor LY49L1

Chain C:



• Molecule 1: Lectin-related NK cell receptor LY49L1



4 Data and refinement statistics (i)

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 29.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.1 (30.00-2.50) 90.1 (29.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.13%)	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)	0.33 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.487 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	2.19	48/1326 (3.6%)	1.84	36/1781 (2.0%)
1	B	2.11	43/1360 (3.2%)	1.77	29/1827 (1.6%)
1	C	2.09	32/1298 (2.5%)	1.81	33/1741 (1.9%)
1	D	2.02	31/1289 (2.4%)	1.83	37/1730 (2.1%)
All	All	2.10	154/5273 (2.9%)	1.81	135/7079 (1.9%)

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

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	146	TRP	CE3-CZ3	12.77	1.60	1.38
1	A	198	TYR	CD2-CE2	11.69	1.56	1.39
1	A	155	TYR	CE2-CZ	10.74	1.52	1.38
1	C	254	CYS	CB-SG	10.60	2.00	1.82
1	B	185	GLU	CD-OE1	9.39	1.35	1.25
1	A	152	LYS	CE-NZ	9.18	1.72	1.49
1	B	143	GLU	CD-OE1	9.10	1.35	1.25
1	B	143	GLU	CG-CD	9.00	1.65	1.51
1	D	258	LYS	CD-CE	8.89	1.73	1.51
1	C	199	TRP	CB-CG	8.83	1.66	1.50
1	B	107	CYS	CB-SG	8.80	1.97	1.82
1	C	149	TYR	CD1-CE1	8.75	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	TYR	CD1-CE1	8.57	1.52	1.39
1	A	146	TRP	CE3-CZ3	8.48	1.52	1.38
1	A	185	GLU	CB-CG	-8.37	1.36	1.52
1	A	179	LYS	CB-CG	7.95	1.74	1.52
1	C	255	ILE	C-O	7.67	1.38	1.23
1	A	185	GLU	CD-OE1	7.59	1.33	1.25
1	A	129	LYS	CD-CE	7.45	1.69	1.51
1	A	183	GLU	CG-CD	7.43	1.63	1.51
1	B	185	GLU	CB-CG	-7.43	1.38	1.52
1	B	198	TYR	CD2-CE2	7.38	1.50	1.39
1	B	180	ILE	CA-CB	-7.37	1.37	1.54
1	B	204	TYR	CD2-CE2	-7.29	1.28	1.39
1	C	252	PHE	N-CA	7.25	1.60	1.46
1	C	254	CYS	CA-C	7.22	1.71	1.52
1	A	180	ILE	CA-CB	-7.19	1.38	1.54
1	A	183	GLU	CB-CG	7.16	1.65	1.52
1	A	199	TRP	CB-CG	7.12	1.63	1.50
1	A	204	TYR	CD2-CE2	-7.10	1.28	1.39
1	B	179	LYS	CD-CE	7.09	1.69	1.51
1	C	146	TRP	CD2-CE2	7.09	1.49	1.41
1	A	187	LYS	CD-CE	7.05	1.68	1.51
1	A	255	ILE	CB-CG2	7.03	1.74	1.52
1	B	152	LYS	CE-NZ	6.99	1.66	1.49
1	D	125	TYR	CD1-CE1	6.98	1.49	1.39
1	A	115	GLU	CG-CD	6.98	1.62	1.51
1	D	183	GLU	CB-CG	6.97	1.65	1.52
1	C	120	GLU	CD-OE1	6.86	1.33	1.25
1	D	248	CYS	C-O	6.86	1.36	1.23
1	C	149	TYR	CG-CD1	6.85	1.48	1.39
1	C	187	LYS	CB-CG	6.84	1.71	1.52
1	D	183	GLU	CG-CD	6.79	1.62	1.51
1	C	145	TYR	C-O	6.69	1.36	1.23
1	A	155	TYR	CD1-CE1	6.67	1.49	1.39
1	A	198	TYR	CD1-CE1	6.61	1.49	1.39
1	B	155	TYR	CD1-CE1	6.59	1.49	1.39
1	A	127	GLU	CG-CD	6.58	1.61	1.51
1	A	204	TYR	CE1-CZ	6.56	1.47	1.38
1	D	256	CYS	CB-SG	6.48	1.93	1.82
1	D	120	GLU	CB-CG	6.47	1.64	1.52
1	A	248	CYS	CB-SG	-6.35	1.71	1.82
1	C	251	SER	CA-CB	-6.35	1.43	1.52
1	D	125	TYR	CE2-CZ	-6.34	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	185	GLU	CD-OE2	-6.29	1.18	1.25
1	B	170	CYS	CB-SG	6.26	1.92	1.82
1	B	157	VAL	CA-CB	-6.22	1.41	1.54
1	C	143	GLU	CB-CG	6.22	1.64	1.52
1	C	203	SER	CB-OG	-6.21	1.34	1.42
1	D	119	LYS	CD-CE	6.18	1.66	1.51
1	C	156	PHE	CD2-CE2	-6.14	1.26	1.39
1	B	154	TYR	CG-CD1	6.13	1.47	1.39
1	D	199	TRP	CB-CG	6.11	1.61	1.50
1	A	259	ARG	CG-CD	6.11	1.67	1.51
