



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:15 PM UTC

PDB ID : 8RJI / pdb_00008rji
Title : HLA A*2402-NF9_5R pMHC complex
Authors : Wall, A.; Motozono, C.; Sewell, A.K.; Rizkallah, P.J.; Fuller, A.
Deposited on : 2023-12-21
Resolution : 2.30 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

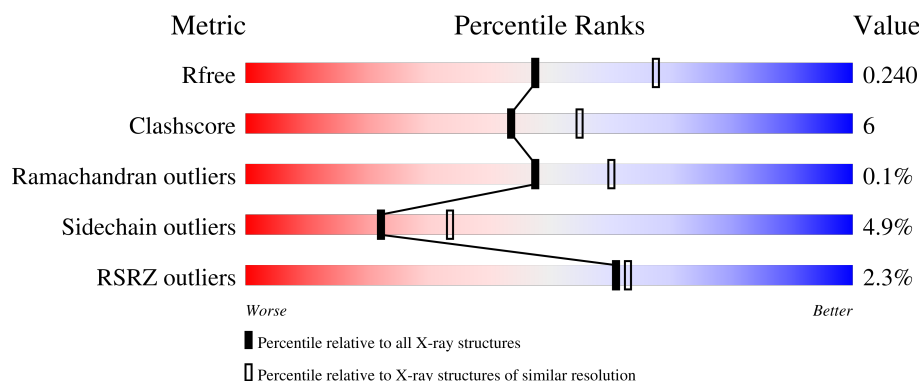
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	3% 85% 14% .
1	D	276	4% 86% 12% .
1	G	276	3% 84% 14% .
1	J	276	85% 14% .
2	B	100	3% 83% 17%

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Mol	Chain	Length	Quality of chain
2	E	100	% 84% 15%
2	H	100	% 76% 24%
2	K	100	2% 81% 18%
3	C	9	67% 33%
3	F	9	89% 11%
3	I	9	11% 56% 44%
3	L	9	44% 56%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13033 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 class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2238	1392	405	431	10			
1	D	276	Total	C	N	O	S	0	0	0
			2238	1392	405	431	10			
1	G	276	Total	C	N	O	S	0	0	0
			2238	1392	405	431	10			
1	J	276	Total	C	N	O	S	0	0	0
			2238	1392	405	431	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	K	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769
K	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			94	62	17	15			
3	F	9	Total	C	N	O	0	0	0
			94	62	17	15			
3	L	9	Total	C	N	O	0	0	0
			94	62	17	15			
3	I	9	Total	C	N	O	0	0	0
			94	62	17	15			

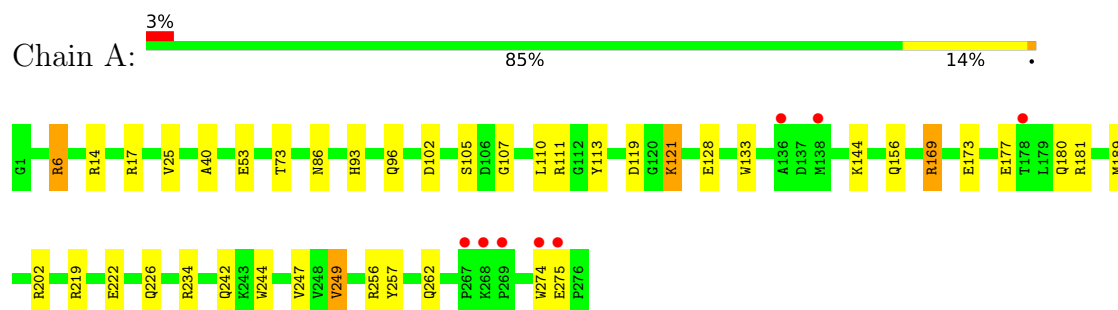
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		
4	B	25	Total	O	0	0
			25	25		
4	C	4	Total	O	0	0
			4	4		
4	D	46	Total	O	0	0
			46	46		
4	E	23	Total	O	0	0
			23	23		
4	G	53	Total	O	0	0
			53	53		
4	H	24	Total	O	0	0
			24	24		
4	J	85	Total	O	0	0
			85	85		
4	K	22	Total	O	0	0
			22	22		
4	L	1	Total	O	0	0
			1	1		
4	I	1	Total	O	0	0
			1	1		

