



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:12 PM UTC

PDB ID : 1S7W / pdb_00001s7w
Title : Crystal structures of the murine class I major histocompatibility complex H-2Db in complex with LCMV-derived gp33 index peptide and three of its escape variants
Authors : Velloso, L.M.; Michaelsson, J.; Ljunggren, H.G.; Schneider, G.; Achour, A.
Deposited on : 2004-01-30
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

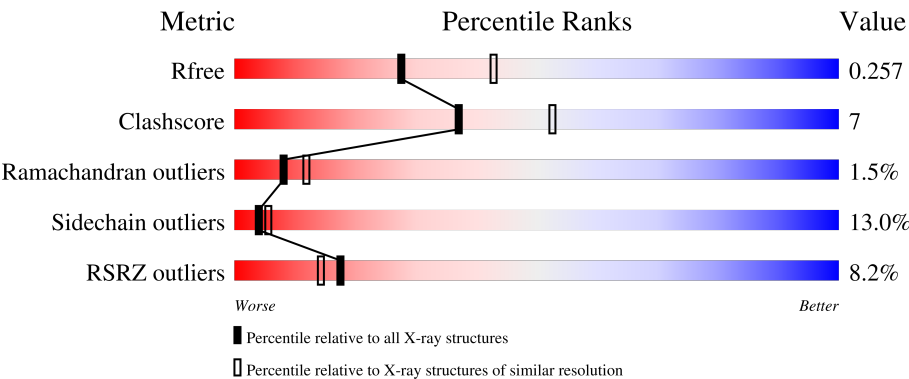
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



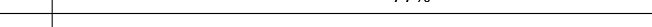
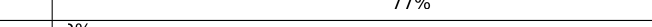
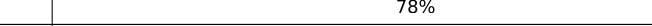
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	7% 60% 16% 5% 18%
1	D	338	5% 64% 14% • 18%
1	G	338	10% 65% 12% • 18%
1	J	338	14% 68% 11% •• 18%
2	B	99	% 72% 20% 6% ••

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Mol	Chain	Length	Quality of chain
2	E	99	 77% 19%
2	H	99	 77% 21%
2	K	99	 78% 20%
3	C	9	 78% 22%
3	F	9	 89% 11%
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 13148 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	1	0
			2269	1432	401	427	9			
1	D	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			
1	G	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			
1	J	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			812	519	137	150	6			
2	E	99	Total	C	N	O	S	0	0	0
			818	523	138	151	6			
2	H	99	Total	C	N	O	S	0	0	0
			818	523	138	151	6			
2	K	99	Total	C	N	O	S	0	0	0
			818	523	138	151	6			

- Molecule 3 is a protein called Glycoprotein 9-residue peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			74	49	11	13	1			
3	F	9	Total	C	N	O	S	0	0	0
			74	49	11	13	1			
3	I	9	Total	C	N	O	S	0	0	0
			74	49	11	13	1			
3	L	9	Total	C	N	O	S	0	0	0
			74	49	11	13	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	LEU	VAL	engineered mutation	UNP P07399
C	9	MET	CYS	SEE REMARK 999	UNP P07399
F	3	LEU	VAL	engineered mutation	UNP P07399
F	9	MET	CYS	SEE REMARK 999	UNP P07399
I	3	LEU	VAL	engineered mutation	UNP P07399
I	9	MET	CYS	SEE REMARK 999	UNP P07399
L	3	LEU	VAL	engineered mutation	UNP P07399
L	9	MET	CYS	SEE REMARK 999	UNP P07399

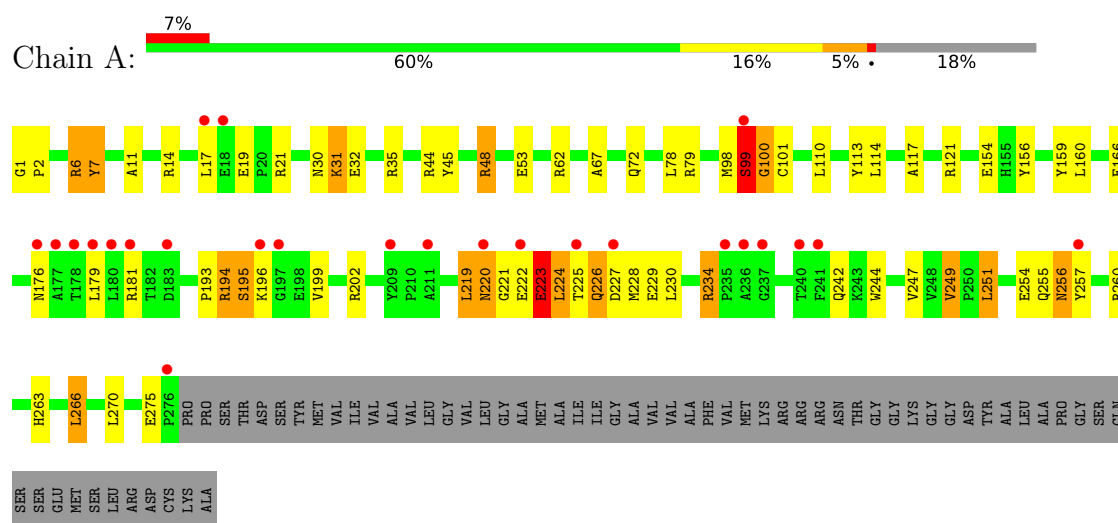
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	87	Total O 87 87	0	0
4	B	57	Total O 57 57	0	0
4	C	2	Total O 2 2	0	0
4	D	80	Total O 80 80	0	0
4	E	35	Total O 35 35	0	0
4	F	3	Total O 3 3	0	0
4	G	84	Total O 84 84	0	0
4	H	44	Total O 44 44	0	0
4	I	2	Total O 2 2	0	0
4	J	83	Total O 83 83	0	0
4	K	44	Total O 44 44	0	0
4	L	4	Total O 4 4	0	0