1	D	166	CYS	CB-SG	6.11	1.92	1.82
1	B	229	ASN	CG-OD1	6.08	1.37	1.24
1	A	183	GLU	CD-OE2	6.07	1.32	1.25
1	A	249	ASP	CB-CG	6.04	1.64	1.51
1	C	120	GLU	CB-CG	6.01	1.63	1.52
1	D	178	LEU	N-CA	-5.99	1.34	1.46
1	C	183	GLU	CD-OE2	5.98	1.32	1.25
1	B	161	LYS	C-O	5.97	1.34	1.23
1	D	156	PHE	CG-CD1	5.95	1.47	1.38
1	B	253	ILE	CA-CB	-5.93	1.41	1.54
1	C	146	TRP	CD1-NE1	5.93	1.48	1.38
1	D	119	LYS	CE-NZ	5.91	1.63	1.49
1	C	126	SER	CB-OG	-5.90	1.34	1.42
1	B	263	PHE	CG-CD2	-5.89	1.29	1.38
1	B	132	SER	CB-OG	-5.88	1.34	1.42
1	B	171	GLN	CB-CG	5.87	1.68	1.52
1	C	179	LYS	CG-CD	5.87	1.72	1.52
1	D	127	GLU	C-O	-5.85	1.12	1.23
1	A	151	ILE	CG1-CD1	5.80	1.90	1.50
1	C	124	TRP	CG-CD1	5.80	1.44	1.36
1	D	160	ARG	CB-CG	5.79	1.68	1.52
1	B	155	TYR	CZ-OH	5.79	1.47	1.37
1	C	216	ASN	CB-CG	5.78	1.64	1.51
1	B	248	CYS	C-O	5.78	1.34	1.23
1	D	195	SER	N-CA	5.75	1.57	1.46
1	A	150	GLY	C-O	-5.74	1.14	1.23
1	B	155	TYR	CD2-CE2	5.73	1.48	1.39
1	B	190	LYS	CD-CE	5.71	1.65	1.51
1	D	127	GLU	CD-OE2	5.71	1.31	1.25
1	A	152	LYS	CG-CD	5.69	1.71	1.52
1	C	231	ARG	CB-CG	5.68	1.67	1.52
1	A	124	TRP	CG-CD1	5.67	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	LEU	C-O	5.67	1.34	1.23
1	B	179	LYS	CE-NZ	5.66	1.63	1.49
1	D	216	ASN	CB-CG	5.65	1.64	1.51
1	D	261	ASP	CB-CG	5.64	1.63	1.51
1	C	204	TYR	N-CA	5.62	1.57	1.46
1	C	147	PHE	CD2-CE2	-5.61	1.28	1.39
1	B	124	TRP	CG-CD1	5.58	1.44	1.36
1	A	193	VAL	CB-CG1	-5.58	1.41	1.52
1	D	198	TYR	CG-CD1	-5.55	1.31	1.39
1	B	259	ARG	CG-CD	5.54	1.65	1.51
1	A	146	TRP	C-O	5.54	1.33	1.23
1	B	136	GLN	CB-CG	5.54	1.67	1.52
1	B	154	TYR	CE2-CZ	5.53	1.45	1.38
1	D	187	LYS	CG-CD	5.49	1.71	1.52
1	A	246	ASP	CB-CG	5.47	1.63	1.51
1	A	183	GLU	CD-OE1	5.47	1.31	1.25
1	B	136	GLN	CG-CD	5.47	1.63	1.51
1	D	126	SER	CB-OG	-5.46	1.35	1.42
1	A	160	ARG	N-CA	5.45	1.57	1.46
1	A	205	ASP	CB-CG	5.44	1.63	1.51
1	B	148	CYS	CB-SG	5.42	1.91	1.82
1	A	249	ASP	CA-C	-5.42	1.38	1.52
1	B	246	ASP	CB-CG	5.41	1.63	1.51
1	A	253	ILE	CA-CB	-5.40	1.42	1.54
1	D	156	PHE	C-O	5.40	1.33	1.23
1	B	226	MET	CG-SD	5.39	1.95	1.81
1	A	156	PHE	C-O	5.39	1.33	1.23
1	A	255	ILE	N-CA	-5.38	1.35	1.46
1	B	231	ARG	CZ-NH2	5.37	1.40	1.33
1	A	155	TYR	CD2-CE2	5.36	1.47	1.39
1	D	147	PHE	CD2-CE2	-5.34	1.28	1.39
1	D	187	LYS	CB-CG	5.31	1.66	1.52
1	C	155	TYR	CD1-CE1	5.30	1.47	1.39
1	B	198	TYR	CA-CB	5.29	1.65	1.53
1	A	249	ASP	C-O	-5.28	1.13	1.23
1	A	115	GLU	CB-CG	5.25	1.62	1.52
1	D	145	TYR	C-O	5.24	1.33	1.23
1	B	187	LYS	CG-CD	5.23	1.70	1.52
1	C	143	GLU	CD-OE1	5.21	1.31	1.25
1	C	149	TYR	CE2-CZ	5.21	1.45	1.38
1	D	179	LYS	CD-CE	5.20	1.64	1.51
1	B	152	LYS	CD-CE	5.18	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	TRP	CA-C	-5.17	1.39	1.52
1	B	130	THR	CB-CG2	5.15	1.69	1.52
1	A	188	PHE	CE1-CZ	5.14	1.47	1.37
1	A	263	PHE	CD2-CE2	5.12	1.49	1.39
1	A	247	ASN	CA-C	-5.10	1.39	1.52
1	B	160	ARG	C-O	-5.07	1.13	1.23
1	B	231	ARG	CB-CG	5.07	1.66	1.52
1	D	200	ILE	CA-CB	-5.07	1.43	1.54
1	C	146	TRP	CG-CD1	5.06	1.43	1.36
1	D	258	LYS	CG-CD	5.06	1.69	1.52
1	A	248	CYS	C-O	5.05	1.32	1.23
1	A	136	GLN	CA-C	5.03	1.66	1.52
1	C	252	PHE	CE1-CZ	5.03	1.47	1.37
1	B	179	LYS	CG-CD	5.01	1.69	1.52
1	B	185	GLU	N-CA	5.01	1.56	1.46
1	D	107	CYS	CB-SG	5.00	1.90	1.82

