



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:52 AM EDT

PDB ID : 1S7U / pdb_00001s7u
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 : 2.20 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:

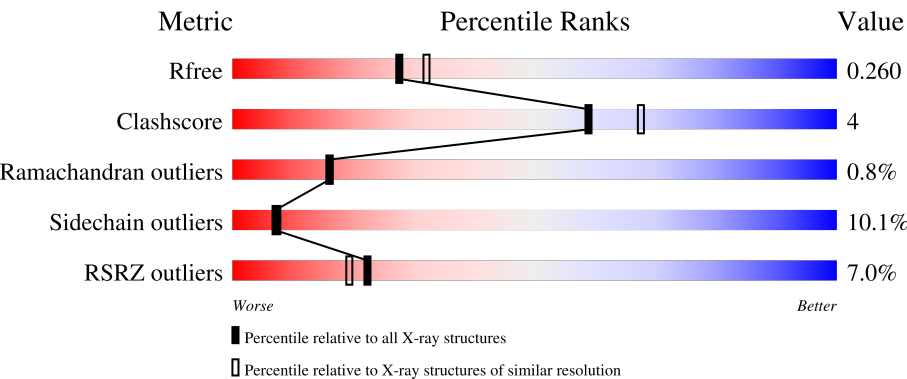
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	5% 69% 11% • 18%
1	D	338	9% 70% 9% • 19%
1	G	338	11% 68% 12% • 19%
1	J	338	6% 68% 11% • 19%
2	B	99	% 78% 20% •

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Mol	Chain	Length	Quality of chain
2	E	99	2% 84% 15%
2	H	99	% 75% 23%
2	K	99	83% 14%
3	C	9	89% 11%
3	F	9	89% 11%
3	I	9	78% 11% 11%
3	L	9	67% 33%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13593 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	0	0
			2264	1430	400	425	9			
1	D	274	Total	C	N	O	S	0	0	0
			2248	1420	398	421	9			
1	G	274	Total	C	N	O	S	0	0	0
			2248	1420	398	421	9			
1	J	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			818	523	138	151	6			
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 Glycoprotein 9-residue peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			
3	F	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			
3	I	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			
3	L	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	9	MET	CYS	SEE REMARK 999	UNP P07399
F	9	MET	CYS	SEE REMARK 999	UNP P07399
I	9	MET	CYS	SEE REMARK 999	UNP P07399
L	9	MET	CYS	SEE REMARK 999	UNP P07399

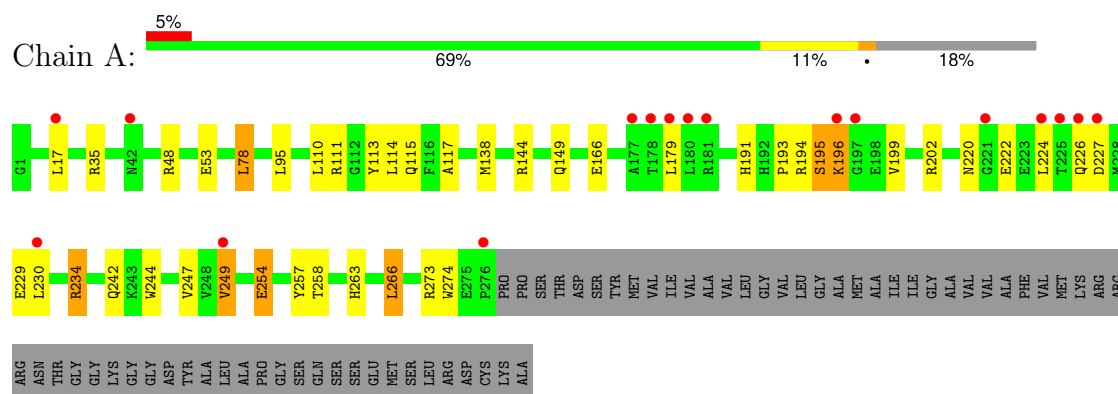
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	168	Total 168	O 168	0	0
4	B	118	Total 118	O 118	0	0
4	C	4	Total 4	O 4	0	0
4	D	163	Total 163	O 163	0	0
4	E	83	Total 83	O 83	0	0
4	F	6	Total 6	O 6	0	0
4	G	140	Total 140	O 140	0	0
4	H	79	Total 79	O 79	0	0
4	I	5	Total 5	O 5	0	0
4	J	152	Total 152	O 152	0	0
4	K	95	Total 95	O 95	0	0
4	L	3	Total 3	O 3	0	0

