



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:40 PM UTC

PDB ID : 8BS7 / pdb_00008bs7
Title : Multimerisation domain of Borna disease virus 1
Authors : Whitehead, J.D.; Grimes, J.M.; Keown, J.R.
Deposited on : 2022-11-24
Resolution : 3.20 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

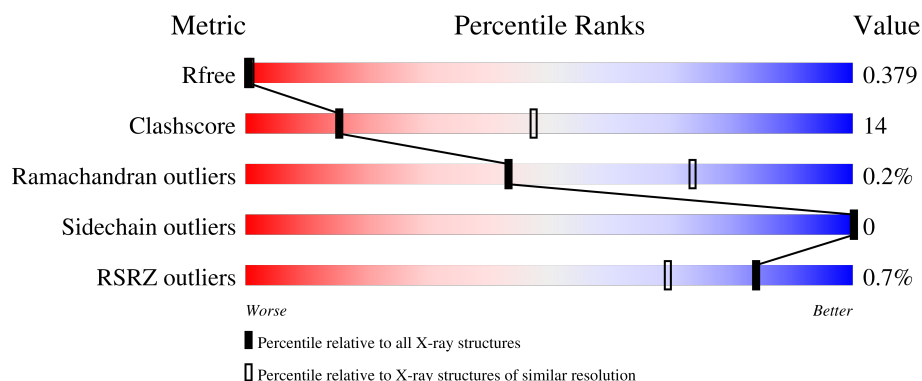
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	217	 23% 8% 69%
1	B	217	 26% 9% 65%
1	C	217	 28% 10% 63%
1	D	217	 27% 9% 63%
1	E	217	 25% 7% 67%

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Mol	Chain	Length	Quality of chain
1	F	217	 28% 6% 66%
1	G	217	 26% 5% 69%
1	H	217	 24% 9% 67%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9095 atoms, of which 4570 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 Phosphoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	68	Total	C	H	N	O	S	0	0	0
			1047	316	524	92	109	6			
1	B	76	Total	C	H	N	O	S	0	0	0
			1167	354	585	99	121	8			
1	C	81	Total	C	H	N	O	S	0	0	0
			1270	384	643	107	128	8			
1	D	80	Total	C	H	N	O	S	0	0	0
			1234	375	621	103	127	8			
1	E	71	Total	C	H	N	O	S	0	0	0
			1092	330	547	95	114	6			
1	F	74	Total	C	H	N	O	S	0	0	0
			1149	347	579	99	117	7			
1	G	68	Total	C	H	N	O	S	0	0	0
			1031	313	514	89	109	6			
1	H	71	Total	C	H	N	O	S	0	0	0
			1105	333	557	96	112	7			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP P0C799
A	-14	HIS	-	expression tag	UNP P0C799
A	-13	HIS	-	expression tag	UNP P0C799
A	-12	HIS	-	expression tag	UNP P0C799
A	-11	HIS	-	expression tag	UNP P0C799
A	-10	HIS	-	expression tag	UNP P0C799
A	-9	HIS	-	expression tag	UNP P0C799
A	-8	HIS	-	expression tag	UNP P0C799
A	-7	HIS	-	expression tag	UNP P0C799
A	-6	GLU	-	expression tag	UNP P0C799
A	-5	ASN	-	expression tag	UNP P0C799
A	-4	LEU	-	expression tag	UNP P0C799
A	-3	TYR	-	expression tag	UNP P0C799