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	246	ASP	CB-CG-OD1	-13.10	106.51	118.30
1	D	117	LEU	CB-CG-CD1	-11.95	90.69	111.00
1	C	231	ARG	NE-CZ-NH1	10.51	125.55	120.30
1	D	196	ASP	CB-CG-OD2	-10.03	109.27	118.30
1	C	236	MET	CA-CB-CG	-9.20	97.66	113.30
1	D	238	LEU	CA-CB-CG	9.13	136.30	115.30
1	A	248	CYS	CA-CB-SG	-8.86	98.06	114.00
1	C	251	SER	CB-CA-C	-8.72	93.54	110.10
1	A	237	LEU	CB-CA-C	-8.64	93.79	110.20
1	A	177	LEU	CB-CG-CD2	8.50	125.45	111.00
1	C	217	GLY	C-N-CD	8.33	145.89	128.40
1	A	191	LEU	CB-CG-CD2	7.97	124.56	111.00
1	D	223	LEU	CB-CG-CD2	7.95	124.52	111.00
1	A	261	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	C	117	LEU	CA-CB-CG	-7.69	97.60	115.30
1	C	208	LYS	N-CA-C	7.66	131.69	111.00
1	C	223	LEU	CA-CB-CG	7.54	132.64	115.30
1	A	177	LEU	CA-CB-CG	7.49	132.53	115.30
1	C	193	VAL	C-N-CD	7.43	144.01	128.40
1	C	246	ASP	CB-CG-OD2	7.42	124.98	118.30
1	D	196	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	235	CYS	CA-CB-SG	-7.16	101.12	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	191	LEU	CA-CB-CG	7.12	131.67	115.30
1	B	255	ILE	CG1-CB-CG2	-7.08	95.83	111.40
1	C	191	LEU	CA-CB-CG	6.97	131.32	115.30
1	C	232	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	237	LEU	CB-CG-CD2	-6.96	99.17	111.00
1	D	177	LEU	CA-CB-CG	6.87	131.10	115.30
1	D	206	ASN	N-CA-C	-6.81	92.60	111.00
1	B	123	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	A	238	LEU	CB-CA-C	-6.76	97.35	110.20
1	D	117	LEU	CB-CG-CD2	-6.73	99.56	111.00
1	A	163	TRP	C-N-CA	-6.70	104.94	121.70
1	D	241	THR	N-CA-C	-6.68	92.97	111.00
1	B	159	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	C	238	LEU	CA-CB-CG	6.62	130.52	115.30
1	C	231	ARG	CG-CD-NE	6.61	125.67	111.80
1	A	205	ASP	CB-CG-OD2	6.60	124.24	118.30
1	D	195	SER	CB-CA-C	-6.56	97.63	110.10
1	B	151	ILE	CG1-CB-CG2	-6.56	96.97	111.40
1	B	237	LEU	CA-CB-CG	-6.43	100.50	115.30
1	D	251	SER	CA-CB-OG	-6.39	93.94	111.20
1	C	191	LEU	CB-CG-CD2	6.38	121.85	111.00
1	B	152	LYS	CD-CE-NZ	-6.34	97.12	111.70
1	C	151	ILE	CG1-CB-CG2	-6.30	97.53	111.40
1	B	223	LEU	CA-CB-CG	-6.30	100.81	115.30
1	D	112	ASP	CB-CG-OD2	6.29	123.96	118.30
1	D	244	ASP	N-CA-CB	-6.25	99.34	110.60
1	D	181	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	B	216	ASN	N-CA-C	6.21	127.76	111.00
1	B	172	ILE	CB-CA-C	-6.20	99.19	111.60
1	C	248	CYS	CA-CB-SG	-6.19	102.86	114.00
1	D	242	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	260	LEU	C-N-CA	-6.13	106.38	121.70
1	B	178	LEU	CA-CB-CG	-6.12	101.22	115.30
1	A	186	LEU	CB-CG-CD2	6.11	121.38	111.00
1	C	113	LEU	CB-CG-CD2	-6.09	100.64	111.00
1	A	181	ASP	N-CA-C	6.09	127.44	111.00
1	A	240	LYS	CD-CE-NZ	-6.07	97.73	111.70
1	B	113	LEU	CA-CB-CG	6.06	129.23	115.30
1	C	216	ASN	N-CA-C	-6.06	94.65	111.00
1	A	181	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	D	232	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	190	LYS	CB-CA-C	-6.03	98.34	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	236	MET	CA-CB-CG	-6.01	103.08	113.30
1	C	235	CYS	CA-CB-SG	-6.00	103.21	114.00