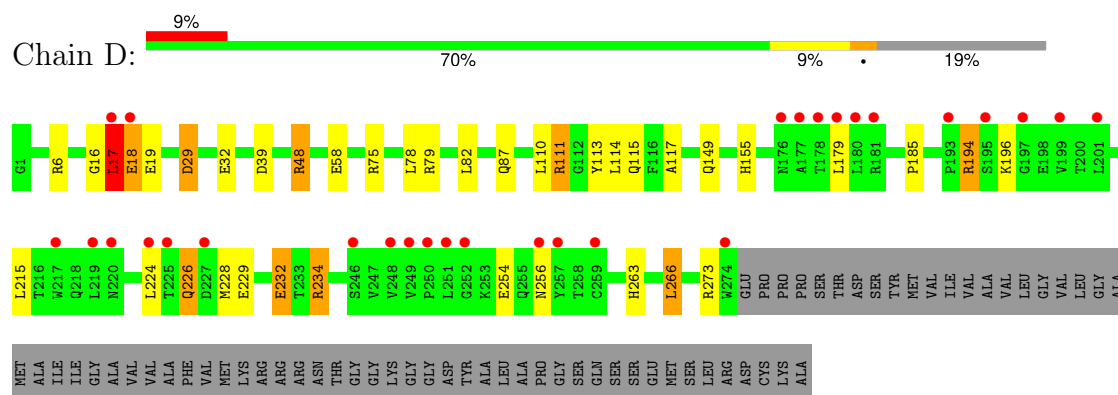
3 Residue-property plots

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

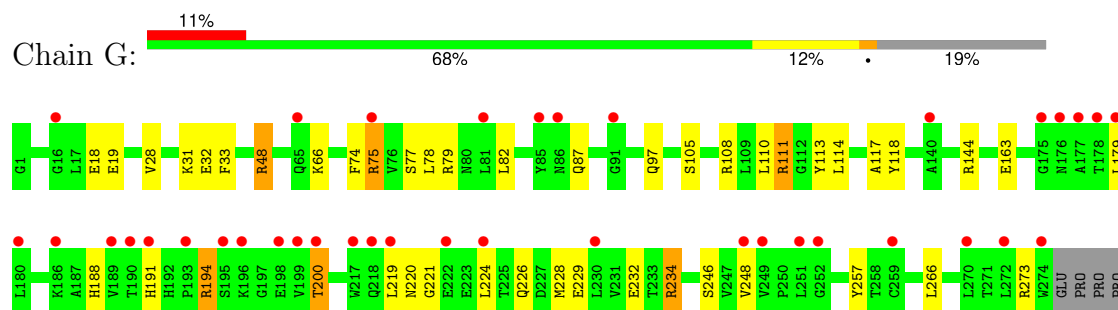
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- 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 3: Glycoprotein 9-residue peptide

Chain F:  89% 11%



- Molecule 3: Glycoprotein 9-residue peptide

Chain I:  78% 11% 11%



- Molecule 3: Glycoprotein 9-residue peptide

Chain L:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.39Å 123.34Å 99.39Å 90.00° 103.17° 90.00°	Depositor
Resolution (Å)	72.70 – 2.20 72.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (72.70-2.20) 99.0 (72.70-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.213 , 0.262 0.213 , 0.260	Depositor DCC
R_{free} test set	5426 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13593	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.83% 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	0.59	1/2331 (0.0%)	0.79	0/3166
1	D	0.57	0/2314	0.78	0/3142
1	G	0.58	0/2314	0.78	0/3142
1	J	0.60	1/2310 (0.0%)	0.77	0/3136
2	B	0.79	1/844 (0.1%)	0.84	0/1146
2	E	0.77	1/847 (0.1%)	0.82	0/1148
2	H	0.62	1/847 (0.1%)	0.76	0/1148
2	K	0.73	1/847 (0.1%)	0.81	0/1148
3	C	0.69	0/74	0.74	0/97
3	F	0.69	0/74	0.88	0/97
3	I	0.69	0/74	0.75	0/97
3	L	0.91	1/74 (1.4%)	1.06	0/97
All	All	0.63	7/12950 (0.1%)	0.79	0/17564

