



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:45 AM UTC

PDB ID : 6L9N / pdb_00006l9n
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

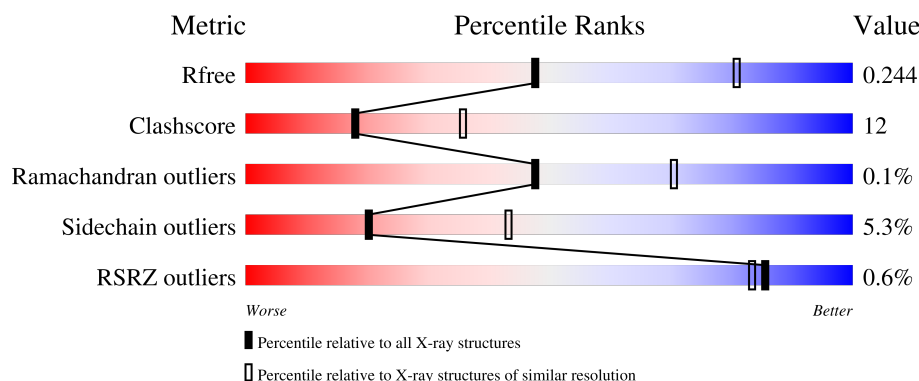
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	278	
1	D	278	
1	G	278	
1	J	278	
2	B	99	

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Mol	Chain	Length	Quality of chain
2	E	99	 77% 17% 6%
2	H	99	 81% 15% 4%
2	K	99	 77% 18% 5%
3	C	9	 78% 22%
3	F	9	 78% 22%
3	I	9	 67% 33%
3	L	9	 89% 11%

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			

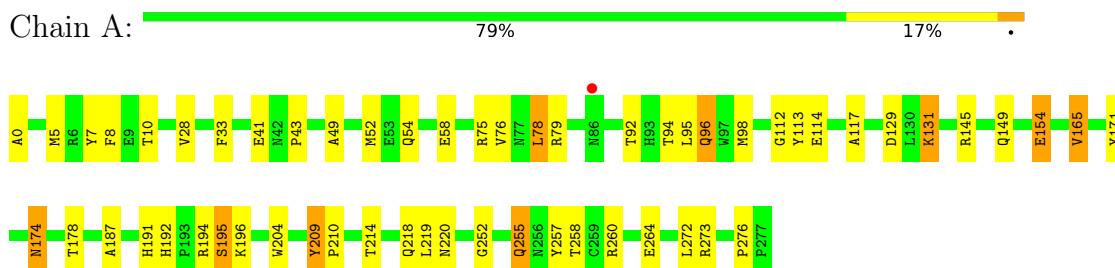
- Molecule 4 is water.

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

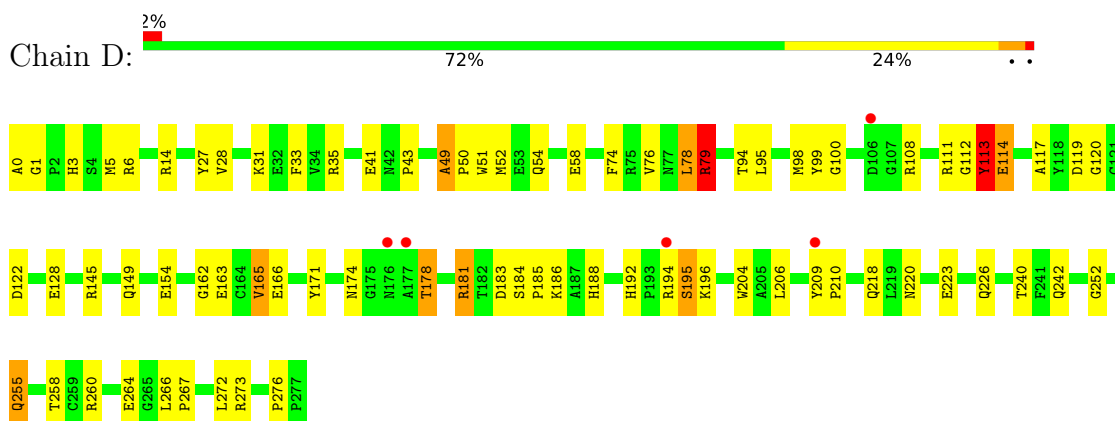
3 Residue-property plots [i](#)

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.