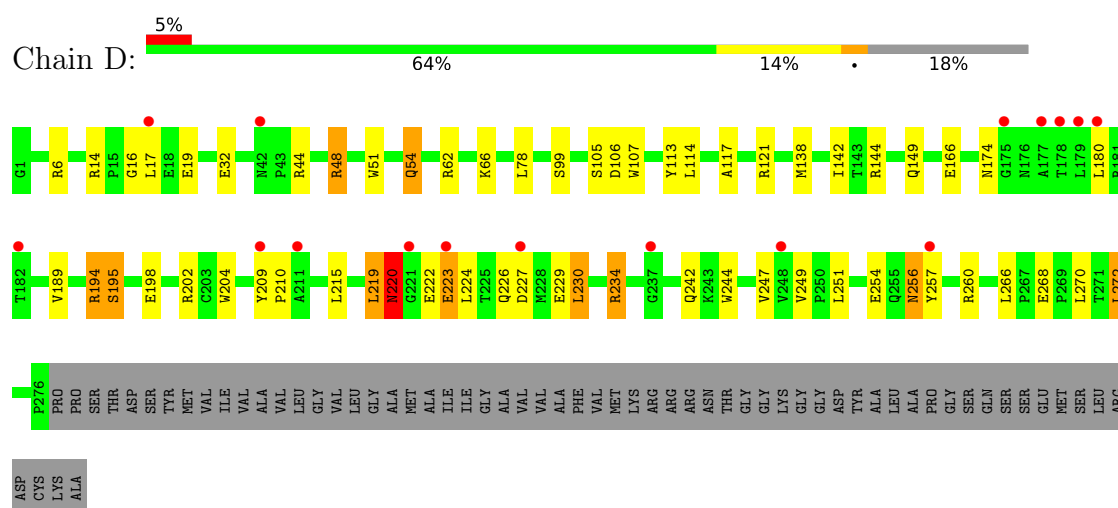
3 Residue-property plots [i](#)

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: H-2 class I histocompatibility antigen, D-B alpha chain

