



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:46 AM UTC

PDB ID : 8IGL / pdb_00008igl
Title : Crystal structure of a major fragment of the ASFV inner capsid protein p150
Authors : Li, H.; Liu, Q.; Xiang, Y.
Deposited on : 2023-02-20
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

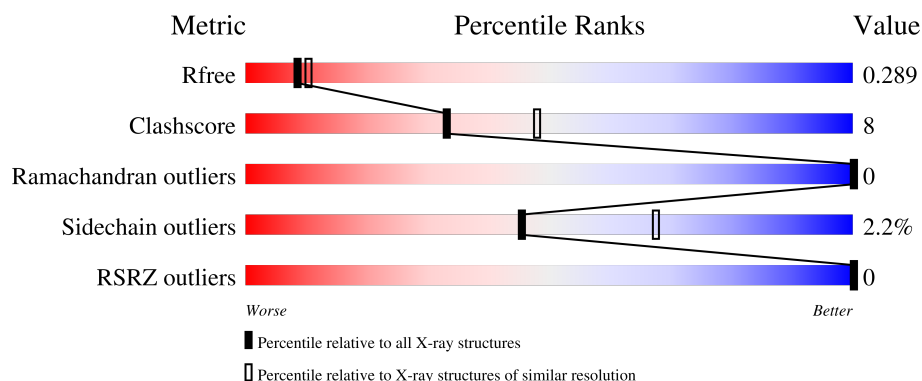
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	883	
1	B	883	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26172 atoms, of which 12696 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 CP2475L.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	793	Total	C	H	N	O	S	0	0	0
			12733	4053	6355	1112	1192	21			
1	B	792	Total	C	H	N	O	S	0	0	0
			12714	4050	6341	1111	1191	21			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-47	MET	-	initiating methionine	UNP A0A2X0THU5
A	-46	HIS	-	expression tag	UNP A0A2X0THU5
A	-45	HIS	-	expression tag	UNP A0A2X0THU5
A	-44	HIS	-	expression tag	UNP A0A2X0THU5
A	-43	HIS	-	expression tag	UNP A0A2X0THU5
A	-42	HIS	-	expression tag	UNP A0A2X0THU5
A	-41	HIS	-	expression tag	UNP A0A2X0THU5
A	-40	HIS	-	expression tag	UNP A0A2X0THU5
A	-39	HIS	-	expression tag	UNP A0A2X0THU5
A	-38	HIS	-	expression tag	UNP A0A2X0THU5
A	-37	HIS	-	expression tag	UNP A0A2X0THU5
A	-36	GLY	-	expression tag	UNP A0A2X0THU5
A	-35	SER	-	expression tag	UNP A0A2X0THU5
A	-34	ASP	-	expression tag	UNP A0A2X0THU5
A	-33	TYR	-	expression tag	UNP A0A2X0THU5
A	-32	LYS	-	expression tag	UNP A0A2X0THU5
A	-31	ASP	-	expression tag	UNP A0A2X0THU5
A	-30	HIS	-	expression tag	UNP A0A2X0THU5
A	-29	ASP	-	expression tag	UNP A0A2X0THU5
A	-28	GLY	-	expression tag	UNP A0A2X0THU5
A	-27	ASP	-	expression tag	UNP A0A2X0THU5
A	-26	TYR	-	expression tag	UNP A0A2X0THU5
A	-25	LYS	-	expression tag	UNP A0A2X0THU5
A	-24	ASP	-	expression tag	UNP A0A2X0THU5
A	-23	HIS	-	expression tag	UNP A0A2X0THU5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	ASP	-	expression tag	UNP A0A2X0THU5
A	-21	ILE	-	expression tag	UNP A0A2X0THU5
A	-20	ASP	-	expression tag	UNP A0A2X0THU5
A	-19	TYR	-	expression tag	UNP A0A2X0THU5
A	-18	LYS	-	expression tag	UNP A0A2X0THU5
A	-17	ASP	-	expression tag	UNP A0A2X0THU5
A	-16	ASP	-	expression tag	UNP A0A2X0THU5
A	-15	ASP	-	expression tag	UNP A0A2X0THU5
A	-14	ASP	-	expression tag	UNP A0A2X0THU5