1	B	114	LEU	CA-CB-CG	5.99	129.08	115.30
1	D	261	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	254	CYS	CB-CA-C	-5.97	98.47	110.40
1	A	180	ILE	CG1-CB-CG2	5.96	124.51	111.40
1	B	233	GLY	N-CA-C	-5.92	98.31	113.10
1	C	186	LEU	CB-CG-CD2	-5.90	100.97	111.00
1	A	202	LEU	CA-CB-CG	-5.87	101.80	115.30
1	C	232	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	253	ILE	CG1-CB-CG2	-5.86	98.50	111.40
1	C	128	THR	CA-CB-CG2	-5.84	104.23	112.40
1	A	236	MET	CG-SD-CE	-5.83	90.87	100.20
1	A	258	LYS	CA-CB-CG	5.82	126.21	113.40
1	A	263	PHE	N-CA-C	-5.81	95.31	111.00
1	B	138	THR	CB-CA-C	-5.78	96.00	111.60
1	A	175	LEU	N-CA-C	-5.72	95.57	111.00
1	B	135	SER	N-CA-CB	-5.71	101.93	110.50
1	D	114	LEU	CA-CB-CG	-5.71	102.18	115.30
1	A	157	VAL	CB-CA-C	-5.71	100.56	111.40
1	C	223	LEU	CB-CG-CD1	5.70	120.70	111.00
1	D	181	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	237	LEU	CB-CA-C	-5.68	99.41	110.20
1	C	166	CYS	CA-CB-SG	5.67	124.20	114.00
1	A	152	LYS	CD-CE-NZ	5.62	124.62	111.70
1	D	125	TYR	CB-CG-CD1	5.60	124.36	121.00
1	B	123	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	D	196	ASP	CB-CA-C	5.58	121.56	110.40
1	A	179	LYS	CB-CA-C	-5.58	99.24	110.40
1	B	205	ASP	CB-CA-C	-5.57	99.25	110.40
1	D	241	THR	CB-CA-C	5.56	126.61	111.60
1	B	236	MET	CG-SD-CE	-5.52	91.37	100.20
1	B	231	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	A	260	LEU	CB-CG-CD2	-5.46	101.72	111.00
1	A	213	TRP	N-CA-C	-5.43	96.33	111.00
1	D	111	ASN	CB-CA-C	5.43	121.26	110.40
1	D	235	CYS	CA-CB-SG	-5.42	104.24	114.00
1	B	253	ILE	CB-CA-C	-5.41	100.77	111.60
1	D	210	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	D	197	SER	N-CA-CB	-5.36	102.46	110.50
1	A	265	HIS	CB-CA-C	5.35	121.11	110.40
1	B	126	SER	CB-CA-C	-5.28	100.06	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	192	LEU	CA-CB-CG	5.28	127.45	115.30
1	B	242	ARG	CG-CD-NE	-5.27	100.73	111.80
1	A	260	LEU	CA-CB-CG	-5.24	103.24	115.30
1	D	240	LYS	N-CA-C	-5.24	96.86	111.00
1	C	177	LEU	CA-CB-CG	5.24	127.34	115.30
1	D	200	ILE	C-N-CA	-5.23	111.32	122.30
1	B	185	GLU	CG-CD-OE2	-5.21	107.87	118.30
1	A	238	LEU	N-CA-C	5.18	125.00	111.00
1	B	143	GLU	CG-CD-OE1	5.17	128.65	118.30
1	D	246	ASP	N-CA-CB	-5.17	101.30	110.60
1	C	221	LEU	CA-CB-CG	-5.16	103.44	115.30
1	B	159	ASP	N-CA-C	-5.13	97.16	111.00
1	A	195	SER	N-CA-CB	-5.12	102.81	110.50
1	C	123	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	D	189	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	B	177	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	D	243	LEU	C-N-CA	-5.10	108.94	121.70
1	D	145	TYR	N-CA-C	-5.09	97.26	111.00
1	C	234	GLY	O-C-N	-5.08	114.58	122.70
1	A	208	LYS	CB-CA-C	5.08	120.56	110.40
1	B	175	LEU	CA-CB-CG	5.07	126.96	115.30
1	C	111	ASN	N-CA-C	5.06	124.66	111.00
1	C	250	LYS	N-CA-C	-5.06	97.34	111.00
1	D	117	LEU	CB-CA-C	-5.04	100.63	110.20
1	C	202	LEU	CA-CB-CG	5.04	126.88	115.30
1	C	260	LEU	CB-CG-CD2	-5.03	102.44	111.00
1	D	163	TRP	CB-CA-C	-5.02	100.36	110.40
1	D	114	LEU	CB-CA-C	-5.01	100.67	110.20
1	A	247	ASN	O-C-N	5.00	130.71	122.70