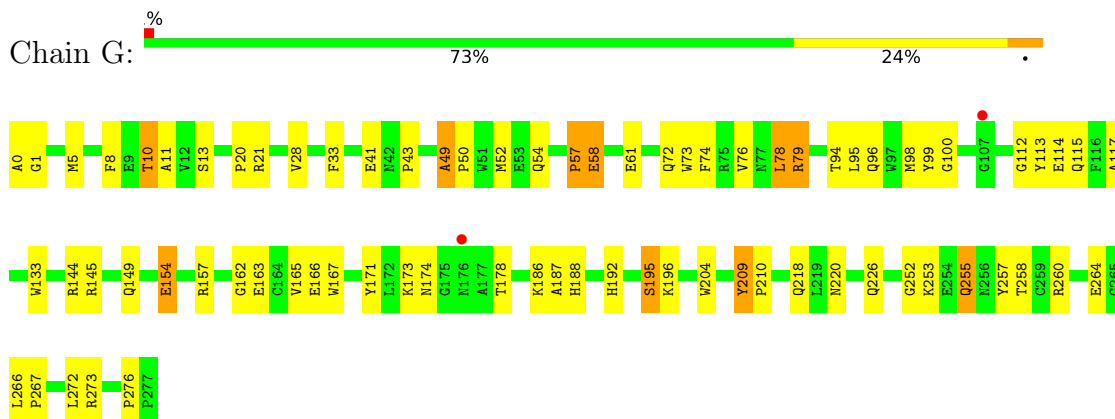
• Molecule 1: MHC



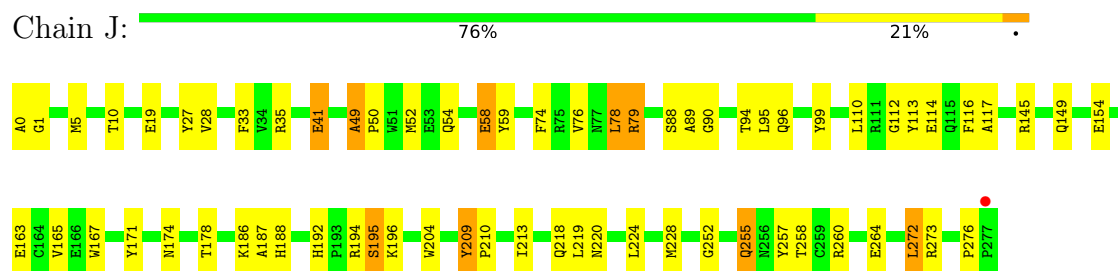
• Molecule 1: MHC



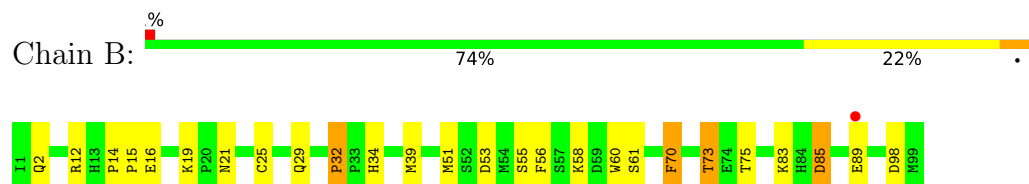
• Molecule 1: MHC



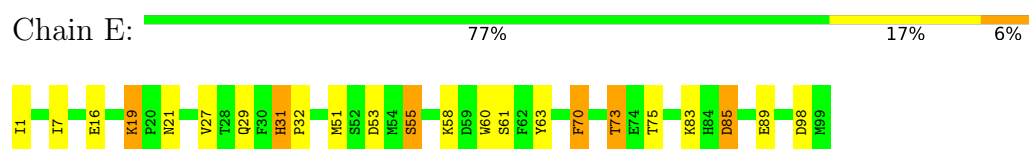
- Molecule 1: MHC



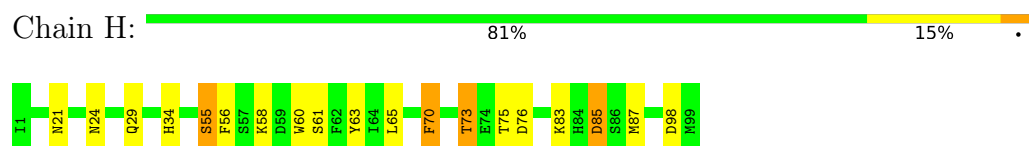
- Molecule 2: b2m



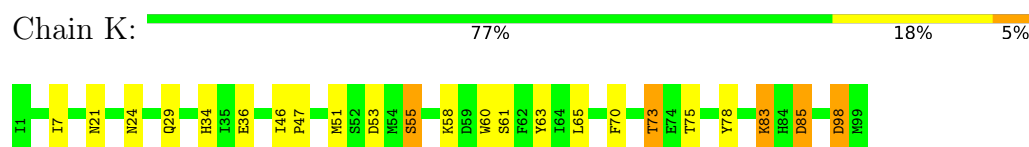
- Molecule 2: b2m



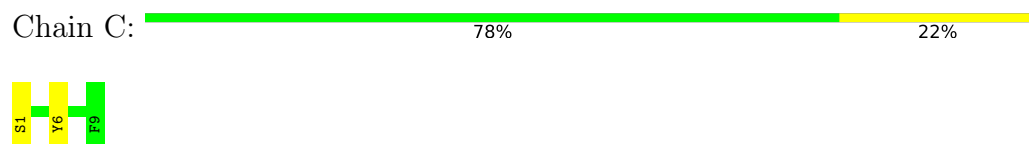
- Molecule 2: b2m



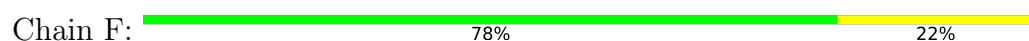
- Molecule 2: b2m



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



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

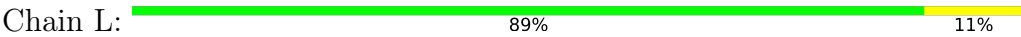




- Molecule 3: SER-PRO-SER-TYR-ALA-TYR-HIS-GLN-PHE



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



4 Data and refinement statistics

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) 97.1 (19.96-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	2007 reflections (3.62%)	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)	0.31 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.12	7/2337 (0.3%)	1.17	7/3180 (0.2%)
1	D	1.18	9/2337 (0.4%)	1.24	11/3180 (0.3%)
1	G	1.22	3/2337 (0.1%)	1.25	13/3180 (0.4%)
1	J	1.12	3/2337 (0.1%)	1.17	9/3180 (0.3%)
2	B	1.04	0/847	1.17	2/1148 (0.2%)
