Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 07:55 AM JST

PDB ID	:	6L9N
Title	:	H2-Ld complexed with A5 peptide
Authors	:	Wei, P.C.; Yin, L.
Deposited on	:	2019-11-10
Resolution	:	2.60 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:

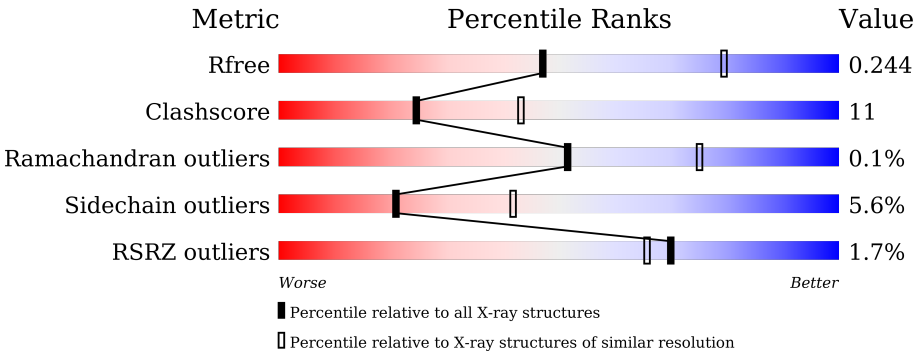
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	278	82% 15%
1	D	278	76% 20%
1	G	278	4% 76% 20%
1	J	278	2% 77% 19%
2	B	99	75% 23%
2	E	99	80% 15%

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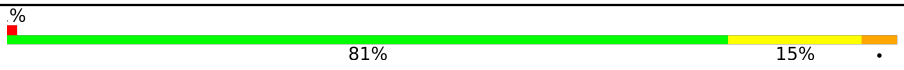
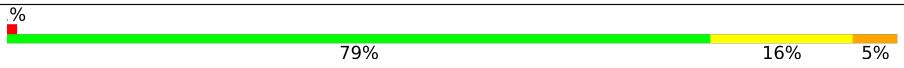
Mol	Chain	Length	Quality of chain
2	H	99	
2	K	99	
3	C	9	
3	F	9	
3	I	9	
3	L	9	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12879 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 MHC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	4	0	0
			2268	1437	395	426	10			
1	D	278	Total	C	N	O	S	4	0	0
			2268	1437	395	426	10			
1	G	278	Total	C	N	O	S	4	0	0
			2268	1437	395	426	10			
1	J	278	Total	C	N	O	S	4	0	0
			2268	1437	395	426	10			

- Molecule 2 is a protein called b2m.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	E	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	H	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	K	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 3 is a protein called SER-PRO-SER-TYR-ALA-TYR-HIS-GLN-PHE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			79	52	12	15			
3	F	9	Total	C	N	O	0	0	0
			79	52	12	15			
3	I	9	Total	C	N	O	0	0	0
			79	52	12	15			
3	L	9	Total	C	N	O	0	0	0
			79	52	12	15			

- Molecule 4 is water.

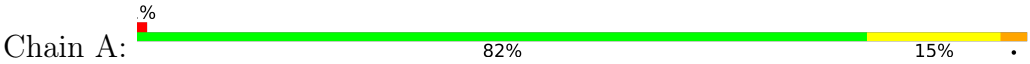
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	38	Total O 38 38	0	0
4	B	26	Total O 26 26	0	0
4	C	2	Total O 2 2	0	0
4	D	40	Total O 40 40	0	0
4	E	21	Total O 21 21	0	0
4	F	2	Total O 2 2	0	0
4	G	15	Total O 15 15	0	0
4	H	11	Total O 11 11	0	0
4	I	2	Total O 2 2	0	0
4	J	26	Total O 26 26	0	0
4	K	22	Total O 22 22	0	0
4	L	2	Total O 2 2	0	0

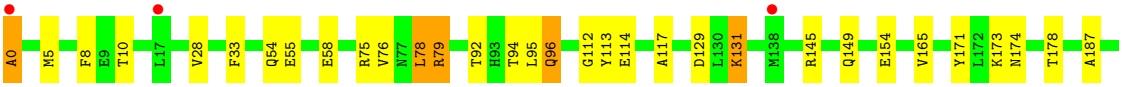
3 Residue-property plots (i)

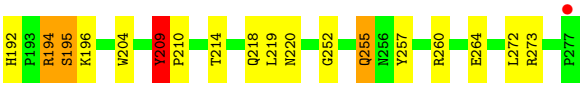
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:

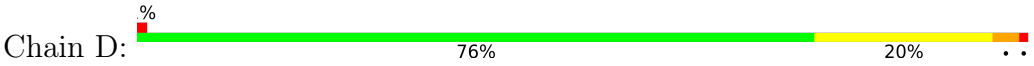


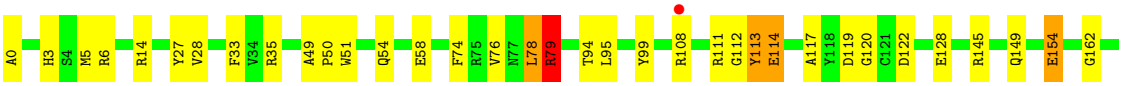


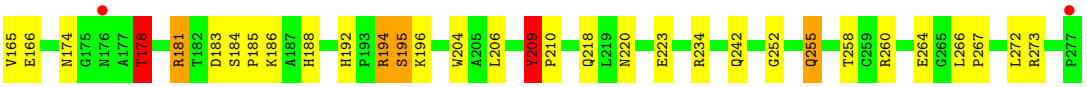


• Molecule 1: MHC

Chain D:

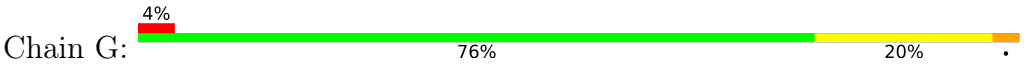


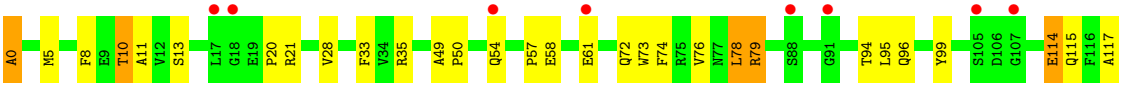


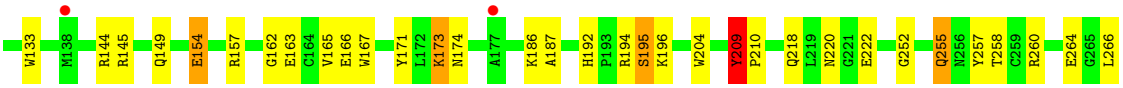


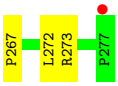
• Molecule 1: MHC

Chain G:



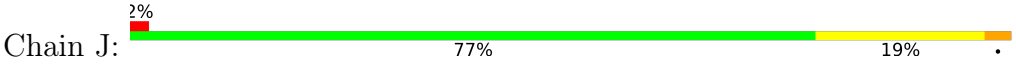


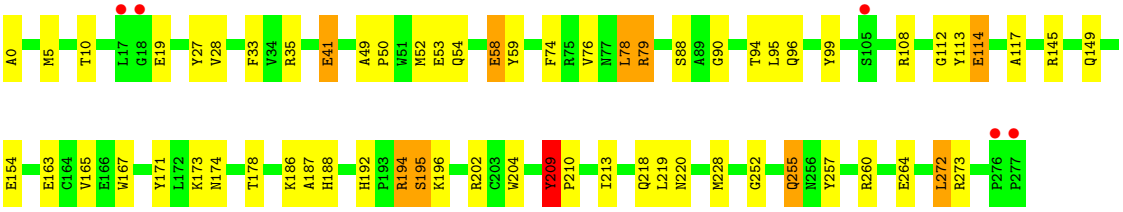




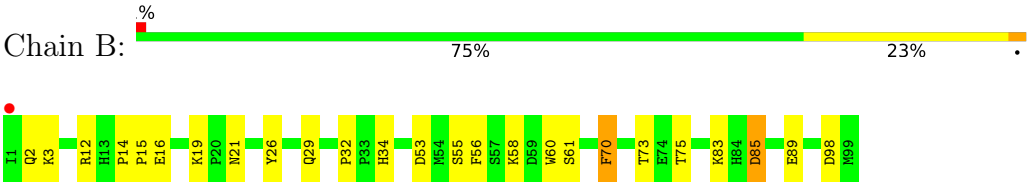
• Molecule 1: MHC

Chain J:

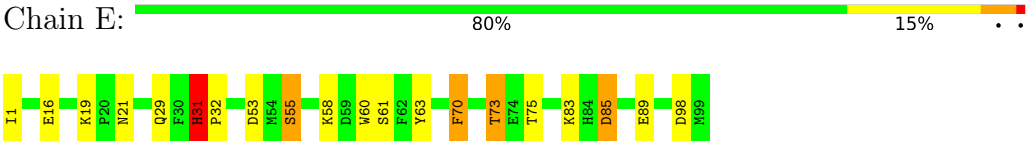




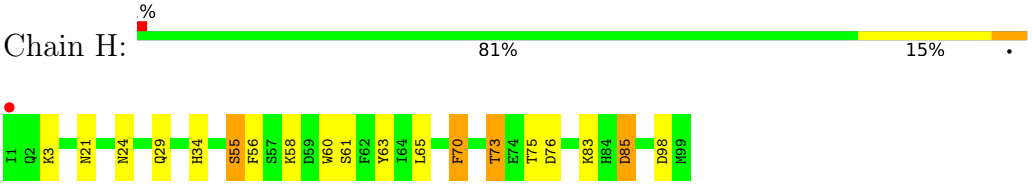
• Molecule 2: b2m



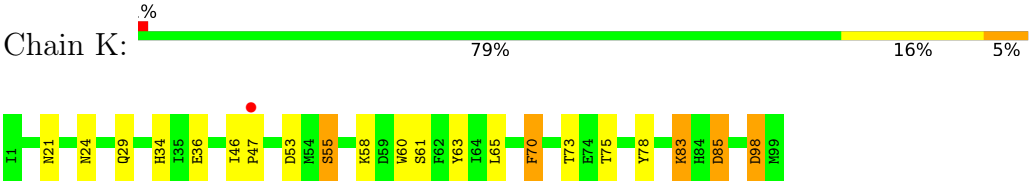
• Molecule 2: b2m



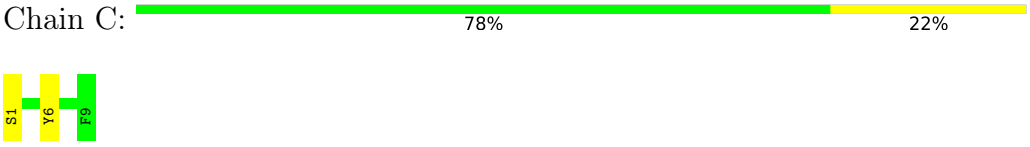
• Molecule 2: b2m



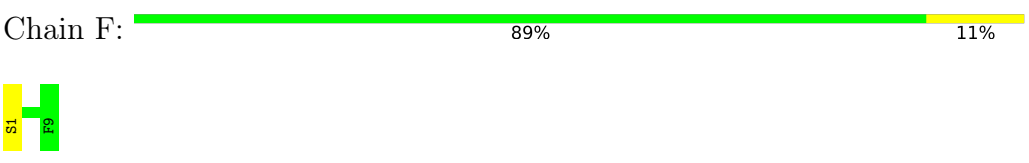
• Molecule 2: b2m



• Molecule 3: SER-PRO-SER-TYR-ALA-TYR-HIS-GLN-PHE



• Molecule 3: SER-PRO-SER-TYR-ALA-TYR-HIS-GLN-PHE

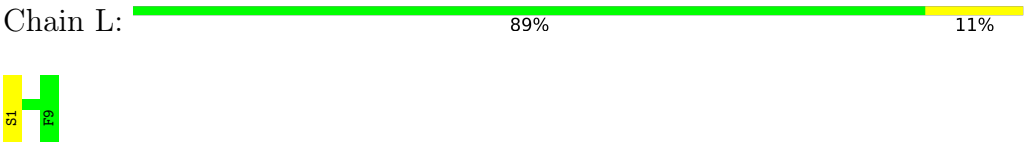


• Molecule 3: SER-PRO-SER-TYR-ALA-TYR-HIS-GLN-PHE

Chain I:

• Molecule 3: SER-PRO-SER-TYR-ALA-TYR-HIS-GLN-PHE

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.96Å 88.44Å 105.81Å 80.99° 75.81° 88.34°	Depositor
Resolution (Å)	19.96 – 2.60 19.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.96-2.60) 97.3 (19.96-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.59Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.209 , 0.254 0.194 , 0.244	Depositor DCC
R_{free} test set	2005 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for h,-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12879	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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	1.04	6/2337 (0.3%)	0.95	6/3180 (0.2%)
1	D	1.11	9/2337 (0.4%)	1.11	12/3180 (0.4%)
1	G	1.15	7/2337 (0.3%)	1.13	8/3180 (0.3%)
1	J	1.06	5/2337 (0.2%)	0.96	8/3180 (0.3%)
2	B	0.94	1/847 (0.1%)	0.82	0/1148
2	E	0.99	3/847 (0.4%)	0.93	3/1148 (0.3%)
2	H	0.94	0/847	0.81	0/1148
2	K	0.91	0/847	0.81	0/1148
3	C	1.58	0/83	0.95	0/111
3	F	0.94	0/83	0.86	0/111
3	I	0.76	0/83	0.79	0/111
3	L	1.14	0/83	0.81	0/111
All	All	1.06	31/13068 (0.2%)	0.99	37/17756 (0.2%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	114	GLU	CD-OE2	-10.10	1.14	1.25
1	A	114	GLU	CD-OE1	-9.56	1.15	1.25
1	D	113	TYR	CG-CD1	-9.11	1.27	1.39
1	D	113	TYR	CG-CD2	-8.98	1.27	1.39
1	D	114	GLU	CD-OE1	-8.92	1.15	1.25
1	J	114	GLU	CD-OE2	-8.79	1.16	1.25
1	D	113	TYR	CE2-CZ	-8.48	1.27	1.38
1	J	114	GLU	CD-OE1	-8.31	1.16	1.25
1	G	115	GLN	CD-NE2	-7.51	1.14	1.32
1	A	114	GLU	CD-OE2	-7.50	1.17	1.25
1	G	154	GLU	CB-CG	-7.48	1.38	1.52
1	D	113	TYR	CE1-CZ	-7.46	1.28	1.38
1	G	114	GLU	CD-OE1	-7.04	1.18	1.25
1	J	209	TYR	CE2-CZ	-6.68	1.29	1.38
1	A	96	GLN	CD-NE2	-6.65	1.16	1.32
2	B	26	TYR	CE1-CZ	6.53	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	89	GLU	CD-OE1	-6.43	1.18	1.25
1	J	41	GLU	CB-CG	-6.04	1.40	1.52
1	A	0	ALA	CA-CB	6.02	1.65	1.52
1	G	0	ALA	CA-CB	5.74	1.64	1.52
1	D	209	TYR	CE2-CZ	-5.56	1.31	1.38
1	A	209	TYR	CE2-CZ	-5.52	1.31	1.38
2	E	31	HIS	ND1-CE1	-5.50	1.21	1.34
2	E	89	GLU	CB-CG	-5.41	1.41	1.52
1	G	115	GLN	CD-OE1	-5.23	1.12	1.24
1	D	154	GLU	CB-CG	-5.22	1.42	1.52
1	G	222	GLU	CD-OE1	-5.21	1.20	1.25
1	J	53	GLU	CD-OE1	-5.18	1.20	1.25
1	D	3	HIS	CD2-NE2	-5.15	1.26	1.38
1	A	55	GLU	CD-OE1	-5.15	1.20	1.25
1	G	114	GLU	CD-OE2	-5.13	1.20	1.25

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	79	ARG	NE-CZ-NH2	24.57	132.59	120.30
1	G	79	ARG	NE-CZ-NH1	-21.48	109.56	120.30
1	D	181	ARG	NE-CZ-NH1	19.92	130.26	120.30
1	D	181	ARG	NE-CZ-NH2	-16.93	111.84	120.30
1	G	79	ARG	CD-NE-CZ	11.01	139.02	123.60
1	D	79	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	D	79	ARG	CG-CD-NE	9.58	131.92	111.80
1	J	114	GLU	OE1-CD-OE2	-9.33	112.10	123.30
1	A	114	GLU	OE1-CD-OE2	-8.62	112.95	123.30
1	D	108	ARG	NE-CZ-NH2	8.07	124.33	120.30
1	J	58	GLU	CA-CB-CG	7.89	130.76	113.40
1	G	222	GLU	OE1-CD-OE2	-7.80	113.93	123.30
1	D	114	GLU	OE1-CD-OE2	-7.78	113.97	123.30
1	D	79	ARG	CD-NE-CZ	7.44	134.01	123.60
2	E	89	GLU	CG-CD-OE2	7.29	132.88	118.30
1	A	79	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	J	79	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	D	178	THR	CA-CB-CG2	-6.87	102.79	112.40
1	G	79	ARG	CG-CD-NE	-6.79	97.55	111.80
1	J	108	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	D	79	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	D	209	TYR	CG-CD2-CE2	6.49	126.49	121.30
1	A	209	TYR	CG-CD2-CE2	6.46	126.47	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	53	GLU	OE1-CD-OE2	-6.41	115.60	123.30
2	E	31	HIS	ND1-CG-CD2	-6.21	97.30	106.00
1	G	209	TYR	CG-CD2-CE2	6.01	126.11	121.30
1	A	55	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	J	209	TYR	CG-CD2-CE2	5.82	125.96	121.30
1	J	79	ARG	CG-CD-NE	5.74	123.86	111.80
1	D	234	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	A	131	LYS	CG-CD-CE	5.59	128.67	111.90
1	J	202	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	D	181	ARG	CD-NE-CZ	5.34	131.08	123.60
1	A	79	ARG	CG-CD-NE	5.15	122.61	111.80
1	G	114	GLU	OE1-CD-OE2	-5.07	117.22	123.30
2	E	89	GLU	CG-CD-OE1	-5.06	108.19	118.30
1	G	35	ARG	NE-CZ-NH1	-5.03	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2268	0	2131	40	0
1	D	2268	0	2131	77	0
1	G	2268	0	2131	66	0
1	J	2268	0	2131	55	2
2	B	821	0	796	17	2
2	E	821	0	796	30	0
2	H	821	0	796	14	0
2	K	821	0	796	20	0
3	C	79	0	66	1	0
3	F	79	0	66	1	0
3	I	79	0	66	4	0
3	L	79	0	66	1	0
4	A	38	0	0	1	0
4	B	26	0	0	3	0
4	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	40	0	0	3	0
4	E	21	0	0	4	0
4	F	2	0	0	0	0
4	G	15	0	0	0	0
4	H	11	0	0	1	0
4	I	2	0	0	0	0
4	J	26	0	0	5	0
4	K	22	0	0	3	0
4	L	2	0	0	0	0
All	All	12879	0	11972	267	2