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	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
1	C	240	LYS	Peptide
1	C	242	ARG	Peptide
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	191	0
1	B	1327	0	1285	144	0
1	C	1267	0	1229	169	0
1	D	1258	0	1221	166	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	642	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 63.

All (642) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:109:PRO:HA	1:A:112:ASP:OD1	1.30	1.23
1:D:205:ASP:HA	1:D:206:ASN:HB2	1.24	1.18
1:C:217:GLY:O	1:C:218:PRO:C	1.81	1.17
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: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:C:113:LEU:HD23	1:C:113:LEU:C	1.87	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: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:D:162:THR:C	1:D:164:SER:H	1.74	0.91
1:B:242:ARG:HG3	1:B:243:LEU:N	1.86	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:C:237:LEU:HD12	1:C:237:LEU:C	1.91	0.89
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: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:C:230:ILE:HD12	1:C:230:ILE:H	1.43	0.82
1:C:243:LEU:H	1:C:243:LEU:CD2	1.92	0.82
1:A:183:GLU:O	1:A:187:LYS:HD3	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:230:ILE:HD12	1:D:230:ILE:N	1.97	0.79
1:C:240:LYS:C	1:C:241:THR:O	2.17	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:A:214:ILE:HD13	1:A:214:ILE:C	2.03	0.78
1:B:189:LEU:HA	1:B:192:LEU:CD2	2.13	0.78
1:C:237:LEU:C	1:C:237:LEU:CD1	2.52	0.77
1:A:230:ILE:C	1:A:232:ASP:H	1.87	0.77
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: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: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: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: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
1:D:162:THR:C	1:D:164:SER:N	2.37	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:214:ILE:O	1:B:215:ASN:C	2.28	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:C:171:GLN:HA	1:C:171:GLN:NE2	2.06	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:C:214:ILE:C	1:C:215:ASN:HD22	1.95	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:C:234:GLY:O	1:C:235:CYS:SG	2.49	0.70
1:B:147:PHE:CD1	1:B:147:PHE:C	2.65	0.69
1:A:236:MET:HE1	1:A:243:LEU:HB3	1.73	0.69
1:B:165:GLY:O	1:B:169:THR:HG23	1.92	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:A:247:ASN:C	1:A:249:ASP:H	1.97	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:D:240:LYS:O	1:D:240:LYS:HG3	1.94	0.68
1:A:168:GLN:O	1:A:172:ILE:HG23	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASN:HD22	1:B:111:ASN:H	1.41	0.68
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:C:160:ARG:O	1:C:161:LYS:CG	2.42	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:B:245:ASN:HD22	1:B:245:ASN:N	1.93	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: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:204:TYR:C	1:B:204:TYR:CD2	2.69	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:D:127:GLU:C	1:D:128:THR:HG23	2.16	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:230:ILE:C	1:A:232:ASP:N	2.48	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
1:D:110:GLY:HA2	1:D:113:LEU:H	1.62	0.64
1:C:151:ILE:CD1	1:C:151:ILE:CG2	2.75	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:B:262:LYS:O	1:B:263:PHE:C	2.36	0.61
1:C:160:ARG:C	1:C:161:LYS:HG3	2.21	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
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:B:120:GLU:O	1:B:121:GLN:C	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:219:SER:HG	1:A:221:LEU:HB3	1.66	0.59
1:D:229:ASN:HA	1:D:230:ILE:HD12	1.84	0.59
1:A:249:ASP:C	1:A:249:ASP:OD1	2.41	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:A:247:ASN:O	1:A:249:ASP:N	2.26	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:152:LYS:NZ	1:A:185:GLU:CD	2.56	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: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:253:ILE:HD13	1:A:253:ILE:CG2	2.34	0.58
1:B:199:TRP:CE3	1:B:237:LEU:HD23	2.39	0.58
1:A:214:ILE:CD1	1:A:214:ILE:C	2.67	0.58
1:C:240:LYS:O	1:C:241:THR:O	2.21	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:C:171:GLN:HA	1:C:171:GLN:HE21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ILE:HG12	1:C:238:LEU:HB2	1.84	0.57