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PHE	-	expression tag	UNP P0C799
A	-1	GLN	-	expression tag	UNP P0C799
A	0	GLY	-	expression tag	UNP P0C799
B	-15	MET	-	initiating methionine	UNP P0C799
B	-14	HIS	-	expression tag	UNP P0C799
B	-13	HIS	-	expression tag	UNP P0C799
B	-12	HIS	-	expression tag	UNP P0C799
B	-11	HIS	-	expression tag	UNP P0C799
B	-10	HIS	-	expression tag	UNP P0C799
B	-9	HIS	-	expression tag	UNP P0C799
B	-8	HIS	-	expression tag	UNP P0C799
B	-7	HIS	-	expression tag	UNP P0C799
B	-6	GLU	-	expression tag	UNP P0C799
B	-5	ASN	-	expression tag	UNP P0C799
B	-4	LEU	-	expression tag	UNP P0C799
B	-3	TYR	-	expression tag	UNP P0C799
B	-2	PHE	-	expression tag	UNP P0C799
B	-1	GLN	-	expression tag	UNP P0C799
B	0	GLY	-	expression tag	UNP P0C799
C	-15	MET	-	initiating methionine	UNP P0C799
C	-14	HIS	-	expression tag	UNP P0C799
C	-13	HIS	-	expression tag	UNP P0C799
C	-12	HIS	-	expression tag	UNP P0C799
C	-11	HIS	-	expression tag	UNP P0C799
C	-10	HIS	-	expression tag	UNP P0C799
C	-9	HIS	-	expression tag	UNP P0C799
C	-8	HIS	-	expression tag	UNP P0C799
C	-7	HIS	-	expression tag	UNP P0C799
C	-6	GLU	-	expression tag	UNP P0C799
C	-5	ASN	-	expression tag	UNP P0C799
C	-4	LEU	-	expression tag	UNP P0C799
C	-3	TYR	-	expression tag	UNP P0C799
C	-2	PHE	-	expression tag	UNP P0C799
C	-1	GLN	-	expression tag	UNP P0C799
C	0	GLY	-	expression tag	UNP P0C799
D	-15	MET	-	initiating methionine	UNP P0C799
D	-14	HIS	-	expression tag	UNP P0C799
D	-13	HIS	-	expression tag	UNP P0C799
D	-12	HIS	-	expression tag	UNP P0C799
D	-11	HIS	-	expression tag	UNP P0C799
D	-10	HIS	-	expression tag	UNP P0C799
D	-9	HIS	-	expression tag	UNP P0C799

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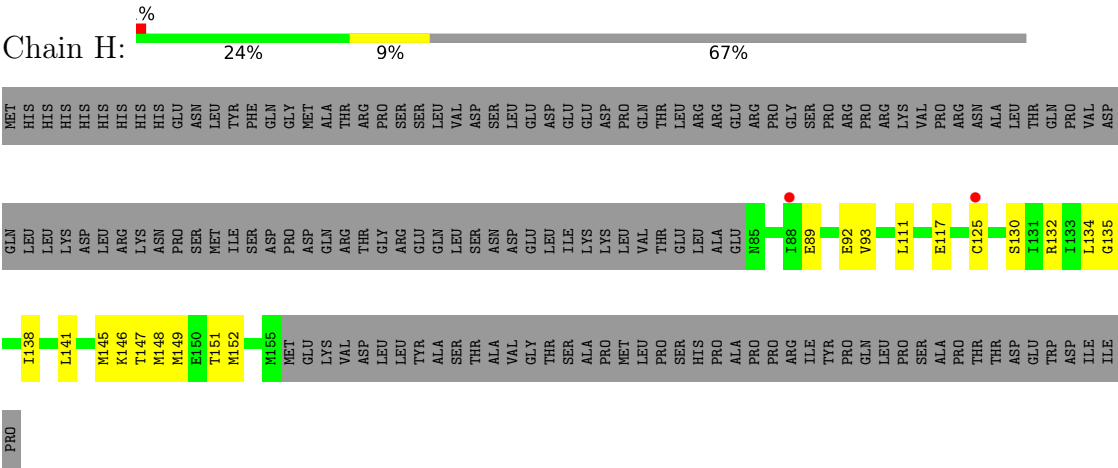
Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	HIS	-	expression tag	UNP P0C799
D	-7	HIS	-	expression tag	UNP P0C799
D	-6	GLU	-	expression tag	UNP P0C799
D	-5	ASN	-	expression tag	UNP P0C799
D	-4	LEU	-	expression tag	UNP P0C799
D	-3	TYR	-	expression tag	UNP P0C799
D	-2	PHE	-	expression tag	UNP P0C799
D	-1	GLN	-	expression tag	UNP P0C799
D	0	GLY	-	expression tag	UNP P0C799
E	-15	MET	-	initiating methionine	UNP P0C799
E	-14	HIS	-	expression tag	UNP P0C799
E	-13	HIS	-	expression tag	UNP P0C799
E	-12	HIS	-	expression tag	UNP P0C799
E	-11	HIS	-	expression tag	UNP P0C799
E	-10	HIS	-	expression tag	UNP P0C799
E	-9	HIS	-	expression tag	UNP P0C799
E	-8	HIS	-	expression tag	UNP P0C799
E	-7	HIS	-	expression tag	UNP P0C799
E	-6	GLU	-	expression tag	UNP P0C799
E	-5	ASN	-	expression tag	UNP P0C799
E	-4	LEU	-	expression tag	UNP P0C799
E	-3	TYR	-	expression tag	UNP P0C799
E	-2	PHE	-	expression tag	UNP P0C799
E	-1	GLN	-	expression tag	UNP P0C799
E	0	GLY	-	expression tag	UNP P0C799
F	-15	MET	-	initiating methionine	UNP P0C799
F	-14	HIS	-	expression tag	UNP P0C799
F	-13	HIS	-	expression tag	UNP P0C799
F	-12	HIS	-	expression tag	UNP P0C799
F	-11	HIS	-	expression tag	UNP P0C799
F	-10	HIS	-	expression tag	UNP P0C799
F	-9	HIS	-	expression tag	UNP P0C799
F	-8	HIS	-	expression tag	UNP P0C799
F	-7	HIS	-	expression tag	UNP P0C799
F	-6	GLU	-	expression tag	UNP P0C799
F	-5	ASN	-	expression tag	UNP P0C799
F	-4	LEU	-	expression tag	UNP P0C799
F	-3	TYR	-	expression tag	UNP P0C799
F	-2	PHE	-	expression tag	UNP P0C799
F	-1	GLN	-	expression tag	UNP P0C799
F	0	GLY	-	expression tag	UNP P0C799
G	-15	MET	-	initiating methionine	UNP P0C799