A	-13	LYS	-	expression tag	UNP A0A2X0THU5
A	-12	GLU	-	expression tag	UNP A0A2X0THU5
A	-11	LEU	-	expression tag	UNP A0A2X0THU5
A	-10	GLU	-	expression tag	UNP A0A2X0THU5
A	-9	ASN	-	expression tag	UNP A0A2X0THU5
A	-8	LEU	-	expression tag	UNP A0A2X0THU5
A	-7	TYR	-	expression tag	UNP A0A2X0THU5
A	-6	PHE	-	expression tag	UNP A0A2X0THU5
A	-5	GLN	-	expression tag	UNP A0A2X0THU5
A	-4	GLY	-	expression tag	UNP A0A2X0THU5
A	-3	ALA	-	expression tag	UNP A0A2X0THU5
A	-2	GLY	-	expression tag	UNP A0A2X0THU5
A	-1	SER	-	expression tag	UNP A0A2X0THU5
A	0	MET	-	expression tag	UNP A0A2X0THU5
B	-47	MET	-	initiating methionine	UNP A0A2X0THU5
B	-46	HIS	-	expression tag	UNP A0A2X0THU5
B	-45	HIS	-	expression tag	UNP A0A2X0THU5
B	-44	HIS	-	expression tag	UNP A0A2X0THU5
B	-43	HIS	-	expression tag	UNP A0A2X0THU5
B	-42	HIS	-	expression tag	UNP A0A2X0THU5
B	-41	HIS	-	expression tag	UNP A0A2X0THU5
B	-40	HIS	-	expression tag	UNP A0A2X0THU5
B	-39	HIS	-	expression tag	UNP A0A2X0THU5
B	-38	HIS	-	expression tag	UNP A0A2X0THU5
B	-37	HIS	-	expression tag	UNP A0A2X0THU5
B	-36	GLY	-	expression tag	UNP A0A2X0THU5
B	-35	SER	-	expression tag	UNP A0A2X0THU5
B	-34	ASP	-	expression tag	UNP A0A2X0THU5
B	-33	TYR	-	expression tag	UNP A0A2X0THU5
B	-32	LYS	-	expression tag	UNP A0A2X0THU5
B	-31	ASP	-	expression tag	UNP A0A2X0THU5
B	-30	HIS	-	expression tag	UNP A0A2X0THU5
B	-29	ASP	-	expression tag	UNP A0A2X0THU5

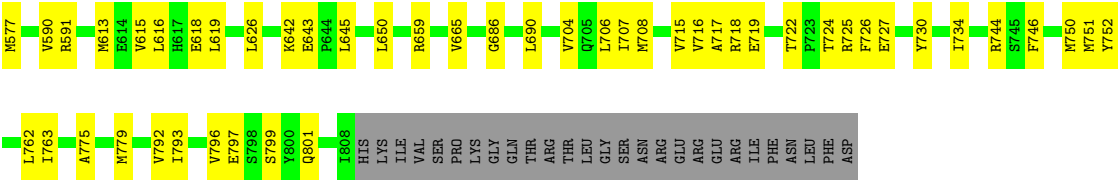
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-28	GLY	-	expression tag	UNP A0A2X0THU5
B	-27	ASP	-	expression tag	UNP A0A2X0THU5
B	-26	TYR	-	expression tag	UNP A0A2X0THU5
B	-25	LYS	-	expression tag	UNP A0A2X0THU5
B	-24	ASP	-	expression tag	UNP A0A2X0THU5
B	-23	HIS	-	expression tag	UNP A0A2X0THU5
B	-22	ASP	-	expression tag	UNP A0A2X0THU5
B	-21	ILE	-	expression tag	UNP A0A2X0THU5
B	-20	ASP	-	expression tag	UNP A0A2X0THU5
B	-19	TYR	-	expression tag	UNP A0A2X0THU5
B	-18	LYS	-	expression tag	UNP A0A2X0THU5
B	-17	ASP	-	expression tag	UNP A0A2X0THU5
B	-16	ASP	-	expression tag	UNP A0A2X0THU5
B	-15	ASP	-	expression tag	UNP A0A2X0THU5
B	-14	ASP	-	expression tag	UNP A0A2X0THU5
B	-13	LYS	-	expression tag	UNP A0A2X0THU5
B	-12	GLU	-	expression tag	UNP A0A2X0THU5
B	-11	LEU	-	expression tag	UNP A0A2X0THU5
B	-10	GLU	-	expression tag	UNP A0A2X0THU5
B	-9	ASN	-	expression tag	UNP A0A2X0THU5