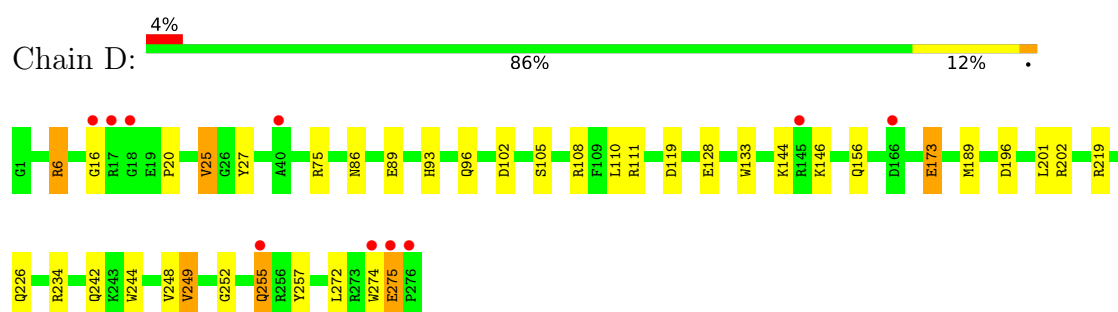
3 Residue-property plots [i](#)

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.

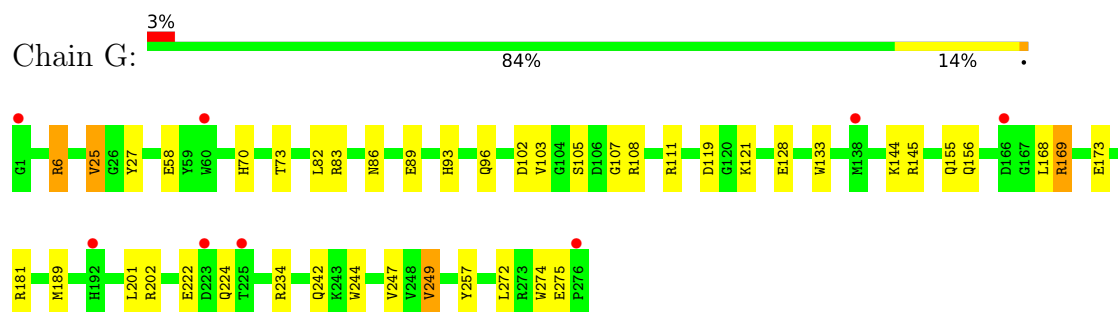
- Molecule 1: MHC class I antigen



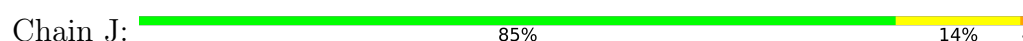
- Molecule 1: MHC class I antigen



- Molecule 1: MHC class I antigen

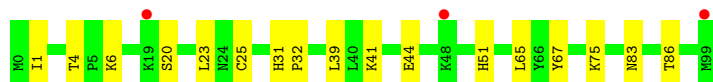
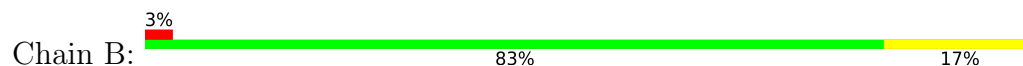