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	HIS	-	expression tag	UNP P0C799
G	-13	HIS	-	expression tag	UNP P0C799
G	-12	HIS	-	expression tag	UNP P0C799
G	-11	HIS	-	expression tag	UNP P0C799
G	-10	HIS	-	expression tag	UNP P0C799
G	-9	HIS	-	expression tag	UNP P0C799
G	-8	HIS	-	expression tag	UNP P0C799
G	-7	HIS	-	expression tag	UNP P0C799
G	-6	GLU	-	expression tag	UNP P0C799
G	-5	ASN	-	expression tag	UNP P0C799
G	-4	LEU	-	expression tag	UNP P0C799
G	-3	TYR	-	expression tag	UNP P0C799
G	-2	PHE	-	expression tag	UNP P0C799
G	-1	GLN	-	expression tag	UNP P0C799
G	0	GLY	-	expression tag	UNP P0C799
H	-15	MET	-	initiating methionine	UNP P0C799
H	-14	HIS	-	expression tag	UNP P0C799
H	-13	HIS	-	expression tag	UNP P0C799
H	-12	HIS	-	expression tag	UNP P0C799
H	-11	HIS	-	expression tag	UNP P0C799
H	-10	HIS	-	expression tag	UNP P0C799
H	-9	HIS	-	expression tag	UNP P0C799
H	-8	HIS	-	expression tag	UNP P0C799
H	-7	HIS	-	expression tag	UNP P0C799
H	-6	GLU	-	expression tag	UNP P0C799
H	-5	ASN	-	expression tag	UNP P0C799
H	-4	LEU	-	expression tag	UNP P0C799
H	-3	TYR	-	expression tag	UNP P0C799
H	-2	PHE	-	expression tag	UNP P0C799
H	-1	GLN	-	expression tag	UNP P0C799
H	0	GLY	-	expression tag	UNP P0C799





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	34.87Å 35.15Å 153.12Å 89.97° 90.01° 90.54°	Depositor
Resolution (Å)	51.04 – 3.20 51.04 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.3 (51.04-3.20) 82.1 (51.04-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.335 , 0.387 0.337 , 0.379	Depositor DCC
R_{free} test set	589 reflections (3.91%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 166.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.367 for -k,h,l 0.367 for k,-h,l 0.397 for h,-k,-l 0.367 for -h,k,-l 0.377 for -h,-k,l 0.377 for -k,-h,-l 0.378 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9095	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 28.46 % 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 1.8354e-03. 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 [i](#)

5.1 Standard geometry [i](#)

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	0.11	0/524	0.26	0/700
1	B	0.12	0/583	0.24	0/777
1	C	0.10	0/628	0.26	0/838
1	D	0.11	0/614	0.26	0/820
1	E	0.11	0/546	0.27	0/730
1	F	0.12	0/571	0.27	0/762
1	G	0.10	0/518	0.24	0/693
1	H	0.11	0/549	0.28	0/732
All	All	0.11	0/4533	0.26	0/6052

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	523	524	524	30	0
1	B	582	585	585	26	0
1	C	627	643	642	24	0
1	D	613	621	620	32	0
1	E	545	547	546	25	0
1	F	570	579	579	21	0
1	G	517	514	513	17	0
1	H	548	557	557	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4525	4570	4566	123	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 14.