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	39	MET	SD-CE	-12.61	1.48	1.79
2	B	39	MET	SD-CE	-11.66	1.50	1.79
2	K	39	MET	SD-CE	-10.07	1.54	1.79
1	A	138	MET	SD-CE	-7.78	1.60	1.79
1	J	138	MET	SD-CE	-6.71	1.62	1.79
2	H	39	MET	SD-CE	-6.41	1.63	1.79
3	L	9	MET	CG-SD	-5.04	1.68	1.80

There are no bond angle outliers.

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	2264	0	2136	17	0
1	D	2248	0	2123	17	0
1	G	2248	0	2123	22	0
1	J	2244	0	2118	18	0
2	B	818	0	791	17	0
2	E	821	0	796	9	0
2	H	821	0	796	10	0
2	K	821	0	796	10	0
3	C	73	0	74	0	0
3	F	73	0	74	1	0
3	I	73	0	74	3	0
3	L	73	0	74	2	0
4	A	168	0	0	2	0
4	B	118	0	0	2	0
4	C	4	0	0	0	0
4	D	163	0	0	2	0
4	E	83	0	0	0	0
4	F	6	0	0	0	0
4	G	140	0	0	5	0
4	H	79	0	0	0	0
4	I	5	0	0	0	0
4	J	152	0	0	4	0
4	K	95	0	0	2	0
4	L	3	0	0	0	0
All	All	13593	0	11975	107	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 4.