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 11.

All (267) 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:D:14:ARG:NH2	4:D:302:HOH:O	1.91	1.02
1:A:220:ASN:HD22	2:E:58:LYS:HB2	1.25	0.98
2:E:85:ASP:OD1	4:E:101:HOH:O	1.80	0.96
2:B:73:THR:HG22	2:B:75:THR:H	1.31	0.94
1:D:178:THR:HG21	1:G:61:GLU:OE2	1.67	0.93
2:K:78:TYR:OH	4:K:101:HOH:O	1.90	0.90
2:E:31:HIS:ND1	2:E:32:PRO:HA	1.89	0.87
1:D:209:TYR:HD2	1:D:210:PRO:HA	1.39	0.87
1:D:181:ARG:HH21	1:G:57:PRO:HG3	1.37	0.86
1:G:209:TYR:HD2	1:G:210:PRO:HA	1.37	0.86
1:G:220:ASN:HD22	2:K:58:LYS:HB2	1.42	0.84
2:B:58:LYS:HB2	1:D:220:ASN:HD22	1.42	0.84
1:J:213:ILE:O	4:J:301:HOH:O	1.94	0.84
1:G:209:TYR:HD2	1:G:210:PRO:CA	1.91	0.83
1:D:112:GLY:C	1:D:113:TYR:HD2	1.81	0.82
2:H:73:THR:HG22	2:H:75:THR:H	1.46	0.81
1:D:209:TYR:HD2	1:D:210:PRO:CA	1.94	0.81
2:E:73:THR:HG22	2:E:75:THR:H	1.46	0.81
1:D:181:ARG:HH21	1:G:57:PRO:CG	1.93	0.80
1:D:79:ARG:HB3	1:D:79:ARG:HH11	1.44	0.80
1:G:209:TYR:CD2	1:G:210:PRO:HA	2.16	0.80
2:B:53:ASP:O	4:B:101:HOH:O	1.99	0.79
2:K:73:THR:HG22	2:K:75:THR:H	1.47	0.78
1:D:128:GLU:OE1	4:D:303:HOH:O	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ARG:HG2	1:D:113:TYR:HE2	1.52	0.75
2:H:58:LYS:HB2	1:J:220:ASN:HD22	1.52	0.75
1:J:209:TYR:HD2	1:J:210:PRO:N	1.86	0.74
1:D:209:TYR:CD2	1:D:210:PRO:HA	2.23	0.73
1:J:0:ALA:N	1:J:264:GLU:OE1	2.22	0.72
1:D:27:TYR:OH	2:E:55:SER:OG	2.08	0.71
1:A:209:TYR:HD2	1:A:210:PRO:N	1.87	0.71
1:A:209:TYR:CD2	1:A:210:PRO:HA	2.25	0.71
2:E:53:ASP:O	4:E:102:HOH:O	2.08	0.71
1:D:78:LEU:HD13	1:D:95:LEU:HB2	1.71	0.71
1:D:181:ARG:NH2	1:G:57:PRO:CD	2.54	0.71
1:J:19:GLU:HB3	4:J:308:HOH:O	1.90	0.70
1:G:76:VAL:HG13	1:G:79:ARG:HH12	1.57	0.70
1:D:112:GLY:C	1:D:113:TYR:CD2	2.65	0.69
1:J:54:GLN:HE21	1:J:174:ASN:HB3	1.57	0.69
1:D:112:GLY:O	1:D:113:TYR:HD2	1.76	0.69
2:K:85:ASP:OD1	2:K:85:ASP:N	2.23	0.68
2:H:85:ASP:OD1	2:H:85:ASP:N	2.25	0.68
1:A:220:ASN:ND2	2:E:58:LYS:HB2	2.04	0.68
2:B:34:HIS:O	4:B:103:HOH:O	2.12	0.68
1:G:78:LEU:HD13	1:G:95:LEU:HB2	1.76	0.67
1:A:195:SER:OG	1:A:196:LYS:N	2.28	0.66
1:J:76:VAL:HA	1:J:79:ARG:HH12	1.59	0.66
1:D:181:ARG:HE	1:G:57:PRO:HB3	1.59	0.66
1:G:195:SER:OG	1:G:196:LYS:N	2.27	0.66
1:D:99:TYR:HB2	1:D:114:GLU:OE2	1.96	0.66
1:D:120:GLY:HA3	2:E:31:HIS:CD2	2.31	0.66
1:D:181:ARG:HH21	1:G:57:PRO:CD	2.09	0.66
1:A:76:VAL:HA	1:A:79:ARG:HH12	1.61	0.65
2:K:34:HIS:O	4:K:102:HOH:O	2.14	0.65
2:H:34:HIS:O	4:H:101:HOH:O	2.15	0.65
1:D:76:VAL:HG13	1:D:79:ARG:HH12	1.61	0.64
1:A:209:TYR:HD2	1:A:210:PRO:CA	2.09	0.64
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.32	0.64
1:A:220:ASN:HD22	2:E:58:LYS:CB	2.04	0.64
1:D:120:GLY:HA3	2:E:31:HIS:HD2	1.63	0.64
2:E:85:ASP:OD1	2:E:85:ASP:N	2.31	0.63
1:D:188:HIS:CD2	1:D:204:TRP:HB2	2.33	0.63
1:A:209:TYR:CD2	1:A:210:PRO:CA	2.82	0.63
2:B:85:ASP:N	2:B:85:ASP:OD1	2.31	0.63
1:D:181:ARG:NE	1:G:57:PRO:HB3	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:209:TYR:CD2	1:J:210:PRO:HA	2.33	0.63
1:J:27:TYR:OH	2:K:55:SER:OG	2.15	0.63
1:G:0:ALA:N	1:G:264:GLU:OE1	2.30	0.63
1:J:79:ARG:HH11	1:J:79:ARG:HB3	1.63	0.62
1:J:209:TYR:HD2	1:J:210:PRO:CA	2.12	0.62
1:J:78:LEU:HD13	1:J:95:LEU:HB2	1.80	0.61
1:G:255:GLN:N	1:G:255:GLN:OE1	2.33	0.61
1:A:255:GLN:HB3	1:A:273:ARG:NH2	2.16	0.61
1:G:220:ASN:ND2	2:K:58:LYS:HB2	2.14	0.61
1:A:255:GLN:OE1	1:A:255:GLN:N	2.34	0.61
1:D:6:ARG:NH2	1:D:113:TYR:CE1	2.69	0.60
1:A:78:LEU:HD13	1:A:95:LEU:HB2	1.82	0.60
2:E:19:LYS:CE	1:G:173:LYS:HE3	2.32	0.60
2:B:58:LYS:HB2	1:D:220:ASN:ND2	2.13	0.60
1:J:54:GLN:NE2	1:J:174:ASN:HB3	2.17	0.59
1:D:181:ARG:HE	1:G:57:PRO:CB	2.15	0.59
1:J:255:GLN:N	1:J:255:GLN:OE1	2.36	0.59
1:G:255:GLN:HB3	1:G:273:ARG:NH2	2.17	0.59
1:A:145:ARG:O	1:A:149:GLN:HG3	2.03	0.58
1:J:76:VAL:HA	1:J:79:ARG:NH1	2.18	0.58
2:E:19:LYS:HE2	1:G:173:LYS:HE3	1.83	0.58
1:A:79:ARG:HH11	1:A:79:ARG:HB3	1.68	0.58
1:A:5:MET:HE1	3:C:1:SER:H2	1.69	0.58