- Molecule 1: MHC class I antigen

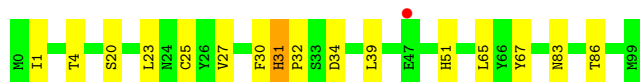
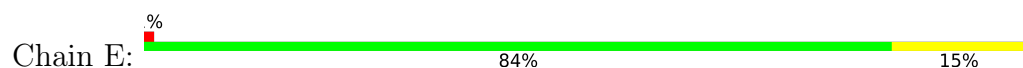




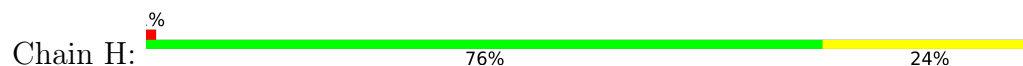
- Molecule 2: Beta-2-microglobulin



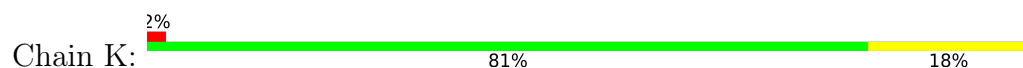
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



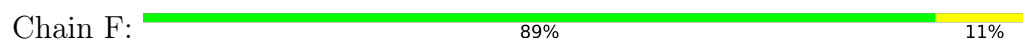
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Spike glycoprotein

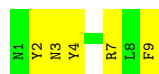


- Molecule 3: Spike glycoprotein



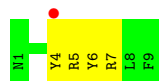
- Molecule 3: Spike glycoprotein

Chain L:  44% 56%



- Molecule 3: Spike glycoprotein

Chain I:  11% 56% 44%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.28Å 77.02Å 111.82Å 90.00° 110.58° 90.00°	Depositor
Resolution (Å)	54.80 – 2.30 54.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (54.80-2.30) 99.7 (54.80-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.217 , 0.265 (Not available) , 0.240	Depositor DCC
R_{free} test set	3590 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13033	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1421e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	1.10	0/2299	1.35	2/3116 (0.1%)
1	D	1.08	0/2299	1.36	0/3116
1	G	1.07	0/2299	1.34	0/3116
1	J	1.14	2/2299 (0.1%)	1.36	1/3116 (0.0%)
2	B	1.05	0/860	1.17	0/1162
2	E	1.08	1/860 (0.1%)	1.20	0/1162
2	H	1.04	0/860	1.18	1/1162 (0.1%)
2	K	1.07	1/860 (0.1%)	1.18	1/1162 (0.1%)
3	C	0.99	0/97	1.33	0/128
3	F	0.89	0/97	1.29	0/128
3	I	0.94	0/97	1.37	0/128
3	L	1.06	0/97	1.34	0/128
All	All	1.08	4/13024 (0.0%)	1.31	5/17624 (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
3	L	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	192	HIS	CE1-NE2	7.92	1.40	1.32
2	E	31	HIS	CE1-NE2	6.86	1.39	1.32
2	K	31	HIS	CE1-NE2	6.59	1.39	1.32
1	J	247	VAL	C-O	5.39	1.29	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	58	GLU	CB-CG-CD	6.67	123.94	112.60
1	A	53	GLU	CA-C-N	6.09	128.44	120.28
1	A	53	GLU	C-N-CA	6.09	128.44	120.28
2	H	71	THR	CB-CA-C	5.51	117.50	110.34
2	K	71	THR	CB-CA-C	5.33	117.26	110.34

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	2	TYR	Mainchain,Peptide

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	2238	0	2095	27	1
1	D	2238	0	2095	33	1
1	G	2238	0	2095	31	1
1	J	2238	0	2095	27	0
2	B	837	0	803	10	0
2	E	837	0	803	9	0
2	H	837	0	803	13	1
2	K	837	0	803	10	0
3	C	94	0	87	3	0
3	F	94	0	87	1	0
3	I	94	0	87	3	0
3	L	94	0	87	3	0
4	A	73	0	0	2	0
4	B	25	0	0	2	0
4	C	4	0	0	1	0
4	D	46	0	0	2	0
4	E	23	0	0	2	0
4	G	53	0	0	0	0
4	H	24	0	0	1	0
4	I	1	0	0	0	0
4	J	85	0	0	5	0
4	K	22	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1	0	0	0	0
All	All	13033	0	11940	150	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 6.