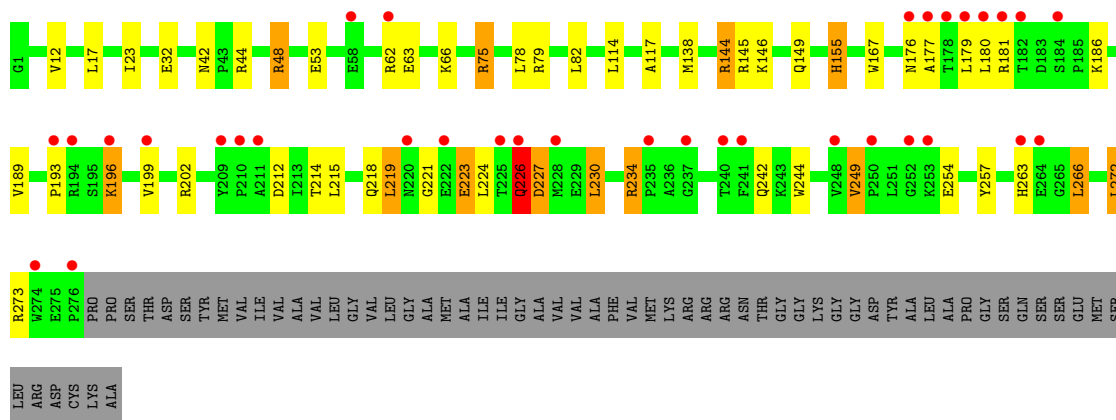


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

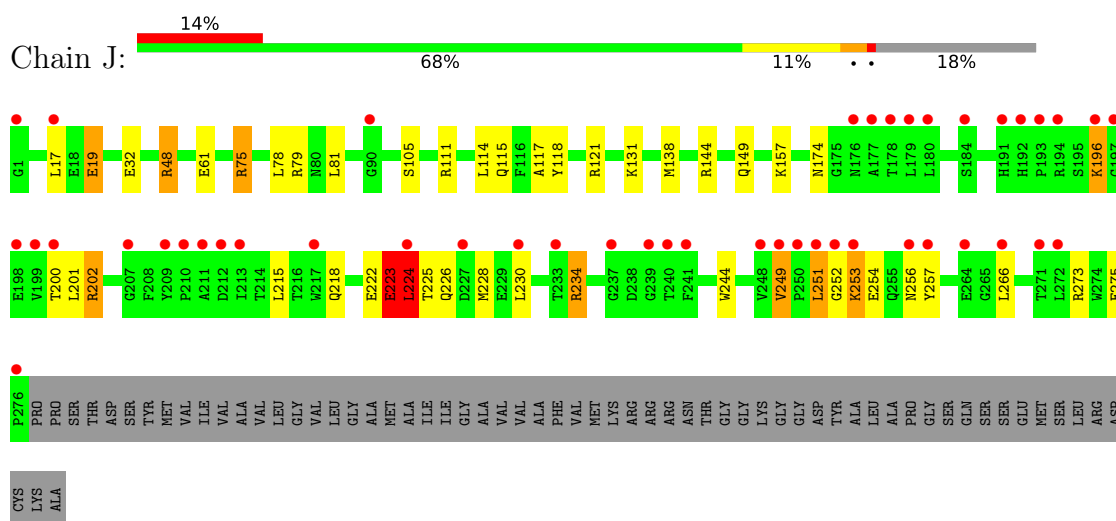


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

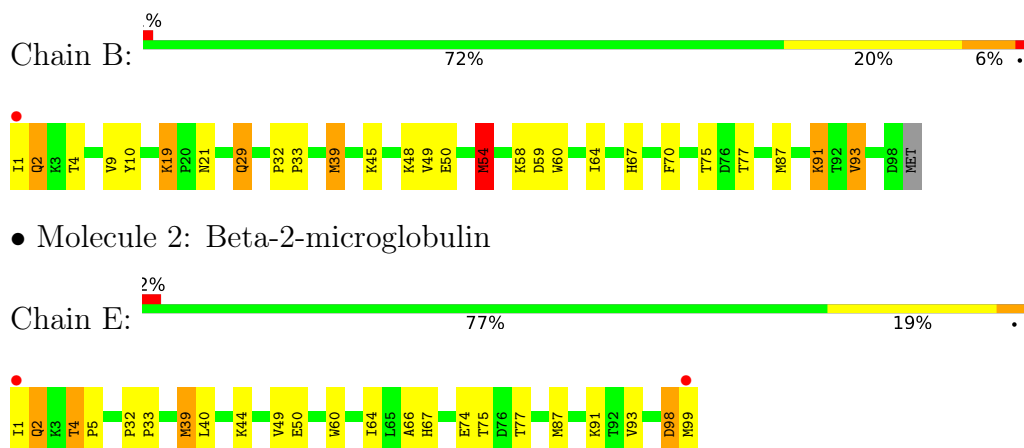




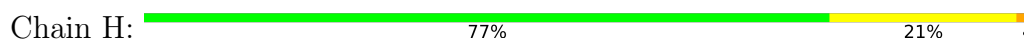
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

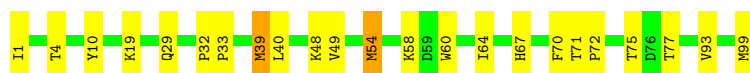


- Molecule 2: Beta-2-microglobulin

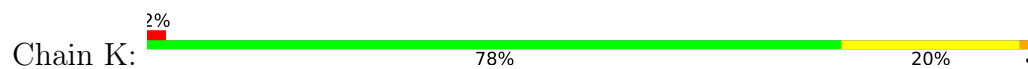


- Molecule 2: Beta-2-microglobulin

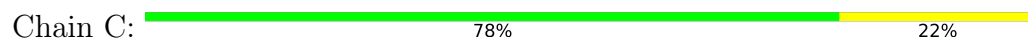




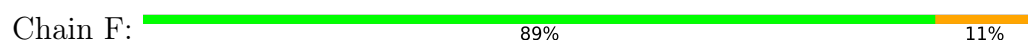
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Glycoprotein 9-residue peptide



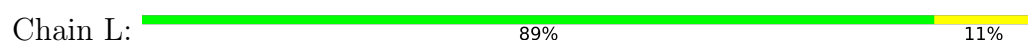
- Molecule 3: Glycoprotein 9-residue peptide



- Molecule 3: Glycoprotein 9-residue peptide



- Molecule 3: Glycoprotein 9-residue peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.25Å 123.30Å 99.30Å 90.00° 103.13° 90.00°	Depositor
Resolution (Å)	19.84 – 2.40 19.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.84-2.40) 99.7 (19.84-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.199 , 0.246 0.213 , 0.257	Depositor DCC
R_{free} test set	1689 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13148	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.15% 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	0.87	0/2337	0.93	3/3174 (0.1%)
1	D	0.83	1/2331 (0.0%)	0.92	1/3166 (0.0%)
1	G	0.85	2/2331 (0.1%)	0.87	0/3166
1	J	0.84	1/2331 (0.0%)	0.90	0/3166
2	B	1.04	2/838 (0.2%)	0.99	0/1138
2	E	1.10	2/844 (0.2%)	0.94	1/1146 (0.1%)
2	H	0.97	1/844 (0.1%)	0.97	0/1146
2	K	0.99	2/844 (0.2%)	0.96	0/1146
3	C	0.93	0/75	1.02	0/98
3	F	0.95	0/75	1.00	0/98
3	I	0.95	0/75	0.99	0/98
3	L	0.72	0/75	1.00	0/98
All	All	0.90	11/13000 (0.1%)	0.92	5/17640 (0.0%)

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	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	39	MET	SD-CE	-14.58	1.43	1.79
2	B	39	MET	SD-CE	-13.13	1.46	1.79
2	K	39	MET	SD-CE	-11.05	1.51	1.79
2	H	39	MET	SD-CE	-10.47	1.53	1.79
1	J	138	MET	SD-CE	-10.45	1.53	1.79
2	E	87	MET	SD-CE	-8.49	1.58	1.79
1	D	138	MET	SD-CE	-8.45	1.58	1.79
1	G	138	MET	SD-CE	-7.00	1.62	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	MET	CG-SD	5.90	1.95	1.80
1	G	144	ARG	NE-CZ	5.33	1.39	1.33
2	K	54	MET	CG-SD	5.32	1.94	1.80

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	CYS	N-CA-C	10.14	124.94	109.23
1	A	196	LYS	N-CA-C	5.48	117.36	110.24
1	D	222	GLU	N-CA-C	5.45	116.81	108.52
2	E	2	GLN	N-CA-C	5.14	118.49	110.32
1	A	7	TYR	N-CA-C	5.10	117.07	108.96

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	6	ARG	Peptide
1	A	98	MET	Mainchain
1	A	99[B]	SER	Mainchain

