



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:03 PM UTC

PDB ID : 1ZHB / pdb_00001zhh
Title : Crystal Structure Of The Murine Class I Major Histocompatibility Complex Of H-2Db, B2-Microglobulin, and a 9-Residue Peptide Derived from rat dopamine beta-monooxygenase
Authors : Sandalova, T.; Michaelsson, J.; Harris, R.A.; Odeberg, J.; Schneider, G.; Karre, K.; Achour, A.
Deposited on : 2005-04-25
Resolution : 2.70 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

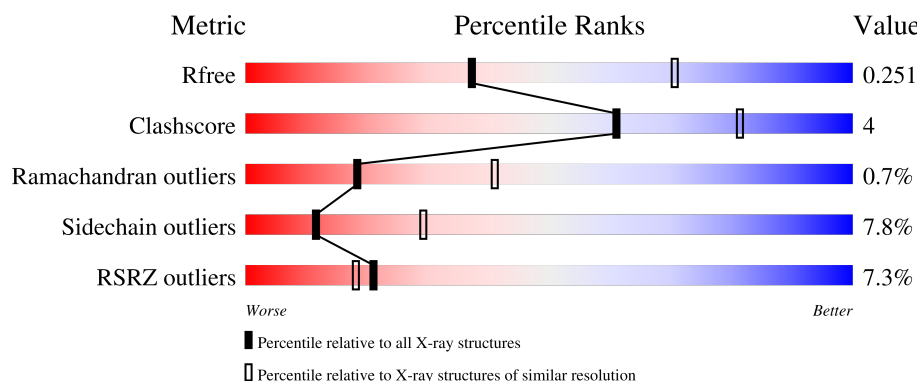
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	276	4% 85% 13% ..
1	D	276	15% 82% 15% ..
1	G	276	11% 83% 14% ..
1	J	276	7% 83% 14% ..
2	B	99	2% 86% 11% .

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Mol	Chain	Length	Quality of chain
2	E	99	% 87% 11%
2	H	99	2% 85% 12%
2	K	99	% 85% 15%
3	C	9	78% 22%
3	F	9	100%
3	I	9	67% 33%
3	L	9	11% 78% 11% 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12661 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	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			
1	D	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			
1	G	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	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
			820	524	138	151	7			
2	E	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	H	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	K	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			

- Molecule 3 is a protein called 9-mer peptide from Dopamine beta-monooxygenase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			74	51	11	12			
3	F	9	Total	C	N	O	0	0	0
			74	51	11	12			
3	I	9	Total	C	N	O	0	0	0
			74	51	11	12			
3	L	9	Total	C	N	O	0	0	0
			74	51	11	12			

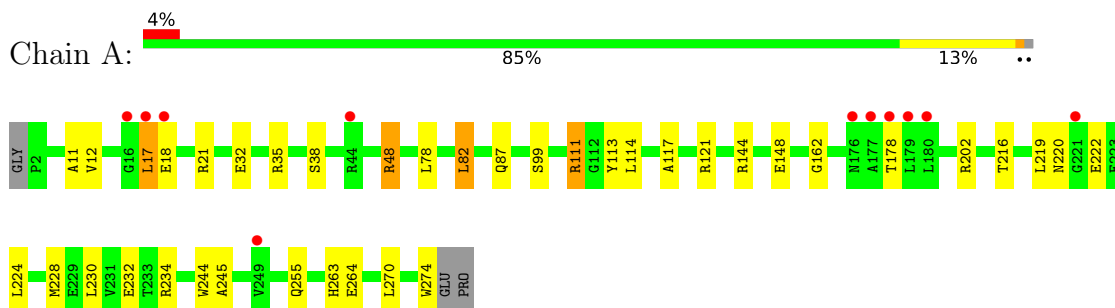
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total 21	O 21	0	0
4	B	7	Total 7	O 7	0	0
4	C	2	Total 2	O 2	0	0
4	D	16	Total 16	O 16	0	0
4	E	9	Total 9	O 9	0	0
4	F	1	Total 1	O 1	0	0
4	G	15	Total 15	O 15	0	0
4	H	10	Total 10	O 10	0	0
4	J	19	Total 19	O 19	0	0
4	K	7	Total 7	O 7	0	0
4	L	2	Total 2	O 2	0	0