All (107) 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:G:77:SER:HB3	4:G:475:HOH:O	1.25	1.25
1:G:77:SER:CB	4:G:475:HOH:O	1.84	1.14
2:B:39:MET:HE2	2:B:49:VAL:HG13	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:MET:HE2	2:H:49:VAL:HG13	1.62	0.81
1:J:142:ILE:HG13	4:J:478:HOH:O	1.81	0.79
1:D:232:GLU:CD	2:E:8:GLN:HE21	1.93	0.77
1:D:32:GLU:OE2	1:D:48:ARG:HD2	1.87	0.74
2:K:39:MET:HE2	2:K:49:VAL:HG13	1.70	0.74
1:G:163:GLU:OE2	3:I:1:LYS:NZ	2.22	0.73
2:B:39:MET:HE1	2:B:67:HIS:C	2.17	0.69
2:B:29:GLN:NE2	2:B:59:ASP:OD2	2.27	0.68
2:K:39:MET:HE1	2:K:67:HIS:C	2.18	0.67
2:E:39:MET:HE2	2:E:49:VAL:HG13	1.77	0.67
1:A:111:ARG:CZ	4:A:418:HOH:O	2.47	0.62
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.35	0.61
2:K:1:ILE:N	4:K:189:HOH:O	2.34	0.60
2:B:39:MET:HE2	2:B:49:VAL:CG1	2.30	0.60
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.38	0.58
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.39	0.58
1:J:32:GLU:OE2	1:J:48:ARG:HD2	2.04	0.57
1:G:188:HIS:ND1	4:G:452:HOH:O	2.32	0.57
2:K:50:GLU:HB2	2:K:67:HIS:CE1	2.40	0.57
2:B:87:MET:HE1	2:B:91:LYS:CD	2.35	0.57
1:D:232:GLU:CD	2:E:8:GLN:NE2	2.62	0.57
1:A:263:HIS:HB3	1:A:266:LEU:HD22	1.87	0.56
2:E:39:MET:CE	2:E:49:VAL:HG13	2.35	0.56
1:J:142:ILE:CD1	4:J:478:HOH:O	2.52	0.56
2:K:31:HIS:CD2	2:K:32:PRO:HA	2.41	0.55
1:A:191:HIS:CE1	1:A:199:VAL:HG21	2.42	0.55
2:B:39:MET:CE	2:B:49:VAL:HG13	2.36	0.55
2:B:87:MET:HE1	2:B:91:LYS:HD3	1.89	0.55
1:D:17:LEU:HB3	4:D:385:HOH:O	2.07	0.54
1:J:234:ARG:HD3	2:K:10:TYR:CE2	2.43	0.54
1:A:230:LEU:HD12	1:A:230:LEU:C	2.33	0.54
2:H:39:MET:HE1	2:H:67:HIS:C	2.33	0.53
1:D:16:GLY:O	1:D:17:LEU:O	2.27	0.53
2:K:39:MET:HE1	2:K:67:HIS:CA	2.39	0.53
1:A:111:ARG:HD3	1:A:113:TYR:CZ	2.43	0.53
2:H:39:MET:CE	2:H:49:VAL:HG13	2.37	0.53
1:J:111:ARG:HD2	1:J:113:TYR:CZ	2.43	0.53
1:A:193:PRO:HA	1:A:199:VAL:HG12	1.92	0.52
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.44	0.52
2:H:73:THR:OG1	2:H:76:ASP:OD2	2.27	0.52
1:D:111:ARG:HD2	1:D:113:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:12:VAL:HG21	4:J:436:HOH:O	2.08	0.52
1:A:234:ARG:HD2	1:A:242:GLN:HB2	1.92	0.52
1:A:254:GLU:HG3	1:A:274:TRP:HD1	1.75	0.52
1:J:142:ILE:CG1	4:J:478:HOH:O	2.49	0.52
1:J:263:HIS:HB3	1:J:266:LEU:HD22	1.92	0.51
2:B:87:MET:HE2	4:B:132:HOH:O	2.11	0.50
2:E:39:MET:HE1	2:E:67:HIS:C	2.36	0.50
1:G:108:ARG:HG2	4:G:384:HOH:O	2.12	0.49
2:H:4:THR:HG22	2:H:86:SER:HB2	1.93	0.49
1:J:32:GLU:OE2	1:J:48:ARG:CD	2.61	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.48
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.50	0.47
2:B:36:GLU:OE1	4:B:214:HOH:O	2.20	0.47
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.49	0.47
1:D:82:LEU:HA	1:D:87:GLN:HE21	1.79	0.47
1:G:144:ARG:HD3	4:G:434:HOH:O	2.14	0.47
1:J:45:TYR:CE2	1:J:67:ALA:HB2	2.50	0.47
1:G:87:GLN:NE2	1:G:118:TYR:OH	2.39	0.47
1:J:230:LEU:C	1:J:230:LEU:HD12	2.40	0.46
1:A:35:ARG:NH2	2:B:54:MET:O	2.40	0.46
1:A:220:ASN:ND2	4:A:489:HOH:O	2.48	0.46
2:H:32:PRO:HB2	2:H:33:PRO:HD2	1.98	0.46
1:A:234:ARG:HD3	2:B:10:TYR:CD2	2.51	0.46
2:B:87:MET:HE1	2:B:91:LYS:HD2	1.98	0.46
1:D:115:GLN:NE2	4:D:500:HOH:O	2.48	0.46
2:E:39:MET:HE1	2:E:67:HIS:CA	2.45	0.45
1:J:249:VAL:HG22	1:J:257:TYR:CZ	2.52	0.45
1:G:74:PHE:HZ	1:G:97:GLN:HE21	1.65	0.45
2:B:39:MET:HE1	2:B:67:HIS:CA	2.47	0.45
2:H:29:GLN:HA	2:H:61:SER:HB2	1.98	0.45
1:J:191:HIS:NE2	1:J:199:VAL:HG21	2.32	0.45
1:A:194:ARG:O	1:A:195:SER:C	2.60	0.45
2:K:39:MET:HE1	2:K:67:HIS:HA	1.99	0.45
1:G:19:GLU:OE1	1:G:75:ARG:NE	2.49	0.44
1:D:263:HIS:HB3	1:D:266:LEU:HD22	1.98	0.44
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.52	0.44
1:G:194:ARG:NH1	1:G:248:VAL:HG12	2.33	0.44
1:G:219:LEU:HD13	1:G:257:TYR:CE1	2.52	0.44
1:D:185:PRO:HD2	1:D:266:LEU:HD13	1.99	0.44
1:J:219:LEU:O	1:J:220:ASN:C	2.62	0.43
2:B:32:PRO:HB2	2:B:33:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:HIS:HE1	3:F:4:TYR:O	2.01	0.43
1:G:66:LYS:NZ	3:I:1:LYS:NZ	2.66	0.43
1:J:155:HIS:HB3	3:L:6:PHE:CZ	2.54	0.43
2:K:4:THR:HG22	4:K:180:HOH:O	2.19	0.43
1:G:28:VAL:HG23	1:G:33:PHE:CE1	2.53	0.43
1:D:6:ARG:NH2	1:D:113:TYR:CE1	2.87	0.43
1:G:200:THR:HG23	1:G:246:SER:HB2	2.00	0.42
2:H:21:ASN:HB3	2:H:70:PHE:CE1	2.54	0.42
1:G:19:GLU:OE1	1:G:75:ARG:CZ	2.67	0.42
1:J:32:GLU:OE2	1:J:35:ARG:HD2	2.19	0.42
1:D:234:ARG:HD3	2:E:10:TYR:CZ	2.55	0.42
1:G:32:GLU:OE2	1:G:48:ARG:HD2	2.20	0.42
1:J:167:TRP:CE2	3:L:1:LYS:HD2	2.56	0.41
1:G:77:SER:HB2	3:I:9:MET:HG2	2.02	0.41
2:B:4:THR:HG22	2:B:86:SER:HB2	2.03	0.41
1:A:78:LEU:HD13	1:A:95:LEU:HB2	2.02	0.41
1:D:18:GLU:HG2	1:D:19:GLU:N	2.36	0.41
1:G:111:ARG:HD2	1:G:113:TYR:CZ	2.56	0.41
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.56	0.40
1:D:194:ARG:HE	1:D:194:ARG:HB3	1.75	0.40
1:G:32:GLU:OE2	1:G:48:ARG:CD	2.70	0.40
1:G:82:LEU:HA	1:G:87:GLN:HE21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/338 (81%)	263 (96%)	8 (3%)	3 (1%)	11	10
1	D	272/338 (80%)	256 (94%)	13 (5%)	3 (1%)	11	10
1	G	272/338 (80%)	257 (94%)	12 (4%)	3 (1%)	11	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	271/338 (80%)	256 (94%)	12 (4%)	3 (1%)	11	10
2	B	97/99 (98%)	95 (98%)	2 (2%)	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%)	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	1505/1784 (84%)	1435 (95%)	58 (4%)	12 (1%)	16	16