1:A:192:HIS:CE1	2:B:98:ASP:HB3	2.39	0.58
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.38	0.58
1:J:99:TYR:HB2	1:J:114:GLU:OE2	2.03	0.57
1:J:209:TYR:CD2	1:J:210:PRO:CA	2.86	0.57
1:D:122:ASP:O	4:D:304:HOH:O	2.17	0.57
1:G:76:VAL:HG13	1:G:79:ARG:NH1	2.20	0.57
1:G:209:TYR:HD2	1:G:210:PRO:N	2.02	0.57
1:D:181:ARG:NE	1:G:57:PRO:CB	2.67	0.56
1:D:79:ARG:HB3	1:D:79:ARG:NH1	2.18	0.56
1:J:54:GLN:HE21	1:J:174:ASN:CB	2.18	0.56
1:D:255:GLN:N	1:D:255:GLN:OE1	2.38	0.56
1:A:187:ALA:HA	1:A:204:TRP:O	2.06	0.56
1:G:145:ARG:O	1:G:149:GLN:HG3	2.05	0.56
1:D:209:TYR:HD2	1:D:210:PRO:N	2.04	0.56
1:A:76:VAL:HA	1:A:79:ARG:NH1	2.21	0.55
1:G:209:TYR:CD2	1:G:210:PRO:CA	2.80	0.55
2:E:31:HIS:ND1	2:E:32:PRO:CA	2.67	0.55
1:D:0:ALA:N	1:D:264:GLU:OE1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:53:ASP:O	4:K:103:HOH:O	2.18	0.55
1:D:178:THR:CG2	1:G:61:GLU:OE2	2.49	0.55
1:D:181:ARG:NH2	1:G:57:PRO:N	2.55	0.54
1:D:119:ASP:C	2:E:31:HIS:HE2	2.11	0.54
1:J:145:ARG:O	1:J:149:GLN:HG3	2.07	0.54
1:J:228:MET:O	4:J:302:HOH:O	2.18	0.54
1:A:0:ALA:N	1:A:264:GLU:OE1	2.34	0.54
1:D:181:ARG:NH2	1:G:57:PRO:CG	2.68	0.54
1:D:181:ARG:NH2	1:G:57:PRO:HD3	2.23	0.54
2:H:73:THR:CG2	2:H:75:THR:H	2.18	0.53
1:A:5:MET:HE3	1:A:171:TYR:CE1	2.44	0.53
1:D:178:THR:HG21	1:G:61:GLU:CD	2.29	0.53
1:J:209:TYR:HD2	1:J:209:TYR:C	2.13	0.53
1:D:209:TYR:CD2	1:D:210:PRO:CA	2.84	0.52
1:G:252:GLY:O	1:G:255:GLN:NE2	2.42	0.52
2:H:21:ASN:HB3	2:H:70:PHE:CE1	2.43	0.52
1:J:163:GLU:HG2	1:J:167:TRP:CD1	2.45	0.52
2:K:24:ASN:HB3	2:K:65:LEU:HD11	1.92	0.52
1:J:264:GLU:HG2	4:J:303:HOH:O	2.09	0.51
1:D:145:ARG:O	1:D:149:GLN:HG3	2.10	0.51
1:D:74:PHE:O	1:D:78:LEU:HB2	2.10	0.51
1:J:252:GLY:O	1:J:255:GLN:NE2	2.42	0.51
2:K:29:GLN:HA	2:K:61:SER:OG	2.10	0.51
1:J:195:SER:OG	1:J:196:LYS:N	2.43	0.51
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.46	0.50
2:E:55:SER:HB3	2:E:63:TYR:CZ	2.47	0.50
1:D:35:ARG:CZ	2:E:53:ASP:CB	2.89	0.50
1:D:178:THR:HG21	1:G:61:GLU:CG	2.42	0.50
1:G:192:HIS:CE1	2:H:98:ASP:HB3	2.47	0.50
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.46	0.50
1:G:54:GLN:NE2	1:G:174:ASN:HB3	2.27	0.50
1:J:218:GLN:NE2	1:J:260:ARG:HG3	2.27	0.50
2:B:73:THR:HG22	2:B:75:THR:N	2.14	0.49
2:H:73:THR:HG22	2:H:75:THR:N	2.23	0.49
1:D:113:TYR:CD2	1:D:113:TYR:N	2.77	0.49
1:D:195:SER:OG	1:D:196:LYS:N	2.45	0.49
1:G:10:THR:HG23	1:G:96:GLN:HG2	1.94	0.49
1:D:218:GLN:NE2	1:D:260:ARG:HG3	2.27	0.49
1:G:74:PHE:O	1:G:78:LEU:HB2	2.13	0.49
1:J:5:MET:HE1	3:L:1:SER:N	2.28	0.49
1:A:8:PHE:HB3	2:B:56:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:73:THR:HG22	2:K:75:THR:N	2.22	0.49
1:G:187:ALA:HA	1:G:204:TRP:O	2.13	0.49
1:A:75:ARG:NH1	4:A:302:HOH:O	2.18	0.49
1:G:163:GLU:HG2	1:G:167:TRP:CD1	2.48	0.49
2:B:29:GLN:HA	2:B:61:SER:OG	2.13	0.48
1:J:54:GLN:HE21	1:J:174:ASN:ND2	2.10	0.48
1:D:5:MET:HE1	3:F:1:SER:H2	1.79	0.48
2:E:1:ILE:N	4:E:106:HOH:O	2.46	0.48
1:J:99:TYR:CB	1:J:114:GLU:OE2	2.62	0.47
1:J:209:TYR:CD2	1:J:209:TYR:C	2.87	0.47
1:A:209:TYR:HD2	1:A:209:TYR:C	2.17	0.47
1:D:99:TYR:CB	1:D:114:GLU:OE2	2.62	0.47
1:G:99:TYR:HB2	1:G:114:GLU:OE2	2.14	0.47
1:A:218:GLN:O	1:A:257:TYR:HA	2.14	0.47
1:J:194:ARG:HD3	1:J:195:SER:HB3	1.96	0.47
1:J:255:GLN:HB3	1:J:273:ARG:NH2	2.29	0.47
1:A:10:THR:HG23	1:A:96:GLN:HG2	1.95	0.47
2:E:73:THR:CG2	2:E:75:THR:H	2.22	0.47
1:D:178:THR:CG2	1:G:61:GLU:HG2	2.44	0.47
1:D:194:ARG:HD3	1:D:195:SER:HB3	1.97	0.47
1:J:187:ALA:HA	1:J:204:TRP:O	2.15	0.47
1:D:186:LYS:HD2	1:D:186:LYS:N	2.29	0.47
1:J:28:VAL:HG23	1:J:33:PHE:CD1	2.49	0.47
1:J:188:HIS:CD2	1:J:204:TRP:HB2	2.50	0.47
1:D:255:GLN:HB3	1:D:273:ARG:NH2	2.29	0.46
1:A:218:GLN:NE2	1:A:260:ARG:HG3	2.30	0.46
2:E:21:ASN:HB3	2:E:70:PHE:CE1	2.50	0.46
2:H:55:SER:HB3	2:H:63:TYR:CZ	2.51	0.46
1:J:74:PHE:O	1:J:78:LEU:HB2	2.16	0.46
1:J:187:ALA:HB1	1:J:272:LEU:HD11	1.98	0.46
1:D:6:ARG:NH2	1:D:113:TYR:HE1	2.13	0.46
1:D:178:THR:CG2	1:G:61:GLU:CG	2.92	0.46