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	2269	0	2138	45	0
1	D	2264	0	2136	36	0
1	G	2264	0	2136	30	0
1	J	2264	0	2136	22	0
2	B	812	0	787	15	0
2	E	818	0	791	12	0
2	H	818	0	791	11	0
2	K	818	0	791	15	0
3	C	74	0	76	2	0
3	F	74	0	76	5	0
3	I	74	0	76	3	0
3	L	74	0	76	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	87	0	0	7	0
4	B	57	0	0	0	0
4	C	2	0	0	0	0
4	D	80	0	0	3	0
4	E	35	0	0	1	0
4	F	3	0	0	0	0
4	G	84	0	0	7	0
4	H	44	0	0	2	0
4	I	2	0	0	0	0
4	J	83	0	0	3	0
4	K	44	0	0	4	0
4	L	4	0	0	0	0
All	All	13148	0	12010	175	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 7.

All (175) 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)
4:G:347:HOH:O	2:H:99:MET:CG	2.01	1.09
1:D:219:LEU:HD13	1:D:257:TYR:OH	1.48	1.09
1:J:144:ARG:HD2	4:J:404:HOH:O	1.62	1.00
1:A:99[A]:SER:OG	1:A:100:GLY:N	1.91	0.96
1:D:219:LEU:HB2	1:D:257:TYR:CE1	2.09	0.87
1:D:219:LEU:CD1	1:D:257:TYR:OH	2.22	0.87
1:A:99[A]:SER:HA	4:A:413:HOH:O	1.83	0.78
1:A:99[B]:SER:HA	4:A:413:HOH:O	1.83	0.77
1:A:1:GLY:N	1:A:2:PRO:HD2	2.00	0.76
1:D:219:LEU:CD1	1:D:257:TYR:CZ	2.69	0.75
1:D:219:LEU:HD13	1:D:257:TYR:CZ	2.22	0.75
1:A:1:GLY:N	1:A:2:PRO:CD	2.51	0.74
2:H:39:MET:HE2	2:H:49:VAL:HG13	1.70	0.74
1:J:75:ARG:HH11	1:J:75:ARG:HG3	1.53	0.72
2:H:77:THR:HG22	4:H:139:HOH:O	1.88	0.71
1:A:99[A]:SER:O	1:A:113:TYR:O	2.10	0.69
2:K:78:TYR:OH	4:K:143:HOH:O	2.09	0.69
1:D:194:ARG:O	1:D:198:GLU:O	2.11	0.69
1:J:234:ARG:HD3	2:K:10:TYR:CE2	2.29	0.67
1:D:219:LEU:CB	1:D:257:TYR:CE1	2.78	0.66
2:B:39:MET:HE1	2:B:67:HIS:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:GLN:HE22	1:D:174:ASN:HB3	1.62	0.65
1:A:1:GLY:H3	1:A:2:PRO:CD	2.09	0.64
1:D:66:LYS:HZ2	3:F:1:LYS:HE3	1.63	0.64
1:J:249:VAL:HG22	1:J:257:TYR:CZ	2.31	0.63
2:B:39:MET:HE1	2:B:67:HIS:CA	2.28	0.63
1:D:256:ASN:C	1:D:256:ASN:HD22	2.05	0.63
2:K:87:MET:HE1	2:K:91:LYS:HD2	1.82	0.62
1:A:6:ARG:HD3	1:A:99[A]:SER:OG	1.99	0.62
1:G:32:GLU:OE2	1:G:48:ARG:HD2	2.00	0.61
2:K:54:MET:HA	4:K:100:HOH:O	2.00	0.61
1:D:142:ILE:HG13	4:D:398:HOH:O	2.01	0.61
2:E:98:ASP:O	2:E:99:MET:C	2.44	0.60
1:A:219:LEU:HD13	1:A:257:TYR:CZ	2.38	0.59
1:D:66:LYS:NZ	3:F:1:LYS:HE3	2.17	0.59
1:A:193:PRO:HA	1:A:199:VAL:HG12	1.85	0.59
2:H:39:MET:HE1	2:H:67:HIS:C	2.27	0.59
1:D:219:LEU:HD12	1:D:257:TYR:CZ	2.38	0.59
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.38	0.58
1:A:99[B]:SER:O	4:A:413:HOH:O	2.11	0.58
1:A:1:GLY:H3	1:A:2:PRO:HD2	1.66	0.58
1:G:249:VAL:HG12	1:G:257:TYR:CZ	2.39	0.58
1:J:75:ARG:HH11	1:J:75:ARG:CG	2.17	0.58
1:D:66:LYS:HZ2	3:F:1:LYS:CE	2.17	0.57
1:G:145:ARG:O	1:G:149:GLN:HG2	2.04	0.57
2:E:39:MET:HE3	2:E:49:VAL:HG13	1.86	0.57
1:A:1:GLY:H2	1:A:2:PRO:HD2	1.69	0.57
1:G:189:VAL:HG23	1:G:272:LEU:HD11	1.88	0.56
1:G:263:HIS:HB3	1:G:266:LEU:HD22	1.88	0.56
2:B:87:MET:HE1	2:B:91:LYS:HD2	1.87	0.56
1:D:66:LYS:NZ	3:F:1:LYS:CE	2.68	0.55
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.42	0.55
1:G:146:LYS:CE	4:G:355:HOH:O	2.53	0.55
1:D:234:ARG:HD2	1:D:242:GLN:HB2	1.89	0.55
1:G:62:ARG:NH2	3:I:1:LYS:HD2	2.21	0.55
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.42	0.55
1:G:176:ASN:OD1	1:G:180:LEU:HD13	2.06	0.54
1:J:202:ARG:HD2	1:J:244:TRP:CE3	2.42	0.54
1:A:6:ARG:HA	1:A:99[A]:SER:OG	2.08	0.54
1:G:63:GLU:O	1:G:66:LYS:HB2	2.07	0.54
1:G:146:LYS:HE3	4:G:355:HOH:O	2.07	0.54
1:A:256:ASN:HD22	1:A:256:ASN:C	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:THR:HG22	4:E:101:HOH:O	2.06	0.54
2:K:39:MET:HE1	2:K:67:HIS:CA	2.38	0.53
1:D:32:GLU:OE2	1:D:48:ARG:HD2	2.09	0.53
1:A:219:LEU:C	1:A:221:GLY:N	2.64	0.53
2:E:39:MET:CE	2:E:49:VAL:HG13	2.38	0.53
1:A:30:ASN:ND2	4:A:416:HOH:O	2.42	0.52
1:D:256:ASN:ND2	1:D:257:TYR:CD2	2.77	0.52
1:J:75:ARG:HG3	1:J:75:ARG:NH1	2.21	0.52
1:J:19:GLU:HG3	1:J:75:ARG:CZ	2.40	0.51
1:J:249:VAL:HG22	1:J:257:TYR:CE2	2.45	0.51
1:A:194:ARG:O	1:A:195:SER:C	2.53	0.51
1:A:199:VAL:HG11	1:A:251:LEU:HD12	1.91	0.51
2:E:39:MET:HE1	2:E:67:HIS:CA	2.40	0.51
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.46	0.51
1:A:224:LEU:HD23	1:A:247:VAL:HG21	1.93	0.51
1:J:32:GLU:OE2	1:J:48:ARG:CD	2.58	0.51
1:D:194:ARG:O	1:D:195:SER:O	2.29	0.51