All (123) 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:B:141:LEU:HD22	1:C:141:LEU:HD21	1.52	0.92
1:E:141:LEU:HD21	1:H:141:LEU:HD23	1.56	0.86
1:A:145:MET:HE2	1:D:145:MET:HE1	1.60	0.83
1:C:109:GLU:OE1	1:H:132:ARG:NH1	2.19	0.75
1:A:147:THR:O	1:A:151:THR:HG23	1.89	0.73
1:C:99:ASP:OD1	1:C:100:ILE:N	2.22	0.72
1:G:147:THR:O	1:G:151:THR:HG23	1.92	0.69
1:E:145:MET:HE1	1:F:145:MET:CG	2.23	0.68
1:E:134:LEU:HD23	1:F:134:LEU:HD21	1.76	0.67
1:D:84:GLU:O	1:D:88:ILE:HD12	1.95	0.67
1:A:145:MET:HE1	1:B:145:MET:SD	2.34	0.67
1:A:134:LEU:HD21	1:D:138:ILE:HD13	1.77	0.66
1:A:145:MET:HE2	1:D:145:MET:CE	2.24	0.66
1:C:134:LEU:HD23	1:D:134:LEU:HD21	1.77	0.66
1:A:145:MET:HE3	1:B:141:LEU:HD21	1.76	0.65
1:B:117:GLU:O	1:B:121:THR:HG23	1.97	0.64
1:C:141:LEU:HD23	1:D:141:LEU:CD1	2.27	0.64
1:F:134:LEU:HD23	1:G:134:LEU:CD1	2.27	0.64
1:A:134:LEU:HD21	1:D:138:ILE:CD1	2.29	0.63
1:E:141:LEU:HG	1:H:145:MET:HE3	1.81	0.62
1:E:148:MET:O	1:E:152:MET:HE3	2.00	0.61
1:F:147:THR:O	1:F:151:THR:HG23	2.01	0.61
1:D:89:GLU:O	1:D:93:VAL:HG23	2.01	0.59
1:D:158:LYS:HA	1:D:161:LEU:HD23	1.86	0.58
1:B:115:GLN:HB3	1:C:114:LEU:HD22	1.85	0.58
1:C:141:LEU:HD23	1:D:141:LEU:HD13	1.85	0.58
1:H:147:THR:O	1:H:151:THR:HG23	2.04	0.58
1:E:145:MET:HE1	1:F:145:MET:HG3	1.85	0.58
1:E:141:LEU:CD2	1:H:141:LEU:HD23	2.32	0.57
1:E:145:MET:HE1	1:F:145:MET:HG2	1.85	0.57
1:G:119:ILE:HD12	1:H:117:GLU:HG2	1.86	0.56
1:E:148:MET:SD	1:H:148:MET:HE2	2.45	0.56
1:H:92:GLU:OE2	1:H:93:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:MET:HE3	1:C:148:MET:SD	2.46	0.55
1:D:147:THR:O	1:D:151:THR:HG23	2.07	0.55
1:E:134:LEU:CD2	1:F:134:LEU:HD21	2.36	0.55
1:A:134:LEU:HD11	1:D:134:LEU:HD23	1.88	0.55
1:A:152:MET:CE	1:B:152:MET:HE2	2.37	0.54
1:B:154:LEU:HD12	1:E:87:MET:SD	2.48	0.54
1:E:141:LEU:HD21	1:H:141:LEU:CD2	2.33	0.54
1:F:134:LEU:HD23	1:G:134:LEU:HD11	1.88	0.54
1:B:136:GLU:OE2	1:B:140:ILE:HD11	2.08	0.53
1:D:146:LYS:O	1:D:149:MET:HG2	2.09	0.53
1:A:145:MET:HE1	1:B:145:MET:CG	2.39	0.53
1:A:138:ILE:CD1	1:B:138:ILE:HD11	2.40	0.52
1:E:147:THR:O	1:E:151:THR:HG23	2.09	0.52
1:F:134:LEU:HD23	1:G:134:LEU:HD13	1.91	0.52
1:B:99:ASP:OD2	1:B:103:ARG:NH2	2.42	0.51
1:A:141:LEU:HD23	1:B:141:LEU:CD1	2.40	0.51
1:C:108:PHE:HD1	1:D:111:LEU:HD11	1.75	0.51
1:C:99:ASP:OD1	1:C:99:ASP:C	2.53	0.51
1:A:149:MET:HE3	1:B:147:THR:HG21	1.92	0.51
1:C:112:SER:O	1:C:116:VAL:HG23	2.11	0.51
1:F:119:ILE:HD12	1:G:117:GLU:HG2	1.93	0.51
1:B:100:ILE:O	1:B:104:ILE:HG13	2.10	0.50
1:C:114:LEU:O	1:C:114:LEU:HD23	2.11	0.50
1:A:152:MET:HE1	1:B:152:MET:HE2	1.93	0.50
1:G:131:ILE:HG21	1:H:130:SER:HB3	1.94	0.50
1:C:137:ASN:HA	1:C:140:ILE:HD12	1.93	0.50
1:E:116:VAL:HG12	1:E:120:GLN:OE1	2.12	0.50
1:D:84:GLU:HG2	1:D:88:ILE:HD11	1.93	0.49
1:B:97:LEU:HD22	1:C:100:ILE:CD1	2.42	0.49
1:C:134:LEU:CD2	1:D:134:LEU:HD21	2.44	0.48
1:G:145:MET:HE2	1:H:145:MET:HG2	1.96	0.48
1:A:134:LEU:HD23	1:A:134:LEU:O	2.14	0.48
1:A:148:MET:HE1	1:D:145:MET:CE	2.43	0.48
1:G:111:LEU:HB3	1:H:111:LEU:HD11	1.94	0.48