2:B:73:THR:CG2	2:B:75:THR:H	2.14	0.46
2:E:1:ILE:HA	4:E:106:HOH:O	2.15	0.46
1:A:219:LEU:HD13	1:A:257:TYR:CZ	2.51	0.46
2:E:16:GLU:OE1	2:E:19:LYS:HD2	2.16	0.46
1:G:5:MET:HE1	1:G:171:TYR:HE1	1.81	0.46
1:G:8:PHE:HB3	2:H:56:PHE:CE2	2.51	0.46
1:G:54:GLN:HE21	1:G:174:ASN:HB3	1.80	0.46
1:G:162:GLY:O	1:G:166:GLU:HG3	2.16	0.46
1:J:186:LYS:N	1:J:186:LYS:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:TRP:HB2	1:G:144:ARG:HG3	1.98	0.46
1:D:35:ARG:NH1	2:E:53:ASP:HB3	2.31	0.45
2:E:73:THR:HG22	2:E:75:THR:N	2.25	0.45
2:B:14:PRO:HA	2:B:15:PRO:HD3	1.78	0.45
1:D:162:GLY:O	1:D:166:GLU:HG3	2.16	0.45
1:D:35:ARG:CZ	2:E:53:ASP:HB2	2.46	0.45
1:A:54:GLN:NE2	1:A:174:ASN:HB3	2.31	0.45
1:D:54:GLN:NE2	1:D:174:ASN:HB3	2.31	0.45
2:H:29:GLN:HA	2:H:61:SER:OG	2.17	0.45
1:J:163:GLU:HG2	1:J:167:TRP:HD1	1.81	0.45
2:K:55:SER:HB3	2:K:63:TYR:CZ	2.52	0.45
1:J:54:GLN:NE2	1:J:174:ASN:CB	2.79	0.45
1:D:35:ARG:CZ	2:E:53:ASP:HB3	2.46	0.45
1:D:206:LEU:HD23	1:D:242:GLN:HG2	1.97	0.45
1:A:79:ARG:HB3	1:A:79:ARG:NH1	2.31	0.45
1:G:73:TRP:CE2	3:I:5:ALA:HB3	2.51	0.45
1:J:54:GLN:HE21	1:J:174:ASN:CG	2.20	0.44
1:D:178:THR:HG21	1:G:61:GLU:HG2	1.99	0.44
2:H:73:THR:HG22	2:H:76:ASP:H	1.83	0.44
2:K:21:ASN:HB3	2:K:70:PHE:CE1	2.53	0.44
1:D:209:TYR:CD2	1:D:210:PRO:N	2.86	0.44
1:D:192:HIS:CE1	2:E:98:ASP:HB3	2.52	0.44
1:G:5:MET:HE1	3:I:1:SER:H2	1.83	0.44
1:A:113:TYR:N	1:A:113:TYR:CD2	2.86	0.44
1:J:28:VAL:HG23	1:J:33:PHE:CE1	2.52	0.44
2:K:73:THR:CG2	2:K:75:THR:H	2.25	0.44
1:D:184:SER:HA	1:D:185:PRO:HD3	1.89	0.43
1:A:252:GLY:O	1:A:255:GLN:NE2	2.47	0.43
2:E:19:LYS:HE3	1:G:173:LYS:HE3	2.01	0.43
1:J:35:ARG:NH1	2:K:53:ASP:HB3	2.34	0.43
1:A:214:THR:HA	1:D:223:GLU:OE2	2.19	0.43
1:J:209:TYR:CE1	4:J:306:HOH:O	2.67	0.43
1:J:112:GLY:C	1:J:113:TYR:CD2	2.92	0.43
1:J:113:TYR:CD2	1:J:113:TYR:N	2.86	0.43
1:G:218:GLN:O	1:G:257:TYR:HA	2.18	0.43
1:J:59:TYR:OH	1:J:171:TYR:OH	2.17	0.43
1:D:28:VAL:HG23	1:D:33:PHE:CE1	2.54	0.43
1:A:209:TYR:CD2	1:A:209:TYR:C	2.92	0.43
1:A:255:GLN:HB3	1:A:273:ARG:HH21	1.81	0.43
1:G:49:ALA:HA	1:G:50:PRO:HD3	1.81	0.42
2:B:16:GLU:OE1	2:B:19:LYS:HD2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:VAL:HG23	1:G:33:PHE:CD1	2.53	0.42
1:J:10:THR:HG23	1:J:96:GLN:HG2	2.01	0.42
1:J:192:HIS:CE1	2:K:98:ASP:HB3	2.55	0.42
1:G:72:GLN:O	1:G:76:VAL:HG23	2.19	0.42
1:J:218:GLN:HE21	1:J:260:ARG:HG3	1.85	0.42
2:B:2:GLN:HG2	2:B:32:PRO:HD3	2.02	0.42
1:G:13:SER:HA	1:G:20:PRO:HB3	2.00	0.42
2:H:24:ASN:HB3	2:H:65:LEU:HD11	2.01	0.42
2:E:29:GLN:HA	2:E:61:SER:OG	2.20	0.41
1:D:206:LEU:CD2	1:D:242:GLN:HG2	2.50	0.41
1:D:266:LEU:HA	1:D:267:PRO:HD3	1.95	0.41
1:G:5:MET:HE1	3:I:1:SER:N	2.36	0.41
1:G:11:ALA:HA	1:G:21:ARG:O	2.19	0.41
1:G:154:GLU:HB3	1:G:157:ARG:NH2	2.35	0.41
3:I:5:ALA:O	3:I:7:HIS:N	2.53	0.41
1:J:219:LEU:HD13	1:J:257:TYR:CE1	2.55	0.41
1:D:54:GLN:HE21	1:D:174:ASN:HB3	1.85	0.41
1:G:186:LYS:HD2	1:G:186:LYS:N	2.34	0.41
1:J:79:ARG:HB3	1:J:79:ARG:NH1	2.32	0.41
1:D:252:GLY:O	1:D:255:GLN:NE2	2.49	0.41
1:A:194:ARG:HD3	1:A:195:SER:HB3	2.03	0.41
1:J:35:ARG:CZ	2:K:53:ASP:CB	2.98	0.41
1:J:49:ALA:HA	1:J:50:PRO:HD3	1.84	0.41
2:K:46:ILE:HA	2:K:47:PRO:HD3	1.93	0.41
1:A:28:VAL:HG23	1:A:33:PHE:CD1	2.56	0.41
1:A:129:ASP:O	1:A:131:LYS:HG3	2.20	0.41
2:B:12:ARG:NH2	4:B:104:HOH:O	2.26	0.41
1:D:51:TRP:HD1	1:G:61:GLU:OE2	2.04	0.41
1:D:181:ARG:NE	1:G:57:PRO:CA	2.84	0.41
1:D:181:ARG:NH1	1:D:183:ASP:OD1	2.51	0.41
1:G:266:LEU:HA	1:G:267:PRO:HD3	1.84	0.41
1:A:54:GLN:HE21	1:A:174:ASN:HB3	1.87	0.41
1:G:218:GLN:NE2	1:G:260:ARG:HG3	2.36	0.41
2:K:36:GLU:OE2	2:K:83:LYS:HE3	2.21	0.41
1:D:49:ALA:HA	1:D:50:PRO:HD3	1.83	0.40
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.55	0.40
1:G:28:VAL:HG23	1:G:33:PHE:CE1	2.56	0.40
1:A:112:GLY:C	1:A:113:TYR:CD2	2.94	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:GLU:OE2	1:J:90:GLY:N[1_564]	1.96	0.24
2:B:89:GLU:OE2	1:J:88:SER:OG[1_564]	2.19	0.01