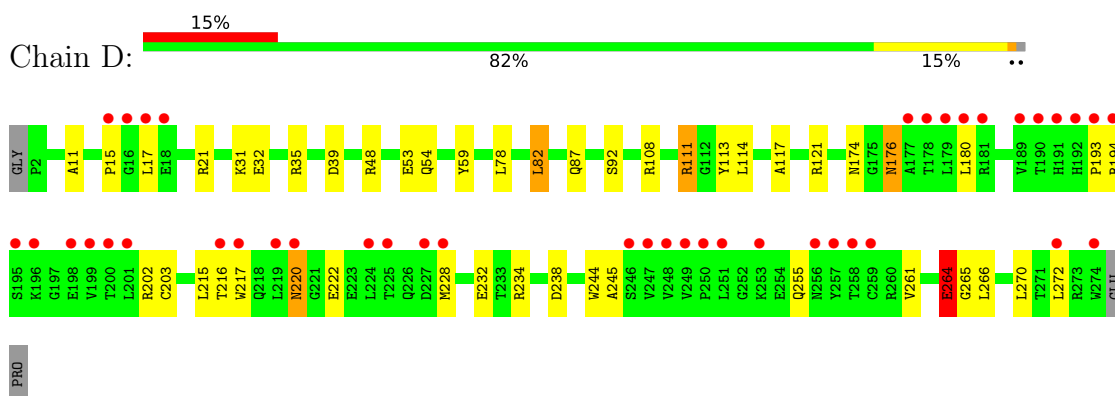
3 Residue-property plots [i](#)

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.

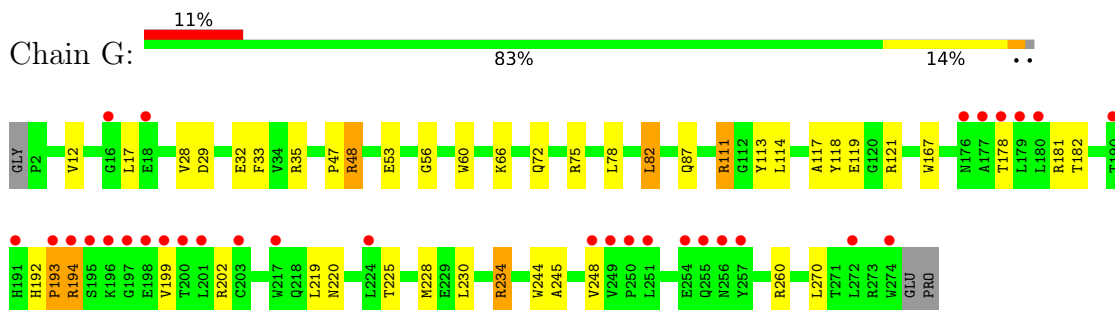
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



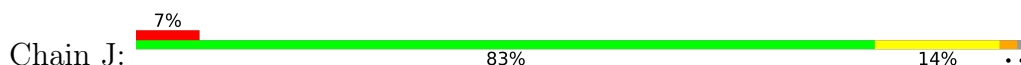
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