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	LYS
1	D	17	LEU
1	J	196	LYS
1	J	220	ASN
1	J	226	GLN
1	A	195	SER
1	D	29	ASP
1	G	220	ASN
1	D	226	GLN
1	A	226	GLN
1	G	194	ARG
1	G	221	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	234/280 (84%)	211 (90%)	23 (10%)	7	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	232/280 (83%)	205 (88%)	27 (12%)	5	5
1	G	232/280 (83%)	211 (91%)	21 (9%)	9	9
1	J	232/280 (83%)	208 (90%)	24 (10%)	7	7
2	B	93/94 (99%)	85 (91%)	8 (9%)	10	10
2	E	94/94 (100%)	84 (89%)	10 (11%)	6	6
2	H	94/94 (100%)	83 (88%)	11 (12%)	5	5
2	K	94/94 (100%)	85 (90%)	9 (10%)	8	8
3	C	7/7 (100%)	6 (86%)	1 (14%)	3	3
3	F	7/7 (100%)	7 (100%)	0	100	100
3	I	7/7 (100%)	6 (86%)	1 (14%)	3	3
3	L	7/7 (100%)	7 (100%)	0	100	100
All	All	1333/1524 (88%)	1198 (90%)	135 (10%)	7	7

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	48	ARG
1	A	53	GLU
1	A	78	LEU
1	A	110	LEU
1	A	114	LEU
1	A	115	GLN
1	A	144	ARG
1	A	149	GLN
1	A	166	GLU
1	A	179	LEU
1	A	196	LYS
1	A	222	GLU
1	A	224	LEU
1	A	227	ASP
1	A	229	GLU
1	A	234	ARG
1	A	247	VAL
1	A	249	VAL
1	A	254	GLU
1	A	258	THR
1	A	266	LEU