1:A:145:MET:HE1	1:B:145:MET:HG2	1.95	0.48
1:E:125:CYS:SG	1:H:125:CYS:HB2	2.54	0.47
1:C:145:MET:CE	1:D:141:LEU:HD22	2.43	0.47
1:G:119:ILE:HD12	1:H:117:GLU:CG	2.45	0.47
1:A:141:LEU:HD23	1:B:141:LEU:HD13	1.97	0.47
1:A:134:LEU:CD1	1:D:134:LEU:HD23	2.45	0.47
1:A:117:GLU:HG2	1:D:119:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:ALA:O	1:F:116:VAL:HG22	2.15	0.47
1:A:134:LEU:HD23	1:A:134:LEU:C	2.40	0.46
1:A:148:MET:HE1	1:D:145:MET:HE2	1.98	0.46
1:A:115:GLN:HE22	1:B:115:GLN:HG3	1.80	0.46
1:E:134:LEU:HD23	1:F:134:LEU:CD2	2.44	0.46
1:E:145:MET:HE2	1:F:141:LEU:CD1	2.46	0.46
1:F:141:LEU:HD23	1:G:141:LEU:CD2	2.46	0.46
1:E:151:THR:OG1	1:E:152:MET:N	2.49	0.46
1:D:88:ILE:HD12	1:D:88:ILE:H	1.82	0.45
1:E:145:MET:SD	1:H:145:MET:HE1	2.56	0.45
1:H:146:LYS:HA	1:H:149:MET:HE3	1.97	0.45
1:B:152:MET:HE1	1:C:152:MET:HE3	1.99	0.45
1:F:107:GLY:O	1:F:111:LEU:HD23	2.17	0.44
1:A:90:ALA:O	1:A:93:VAL:HG12	2.17	0.44
1:G:152:MET:SD	1:H:152:MET:HE1	2.58	0.44
1:A:91:GLU:O	1:A:94:ARG:HG2	2.18	0.44
1:A:138:ILE:HD13	1:B:138:ILE:HD11	2.00	0.44
1:E:134:LEU:CD1	1:H:135:GLY:HA2	2.48	0.44
1:F:141:LEU:HD23	1:G:141:LEU:HD21	1.99	0.44
1:C:141:LEU:HD23	1:D:141:LEU:HD11	1.98	0.44
1:A:114:LEU:HD21	1:D:116:VAL:HG23	2.00	0.43
1:G:135:GLY:HA2	1:H:134:LEU:CD1	2.48	0.43
1:G:141:LEU:CD2	1:H:141:LEU:HD21	2.47	0.43
1:C:138:ILE:CD1	1:D:138:ILE:HD11	2.48	0.43
1:F:82:LEU:O	1:F:82:LEU:HD23	2.18	0.43
1:H:89:GLU:O	1:H:92:GLU:HG3	2.19	0.43
1:D:142:ASP:HA	1:D:145:MET:HG3	2.01	0.43
1:F:145:MET:HE1	1:G:145:MET:CG	2.48	0.43
1:E:112:SER:O	1:E:116:VAL:HG23	2.18	0.42
1:H:148:MET:O	1:H:152:MET:HG2	2.18	0.42
1:E:145:MET:HE2	1:F:141:LEU:HD12	2.02	0.42
1:B:145:MET:HE3	1:C:144:SER:HB2	2.02	0.42
1:A:148:MET:CE	1:D:145:MET:HE2	2.50	0.42
1:F:90:ALA:O	1:F:93:VAL:HG12	2.19	0.42
1:E:129:ASP:O	1:E:133:ILE:HG13	2.19	0.42
1:F:115:GLN:HE21	1:G:111:LEU:HD22	1.84	0.42
1:D:93:VAL:HG12	1:D:97:LEU:HD13	2.01	0.41
1:E:89:GLU:O	1:E:93:VAL:HG23	2.20	0.41
1:D:161:LEU:O	1:D:162:LEU:C	2.63	0.41
1:B:113:ALA:O	1:B:117:GLU:HG3	2.21	0.41
1:C:115:GLN:OE1	1:D:111:LEU:HD22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:HG3	1:A:133:ILE:N	2.36	0.41
1:A:134:LEU:CD2	1:D:138:ILE:HD13	2.47	0.40
1:B:155:MET:HE3	1:B:155:MET:HB2	2.01	0.40
1:C:85:ASN:O	1:C:89:GLU:HG2	2.21	0.40
1:C:155:MET:HE3	1:D:155:MET:HE1	2.02	0.40
1:B:156:MET:HE3	1:B:156:MET:HA	2.03	0.40
1:C:161:LEU:HD23	1:C:161:LEU:N	2.36	0.40
1:E:134:LEU:CD1	1:H:138:ILE:HD12	2.52	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	66/217 (30%)	66 (100%)	0	0	100	100
1	B	74/217 (34%)	74 (100%)	0	0	100	100
1	C	79/217 (36%)	78 (99%)	1 (1%)	0	100	100
1	D	78/217 (36%)	77 (99%)	0	1 (1%)	9	40
1	E	69/217 (32%)	68 (99%)	1 (1%)	0	100	100
1	F	72/217 (33%)	72 (100%)	0	0	100	100
1	G	66/217 (30%)	66 (100%)	0	0	100	100
1	H	69/217 (32%)	69 (100%)	0	0	100	100
All	All	573/1736 (33%)	570 (100%)	2 (0%)	1 (0%)	43	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	161	LEU