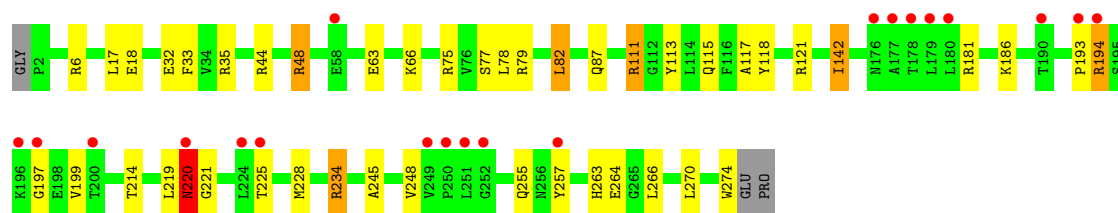


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

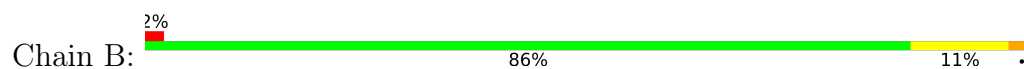


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

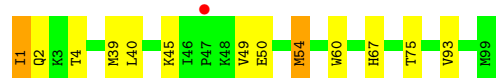
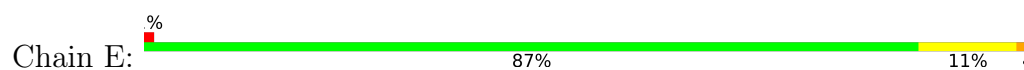




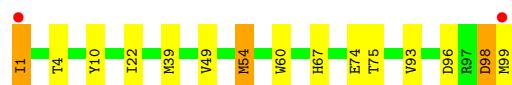
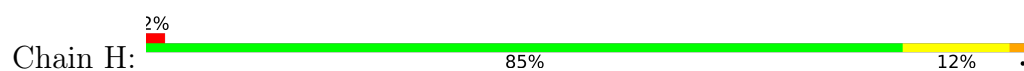
● Molecule 2: Beta-2-microglobulin



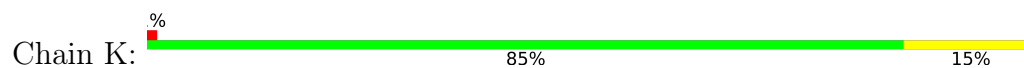
● Molecule 2: Beta-2-microglobulin



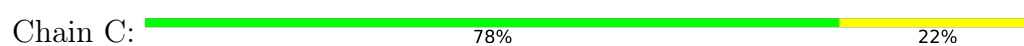
● Molecule 2: Beta-2-microglobulin



● Molecule 2: Beta-2-microglobulin



● Molecule 3: 9-mer peptide from Dopamine beta-monooxygenase



● Molecule 3: 9-mer peptide from Dopamine beta-monooxygenase



There are no outlier residues recorded for this chain.

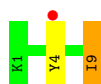
● Molecule 3: 9-mer peptide from Dopamine beta-monooxygenase

Chain I:  67% 33%



- Molecule 3: 9-mer peptide from Dopamine beta-monooxygenase

Chain L:  11% 78% 11% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.06Å 122.72Å 99.40Å 90.00° 103.00° 90.00°	Depositor
Resolution (Å)	24.92 – 2.70 24.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.92-2.70) 93.6 (24.92-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.225 , 0.262 0.240 , 0.251	Depositor DCC
R_{free} test set	2231 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.5	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	12661	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.34% 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	0.85	0/2310	0.86	1/3136 (0.0%)
1	D	0.81	0/2310	0.82	0/3136
1	G	0.84	0/2310	0.86	4/3136 (0.1%)
1	J	0.78	0/2310	0.84	0/3136
2	B	0.91	0/846	0.92	0/1147
2	E	0.86	0/846	0.86	0/1147
2	H	0.88	1/846 (0.1%)	0.89	0/1147
2	K	0.85	0/846	0.89	0/1147
3	C	0.77	0/76	1.05	0/102
3	F	0.91	0/76	0.92	0/102
3	I	0.90	0/76	0.97	0/102
3	L	0.93	0/76	1.01	1/102 (1.0%)
All	All	0.84	1/12928 (0.0%)	0.86	6/17540 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	98	ASP	CA-C	5.71	1.58	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	192	HIS	CA-C-N	7.43	129.13	119.84
1	G	192	HIS	C-N-CA	7.43	129.13	119.84
1	G	56	GLY	CA-C-N	5.74	125.60	119.28
1	G	56	GLY	C-N-CA	5.74	125.60	119.28
3	L	4	TYR	CB-CA-C	-5.32	101.56	110.29
1	A	162	GLY	N-CA-C	5.18	114.93	110.21