1:J:32:GLU:OE2	1:J:48:ARG:HD2	2.11	0.50
1:A:35:ARG:NH2	2:B:54:MET:O	2.45	0.50
1:G:63:GLU:OE2	1:G:66:LYS:NZ	2.45	0.50
2:K:39:MET:CE	2:K:49:VAL:HG13	2.41	0.50
1:A:263:HIS:HB3	1:A:266:LEU:HD22	1.94	0.49
3:C:5:ASN:O	2:K:75:THR:HG21	2.11	0.49
2:K:91:LYS:NZ	4:K:120:HOH:O	2.45	0.48
1:D:202:ARG:HG2	1:D:204:TRP:NE1	2.27	0.48
1:D:260:ARG:HA	1:D:270:LEU:O	2.14	0.48
2:B:29:GLN:NE2	2:B:59:ASP:OD2	2.46	0.48
1:A:31:LYS:HD3	1:A:179:LEU:HD21	1.94	0.48
1:A:223:GLU:HA	4:A:386:HOH:O	2.14	0.48
1:D:6:ARG:NH2	1:D:113:TYR:CE1	2.81	0.48
1:G:62:ARG:HG3	4:G:395:HOH:O	2.13	0.48
1:G:226:GLN:O	1:G:227:ASP:C	2.57	0.48
1:A:62:ARG:HG3	2:K:94:TYR:CE1	2.48	0.47
2:E:32:PRO:HB2	2:E:33:PRO:HD2	1.97	0.47
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.48	0.47
1:D:230:LEU:C	1:D:230:LEU:HD12	2.39	0.47
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.49	0.47
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.49	0.47
1:G:234:ARG:HD2	1:G:242:GLN:HB2	1.97	0.47
1:J:251:LEU:HD23	1:J:252:GLY:H	1.80	0.47
1:A:230:LEU:HD12	1:A:230:LEU:C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLN:O	1:A:226:GLN:HG2	2.16	0.46
1:G:23:ILE:HD12	2:H:54:MET:SD	2.56	0.46
1:J:201:LEU:CD1	1:J:249:VAL:HG21	2.45	0.46
2:K:39:MET:HE1	2:K:67:HIS:C	2.40	0.46
1:G:75:ARG:HG3	4:G:399:HOH:O	2.16	0.46
1:A:219:LEU:C	1:A:221:GLY:H	2.24	0.46
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.51	0.46
1:G:42:ASN:ND2	1:G:44:ARG:HD2	2.31	0.46
2:K:99:MET:CG	4:K:114:HOH:O	2.63	0.46
2:H:75:THR:HG22	4:H:105:HOH:O	2.15	0.45
2:E:50:GLU:HB2	2:E:67:HIS:CE1	2.51	0.45
1:J:223:GLU:O	1:J:224:LEU:HB2	2.17	0.45
2:K:32:PRO:HB2	2:K:33:PRO:HD2	1.99	0.45
2:E:39:MET:HE1	2:E:67:HIS:HA	1.99	0.45
1:G:12:VAL:HG13	4:G:381:HOH:O	2.17	0.45
1:G:219:LEU:O	1:G:219:LEU:HG	2.17	0.45
2:B:19:LYS:HE3	2:B:19:LYS:HB3	1.82	0.45
1:D:219:LEU:HB2	1:D:257:TYR:CD1	2.49	0.45
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.51	0.45
1:A:194:ARG:HG2	1:A:195:SER:N	2.32	0.44
1:A:156:TYR:O	1:A:160:LEU:HG	2.18	0.44
1:D:17:LEU:N	4:D:383:HOH:O	2.51	0.44
1:D:66:LYS:NZ	3:F:1:LYS:HE2	2.32	0.44
2:H:32:PRO:HB2	2:H:33:PRO:HD2	1.99	0.44
2:B:50:GLU:HB2	2:B:67:HIS:CE1	2.53	0.44
1:D:32:GLU:OE2	1:D:48:ARG:CD	2.66	0.44
1:J:225:THR:HG23	1:J:228:MET:HE2	1.99	0.44
1:A:159:TYR:CG	3:C:3:LEU:HD13	2.53	0.43
1:A:234:ARG:HD2	1:A:242:GLN:HB2	2.00	0.43
1:D:189:VAL:HG23	1:D:272:LEU:HD13	2.00	0.43
2:H:39:MET:CE	2:H:49:VAL:HG13	2.43	0.43
1:J:131:LYS:NZ	1:J:157:LYS:HE3	2.32	0.43
1:G:219:LEU:C	1:G:221:GLY:N	2.76	0.43
2:B:39:MET:HE3	2:B:49:VAL:HG13	1.99	0.43
2:E:39:MET:HE2	2:E:66:ALA:HB1	2.01	0.43
1:G:230:LEU:C	1:G:230:LEU:HD12	2.44	0.43
1:G:214:THR:C	1:G:215:LEU:HD12	2.43	0.43
2:B:9:VAL:HG23	2:B:93:VAL:HG22	2.01	0.43
1:A:99[A]:SER:CA	4:A:413:HOH:O	2.56	0.43
1:G:155:HIS:CD2	1:G:155:HIS:C	2.97	0.43
1:A:7:TYR:N	1:A:99[A]:SER:HB2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99[B]:SER:CA	4:A:413:HOH:O	2.56	0.42
1:J:144:ARG:CD	4:J:404:HOH:O	2.42	0.42
2:K:39:MET:HE3	2:K:49:VAL:HG13	2.00	0.42
1:J:32:GLU:OE2	1:J:48:ARG:HD3	2.19	0.42
1:A:45:TYR:CE2	1:A:67:ALA:HB2	2.55	0.42
1:D:219:LEU:HG	1:D:220:ASN:HB2	2.02	0.42
2:E:39:MET:HE1	2:E:67:HIS:C	2.45	0.42
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.54	0.41
1:G:193:PRO:HA	1:G:199:VAL:HG12	2.02	0.41
2:E:4:THR:HA	2:E:5:PRO:HD3	1.91	0.41
1:D:106:ASP:O	1:D:107:TRP:HB2	2.20	0.41
1:D:144:ARG:NH2	4:D:404:HOH:O	2.53	0.41
1:D:209:TYR:CD1	1:D:210:PRO:HA	2.55	0.41
2:H:71:THR:HA	2:H:72:PRO:HD2	1.95	0.41
1:G:167:TRP:CE2	3:I:1:LYS:HD3	2.55	0.41
1:A:11:ALA:HA	1:A:21:ARG:O	2.20	0.41
1:D:51:TRP:O	1:D:54:GLN:NE2	2.44	0.41
2:K:10:TYR:CD1	2:K:10:TYR:N	2.88	0.41
1:J:81:LEU:HD13	1:J:118:TYR:CD1	2.55	0.41
1:A:234:ARG:HD3	2:B:10:TYR:CD2	2.56	0.41
2:B:2:GLN:H	2:B:2:GLN:HG2	1.69	0.41
1:J:75:ARG:NH1	4:J:353:HOH:O	2.54	0.41
1:J:230:LEU:C	1:J:230:LEU:HD12	2.46	0.41
1:G:66:LYS:HG2	3:I:4:TYR:CE1	2.56	0.40
1:G:146:LYS:NZ	4:G:355:HOH:O	2.53	0.40
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.56	0.40
2:B:32:PRO:HB2	2:B:33:PRO:HD2	2.03	0.40
1:A:32:GLU:OE2	1:A:48:ARG:HD2	2.21	0.40
1:D:219:LEU:HB2	1:D:257:TYR:CZ	2.53	0.40