2	E	1.24	5/847 (0.6%)	1.31	8/1148 (0.7%)
2	H	1.03	0/847	1.17	0/1148
2	K	1.03	0/847	1.18	1/1148 (0.1%)
3	C	1.38	0/83	1.34	0/111
3	F	1.10	0/83	1.53	3/111 (2.7%)
3	I	0.85	0/83	1.03	0/111
3	L	1.16	0/83	1.08	0/111
All	All	1.14	27/13068 (0.2%)	1.21	54/17756 (0.3%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	31	HIS	ND1-CE1	-11.55	1.21	1.32
1	D	3	HIS	CD2-NE2	-10.22	1.26	1.37
2	E	31	HIS	CE1-NE2	10.20	1.42	1.32
1	G	115	GLN	CD-NE2	-9.13	1.14	1.33
1	D	3	HIS	CE1-NE2	8.34	1.40	1.32
1	A	96	GLN	CD-NE2	-8.11	1.16	1.33
2	E	31	HIS	CD2-NE2	-7.78	1.29	1.37
1	A	191	HIS	CG-ND1	-7.37	1.30	1.38
1	D	165	VAL	CA-CB	7.14	1.63	1.54
2	E	31	HIS	CG-ND1	6.11	1.45	1.38
1	G	276	PRO	CA-C	5.97	1.57	1.52
1	J	276	PRO	CA-C	5.87	1.57	1.52
1	G	115	GLN	CD-OE1	-5.84	1.12	1.23
1	D	113	TYR	CG-CD1	-5.74	1.27	1.39
1	D	114	GLU	CD-OE2	-5.69	1.14	1.25
1	J	224	LEU	C-O	5.66	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	113	TYR	CG-CD2	-5.65	1.27	1.39
1	D	276	PRO	CA-C	5.54	1.57	1.52
1	A	191	HIS	CG-CD2	5.51	1.42	1.35
1	D	240	THR	CA-CB	5.44	1.61	1.53
1	A	276	PRO	CA-C	5.41	1.57	1.52
1	A	114	GLU	CD-OE1	-5.38	1.15	1.25
2	E	19	LYS	CA-C	5.28	1.58	1.52
1	A	96	GLN	CD-OE1	-5.19	1.13	1.23
1	A	154	GLU	CA-C	-5.13	1.46	1.52
1	J	116	PHE	C-O	5.07	1.30	1.23
1	D	114	GLU	CD-OE1	-5.01	1.15	1.25