B	-8	LEU	-	expression tag	UNP A0A2X0THU5
B	-7	TYR	-	expression tag	UNP A0A2X0THU5
B	-6	PHE	-	expression tag	UNP A0A2X0THU5
B	-5	GLN	-	expression tag	UNP A0A2X0THU5
B	-4	GLY	-	expression tag	UNP A0A2X0THU5
B	-3	ALA	-	expression tag	UNP A0A2X0THU5
B	-2	GLY	-	expression tag	UNP A0A2X0THU5
B	-1	SER	-	expression tag	UNP A0A2X0THU5
B	0	MET	-	expression tag	UNP A0A2X0THU5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	370	Total O 370 370	0	0
2	B	355	Total O 355 355	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.44Å 65.60Å 115.01Å 99.21° 92.70° 90.16°	Depositor
Resolution (Å)	32.54 – 2.40 32.54 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (32.54-2.40) 95.2 (32.54-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.97 (at 2.29Å)	Xtriage
Refinement program	PHENIX Version 1.20.1-4487	Depositor
R, R_{free}	0.238 , 0.283 0.246 , 0.289	Depositor DCC
R_{free} test set	3287 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	9.5	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 13.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	26172	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	6/6502 (0.1%)	0.56	5/8823 (0.1%)
1	B	0.28	2/6496 (0.0%)	0.50	7/8813 (0.1%)
All	All	0.32	8/12998 (0.1%)	0.53	12/17636 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	700	ASP	C-O	-7.69	1.14	1.24
1	B	490	TYR	C-O	-6.49	1.16	1.24
1	A	165	GLN	C-O	-6.38	1.16	1.24
1	A	466	ARG	C-O	-6.20	1.16	1.24
1	A	702	PRO	C-O	-5.64	1.16	1.24
1	A	586	THR	C-O	-5.50	1.16	1.23
1	A	689	LYS	C-O	-5.06	1.18	1.24
1	B	134	LEU	C-O	-5.02	1.18	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	GLN	N-CA-C	7.04	120.72	109.24
1	B	338	ARG	CA-C-O	-6.72	113.94	121.40
1	B	690	LEU	CA-C-N	6.29	129.87	120.31
1	B	690	LEU	C-N-CA	6.29	129.87	120.31
1	B	643	GLU	CA-C-N	5.67	125.43	119.76
1	B	643	GLU	C-N-CA	5.67	125.43	119.76
1	A	550	ASN	CB-CA-C	5.47	119.24	110.16
1	A	173	THR	CA-C-O	-5.22	115.87	121.56
1	A	585	ASN	N-CA-CB	-5.21	103.53	111.66
1	A	385	ARG	CB-CA-C	5.19	119.11	111.17
1	A	343	GLN	CA-CB-CG	5.11	124.32	114.10
1	B	488	PRO	CA-C-O	-5.10	115.64	121.56

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	6378	6355	6353	97	0
1	B	6373	6341	6347	103	0
2	A	370	0	0	31	0
2	B	355	0	0	26	0
All	All	13476	12696	12700	199	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 8.