There are no symmetry-related clashes.

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	275/338 (81%)	259 (94%)	9 (3%)	7 (2%)	4	5
1	D	274/338 (81%)	258 (94%)	12 (4%)	4 (2%)	8	12
1	G	274/338 (81%)	259 (94%)	10 (4%)	5 (2%)	6	9
1	J	274/338 (81%)	250 (91%)	18 (7%)	6 (2%)	5	6
2	B	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
2	E	97/99 (98%)	93 (96%)	3 (3%)	1 (1%)	12	20
2	H	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	K	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
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	1512/1784 (85%)	1426 (94%)	63 (4%)	23 (2%)	8	12

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99[A]	SER
1	A	99[B]	SER
1	G	227	ASP
1	J	196	LYS
1	J	253	LYS
1	A	100	GLY
1	G	196	LYS
1	J	223	GLU
1	D	195	SER
1	D	223	GLU
2	E	98	ASP
1	G	177	ALA
1	G	223	GLU
1	J	174	ASN
1	J	226	GLN
1	A	195	SER
1	A	223	GLU
1	D	220	ASN
1	G	226	GLN
1	J	224	LEU
1	A	220	ASN
1	A	222	GLU

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Mol	Chain	Res	Type
1	D	16	GLY

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	235/280 (84%)	198 (84%)	37 (16%)	2	3
1	D	234/280 (84%)	201 (86%)	33 (14%)	3	4
1	G	234/280 (84%)	207 (88%)	27 (12%)	5	8
1	J	234/280 (84%)	204 (87%)	30 (13%)	4	6
2	B	93/94 (99%)	79 (85%)	14 (15%)	3	3
2	E	93/94 (99%)	82 (88%)	11 (12%)	5	7
2	H	93/94 (99%)	82 (88%)	11 (12%)	5	7
2	K	93/94 (99%)	85 (91%)	8 (9%)	10	16
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	6 (86%)	1 (14%)	3	4
3	I	7/7 (100%)	6 (86%)	1 (14%)	3	4
3	L	7/7 (100%)	6 (86%)	1 (14%)	3	4
All	All	1337/1524 (88%)	1163 (87%)	174 (13%)	4	5