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	79	ARG	NE-CZ-NH2	14.87	132.59	119.20
1	G	79	ARG	NE-CZ-NH1	-11.94	109.56	121.50
1	G	79	ARG	CD-NE-CZ	10.44	139.02	124.40
2	E	31	HIS	CG-CD2-NE2	9.72	116.92	107.20
1	D	79	ARG	CG-CD-NE	9.05	131.92	112.00
2	E	31	HIS	ND1-CG-CD2	-8.80	97.30	106.10
1	D	181	ARG	NE-CZ-NH1	8.76	130.26	121.50
1	J	58	GLU	CA-CB-CG	8.33	130.76	114.10
1	D	181	ARG	NE-CZ-NH2	-8.18	111.84	119.20
1	A	131	LYS	CG-CD-CE	7.55	128.67	111.30
1	J	1	GLY	CA-C-N	7.30	127.30	119.78
1	J	1	GLY	C-N-CA	7.30	127.30	119.78
2	E	89	GLU	CB-CG-CD	7.02	124.53	112.60
3	F	1	SER	CA-C-N	6.95	127.12	120.31
3	F	1	SER	C-N-CA	6.95	127.12	120.31
1	D	79	ARG	CD-NE-CZ	6.87	134.01	124.40
1	D	1	GLY	CA-C-N	6.74	126.72	119.78
1	D	1	GLY	C-N-CA	6.74	126.72	119.78
2	E	31	HIS	CB-CG-CD2	6.65	139.85	131.20
1	G	79	ARG	CG-CD-NE	-6.57	97.55	112.00
1	G	100	GLY	N-CA-C	6.38	119.05	110.43
2	E	89	GLU	CG-CD-OE2	6.30	132.88	118.40
1	G	154	GLU	CB-CG-CD	6.25	123.23	112.60
1	G	57	PRO	CB-CA-C	-6.23	103.00	111.85
1	J	58	GLU	CB-CG-CD	6.22	123.17	112.60
1	J	49	ALA	CA-C-N	6.11	126.00	119.28
1	J	49	ALA	C-N-CA	6.11	126.00	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	49	ALA	CA-C-N	6.10	125.82	119.05
1	G	49	ALA	C-N-CA	6.10	125.82	119.05
1	D	108	ARG	NE-CZ-NH2	5.71	124.33	119.20
1	J	89	ALA	N-CA-C	5.67	120.06	113.20
1	A	49	ALA	CA-C-N	5.65	125.32	119.05
1	A	49	ALA	C-N-CA	5.65	125.32	119.05
2	K	7	ILE	N-CA-C	5.63	116.00	108.11
2	E	31	HIS	CE1-NE2-CD2	-5.50	103.50	109.00
1	G	58	GLU	N-CA-C	-5.49	105.31	112.23
2	E	27	VAL	N-CA-C	5.46	115.71	107.80
1	J	79	ARG	CG-CD-NE	5.39	123.86	112.00
3	F	2	PRO	CA-C-O	-5.37	115.46	122.12
1	G	58	GLU	N-CA-CB	-5.35	102.06	110.30
2	B	32	PRO	CA-C-N	5.35	124.96	119.56
2	B	32	PRO	C-N-CA	5.35	124.96	119.56
1	D	100	GLY	N-CA-C	5.33	117.63	110.43
2	E	7	ILE	N-CA-C	5.28	115.50	108.11
1	A	191	HIS	ND1-CE1-NE2	-5.28	103.12	108.40
1	A	165	VAL	N-CA-C	5.26	115.47	110.42
1	A	174	ASN	N-CA-C	5.25	117.08	111.36
1	J	41	GLU	CB-CA-C	5.19	120.09	109.67
1	G	1	GLY	CA-C-N	5.14	125.07	119.78
1	G	1	GLY	C-N-CA	5.14	125.07	119.78
1	D	49	ALA	CA-C-N	5.10	124.89	119.28
1	D	49	ALA	C-N-CA	5.10	124.89	119.28
1	D	163	GLU	N-CA-C	5.04	117.15	111.11
1	A	131	LYS	CB-CG-CD	5.02	122.84	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2268	0	2131	47	0
1	D	2268	0	2131	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2268	0	2131	73	0
1	J	2268	0	2131	59	2
2	B	821	0	796	21	2
2	E	821	0	796	33	0
2	H	821	0	796	17	0
2	K	821	0	796	21	0
3	C	79	0	66	1	0
3	F	79	0	66	0	0
3	I	79	0	66	2	0
3	L	79	0	66	1	0
4	A	38	0	0	1	0
4	B	26	0	0	4	0
4	C	2	0	0	0	0
4	D	40	0	0	4	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	299	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 12.