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	2244	0	2118	17	0
1	D	2244	0	2118	20	0
1	G	2244	0	2118	24	0
1	J	2244	0	2118	22	0
2	B	820	0	796	6	0
2	E	820	0	796	6	0
2	H	820	0	796	15	0
2	K	820	0	796	6	0
3	C	74	0	78	0	0
3	F	74	0	78	0	0
3	I	74	0	78	2	0
3	L	74	0	78	1	0
4	A	21	0	0	0	0
4	B	7	0	0	0	0
4	C	2	0	0	0	0
4	D	16	0	0	0	0
4	E	9	0	0	0	0
4	F	1	0	0	0	0
4	G	15	0	0	0	0
4	H	10	0	0	0	0
4	J	19	0	0	1	0
4	K	7	0	0	0	0
4	L	2	0	0	0	0
All	All	12661	0	11968	104	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 (104) 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:264:GLU:O	1:D:266:LEU:N	2.12	0.82
2:H:96:ASP:CB	2:H:99:MET:C	2.56	0.79
2:H:96:ASP:HB3	2:H:99:MET:C	2.09	0.78
2:B:39:MET:HE1	2:B:67:HIS:HA	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:96:ASP:CG	2:H:99:MET:C	2.58	0.72
1:G:35:ARG:HD2	1:G:48:ARG:HD2	1.73	0.71
1:J:32:GLU:OE2	1:J:48:ARG:HD2	1.91	0.70
2:H:1:ILE:O	2:H:1:ILE:HG23	1.90	0.69
1:J:111:ARG:HD2	1:J:113:TYR:CZ	2.27	0.68
1:J:87:GLN:NE2	1:J:118:TYR:OH	2.24	0.66
2:H:96:ASP:CG	2:H:99:MET:H	2.03	0.65
1:A:17:LEU:HG	1:A:18:GLU:H	1.63	0.64
1:J:228:MET:HE3	1:J:245:ALA:HB1	1.83	0.61
1:A:263:HIS:ND1	1:A:264:GLU:O	2.34	0.61
1:D:32:GLU:OE2	1:D:48:ARG:HD2	2.01	0.61
1:A:35:ARG:NH2	2:B:54:MET:O	2.34	0.59
1:G:32:GLU:OE2	1:G:48:ARG:HD2	2.02	0.58
1:G:87:GLN:NE2	1:G:118:TYR:OH	2.25	0.58
1:D:111:ARG:HD2	1:D:113:TYR:CZ	2.38	0.58
1:A:111:ARG:HD2	1:A:113:TYR:CZ	2.39	0.57
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.39	0.57
2:E:1:ILE:O	2:E:1:ILE:HG23	2.05	0.56
2:B:1:ILE:HG23	2:B:1:ILE:O	2.05	0.56
1:G:35:ARG:NH2	2:H:54:MET:O	2.40	0.55
1:G:82:LEU:HA	1:G:87:GLN:HE21	1.71	0.55
1:D:228:MET:HE2	1:D:245:ALA:HB1	1.89	0.55
1:G:111:ARG:HD2	1:G:113:TYR:CZ	2.42	0.55
1:D:15:PRO:HD3	1:D:92:SER:OG	2.07	0.54
2:K:39:MET:HE1	2:K:67:HIS:C	2.32	0.54
1:D:35:ARG:NH2	2:E:54:MET:O	2.39	0.54
1:G:167:TRP:CZ2	3:I:1:LYS:HE3	2.43	0.53
1:A:17:LEU:CG	1:A:18:GLU:H	2.21	0.53
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.43	0.53
1:J:82:LEU:HA	1:J:87:GLN:HE21	1.73	0.52
2:B:39:MET:HE1	2:B:67:HIS:CA	2.38	0.52
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.45	0.52
1:D:261:VAL:HB	1:D:270:LEU:HB2	1.92	0.52
1:J:194:ARG:HG3	1:J:199:VAL:HG12	1.92	0.51
1:D:203:CYS:HB2	1:D:217:TRP:CZ2	2.45	0.51
2:E:39:MET:HE2	2:E:49:VAL:HG13	1.93	0.51
2:E:40:LEU:HD23	2:E:45:LYS:HA	1.93	0.51
2:H:39:MET:HE1	2:H:67:HIS:CA	2.41	0.50
1:D:54:GLN:HE22	1:D:174:ASN:HB3	1.77	0.50
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.47	0.50
1:J:63:GLU:OE2	1:J:66:LYS:NZ	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:HD3	1:A:148:GLU:OE2	2.12	0.49
1:A:32:GLU:OE2	1:A:48:ARG:HD2	2.13	0.49
2:K:79:ALA:HB2	2:K:94:TYR:CD1	2.48	0.49
2:B:59:ASP:O	2:B:60:TRP:HB2	2.13	0.48
1:J:75:ARG:HD2	4:J:283:HOH:O	2.13	0.48
1:D:202:ARG:HD2	1:D:244:TRP:CE3	2.49	0.48