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	LEU
1	A	19	GLU
1	A	31	LYS
1	A	44	ARG
1	A	48	ARG
1	A	53	GLU
1	A	72	GLN
1	A	78	LEU

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Mol	Chain	Res	Type
1	A	79	ARG
1	A	110	LEU
1	A	114	LEU
1	A	121	ARG
1	A	154	GLU
1	A	166	GLU
1	A	176	ASN
1	A	181	ARG
1	A	194	ARG
1	A	219	LEU
1	A	220	ASN
1	A	223	GLU
1	A	224	LEU
1	A	225	THR
1	A	226	GLN
1	A	227	ASP
1	A	228	MET
1	A	229	GLU
1	A	234	ARG
1	A	249	VAL
1	A	251	LEU
1	A	254	GLU
1	A	255	GLN
1	A	256	ASN
1	A	260	ARG
1	A	266	LEU
1	A	270	LEU
1	A	275	GLU
2	B	1	ILE
2	B	2	GLN
2	B	4	THR
2	B	19	LYS
2	B	29	GLN
2	B	45	LYS
2	B	48	LYS
2	B	54	MET
2	B	58	LYS
2	B	64	ILE
2	B	75	THR
2	B	77	THR
2	B	91	LYS
2	B	93	VAL

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Mol	Chain	Res	Type
1	D	14	ARG
1	D	19	GLU
1	D	44	ARG
1	D	48	ARG
1	D	54	GLN
1	D	62	ARG
1	D	78	LEU
1	D	99	SER
1	D	105	SER
1	D	114	LEU
1	D	121	ARG
1	D	149	GLN
1	D	166	GLU
1	D	180	LEU
1	D	194	ARG
1	D	215	LEU
1	D	219	LEU
1	D	220	ASN
1	D	223	GLU
1	D	224	LEU
1	D	226	GLN
1	D	227	ASP
1	D	229	GLU
1	D	230	LEU
1	D	234	ARG
1	D	247	VAL
1	D	249	VAL
1	D	251	LEU
1	D	254	GLU
1	D	256	ASN
1	D	266	LEU
1	D	268	GLU
1	D	272	LEU
2	E	1	ILE
2	E	2	GLN
2	E	4	THR
2	E	40	LEU
2	E	44	LYS
2	E	64	ILE
2	E	74	GLU
2	E	75	THR
2	E	77	THR

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Mol	Chain	Res	Type
2	E	91	LYS
2	E	93	VAL
3	F	1	LYS
1	G	17	LEU
1	G	48	ARG
1	G	53	GLU
1	G	75	ARG
1	G	78	LEU
1	G	79	ARG
1	G	82	LEU
1	G	114	LEU
1	G	144	ARG
1	G	155	HIS
1	G	179	LEU
1	G	181	ARG
1	G	186	LYS
1	G	196	LYS
1	G	212	ASP
1	G	218	GLN
1	G	219	LEU
1	G	223	GLU
1	G	224	LEU
1	G	226	GLN
1	G	230	LEU
1	G	234	ARG
1	G	249	VAL
1	G	254	GLU
1	G	266	LEU
1	G	272	LEU
1	G	273	ARG
2	H	1	ILE
2	H	4	THR
2	H	19	LYS
2	H	29	GLN
2	H	40	LEU
2	H	48	LYS
2	H	54	MET
2	H	58	LYS
2	H	64	ILE
2	H	70	PHE
2	H	93	VAL
3	I	3	LEU