All (150) 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:155:GLN:OE1	3:I:7:ARG:NH1	2.02	0.92
1:D:255:GLN:CD	1:D:255:GLN:H	1.83	0.86
1:D:255:GLN:HG2	1:G:83:ARG:O	1.80	0.80
2:K:4:THR:HG22	2:K:86:THR:HB	1.68	0.75
1:D:173:GLU:OE1	1:D:173:GLU:HA	1.87	0.74
1:D:255:GLN:CG	1:G:83:ARG:O	2.36	0.73
2:K:3:ARG:HD3	4:K:107:HOH:O	1.88	0.72
1:G:189:MET:HE2	1:G:274:TRP:HB2	1.72	0.72
2:H:4:THR:HG22	2:H:86:THR:HB	1.72	0.71
1:D:275:GLU:HG3	4:D:346:HOH:O	1.88	0.71
2:B:4:THR:HG22	2:B:86:THR:HB	1.73	0.71
2:E:4:THR:HG22	2:E:86:THR:HB	1.73	0.71
1:G:234:ARG:HE	1:G:242:GLN:HE21	1.40	0.69
1:D:189:MET:HE2	1:D:274:TRP:HB2	1.75	0.68
2:B:41:LYS:O	2:B:44:GLU:HG2	1.94	0.67
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.30	0.67
2:B:31:HIS:HD2	4:B:106:HOH:O	1.80	0.65
1:A:189:MET:HE2	1:A:274:TRP:HB2	1.79	0.65
1:A:73:THR:HG21	3:C:6:TYR:HB3	1.79	0.64
1:G:202:ARG:HD3	1:G:244:TRP:CE3	2.32	0.64
1:J:234:ARG:HE	1:J:242:GLN:HE21	1.46	0.63
1:J:202:ARG:HD3	1:J:244:TRP:CE3	2.35	0.62
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.35	0.61
1:J:151:HIS:HD2	4:J:309:HOH:O	1.83	0.60
1:J:93:HIS:HD2	1:J:119:ASP:OD2	1.85	0.59
1:D:96:GLN:OE1	2:E:31:HIS:HE1	1.86	0.59
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.38	0.59
1:D:93:HIS:HD2	1:D:119:ASP:OD2	1.86	0.59
1:A:180:GLN:HA	4:A:371:HOH:O	2.03	0.58
3:C:5:ARG:HD2	4:C:104:HOH:O	2.02	0.58
1:G:156:GLN:HA	1:G:156:GLN:OE1	2.03	0.58
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ARG:HE	1:D:242:GLN:HE21	1.51	0.58
1:D:219:ARG:NH1	4:D:301:HOH:O	2.17	0.58
1:J:156:GLN:OE1	1:J:156:GLN:HA	2.03	0.58
1:D:156:GLN:HA	1:D:156:GLN:OE1	2.03	0.57
1:G:6:ARG:NH2	1:G:102:ASP:OD1	2.33	0.57
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.53	0.57
1:J:249:VAL:HG22	1:J:257:TYR:CE1	2.40	0.57
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.87	0.56
1:G:93:HIS:HD2	1:G:119:ASP:OD2	1.89	0.56
1:J:111:ARG:NE	1:J:128:GLU:HG3	2.20	0.56
1:J:6:ARG:NH2	1:J:102:ASP:OD1	2.37	0.56
1:A:177:GLU:OE1	1:A:177:GLU:HA	2.06	0.55
1:G:73:THR:HG21	3:I:6:TYR:HB3	1.88	0.55
1:G:96:GLN:OE1	2:H:31:HIS:HE1	1.88	0.55
1:A:156:GLN:HA	1:A:156:GLN:OE1	2.06	0.55
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.36	0.55
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.42	0.55
1:J:202:ARG:HD2	1:J:244:TRP:CD2	2.41	0.55
2:K:25:CYS:HB2	2:K:39:LEU:HD21	1.89	0.54
1:D:111:ARG:NE	1:D:128:GLU:HG3	2.22	0.54
1:J:151:HIS:CD2	4:J:309:HOH:O	2.59	0.54
1:D:252:GLY:O	1:G:83:ARG:NH1	2.41	0.54
1:A:133:TRP:O	1:A:144:LYS:HE3	2.08	0.54
1:D:133:TRP:O	1:D:144:LYS:HE3	2.07	0.54
1:G:121:LYS:CG	2:H:1:ILE:HD12	2.38	0.54
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.43	0.54
1:J:54:GLN:HG3	4:J:342:HOH:O	2.09	0.53
1:J:133:TRP:O	1:J:144:LYS:HE3	2.09	0.53
1:J:138:MET:HG2	4:J:330:HOH:O	2.09	0.53
1:G:249:VAL:HG22	1:G:257:TYR:CZ	2.44	0.53
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.45	0.52
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.45	0.52
1:G:121:LYS:HG3	2:H:1:ILE:HD12	1.91	0.51
2:H:41:LYS:O	2:H:44:GLU:HG2	2.10	0.51
1:D:146:LYS:NZ	3:F:9:PHE:O	2.43	0.51
1:D:6:ARG:NH2	1:D:102:ASP:OD1	2.35	0.51
2:H:41:LYS:O	2:H:44:GLU:CG	2.59	0.51
2:H:25:CYS:HB2	2:H:39:LEU:HD21	1.93	0.50
1:G:133:TRP:O	1:G:144:LYS:HE3	2.11	0.50
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.93	0.50
1:G:111:ARG:NE	1:G:128:GLU:HG3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:HIS:CD2	4:B:106:HOH:O	2.59	0.50