2:H:39:MET:HE1	2:H:67:HIS:C	2.38	0.48
2:E:50:GLU:HB2	2:E:67:HIS:CE1	2.49	0.48
1:J:219:LEU:C	1:J:220:ASN:HD22	2.22	0.48
1:A:230:LEU:HD12	1:A:230:LEU:C	2.39	0.48
1:G:234:ARG:HD3	2:H:10:TYR:CZ	2.48	0.48
1:J:6:ARG:NH2	1:J:113:TYR:CE2	2.82	0.48
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.49	0.47
1:J:266:LEU:HD21	1:J:270:LEU:HG	1.96	0.47
1:J:255:GLN:HE22	1:J:274:TRP:C	2.22	0.47
1:G:260:ARG:HA	1:G:270:LEU:O	2.15	0.47
1:G:72:GLN:HE22	1:G:75:ARG:NH1	2.13	0.47
2:H:1:ILE:O	2:H:1:ILE:CG2	2.59	0.47
1:A:216:THR:HA	1:A:228:MET:HE1	1.96	0.46
1:A:11:ALA:HA	1:A:21:ARG:O	2.15	0.46
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.50	0.46
1:G:230:LEU:HD12	1:G:230:LEU:O	2.16	0.46
1:G:118:TYR:CD2	1:G:119:GLU:HG2	2.51	0.45
1:J:263:HIS:ND1	1:J:264:GLU:O	2.46	0.45
1:A:228:MET:HE2	1:A:245:ALA:HB1	1.97	0.45
1:G:47:PRO:HG3	1:G:60:TRP:CZ2	2.51	0.45
1:D:108:ARG:NE	1:J:214:THR:HG21	2.31	0.45
1:G:66:LYS:HD2	3:I:2:ALA:HB3	1.99	0.45
1:G:219:LEU:O	1:G:220:ASN:C	2.60	0.44
1:A:219:LEU:HB2	1:A:224:LEU:HD11	1.98	0.44
1:G:228:MET:CE	1:G:245:ALA:HB1	2.47	0.44
1:A:82:LEU:HA	1:A:87:GLN:HE21	1.83	0.44
1:A:255:GLN:HE22	1:A:274:TRP:HB3	1.83	0.44
1:D:220:ASN:O	1:D:220:ASN:OD1	2.36	0.44
2:H:39:MET:HE1	2:H:67:HIS:HA	1.99	0.44
1:D:216:THR:HA	1:D:228:MET:HE1	2.00	0.43
1:D:238:ASP:OD1	1:D:238:ASP:C	2.62	0.43
2:K:39:MET:HE1	2:K:67:HIS:CA	2.49	0.43
1:J:33:PHE:C	1:J:48:ARG:HB2	2.43	0.43
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.54	0.42
1:J:234:ARG:HD3	2:K:10:TYR:CZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:111:ARG:HD2	1:J:113:TYR:OH	2.18	0.42
1:D:82:LEU:HA	1:D:87:GLN:HE21	1.85	0.42
2:H:39:MET:CE	2:H:49:VAL:HG13	2.49	0.42
1:J:35:ARG:NH2	2:K:54:MET:O	2.51	0.42
1:J:77:SER:HB3	3:L:9:ILE:HB	2.02	0.42
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.55	0.42
1:D:11:ALA:HA	1:D:21:ARG:O	2.19	0.41
1:D:176:ASN:O	1:D:180:LEU:HB2	2.20	0.41
1:J:142:ILE:N	1:J:142:ILE:HD13	2.35	0.41
1:A:263:HIS:C	1:A:264:GLU:O	2.63	0.41
1:G:28:VAL:HG23	1:G:33:PHE:CE1	2.56	0.41
1:G:33:PHE:C	1:G:48:ARG:HB2	2.46	0.41
1:G:32:GLU:OE2	1:G:35:ARG:HD2	2.22	0.40
1:J:219:LEU:HD13	1:J:257:TYR:CZ	2.57	0.40
1:D:59:TYR:CD1	1:D:59:TYR:C	2.99	0.40
1:G:28:VAL:O	1:G:29:ASP:C	2.64	0.40
1:G:193:PRO:O	1:G:199:VAL:HA	2.21	0.40
2:H:39:MET:HE2	2:H:49:VAL:HG13	2.02	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	271/276 (98%)	259 (96%)	11 (4%)	1 (0%)	30	54
1	D	271/276 (98%)	253 (93%)	15 (6%)	3 (1%)	11	29
1	G	271/276 (98%)	256 (94%)	13 (5%)	2 (1%)	18	41
1	J	271/276 (98%)	258 (95%)	9 (3%)	4 (2%)	8	22
2	B	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
2	E	97/99 (98%)	95 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	K	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	I	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1500/1536 (98%)	1425 (95%)	64 (4%)	11 (1%)	18	41