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Mol	Chain	Res	Type
1	A	273	ARG
2	B	1	ILE
2	B	2	GLN
2	B	19	LYS
2	B	29	GLN
2	B	64	ILE
2	B	69	GLU
2	B	75	THR
2	B	93	VAL
3	C	1	LYS
1	D	17	LEU
1	D	18	GLU
1	D	29	ASP
1	D	39	ASP
1	D	48	ARG
1	D	58	GLU
1	D	75	ARG
1	D	78	LEU
1	D	79	ARG
1	D	110	LEU
1	D	111	ARG
1	D	114	LEU
1	D	149	GLN
1	D	179	LEU
1	D	194	ARG
1	D	196	LYS
1	D	215	LEU
1	D	224	LEU
1	D	226	GLN
1	D	228	MET
1	D	229	GLU
1	D	232	GLU
1	D	234	ARG
1	D	254	GLU
1	D	256	ASN
1	D	266	LEU
1	D	273	ARG
2	E	1	ILE
2	E	2	GLN
2	E	4	THR
2	E	22	ILE
2	E	64	ILE

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Mol	Chain	Res	Type
2	E	74	GLU
2	E	75	THR
2	E	77	THR
2	E	91	LYS
2	E	93	VAL
1	G	18	GLU
1	G	31	LYS
1	G	48	ARG
1	G	75	ARG
1	G	78	LEU
1	G	79	ARG
1	G	105	SER
1	G	110	LEU
1	G	111	ARG
1	G	114	LEU
1	G	179	LEU
1	G	191	HIS
1	G	200	THR
1	G	224	LEU
1	G	226	GLN
1	G	228	MET
1	G	229	GLU
1	G	232	GLU
1	G	234	ARG
1	G	266	LEU
1	G	273	ARG
2	H	1	ILE
2	H	19	LYS
2	H	22	ILE
2	H	29	GLN
2	H	48	LYS
2	H	54	MET
2	H	64	ILE
2	H	74	GLU
2	H	75	THR
2	H	91	LYS
2	H	93	VAL
3	I	1	LYS
1	J	17	LEU
1	J	48	ARG
1	J	53	GLU
1	J	62	ARG

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Mol	Chain	Res	Type
1	J	78	LEU
1	J	110	LEU
1	J	111	ARG
1	J	114	LEU
1	J	144	ARG
1	J	154	GLU
1	J	163	GLU
1	J	179	LEU
1	J	181	ARG
1	J	194	ARG
1	J	196	LYS
1	J	222	GLU
1	J	224	LEU
1	J	226	GLN
1	J	228	MET
1	J	229	GLU
1	J	234	ARG
1	J	254	GLU
1	J	266	LEU
1	J	273	ARG
2	K	1	ILE
2	K	4	THR
2	K	22	ILE
2	K	44	LYS
2	K	48	LYS
2	K	54	MET
2	K	64	ILE
2	K	75	THR
2	K	93	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	97	GLN
1	A	220	ASN
1	A	256	ASN
2	B	13	HIS
2	B	29	GLN
2	B	38	GLN
3	C	5	ASN
1	D	54	GLN