1:D:114:LEU:O	1:D:115:GLU:C	2.43	0.57
1:D:216:ASN:O	1:D:217:GLY:O	2.23	0.57
1:C:113:LEU:C	1:C:113:LEU:CD2	2.64	0.57
1:D:151:ILE:C	1:D:260:LEU:HD23	2.25	0.57
1:C:182:ASN:O	1:C:183:GLU:C	2.44	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:D:195:SER:O	1:D:196:ASP:HB2	2.05	0.57
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:182:ASN:O	1:D:183:GLU:C	2.42	0.56
1:D:185:GLU:HG2	1:D:185:GLU:O	2.04	0.56
1:D:203:SER:HB2	1:D:234:GLY:O	2.05	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:CE3	2.79	0.56
1:C:200:ILE:HD11	1:C:255:ILE:HD12	1.88	0.56
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:A:247:ASN:C	1:A:249:ASP:N	2.58	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:114:LEU:O	1:A:115:GLU:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASN:O	1:A:115:GLU:CG	2.43	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: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:205:ASP:CG	1:D:206:ASN:HB3	2.26	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:A:224:ASN:C	1:A:224:ASN:ND2	2.61	0.54
1:A:233:GLY:HA3	1:A:246:ASP:C	2.27	0.54
1:C:171:GLN:C	1:C:173:SER:H	2.10	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:D:178:LEU:HD22	1:D:255:ILE:CG2	2.37	0.54
1:B:236:MET:SD	1:B:244:ASP:C	2.87	0.53
1:D:242:ARG:HG2	1:D:243:LEU:O	2.08	0.53
1:A:225:THR:C	1:A:227:LYS:H	2.10	0.53
1:D:236:MET:HG3	1:D:237:LEU:N	2.23	0.53
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:C:247:ASN:C	1:C:249:ASP:H	2.10	0.53
1:B:114:LEU:HD12	1:B:118:HIS:HE1	1.74	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: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:A:137:HIS:O	1:A:138:THR:C	2.47	0.52
1:B:168:GLN:O	1:B:172:ILE:HG13	2.09	0.52
1:D:110:GLY:C	1:D:113:LEU:H	2.13	0.52
1:C:179:LYS:HD2	1:C:179:LYS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ASP:O	1:C:182:ASN:CB	2.45	0.52
1:D:127:GLU:C	1:D:128:THR:CG2	2.77	0.52
1:A:200:ILE:HG23	1:A:238:LEU:CD1	2.39	0.52
1:B:147:PHE:C	1:B:147:PHE:HD1	2.11	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:C:166:CYS:O	1:C:167:LYS:C	2.47	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:144:LYS:NZ	1:A:155:TYR:OH	2.31	0.52
1:A:147:PHE:CD1	1:A:147:PHE:C	2.82	0.52
1:A:200:ILE:HG21	1:A:238:LEU:HD11	1.91	0.52
1:A:214:ILE:O	1:A:214:ILE:HG12	2.09	0.51
1:C:215:ASN:O	1:C:216:ASN:HB2	2.10	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:C	1:C:211:TRP:HE3	2.12	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:C:247:ASN:C	1:C:249:ASP:N	2.62	0.51
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:211:TRP:HD1	1:D:225:THR:HG1	1.57	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: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:C:229:ASN:O	1:C:232:ASP:HB2	2.11	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:B:194:PRO:O	1:B:195:SER:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:134:SER:C	1:A:136:GLN:H	2.15	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:261:ASP:OD2	1:C:261:ASP:N	2.38	0.50
1:B:118:HIS:O	1:B:119:LYS:C	2.49	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:D:125:TYR:O	1:D:126:SER:C	2.49	0.49
1:D:160:ARG:O	1:D:161:LYS:CG	2.60	0.49
1:D:171:GLN:O	1:D:174:SER:N	2.44	0.49
1:A:111:ASN:C	1:A:115:GLU:HG3	2.28	0.49
1:D:127:GLU:O	1:D:128:THR:CG2	2.61	0.49
1:D:261:ASP:O	1:D:262:LYS:CB	2.51	0.49
1:B:233:GLY:HA3	1:B:246:ASP:C	2.33	0.49
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:C:124:TRP:O	1:C:125:TYR:C	2.51	0.49
1:B:119:LYS:O	1:B:120:GLU:C	2.50	0.49
1:D:123:ARG:O	1:D:124:TRP:C	2.49	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:151:ILE:H	1:A:151:ILE:HD13	1.71	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:189:LEU:O	1:C:190:LYS:C	2.50	0.48
1:C:214:ILE:C	1:C:215:ASN:ND2	2.65	0.48
1:C:215:ASN:HD22	1:C:215:ASN:N	2.10	0.48
1:B:113:LEU:CD1	1:D:113:LEU:CD2	2.91	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:179:LYS:H	1:C:179:LYS:CD	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:SER:HB2	1:C:237:LEU:HD22	1.96	0.48
1:C:228:TYR:CZ	1:C:236:MET:CE	2.97	0.48
1:C:160:ARG:C	1:C:161:LYS:CG	2.82	0.47
1:A:114:LEU:C	1:A:116:SER:N	2.67	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: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:117:LEU:O	1:A:118:HIS:C	2.51	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:225:THR:C	1:A:227:LYS:N	2.68	0.47
1:B:147:PHE:CD1	1:B:147:PHE:O	2.68	0.46