3:C:5:ARG:HG3	3:C:5:ARG:HH11	1.77	0.49
2:K:31:HIS:HD2	4:K:113:HOH:O	1.94	0.49
1:D:108:ARG:NH2	1:D:108:ARG:HG2	2.27	0.49
1:A:111:ARG:NE	1:A:128:GLU:HG3	2.28	0.49
1:D:234:ARG:HE	1:D:242:GLN:NE2	2.10	0.48
2:K:31:HIS:CD2	2:K:32:PRO:HA	2.47	0.48
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.94	0.48
1:J:273:ARG:NH1	4:J:303:HOH:O	2.41	0.48
1:J:234:ARG:HE	1:J:242:GLN:NE2	2.10	0.47
1:A:202:ARG:CD	1:A:244:TRP:CD2	2.98	0.47
1:A:189:MET:CE	1:A:274:TRP:HB2	2.44	0.47
1:D:202:ARG:CD	1:D:244:TRP:CD2	2.97	0.47
1:A:121:LYS:HG3	2:B:1:ILE:HD12	1.97	0.47
1:D:108:ARG:HG2	1:D:108:ARG:HH21	1.79	0.47
1:G:249:VAL:HG22	1:G:257:TYR:CE1	2.49	0.47
1:D:255:GLN:HG3	1:G:83:ARG:O	2.15	0.46
2:K:23:LEU:O	2:K:67:TYR:HA	2.15	0.46
2:B:31:HIS:CD2	2:B:32:PRO:HA	2.50	0.46
1:G:189:MET:CE	1:G:274:TRP:HB2	2.42	0.46
1:G:202:ARG:CD	1:G:244:TRP:CD2	2.98	0.46
2:H:31:HIS:CD2	2:H:32:PRO:HA	2.50	0.46
1:J:96:GLN:OE1	2:K:31:HIS:HE1	1.97	0.46
1:J:143:THR:HG23	3:L:9:PHE:HA	1.98	0.46
2:E:31:HIS:CD2	2:E:32:PRO:HA	2.51	0.46
1:J:155:GLN:HE22	3:L:7:ARG:NH1	2.14	0.46
2:E:31:HIS:HD2	4:E:121:HOH:O	1.98	0.46
1:G:103:VAL:HG13	1:G:168:LEU:HD23	1.99	0.45
2:K:3:ARG:CD	4:K:107:HOH:O	2.53	0.45
1:A:234:ARG:HE	1:A:242:GLN:NE2	2.13	0.45
1:A:107:GLY:O	1:A:169:ARG:HD2	2.16	0.45
1:J:202:ARG:CD	1:J:244:TRP:CD2	2.98	0.45
2:B:51:HIS:HA	2:B:65:LEU:O	2.16	0.45
2:H:27:VAL:HG23	2:H:30:PHE:CE1	2.52	0.45
1:A:226:GLN:NE2	1:A:226:GLN:HA	2.32	0.44
1:D:196:ASP:HA	1:G:145:ARG:HB3	1.98	0.44
1:D:189:MET:HE3	1:D:201:LEU:HD13	2.00	0.44
2:E:23:LEU:O	2:E:67:TYR:HA	2.17	0.44
2:E:51:HIS:HA	2:E:65:LEU:O	2.17	0.44
1:J:249:VAL:HG22	1:J:257:TYR:CZ	2.53	0.44
2:H:23:LEU:O	2:H:67:TYR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:HG22	1:A:257:TYR:CE1	2.53	0.43
2:E:27:VAL:HG23	2:E:30:PHE:CE1	2.54	0.43
1:D:189:MET:CE	1:D:201:LEU:HD13	2.48	0.43
1:G:25:VAL:CG1	1:G:27:TYR:HE1	2.30	0.43
1:A:40:ALA:HB3	4:A:315:HOH:O	2.18	0.43
2:B:23:LEU:O	2:B:67:TYR:HA	2.18	0.43
1:J:130:LEU:HB2	1:J:157:ARG:HD2	2.00	0.43
2:H:51:HIS:HA	2:H:65:LEU:O	2.18	0.43
1:D:189:MET:CE	1:D:274:TRP:HB2	2.46	0.42
1:G:234:ARG:HE	1:G:242:GLN:NE2	2.14	0.42
2:H:99:MET:HE2	4:H:123:HOH:O	2.20	0.42
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.90	0.42
2:K:51:HIS:HA	2:K:65:LEU:O	2.19	0.42
2:E:31:HIS:CD2	4:E:121:HOH:O	2.71	0.42
1:A:111:ARG:HG2	1:A:113:TYR:OH	2.20	0.42
1:D:20:PRO:HG2	1:D:75:ARG:HG2	2.01	0.42
1:D:110:LEU:HD12	1:D:110:LEU:HA	1.92	0.42
1:G:189:MET:CE	1:G:201:LEU:HD13	2.49	0.42
1:D:25:VAL:CG1	1:D:27:TYR:HE1	2.33	0.42
1:D:249:VAL:HG22	1:D:257:TYR:CE1	2.55	0.41
1:D:226:GLN:NE2	1:D:226:GLN:HA	2.33	0.41
1:G:107:GLY:O	1:G:169:ARG:HD2	2.19	0.41
1:J:187:THR:HB	1:J:272:LEU:HD11	2.01	0.41
1:G:181:ARG:O	1:G:181:ARG:HG2	2.20	0.41
1:J:163:THR:HG21	3:L:4:TYR:OH	2.21	0.41
1:J:110:LEU:HD12	1:J:110:LEU:HA	1.91	0.41
1:A:219:ARG:HD2	1:A:256:ARG:NH1	2.36	0.41
1:J:54:GLN:H	1:J:54:GLN:HG2	1.77	0.41
1:J:201:LEU:O	1:J:246:ALA:HA	2.21	0.41
2:K:27:VAL:HG23	2:K:30:PHE:CE1	2.56	0.41
1:A:14:ARG:HB2	1:A:17:ARG:HE	1.86	0.40
1:G:70:HIS:HB2	3:I:6:TYR:CE2	2.56	0.40
1:G:82:LEU:HD23	1:G:82:LEU:HA	1.96	0.40
2:H:41:LYS:O	2:H:44:GLU:HG3	2.21	0.40
1:A:181:ARG:O	1:A:181:ARG:HG2	2.20	0.40
1:J:103:VAL:HG13	1:J:168:LEU:HD23	2.03	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)
1:A:262:GLN:NE2	1:D:16:GLY:O[2_646]	2.11	0.09
1:G:108:ARG:NH1	2:H:85:VAL:O[2_546]	2.17	0.03