All (299) 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:31:LYS:NZ	4:D:301:HOH:O	1.86	1.04
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:112:GLY:C	1:D:113:TYR:HD2	1.81	0.87
1:D:181:ARG:HH21	1:G:57:PRO:HG3	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:112:GLY:C	1:D:113:TYR:CD2	2.65	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: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:G:5:MET:HE1	1:G:171:TYR:HE1	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:5:MET:HE1	1:D:171:TYR:HE1	1.62	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
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:5:MET:HE1	1:A:171:TYR:HE1	1.64	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:D:119:ASP:C	2:E:31:HIS:HE2	2.11	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:192:HIS:CE1	2:B:98:ASP:HB3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:178:THR:HG21	1:G:61:GLU:CD	2.29	0.57
1:J:5:MET:HE1	1:J:171:TYR:HE1	1.68	0.57
1:J:209:TYR:HD2	1:J:209:TYR:C	2.13	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
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: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:HE1	3:C:1:SER:H2	1.74	0.53
1:A:209:TYR:HD2	1:A:209:TYR:C	2.17	0.52
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:G:52:MET:HE1	1:G:171:TYR:CE2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:29:GLN:HA	2:K:61:SER:OG	2.10	0.51
1:A:52:MET:HE1	1:A:171:TYR:CE2	2.45	0.51
2:B:58:LYS:NZ	4:B:106:HOH:O	2.39	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:J:52:MET:HE1	1:J:171:TYR:CE2	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:J:209:TYR:CD2	1:J:209:TYR:C	2.87	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:J:54:GLN:HE21	1:J:174:ASN:CG	2.20	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:A:8:PHE:HB3	2:B:56:PHE:CE2	2.47	0.49
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
2:E:1:ILE:N	4:E:106:HOH:O	2.46	0.48
1:J:112:GLY:C	1:J:113:TYR:CD2	2.92	0.48
1:J:99:TYR:CB	1:J:114:GLU:OE2	2.62	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
1:A:209:TYR:CD2	1:A:209:TYR:C	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:5:MET:HE1	1:G:171:TYR:CE1	2.45	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:G:98:MET:HE2	2:H:60:TRP:CH2	2.50	0.46
1:D:178:THR:CG2	1:G:61:GLU:CG	2.92	0.46
1:A:98:MET:HE2	2:B:60:TRP:CH2	2.51	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: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
1:G:133:TRP:HB2	1:G:144:ARG:HG3	1.98	0.46
1:D:52:MET:HE1	1:D:171:TYR:CE2	2.51	0.46
1:D:35:ARG:NH1	2:E:53:ASP:HB3	2.31	0.45