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	276/278 (99%)	271 (98%)	5 (2%)	0	100	100
1	D	276/278 (99%)	271 (98%)	5 (2%)	0	100	100
1	G	276/278 (99%)	270 (98%)	6 (2%)	0	100	100
1	J	276/278 (99%)	270 (98%)	6 (2%)	0	100	100
2	B	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
2	E	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	H	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	K	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	5 (71%)	1 (14%)	1 (14%)	0	0
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1520/1544 (98%)	1485 (98%)	34 (2%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	6	TYR

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	232/232 (100%)	219 (94%)	13 (6%)	21 42
1	D	232/232 (100%)	219 (94%)	13 (6%)	21 42
1	G	232/232 (100%)	220 (95%)	12 (5%)	23 46
1	J	232/232 (100%)	218 (94%)	14 (6%)	19 39
2	B	94/94 (100%)	89 (95%)	5 (5%)	22 45
2	E	94/94 (100%)	88 (94%)	6 (6%)	17 35
2	H	94/94 (100%)	88 (94%)	6 (6%)	17 35
2	K	94/94 (100%)	89 (95%)	5 (5%)	22 45
3	C	8/8 (100%)	8 (100%)	0	100 100
3	F	8/8 (100%)	8 (100%)	0	100 100
3	I	8/8 (100%)	7 (88%)	1 (12%)	4 8
3	L	8/8 (100%)	8 (100%)	0	100 100
All	All	1336/1336 (100%)	1261 (94%)	75 (6%)	21 42