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	274/276 (99%)	263 (96%)	11 (4%)	0	100	100
1	D	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
1	G	274/276 (99%)	263 (96%)	11 (4%)	0	100	100
1	J	274/276 (99%)	265 (97%)	9 (3%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	E	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	H	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	K	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
3	I	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
3	L	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
All	All	1516/1540 (98%)	1463 (96%)	51 (3%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	3	ASN
3	I	5	ARG

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%)	221 (95%)	11 (5%)	23	35
1	D	232/232 (100%)	221 (95%)	11 (5%)	23	35
1	G	232/232 (100%)	218 (94%)	14 (6%)	17	25
1	J	232/232 (100%)	223 (96%)	9 (4%)	28	43
2	B	95/95 (100%)	91 (96%)	4 (4%)	26	40
2	E	95/95 (100%)	91 (96%)	4 (4%)	26	40
2	H	95/95 (100%)	89 (94%)	6 (6%)	16	23
2	K	95/95 (100%)	90 (95%)	5 (5%)	20	30
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	7
3	F	9/9 (100%)	9 (100%)	0	100	100
3	I	9/9 (100%)	8 (89%)	1 (11%)	6	7
3	L	9/9 (100%)	9 (100%)	0	100	100
All	All	1344/1344 (100%)	1278 (95%)	66 (5%)	22	34