All (199) 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:751:MET:SD	2:B:1100:HOH:O	2.30	0.90
1:B:206:ASP:HB3	1:B:209:ILE:HD12	1.54	0.90
1:B:613:MET:HE3	1:B:613:MET:HA	1.61	0.81
1:B:722:THR:HG22	2:B:979:HOH:O	1.82	0.77
1:B:650:LEU:HD22	1:B:792:VAL:HG13	1.67	0.76
1:B:388:MET:SD	2:B:1137:HOH:O	2.43	0.75
1:A:617:HIS:ND1	2:A:902:HOH:O	2.21	0.74
1:B:420:ASN:ND2	2:B:902:HOH:O	2.20	0.74
1:B:112:LEU:HD21	1:B:275:LEU:HD21	1.69	0.74
1:A:281:ARG:HD3	2:A:1023:HOH:O	1.87	0.73
1:B:97:GLU:OE2	1:B:275:LEU:HB2	1.90	0.72
1:B:163:MET:HE3	1:B:186:LEU:HD22	1.74	0.69
1:A:423:PHE:HA	2:A:980:HOH:O	1.92	0.69
1:A:317:ASN:ND2	2:A:909:HOH:O	2.26	0.69
1:B:466:ARG:NH1	2:B:909:HOH:O	2.26	0.69
1:A:452:GLU:HG3	1:A:596:ALA:HB1	1.75	0.68
1:B:411:TYR:HB3	1:B:414:LEU:HD13	1.74	0.67
1:A:330:ASP:OD2	1:A:373:ARG:NH2	2.26	0.67
1:B:414:LEU:HD12	1:B:615:VAL:HG21	1.76	0.67
1:B:311:PHE:CB	1:B:388:MET:HE2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:MET:HE1	1:B:616:LEU:HD23	1.76	0.66
1:B:659:ARG:NH1	2:B:915:HOH:O	2.29	0.66
1:B:83:ILE:HD11	1:B:110:GLU:HG3	1.78	0.65
1:A:394:LEU:HD21	1:A:505:MET:HE2	1.80	0.64
1:B:339:THR:HG21	1:B:563:LEU:CD1	2.27	0.64
1:B:550:ASN:ND2	2:B:917:HOH:O	2.31	0.64
1:A:626:LEU:HD12	1:A:796:VAL:HG21	1.80	0.63
1:A:715:VAL:HG22	1:A:719:GLU:OE1	1.98	0.62
1:A:474:GLN:HA	2:A:914:HOH:O	1.98	0.62
1:A:16:LEU:HD13	1:A:191:MET:SD	2.39	0.62
1:B:97:GLU:OE2	1:B:275:LEU:CB	2.48	0.62
1:B:465:GLN:OE1	1:B:466:ARG:NH2	2.33	0.62
1:B:412:LEU:HD13	1:B:480:LEU:HD13	1.81	0.61
1:B:174:ALA:HB3	1:B:264:THR:HA	1.82	0.60
1:A:487:ILE:HG23	1:A:491:LEU:HD23	1.84	0.60
1:A:156:MET:HE1	1:A:739:PHE:HZ	1.66	0.60
1:B:89:MET:HE1	1:B:315:LEU:HD11	1.84	0.59
1:B:722:THR:HG23	1:B:725:ARG:H	1.67	0.59
1:A:106:ASN:HA	1:A:282:ARG:HD2	1.85	0.59
1:B:89:MET:HE2	1:B:535:LEU:HD13	1.84	0.59
1:A:329:GLY:N	2:A:919:HOH:O	2.32	0.58
1:A:447:ARG:C	1:A:579:LEU:HD21	2.28	0.58
1:B:19:ILE:O	1:B:23:LEU:HD13	2.03	0.58
1:B:591:ARG:NH2	2:B:919:HOH:O	2.35	0.58