1:B:205:ASP:OD1	1:B:205:ASP:C	2.54	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:D:213:TRP:O	1:D:214:ILE:C	2.53	0.46
1:C:210:ASP:OD2	1:C:211:TRP:N	2.48	0.46
1:D:143:GLU:HB3	1:D:144:LYS:HE3	1.97	0.46
1:D:234:GLY:C	1:D:235:CYS:SG	2.93	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:C:195:SER:HB2	1:C:240:LYS:CE	2.45	0.46
1:C:199:TRP:C	1:C:200:ILE:HD13	2.36	0.46
1:B:120:GLU:O	1:B:122:ASN:N	2.48	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:147:PHE:CD1	1:C:147:PHE:C	2.90	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:A:205:ASP:CG	1:A:206:ASN:H	2.19	0.45
1:B:108:ARG:O	1:B:109:PRO:C	2.55	0.45
1:B:111:ASN:ND2	1:B:111:ASN:N	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:TYR:HB3	1:C:154:TYR:HE1	1.81	0.45
1:A:207:LYS:O	1:A:208:LYS:C	2.52	0.45
1:A:236:MET:CE	1:A:243:LEU:HB3	2.45	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:188:PHE:C	1:B:192:LEU:HD22	2.26	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: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:150:GLY:HA2	1:D:124:TRP:CE2	2.52	0.45
1:C:128:THR:C	1:C:129:LYS:O	2.53	0.45
1:D:204:TYR:OH	1:D:209:LYS:HA	2.17	0.45
1:A:119:LYS:C	1:A:121:GLN:N	2.64	0.45
1:D:178:LEU:HD22	1:D:255:ILE:HG21	1.99	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:B:224:ASN:O	1:B:224:ASN:CG	2.55	0.45
1:D:164:SER:C	1:D:166:CYS:N	2.68	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: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: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:A:162:THR:C	1:A:199:TRP:NE1	2.71	0.44
1:B:105:ILE:HG21	1:D:111:ASN:OD1	2.17	0.44
1:A:249:ASP:OD1	1:A:250:LYS:N	2.51	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:B:129:LYS:C	1:B:130:THR:CG2	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:213:TRP:C	1:B:214:ILE:O	2.53	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
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:B:113:LEU:HD13	1:D:113:LEU:HD21	2.01	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:C:160:ARG:HA	1:C:252:PHE:C	2.39	0.43
1:D:234:GLY:C	1:D:248:CYS:SG	2.97	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: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:D:199:TRP:CZ3	1:D:235:CYS:HB3	2.54	0.42
1:C:167:LYS:O	1:C:168:GLN:C	2.57	0.42
1:A:166:CYS:O	1:A:167:LYS:C	2.57	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:D:171:GLN:C	1:D:173:SER:N	2.73	0.42
1:A:200:ILE:HG13	1:A:213:TRP:HZ3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:259:ARG:O	1:A:260:LEU:C	2.57	0.42
1:B:166:CYS:O	1:B:167:LYS:C	2.57	0.42
1:C:170:CYS:HB3	1:C:176:SER:N	2.35	0.42
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:D:186:LEU:O	1:D:187:LYS:C	2.59	0.42
1:D:247:ASN:C	1:D:249:ASP:H	2.23	0.42
1:A:185:GLU:O	1:A:186:LEU:C	2.56	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:C:205:ASP:O	1:C:206:ASN:C	2.56	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: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:121:GLN:C	1:B:121:GLN:CD	2.79	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:B:219:SER:C	1:B:221:LEU:H	2.23	0.41
1:C:147:PHE:CZ	1:C:192:LEU:HD12	2.56	0.41
1:C:171:GLN:C	1:C:173:SER:N	2.74	0.41
1:C:236:MET:HB2	1:C:236:MET:HE2	1.79	0.41
1:C:237:LEU:HD13	1:C:238:LEU:C	2.40	0.41
1:D:179:LYS:HA	1:D:213:TRP:CZ3	2.55	0.41
1:D:250:LYS:C	1:D:251:SER:HG	2.23	0.41
1:A:241:THR:C	1:A:242:ARG:HG3	2.40	0.41
1:C:230:ILE:O	1:C:231:ARG:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ARG:NH1	1:B:242:ARG:CG	2.83	0.41
1:B:129:LYS:C	1:B:130:THR:HG23	2.41	0.41
1:B:133:ASP:C	1:B:134:SER:O	2.56	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:A:172:ILE:HG12	1:A:173:SER:N	2.34	0.41
1:C:226:MET:O	1:C:226:MET:CG	2.69	0.41
1:B:135:SER:C	1:B:137:HIS:H	2.24	0.40
1:D:142:PHE:CZ	1:D:160:ARG:NH1	2.89	0.40
1:A:173:SER:O	1:A:174:SER:HB2	2.21	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:A:198:TYR:HD2	1:A:253:ILE:CG2	2.34	0.40
1:A:205:ASP:CG	1:A:206:ASN:N	2.73	0.40
1:B:162:THR:O	1:B:163:TRP:C	2.60	0.40
1:C:229:ASN:HD21	1:C:231:ARG:HE	1.69	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: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%)	1 0
1	B	159/190 (84%)	114 (72%)	24 (15%)	21 (13%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Res	Type
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
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 (i)