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Mol	Chain	Res	Type
1	J	17	LEU
1	J	19	GLU
1	J	48	ARG
1	J	61	GLU
1	J	75	ARG
1	J	78	LEU
1	J	79	ARG
1	J	105	SER
1	J	111	ARG
1	J	114	LEU
1	J	115	GLN
1	J	121	ARG
1	J	149	GLN
1	J	196	LYS
1	J	200	THR
1	J	202	ARG
1	J	215	LEU
1	J	218	GLN
1	J	222	GLU
1	J	223	GLU
1	J	224	LEU
1	J	234	ARG
1	J	249	VAL
1	J	251	LEU
1	J	253	LYS
1	J	254	GLU
1	J	256	ASN
1	J	266	LEU
1	J	273	ARG
1	J	275	GLU
2	K	1	ILE
2	K	4	THR
2	K	22	ILE
2	K	29	GLN
2	K	45	LYS
2	K	48	LYS
2	K	64	ILE
2	K	93	VAL
3	L	3	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	54	GLN
1	A	97	GLN
1	A	176	ASN
1	A	191	HIS
1	A	192	HIS
1	A	255	GLN
1	A	256	ASN
2	B	29	GLN
2	B	38	GLN
3	C	5	ASN
1	D	54	GLN
1	D	97	GLN
1	D	176	ASN
1	D	192	HIS
1	D	255	GLN
1	D	256	ASN
2	E	13	HIS
2	E	34	HIS
2	E	38	GLN
3	F	5	ASN
1	G	97	GLN
1	G	149	GLN
1	G	155	HIS
1	G	192	HIS
1	G	218	GLN
1	G	226	GLN
2	H	31	HIS
3	I	5	ASN
1	J	97	GLN
1	J	191	HIS
1	J	218	GLN
1	J	220	ASN
1	J	226	GLN
3	L	5	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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, 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	276/338 (81%)	0.31	25 (9%) 15 12	8, 20, 46, 56	1 (0%)
1	D	276/338 (81%)	0.27	16 (5%) 29 25	8, 23, 54, 64	0
1	G	276/338 (81%)	0.52	34 (12%) 8 6	6, 23, 48, 59	0
1	J	276/338 (81%)	0.66	46 (16%) 4 3	11, 28, 60, 66	0
2	B	98/99 (98%)	-0.39	1 (1%) 79 76	9, 16, 23, 28	0
2	E	99/99 (100%)	-0.27	2 (2%) 65 60	8, 18, 26, 29	0
2	H	99/99 (100%)	-0.32	0 100 100	10, 18, 27, 32	0
2	K	99/99 (100%)	-0.12	2 (2%) 65 60	12, 25, 34, 40	0
3	C	9/9 (100%)	-0.55	0 100 100	11, 13, 17, 17	0
3	F	9/9 (100%)	-0.37	0 100 100	13, 18, 25, 30	0
3	I	9/9 (100%)	0.16	0 100 100	13, 18, 24, 28	0
3	L	9/9 (100%)	-0.29	0 100 100	35, 37, 45, 46	0
All	All	1535/1784 (86%)	0.24	126 (8%) 17 14	6, 22, 53, 66	1 (0%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	ALA	9.3
1	D	177	ALA	7.7
1	J	178	THR	6.5
1	G	179	LEU	6.2
1	J	177	ALA	4.9
1	A	178	THR	4.7
1	J	209	TYR	4.6
1	A	180	LEU	4.6
1	D	180	LEU	4.6
1	D	179	LEU	4.3
1	J	199	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	J	179	LEU	4.3
1	G	177	ALA	4.2
1	A	227	ASP	4.2
1	G	237	GLY	4.2
1	J	196	LYS	4.2
1	J	252	GLY	4.0
1	D	257	TYR	3.9
1	A	237	GLY	3.9
1	G	180	LEU	3.8
1	G	178	THR	3.8
1	J	251	LEU	3.7
1	A	179	LEU	3.7
1	G	209	TYR	3.7
1	D	178	THR	3.6
1	A	99[A]	SER	3.6
1	J	180	LEU	3.5
1	G	58	GLU	3.5
1	J	248	VAL	3.5
1	J	253	LYS	3.5
1	J	224	LEU	3.4
1	G	240	THR	3.4
1	G	182	THR	3.4
1	J	249	VAL	3.3
1	G	252	GLY	3.3
1	J	184	SER	3.3
1	A	211	ALA	3.3
1	J	210	PRO	3.3
1	J	230	LEU	3.3
1	D	17	LEU	3.2
1	J	200	THR	3.2
1	J	197	GLY	3.2
1	G	211	ALA	3.1
1	A	209	TYR	3.1
2	E	1	ILE	3.1
1	J	239	GLY	3.0
1	J	17	LEU	3.0
1	G	241	PHE	3.0
1	A	222	GLU	3.0
1	A	235	PRO	3.0
1	G	62	ARG	3.0
1	J	241	PHE	2.9
1	J	176	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	199	VAL	2.9
1	J	250	PRO	2.9
1	J	237	GLY	2.9
1	G	264	GLU	2.9
1	D	42	ASN	2.8
1	J	90	GLY	2.8
1	G	210	PRO	2.8
1	G	220	ASN	2.8
1	J	266	LEU	2.7
1	G	196	LYS	2.7
1	A	196	LYS	2.7
1	J	276	PRO	2.7
1	J	193	PRO	2.7
1	G	194	ARG	2.7
1	A	276	PRO	2.6
1	D	211	ALA	2.6
1	A	240	THR	2.6
1	G	235	PRO	2.5
2	K	1	ILE	2.5
1	J	211	ALA	2.5
1	G	184	SER	2.5
1	D	175	GLY	2.5
1	D	237	GLY	2.5
1	D	223	GLU	2.5
1	G	248	VAL	2.5
1	J	191	HIS	2.5
1	D	248	VAL	2.5
1	J	256	ASN	2.5
1	J	271	THR	2.5
2	K	99	MET	2.4
1	D	221	GLY	2.4
1	G	225	THR	2.4
1	A	197	GLY	2.4
1	G	222	GLU	2.4
1	A	18	GLU	2.3
1	J	233	THR	2.3
1	G	181	ARG	2.3
1	G	226	GLN	2.3
1	A	17	LEU	2.3
1	G	193	PRO	2.3
1	G	276	PRO	2.3
1	G	253	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	220	ASN	2.2
1	G	263	HIS	2.2
1	J	192	HIS	2.2
1	J	212	ASP	2.2
1	A	225	THR	2.2
1	J	272	LEU	2.2
2	E	99	MET	2.2
1	J	213	ILE	2.2
1	J	227	ASP	2.2
1	D	182	THR	2.2
1	J	1	GLY	2.2
1	J	198	GLU	2.2
1	J	194	ARG	2.2
1	G	176	ASN	2.2
1	A	257	TYR	2.2
1	J	207	GLY	2.2
1	D	227	ASP	2.2
1	A	176	ASN	2.1
1	A	241	PHE	2.1
1	A	236	ALA	2.1
1	G	274	TRP	2.1
1	J	264	GLU	2.1
1	D	209	TYR	2.1
1	J	257	TYR	2.1
1	A	181	ARG	2.1
1	J	240	THR	2.1
1	A	183	ASP	2.1
1	G	250	PRO	2.0
2	B	1	ILE	2.0
1	J	217	TRP	2.0
1	G	228	MET	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.