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	193	PRO
1	G	194	ARG
1	A	17	LEU
1	D	265	GLY
3	C	6	TYR
1	D	264	GLU
1	J	193	PRO
1	J	220	ASN
1	D	193	PRO
1	J	197	GLY
1	J	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	232/234 (99%)	217 (94%)	15 (6%)	15	37
1	D	232/234 (99%)	213 (92%)	19 (8%)	10	27
1	G	232/234 (99%)	216 (93%)	16 (7%)	14	34
1	J	232/234 (99%)	214 (92%)	18 (8%)	11	29
2	B	94/94 (100%)	83 (88%)	11 (12%)	5	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	94/94 (100%)	88 (94%)	6 (6%)	16	38
2	H	94/94 (100%)	86 (92%)	8 (8%)	10	25
2	K	94/94 (100%)	86 (92%)	8 (8%)	10	25
3	C	7/7 (100%)	6 (86%)	1 (14%)	3	8
3	F	7/7 (100%)	7 (100%)	0	100	100
3	I	7/7 (100%)	6 (86%)	1 (14%)	3	8
3	L	7/7 (100%)	6 (86%)	1 (14%)	3	8
All	All	1332/1340 (99%)	1228 (92%)	104 (8%)	11	29

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	38	SER
1	A	48	ARG
1	A	78	LEU
1	A	82	LEU
1	A	99	SER
1	A	111	ARG
1	A	114	LEU
1	A	121	ARG
1	A	178	THR
1	A	220	ASN
1	A	222	GLU
1	A	232	GLU
1	A	234	ARG
1	A	270	LEU
2	B	1	ILE
2	B	4	THR
2	B	29	GLN
2	B	39	MET
2	B	54	MET
2	B	64	ILE
2	B	70	PHE
2	B	74	GLU
2	B	75	THR
2	B	83	LYS
2	B	93	VAL
3	C	1	LYS
1	D	17	LEU