1:G:98:MET:HE2	2:H:60:TRP:CZ3	2.51	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:A:5:MET:HE3	1:A:33:PHE:CZ	2.52	0.45
1:A:112:GLY:C	1:A:113:TYR:CD2	2.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:5:MET:HE3	1:D:33:PHE:CZ	2.52	0.44
1:J:54:GLN:NE2	1:J:174:ASN:CG	2.75	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
2:H:87:MET:HE3	2:H:87:MET:HB2	1.80	0.44
2:B:51:MET:HE2	2:B:51:MET:HB2	1.95	0.44
1:D:192:HIS:CE1	2:E:98:ASP:HB3	2.52	0.44
1:G:188:HIS:CD2	1:G:188:HIS:C	2.94	0.44
1:A:5:MET:HE2	1:A:7:TYR:CE1	2.52	0.44
1:D:5:MET:HE1	1:D:171:TYR:CE1	2.47	0.44
1:J:5:MET:HE3	1:J:33:PHE:CZ	2.52	0.44
1:A:113:TYR:CD2	1:A:113:TYR:N	2.86	0.44
1:G:253:LYS:C	1:G:255:GLN:OE1	2.61	0.44
1:J:28:VAL:HG23	1:J:33:PHE:CE1	2.52	0.44
1:A:255:GLN:H	1:A:255:GLN:CD	2.26	0.44
2:K:73:THR:CG2	2:K:75:THR:H	2.25	0.44
1:G:41:GLU:C	1:G:43:PRO:HD3	2.43	0.44
1:D:41:GLU:C	1:D:43:PRO:HD3	2.43	0.43
1:D:184:SER:HA	1:D:185:PRO:HD3	1.89	0.43
1:A:5:MET:HE3	1:A:33:PHE:HZ	1.83	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:D:209:TYR:CD2	1:D:209:TYR:C	2.97	0.43
1:A:214:THR:HA	1:D:223:GLU:OE2	2.19	0.43
1:D:113:TYR:CD2	1:D:113:TYR:N	2.77	0.43
1:J:209:TYR:CE1	4:J:306:HOH:O	2.67	0.43
2:E:51:MET:HE2	2:E:51:MET:HB2	1.90	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:98:MET:HE2	2:E:60:TRP:CH2	2.56	0.41
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: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:G:255:GLN:H	1:G:255:GLN:CD	2.28	0.41
1:A:194:ARG:HD3	1:A:195:SER:HB3	2.03	0.41
2:B:25:CYS:HB2	2:B:39:MET:HE3	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:G:112:GLY:C	1:G:113:TYR:CD2	2.99	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:98:MET:HE2	2:E:60:TRP:CZ3	2.56	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:41:GLU:C	1:A:43:PRO:HD3	2.46	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
2:K:51:MET:HE2	2:K:51:MET:HB2	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:MET:HE1	3:L:1:SER:N	2.37	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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	6	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/232 (100%)	220 (95%)	12 (5%)	21	44
1	D	232/232 (100%)	219 (94%)	13 (6%)	19	40
1	G	232/232 (100%)	220 (95%)	12 (5%)	21	44
1	J	232/232 (100%)	219 (94%)	13 (6%)	19	40
2	B	94/94 (100%)	89 (95%)	5 (5%)	20	43
2	E	94/94 (100%)	89 (95%)	5 (5%)	20	43
2	H	94/94 (100%)	89 (95%)	5 (5%)	20	43
2	K	94/94 (100%)	89 (95%)	5 (5%)	20	43
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	9
3	L	8/8 (100%)	8 (100%)	0	100	100
All	All	1336/1336 (100%)	1265 (95%)	71 (5%)	20	43