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	25	VAL
1	A	86	ASN
1	A	105	SER
1	A	121	LYS
1	A	169	ARG
1	A	173	GLU
1	A	222	GLU
1	A	247	VAL
1	A	249	VAL
1	A	275	GLU
2	B	6	LYS
2	B	20	SER
2	B	75	LYS

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Mol	Chain	Res	Type
2	B	83	ASN
3	C	4	TYR
1	D	6	ARG
1	D	25	VAL
1	D	86	ASN
1	D	89	GLU
1	D	105	SER
1	D	173	GLU
1	D	248	VAL
1	D	249	VAL
1	D	255	GLN
1	D	272	LEU
1	D	275	GLU
2	E	1	ILE
2	E	20	SER
2	E	34	ASP
2	E	83	ASN
1	G	6	ARG
1	G	25	VAL
1	G	58	GLU
1	G	86	ASN
1	G	89	GLU
1	G	105	SER
1	G	169	ARG
1	G	173	GLU
1	G	222	GLU
1	G	224	GLN
1	G	247	VAL
1	G	249	VAL
1	G	272	LEU
1	G	275	GLU
2	H	6	LYS
2	H	20	SER
2	H	48	LYS
2	H	74	GLU
2	H	75	LYS
2	H	83	ASN
1	J	6	ARG
1	J	25	VAL
1	J	54	GLN
1	J	86	ASN
1	J	89	GLU