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Mol	Chain	Res	Type
1	D	31	LYS
1	D	39	ASP
1	D	53	GLU
1	D	78	LEU
1	D	82	LEU
1	D	111	ARG
1	D	114	LEU
1	D	121	ARG
1	D	176	ASN
1	D	194	ARG
1	D	215	LEU
1	D	220	ASN
1	D	222	GLU
1	D	232	GLU
1	D	234	ARG
1	D	255	GLN
1	D	264	GLU
1	D	272	LEU
2	E	1	ILE
2	E	2	GLN
2	E	4	THR
2	E	54	MET
2	E	75	THR
2	E	93	VAL
1	G	12	VAL
1	G	17	LEU
1	G	48	ARG
1	G	53	GLU
1	G	78	LEU
1	G	82	LEU
1	G	111	ARG
1	G	114	LEU
1	G	121	ARG
1	G	178	THR
1	G	181	ARG
1	G	182	THR
1	G	194	ARG
1	G	225	THR
1	G	234	ARG
1	G	248	VAL
2	H	1	ILE
2	H	4	THR

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Mol	Chain	Res	Type
2	H	22	ILE
2	H	54	MET
2	H	74	GLU
2	H	75	THR
2	H	93	VAL
2	H	98	ASP
3	I	9	ILE
1	J	17	LEU
1	J	18	GLU
1	J	44	ARG
1	J	48	ARG
1	J	78	LEU
1	J	79	ARG
1	J	82	LEU
1	J	111	ARG
1	J	115	GLN
1	J	121	ARG
1	J	142	ILE
1	J	181	ARG
1	J	186	LYS
1	J	194	ARG
1	J	220	ASN
1	J	225	THR
1	J	234	ARG
1	J	248	VAL
2	K	1	ILE
2	K	2	GLN
2	K	4	THR
2	K	29	GLN
2	K	64	ILE
2	K	74	GLU
2	K	75	THR
2	K	93	VAL
3	L	9	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	65	GLN
1	A	87	GLN
1	A	97	GLN

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Mol	Chain	Res	Type
1	A	176	ASN
1	A	255	GLN
2	B	8	GLN
2	B	38	GLN
2	B	67	HIS
3	C	5	ASN
1	D	54	GLN
1	D	87	GLN
1	D	97	GLN
1	D	226	GLN
2	E	13	HIS
2	E	38	GLN
3	F	5	ASN
1	G	72	GLN
1	G	87	GLN
1	G	97	GLN
1	G	220	ASN
1	G	226	GLN
2	H	13	HIS
2	H	34	HIS
2	H	38	GLN
2	H	67	HIS
3	I	5	ASN
1	J	54	GLN
1	J	87	GLN
1	J	97	GLN
1	J	155	HIS
1	J	220	ASN
1	J	255	GLN
2	K	34	HIS
2	K	67	HIS
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 ⓘ