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Mol	Chain	Res	Type
1	D	97	GLN
1	D	155	HIS
2	E	8	GLN
2	E	13	HIS
2	E	38	GLN
3	F	5	ASN
1	G	87	GLN
1	G	96	GLN
1	G	97	GLN
1	G	188	HIS
1	G	218	GLN
1	G	256	ASN
2	H	13	HIS
3	I	5	ASN
1	J	54	GLN
1	J	72	GLN
1	J	97	GLN
1	J	188	HIS
1	J	255	GLN
2	K	13	HIS
2	K	67	HIS
3	L	5	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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%)	0.37	17 (6%) 26 23	12, 25, 56, 64	0
1	D	274/338 (81%)	0.57	29 (10%) 11 8	12, 25, 53, 64	0
1	G	274/338 (81%)	0.85	38 (13%) 6 5	12, 25, 53, 64	0
1	J	273/338 (80%)	0.50	19 (6%) 22 19	12, 25, 53, 64	0
2	B	99/99 (100%)	-0.16	1 (1%) 79 77	14, 23, 29, 33	0
2	E	99/99 (100%)	0.10	2 (2%) 65 62	14, 23, 30, 33	0
2	H	99/99 (100%)	0.18	1 (1%) 79 77	13, 23, 30, 36	0
2	K	99/99 (100%)	-0.15	0 100 100	14, 23, 30, 33	0
3	C	9/9 (100%)	-0.15	0 100 100	15, 17, 21, 22	0
3	F	9/9 (100%)	-0.54	0 100 100	14, 17, 21, 22	0
3	I	9/9 (100%)	0.04	0 100 100	14, 17, 21, 23	0
3	L	9/9 (100%)	0.77	0 100 100	15, 17, 21, 23	0
All	All	1529/1784 (85%)	0.41	107 (6%) 22 19	12, 24, 52, 64	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	177	ALA	5.5
1	G	178	THR	5.1
1	D	177	ALA	5.0
1	J	180	LEU	4.8
1	A	177	ALA	4.8
1	G	179	LEU	4.6
1	J	274	TRP	4.5
1	A	227	ASP	4.5
1	J	177	ALA	4.2
1	D	180	LEU	4.2
1	G	176	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	179	LEU	3.9
1	G	252	GLY	3.9
1	J	178	THR	3.8
1	A	179	LEU	3.8
1	J	179	LEU	3.8
1	G	251	LEU	3.7
1	A	180	LEU	3.6
1	D	17	LEU	3.5
1	G	274	TRP	3.5
1	G	180	LEU	3.5
1	G	200	THR	3.5
1	D	249	VAL	3.4
1	D	224	LEU	3.4
1	G	272	LEU	3.4
1	D	176	ASN	3.4
1	J	224	LEU	3.3
1	D	248	VAL	3.2
1	D	201	LEU	3.1
1	D	178	THR	3.1
2	B	1	ILE	3.0
1	J	197	GLY	3.0
1	D	193	PRO	3.0
1	G	249	VAL	3.0
1	D	257	TYR	3.0
1	A	196	LYS	3.0
1	J	196	LYS	3.0
1	G	217	TRP	3.0
1	D	274	TRP	3.0
1	G	91	GLY	2.9
1	G	270	LEU	2.9
2	E	1	ILE	2.9
1	D	217	TRP	2.9
1	A	225	THR	2.9
2	H	99	MET	2.9
1	A	42	ASN	2.9
1	D	252	GLY	2.8
1	G	224	LEU	2.8
1	D	256	ASN	2.8
1	G	222	GLU	2.8
1	D	259	CYS	2.8
1	G	195	SER	2.8
1	J	225	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	276	PRO	2.7
1	D	219	LEU	2.7
1	D	225	THR	2.7
1	D	18	GLU	2.7
1	G	140	ALA	2.6
1	G	175	GLY	2.6
1	A	224	LEU	2.5
1	G	75	ARG	2.5
1	D	227	ASP	2.5
1	J	190	THR	2.5
1	G	189	VAL	2.4
1	D	195	SER	2.4
1	D	181	ARG	2.4
1	A	249	VAL	2.4
1	A	230	LEU	2.4
1	G	86	ASN	2.3
1	D	197	GLY	2.3
1	G	81	LEU	2.3
1	A	221	GLY	2.3
1	G	191	HIS	2.3
1	G	198	GLU	2.3
1	G	199	VAL	2.3
2	E	47	PRO	2.2
1	J	272	LEU	2.2
1	D	220	ASN	2.2
1	G	190	THR	2.2
1	A	17	LEU	2.2
1	J	17	LEU	2.2
1	G	248	VAL	2.2
1	G	259	CYS	2.2
1	A	181	ARG	2.1
1	G	193	PRO	2.1
1	J	219	LEU	2.1
1	D	250	PRO	2.1
1	J	221	GLY	2.1
1	J	198	GLU	2.1
1	G	85	TYR	2.1
1	J	59	TYR	2.1
1	J	193	PRO	2.1
1	A	178	THR	2.1
1	G	65	GLN	2.1
1	G	230	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	197	GLY	2.1
1	G	186	LYS	2.0
1	D	246	SER	2.0
1	J	54	GLN	2.0
1	D	251	LEU	2.0
1	G	219	LEU	2.0
1	D	199	VAL	2.0
1	G	16	GLY	2.0
1	G	196	LYS	2.0
1	A	226	GLN	2.0
1	G	218	GLN	2.0
1	J	220	ASN	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.