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Mol	Chain	Res	Type
1	J	105	SER
1	J	248	VAL
1	J	249	VAL
1	J	251	SER
2	K	1	ILE
2	K	20	SER
2	K	48	LYS
2	K	75	LYS
2	K	83	ASN
3	I	4	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	72	GLN
1	A	93	HIS
1	A	141	GLN
1	A	174	ASN
1	A	180	GLN
1	A	188	HIS
1	A	192	HIS
1	A	218	GLN
1	A	226	GLN
1	A	242	GLN
1	A	262	GLN
2	B	13	HIS
2	B	31	HIS
2	B	83	ASN
1	D	43	GLN
1	D	93	HIS
1	D	114	HIS
1	D	141	GLN
1	D	155	GLN
1	D	174	ASN
1	D	180	GLN
1	D	197	HIS
1	D	226	GLN
1	D	242	GLN
2	E	13	HIS
2	E	31	HIS
2	E	83	ASN

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Mol	Chain	Res	Type
1	G	43	GLN
1	G	93	HIS
1	G	141	GLN
1	G	174	ASN
1	G	180	GLN
1	G	192	HIS
1	G	218	GLN
1	G	242	GLN
1	G	255	GLN
2	H	13	HIS
2	H	31	HIS
2	H	83	ASN
1	J	43	GLN
1	J	93	HIS
1	J	141	GLN
1	J	151	HIS
1	J	155	GLN
1	J	174	ASN
1	J	180	GLN
1	J	242	GLN
2	K	13	HIS
2	K	31	HIS
2	K	83	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	276/276 (100%)	0.24	8 (2%) 53 56	20, 37, 61, 82	0
1	D	276/276 (100%)	0.40	10 (3%) 46 48	22, 43, 72, 90	0
1	G	276/276 (100%)	0.38	8 (2%) 53 56	24, 43, 67, 80	0
1	J	276/276 (100%)	0.12	1 (0%) 88 89	20, 35, 58, 81	0
2	B	100/100 (100%)	0.30	3 (3%) 52 54	20, 41, 73, 81	0
2	E	100/100 (100%)	0.10	1 (1%) 79 80	20, 33, 54, 64	0
2	H	100/100 (100%)	0.39	1 (1%) 79 80	25, 44, 70, 80	0
2	K	100/100 (100%)	0.36	2 (2%) 65 66	20, 41, 80, 102	0
3	C	9/9 (100%)	-0.09	0 100 100	23, 29, 38, 40	0
3	F	9/9 (100%)	0.44	0 100 100	34, 43, 54, 58	0
3	I	9/9 (100%)	0.64	1 (11%) 10 11	34, 40, 56, 65	0
3	L	9/9 (100%)	0.11	0 100 100	27, 34, 46, 50	0
All	All	1540/1540 (100%)	0.29	35 (2%) 61 63	20, 39, 68, 102	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	GLY	3.8
1	D	16	GLY	3.6
1	D	40	ALA	3.4
2	K	75	LYS	3.1
1	A	269	PRO	2.9
1	D	275	GLU	2.9
1	G	276	PRO	2.8
1	A	267	PRO	2.8
1	G	192	HIS	2.7
1	A	178	THR	2.6
1	D	17	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	138	MET	2.6
1	G	138	MET	2.6
1	G	225	THR	2.6
2	B	48	LYS	2.6
1	A	268	LYS	2.5
1	D	274	TRP	2.5
1	G	166	ASP	2.4
1	A	275	GLU	2.3
1	A	274	TRP	2.3
1	J	267	PRO	2.3
1	D	255	GLN	2.3
1	D	166	ASP	2.2
2	H	88	SER	2.2
2	B	19	LYS	2.2
1	G	223	ASP	2.1
2	E	47	GLU	2.1
3	I	4	TYR	2.1
1	G	60	TRP	2.1
1	D	145	ARG	2.1
2	B	99	MET	2.1
1	D	276	PRO	2.1
2	K	18	GLY	2.1
1	A	136	ALA	2.0
1	G	1	GLY	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.