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	273/276 (98%)	0.38	11 (4%) 42 38	28, 45, 84, 89	0
1	D	273/276 (98%)	0.72	42 (15%) 5 4	28, 45, 84, 90	0
1	G	273/276 (98%)	0.52	31 (11%) 10 8	28, 45, 84, 90	0
1	J	273/276 (98%)	0.53	20 (7%) 21 18	30, 45, 84, 91	0
2	B	99/99 (100%)	0.12	2 (2%) 65 62	34, 45, 54, 59	0
2	E	99/99 (100%)	0.24	1 (1%) 79 78	34, 45, 54, 60	0
2	H	99/99 (100%)	0.30	2 (2%) 65 62	33, 45, 54, 63	0
2	K	99/99 (100%)	0.14	1 (1%) 79 78	34, 45, 55, 60	0
3	C	9/9 (100%)	0.05	0 100 100	33, 35, 39, 39	0
3	F	9/9 (100%)	0.54	0 100 100	33, 36, 39, 40	0
3	I	9/9 (100%)	-0.03	0 100 100	33, 35, 39, 39	0
3	L	9/9 (100%)	0.48	1 (11%) 10 8	33, 36, 40, 40	0
All	All	1524/1536 (99%)	0.44	111 (7%) 21 18	28, 45, 83, 91	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	178	THR	7.0
1	D	177	ALA	6.6
1	G	177	ALA	6.5
1	D	249	VAL	6.0
1	J	179	LEU	5.8
2	H	99	MET	5.6
1	D	180	LEU	5.1
1	G	249	VAL	4.9
1	D	201	LEU	4.9
1	D	178	THR	4.7
1	J	177	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	177	ALA	4.6
1	G	179	LEU	4.5
1	D	248	VAL	4.4
1	A	179	LEU	4.3
1	D	193	PRO	4.3
1	D	190	THR	4.1
1	G	198	GLU	3.9
1	D	194	ARG	3.8
1	J	178	THR	3.8
1	G	248	VAL	3.8
1	A	18	GLU	3.7
1	D	217	TRP	3.7
1	D	17	LEU	3.7
1	D	199	VAL	3.7
1	G	251	LEU	3.5
1	A	178	THR	3.5
1	J	193	PRO	3.5
1	G	250	PRO	3.5
1	G	197	GLY	3.4
1	J	225	THR	3.4
1	D	179	LEU	3.3
1	J	224	LEU	3.3
1	D	196	LYS	3.3
1	J	197	GLY	3.2
1	A	16	GLY	3.2
1	D	195	SER	3.2
1	J	180	LEU	3.1
1	A	180	LEU	3.1
1	G	199	VAL	3.0
1	D	257	TYR	3.0
1	G	257	TYR	2.9
1	D	16	GLY	2.9
1	G	274	TRP	2.9
1	D	250	PRO	2.8
1	J	196	LYS	2.8
1	D	274	TRP	2.8
1	J	176	ASN	2.8
1	D	15	PRO	2.7
1	D	259	CYS	2.7
1	D	224	LEU	2.7
1	D	258	THR	2.7
1	G	217	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	227	ASP	2.7
1	J	257	TYR	2.7
1	A	249	VAL	2.7
1	G	193	PRO	2.7
1	D	246	SER	2.6
1	A	221	GLY	2.6
1	G	196	LYS	2.6
1	G	195	SER	2.6
1	J	58	GLU	2.6
1	J	250	PRO	2.6
1	G	190	THR	2.6
2	E	47	PRO	2.6
1	J	190	THR	2.5
1	D	225	THR	2.5
1	A	17	LEU	2.5
1	G	224	LEU	2.5
1	D	18	GLU	2.5
2	H	1	ILE	2.5
1	D	192	HIS	2.5
1	J	251	LEU	2.5
1	G	191	HIS	2.5
1	D	272	LEU	2.4
1	G	203	CYS	2.4
1	D	198	GLU	2.4
1	G	254	GLU	2.4
1	J	249	VAL	2.4
1	G	194	ARG	2.4
1	D	200	THR	2.4
1	G	272	LEU	2.4
1	D	191	HIS	2.4
1	J	194	ARG	2.4
1	G	180	LEU	2.4
1	G	18	GLU	2.4
1	D	189	VAL	2.4
1	J	200	THR	2.3
1	J	220	ASN	2.3
1	A	176	ASN	2.3
1	G	256	ASN	2.3
1	D	219	LEU	2.3
1	D	251	LEU	2.3
1	G	200	THR	2.2
1	D	220	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1	ILE	2.2
1	G	16	GLY	2.2
2	B	74	GLU	2.2
1	G	201	LEU	2.2
1	D	247	VAL	2.2
1	D	181	ARG	2.1
1	D	216	THR	2.1
1	D	253	LYS	2.1
1	G	255	GLN	2.1
1	D	228	MET	2.1
1	G	176	ASN	2.1
3	L	4	TYR	2.1
2	K	1	ILE	2.1
1	D	256	ASN	2.1
1	J	252	GLY	2.0
1	A	44	ARG	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.