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	78	LEU
1	A	92	THR
1	A	94	THR
1	A	154	GLU
1	A	165	VAL
1	A	173	LYS
1	A	178	THR
1	A	194	ARG
1	A	195	SER
1	A	209	TYR
1	A	255	GLN
1	A	272	LEU
2	B	3	LYS

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Mol	Chain	Res	Type
2	B	55	SER
2	B	70	PHE
2	B	83	LYS
2	B	85	ASP
1	D	58	GLU
1	D	78	LEU
1	D	79	ARG
1	D	94	THR
1	D	154	GLU
1	D	165	VAL
1	D	178	THR
1	D	194	ARG
1	D	195	SER
1	D	209	TYR
1	D	255	GLN
1	D	258	THR
1	D	272	LEU
2	E	31	HIS
2	E	55	SER
2	E	70	PHE
2	E	73	THR
2	E	83	LYS
2	E	85	ASP
1	G	10	THR
1	G	58	GLU
1	G	78	LEU
1	G	94	THR
1	G	165	VAL
1	G	173	LYS
1	G	194	ARG
1	G	195	SER
1	G	209	TYR
1	G	255	GLN
1	G	258	THR
1	G	272	LEU
2	H	3	LYS
2	H	55	SER
2	H	70	PHE
2	H	73	THR
2	H	83	LYS
2	H	85	ASP
3	I	3	SER

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Mol	Chain	Res	Type
1	J	41	GLU
1	J	52	MET
1	J	58	GLU
1	J	78	LEU
1	J	94	THR
1	J	154	GLU
1	J	165	VAL
1	J	173	LYS
1	J	178	THR
1	J	194	ARG
1	J	195	SER
1	J	209	TYR
1	J	255	GLN
1	J	272	LEU
2	K	55	SER
2	K	70	PHE
2	K	83	LYS
2	K	85	ASP
2	K	98	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	220	ASN
1	D	188	HIS
1	G	54	GLN
1	J	54	GLN

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 monosaccharides 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	278/278 (100%)	-0.25	4 (1%) 75 71	26, 42, 83, 116	1 (0%)
1	D	278/278 (100%)	-0.26	3 (1%) 80 78	29, 44, 86, 117	1 (0%)
1	G	278/278 (100%)	-0.01	11 (3%) 38 31	30, 49, 88, 118	1 (0%)
1	J	278/278 (100%)	-0.18	5 (1%) 68 64	29, 47, 87, 117	1 (0%)
2	B	99/99 (100%)	-0.34	1 (1%) 82 80	28, 41, 78, 96	0
2	E	99/99 (100%)	-0.33	0 100 100	31, 44, 80, 97	0
2	H	99/99 (100%)	-0.41	1 (1%) 82 80	28, 43, 79, 96	0
2	K	99/99 (100%)	-0.23	1 (1%) 82 80	32, 47, 82, 100	0
3	C	9/9 (100%)	-0.41	0 100 100	30, 35, 44, 57	0
3	F	9/9 (100%)	-0.30	0 100 100	38, 44, 64, 65	0
3	I	9/9 (100%)	-0.15	0 100 100	49, 63, 72, 74	0
3	L	9/9 (100%)	-0.31	0 100 100	36, 44, 60, 65	0
All	All	1544/1544 (100%)	-0.22	26 (1%) 70 66	26, 45, 85, 118	4 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	107	GLY	5.0
1	G	277	PRO	3.8
1	J	18	GLY	3.5
1	J	277	PRO	3.4
1	J	105	SER	3.3
1	A	277	PRO	3.2
1	D	277	PRO	3.1
1	G	138	MET	3.0
1	A	0	ALA	3.0
1	G	17	LEU	2.8
1	G	91	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	1	ILE	2.8
1	D	108	ARG	2.7
1	A	138	MET	2.6
1	J	17	LEU	2.6
1	G	88	SER	2.5
2	K	47	PRO	2.5
1	G	54	GLN	2.5
1	G	105	SER	2.4
2	H	1	ILE	2.4
1	A	17	LEU	2.4
1	G	177	ALA	2.3
1	D	176	ASN	2.2
1	J	276	PRO	2.2
1	G	61	GLU	2.2
1	G	18	GLY	2.2

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.