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	59/196 (30%)	59 (100%)	0	100	100
1	B	65/196 (33%)	65 (100%)	0	100	100
1	C	71/196 (36%)	71 (100%)	0	100	100
1	D	69/196 (35%)	69 (100%)	0	100	100
1	E	61/196 (31%)	61 (100%)	0	100	100
1	F	64/196 (33%)	64 (100%)	0	100	100
1	G	58/196 (30%)	58 (100%)	0	100	100
1	H	62/196 (32%)	62 (100%)	0	100	100
All	All	509/1568 (32%)	509 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	137	ASN
1	B	85	ASN
1	C	85	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	68/217 (31%)	-0.64	0 100 100	33, 42, 57, 63	0
1	B	76/217 (35%)	-0.36	0 100 100	31, 44, 66, 81	0
1	C	81/217 (37%)	-0.43	0 100 100	33, 44, 69, 76	0
1	D	80/217 (36%)	-0.54	0 100 100	29, 46, 74, 94	0
1	E	71/217 (32%)	-0.35	2 (2%) 55 35	31, 43, 72, 102	0
1	F	74/217 (34%)	-0.45	0 100 100	36, 45, 73, 92	0
1	G	68/217 (31%)	-0.45	0 100 100	32, 42, 55, 61	0
1	H	71/217 (32%)	-0.34	2 (2%) 55 35	31, 45, 67, 92	0
All	All	589/1736 (33%)	-0.44	4 (0%) 84 69	29, 44, 71, 102	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	125	CYS	2.5
1	E	131	ILE	2.4
1	E	138	ILE	2.4
1	H	88	ILE	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.