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%)	105 (72%)	40 (28%)	0 0
1	B	149/177 (84%)	118 (79%)	31 (21%)	1 2
1	C	142/177 (80%)	100 (70%)	42 (30%)	0 0
1	D	141/177 (80%)	98 (70%)	43 (30%)	0 0
All	All	577/708 (82%)	421 (73%)	156 (27%)	0 0

All (156) 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	121	GLN
1	A	122	ASN
1	A	126	SER
1	A	129	LYS
1	A	137	HIS
1	A	145	TYR
1	A	151	ILE
1	A	152	LYS
1	A	161	LYS
1	A	172	ILE
1	A	177	LEU
1	A	179	LYS
1	A	183	GLU
1	A	189	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	229	ASN

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Mol	Chain	Res	Type
1	A	232	ASP
1	A	238	LEU
1	A	241	THR
1	A	242	ARG
1	A	245	ASN
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
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	155	TYR
1	B	169	THR
1	B	173	SER
1	B	176	SER
1	B	179	LYS
1	B	183	GLU
1	B	192	LEU
1	B	207	LYS
1	B	208	LYS
1	B	214	ILE
1	B	221	LEU
1	B	226	MET
1	B	229	ASN
1	B	241	THR
1	B	242	ARG
1	B	245	ASN
1	B	249	ASP
1	B	251	SER
1	B	259	ARG
1	B	260	LEU

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Mol	Chain	Res	Type
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	132	SER
1	C	133	ASP
1	C	140	ARG
1	C	142	PHE
1	C	143	GLU
1	C	144	LYS
1	C	158	MET
1	C	159	ASP
1	C	164	SER
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	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	231	ARG
1	C	236	MET
1	C	237	LEU
1	C	242	ARG
1	C	243	LEU
1	C	244	ASP
1	C	250	LYS
1	C	251	SER
1	C	260	LEU

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Mol	Chain	Res	Type
1	C	265	HIS
1	D	108	ARG
1	D	115	GLU
1	D	116	SER
1	D	120	GLU
1	D	131	PHE
1	D	142	PHE
1	D	144	LYS
1	D	152	LYS
1	D	158	MET
1	D	159	ASP
1	D	164	SER
1	D	169	THR
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	199	TRP
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	237	LEU
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

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Mol	Chain	Res	Type
1	D	261	ASP
1	D	262	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	122	ASN
1	A	216	ASN
1	A	224	ASN
1	A	229	ASN
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	D	121	GLN
1	D	224	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

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, 95^{th} 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	157/190 (82%)	0.02	1 (0%)	89	90	37, 55, 79, 85	0
1	B	161/190 (84%)	0.24	8 (4%)	28	30	37, 56, 86, 119	0
1	C	154/190 (81%)	0.08	6 (3%)	39	42	36, 58, 88, 99	0
1	D	152/190 (80%)	0.16	3 (1%)	65	68	36, 56, 89, 116	0
All	All	624/760 (82%)	0.13	18 (2%)	51	55	36, 56, 86, 119	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	ILE	7.9
1	D	141	GLY	6.9
1	B	110	GLY	6.5
1	B	226	MET	4.9
1	B	108	ARG	4.8
1	B	109	PRO	4.0
1	D	107	CYS	3.7
1	C	109	PRO	3.7
1	B	107	CYS	2.7
1	C	223	LEU	2.7
1	C	222	ALA	2.6
1	C	226	MET	2.5
1	B	215	ASN	2.5
1	C	135	SER	2.3
1	A	211	TRP	2.3
1	D	168	GLN	2.1
1	B	230	ILE	2.1
1	C	204	TYR	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 monosaccharides 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.