All (71) 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	178	THR
1	A	195	SER
1	A	209	TYR
1	A	255	GLN

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Mol	Chain	Res	Type
1	A	258	THR
1	A	272	LEU
2	B	55	SER
2	B	70	PHE
2	B	73	THR
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	113	TYR
1	D	154	GLU
1	D	165	VAL
1	D	178	THR
1	D	195	SER
1	D	226	GLN
1	D	255	GLN
1	D	258	THR
1	D	272	LEU
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	178	THR
1	G	195	SER
1	G	209	TYR
1	G	226	GLN
1	G	255	GLN
1	G	258	THR
1	G	272	LEU
2	H	55	SER
2	H	70	PHE
2	H	73	THR
2	H	83	LYS
2	H	85	ASP

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Mol	Chain	Res	Type
3	I	3	SER
1	J	41	GLU
1	J	58	GLU
1	J	78	LEU
1	J	94	THR
1	J	110	LEU
1	J	154	GLU
1	J	165	VAL
1	J	178	THR
1	J	195	SER
1	J	209	TYR
1	J	255	GLN
1	J	258	THR
1	J	272	LEU
2	K	55	SER
2	K	73	THR
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 (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	220	ASN
2	B	13	HIS
2	B	29	GLN
1	D	48	GLN
1	D	115	GLN
1	D	192	HIS
2	E	29	GLN
1	G	48	GLN
1	G	65	GLN
2	H	13	HIS
2	H	29	GLN
1	J	48	GLN
1	J	54	GLN
1	J	96	GLN
1	J	188	HIS
2	K	29	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	278/278 (100%)	-0.28	1 (0%) 88 86	26, 42, 83, 116	1 (0%)
1	D	278/278 (100%)	-0.15	5 (1%) 67 63	29, 44, 86, 117	1 (0%)
1	G	278/278 (100%)	0.00	2 (0%) 84 82	30, 49, 88, 118	1 (0%)
1	J	278/278 (100%)	-0.30	1 (0%) 88 86	29, 47, 87, 117	1 (0%)
2	B	99/99 (100%)	-0.49	1 (1%) 79 76	28, 41, 78, 96	0
2	E	99/99 (100%)	-0.35	0 100 100	31, 44, 80, 97	0
2	H	99/99 (100%)	-0.52	0 100 100	28, 43, 79, 96	0
2	K	99/99 (100%)	-0.40	0 100 100	32, 47, 82, 100	0
3	C	9/9 (100%)	-0.77	0 100 100	30, 35, 44, 57	0
3	F	9/9 (100%)	-0.52	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%)	-0.69	0 100 100	36, 44, 60, 65	0
All	All	1544/1544 (100%)	-0.26	10 (0%) 85 83	26, 45, 85, 118	4 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	177	ALA	3.4
1	D	194	ARG	2.8
1	J	277	PRO	2.6
1	D	209	TYR	2.6
1	D	176	ASN	2.5
1	G	107	GLY	2.3
1	D	106	ASP	2.3
1	A	86	ASN	2.1
1	G	176	ASN	2.1
2	B	89	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.