1:B:311:PHE:HB3	1:B:388:MET:HE2	1.86	0.57
1:A:453:GLN:HA	2:A:1120:HOH:O	2.04	0.57
1:B:451:THR:OG1	1:B:574:VAL:O	2.22	0.57
1:B:166:VAL:HG22	1:B:178:LEU:HD22	1.87	0.57
1:B:235:LYS:O	1:B:235:LYS:HD3	2.05	0.57
1:A:625:TYR:CE1	1:A:626:LEU:HD23	2.40	0.56
1:A:2:ILE:N	2:A:931:HOH:O	2.39	0.56
1:B:60:ILE:HB	2:B:992:HOH:O	2.06	0.56
1:A:730:TYR:O	1:A:734:ILE:HG12	2.06	0.55
1:B:216:ARG:HG3	1:B:216:ARG:HH11	1.69	0.55
1:A:448:GLY:HA2	1:A:579:LEU:HD23	1.88	0.55
1:A:452:GLU:CG	1:A:596:ALA:HB1	2.36	0.55
1:B:645:LEU:HD11	1:B:801:GLN:HB3	1.89	0.55
1:A:404:ASP:OD1	1:A:490:TYR:OH	2.24	0.55
1:A:280:GLN:NE2	2:A:933:HOH:O	2.40	0.55
1:A:631:HIS:HA	2:A:1145:HOH:O	2.06	0.55
1:A:392:ASN:OD1	1:A:460:LEU:HD12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:VAL:HG12	1:B:717:ALA:N	2.22	0.54
1:A:281:ARG:N	2:A:926:HOH:O	2.38	0.54
1:A:484:LEU:HD22	1:A:618:GLU:HG2	1.90	0.54
1:B:370:ARG:NH2	2:B:930:HOH:O	2.40	0.53
1:B:339:THR:HG21	1:B:563:LEU:HD11	1.90	0.53
1:A:563:LEU:HB2	2:A:953:HOH:O	2.10	0.52
1:B:555:GLY:HA3	2:B:939:HOH:O	2.09	0.52
1:B:626:LEU:HA	1:B:686:GLY:HA3	1.91	0.52
1:B:47:ARG:NH1	2:B:931:HOH:O	2.41	0.52
1:A:645:LEU:HD11	1:A:801:GLN:HB3	1.92	0.52
1:A:101:ALA:HB2	2:A:1013:HOH:O	2.09	0.51
1:B:500:PRO:HG3	1:B:616:LEU:HD21	1.92	0.51
1:A:166:VAL:HG22	1:A:178:LEU:HD22	1.92	0.51
1:A:738:ARG:HG2	2:A:1188:HOH:O	2.10	0.51
1:A:195:LYS:HD2	2:A:1244:HOH:O	2.09	0.51
1:B:422:ASN:N	2:B:926:HOH:O	2.37	0.51
1:A:388:MET:HE3	1:A:455:VAL:HA	1.93	0.51
1:B:10:ILE:HG21	2:B:928:HOH:O	2.10	0.51
1:A:74:ARG:N	2:A:924:HOH:O	2.35	0.51
1:B:730:TYR:O	1:B:734:ILE:HG12	2.11	0.51
1:A:89:MET:SD	1:A:315:LEU:HD11	2.51	0.51
1:A:661:GLU:HG2	2:A:929:HOH:O	2.11	0.50
1:B:172:SER:HA	2:B:1039:HOH:O	2.11	0.50
1:A:292:ASN:O	1:B:521:GLN:OE1	2.30	0.50
1:B:562:ALA:C	1:B:563:LEU:HD22	2.37	0.50
1:A:315:LEU:HD22	1:A:315:LEU:O	2.10	0.50
1:A:328:LEU:HD23	1:A:371:ARG:HB2	1.92	0.50
1:B:82:GLU:HG3	1:B:85:MET:HB2	1.93	0.50
1:A:619:LEU:HA	2:A:974:HOH:O	2.12	0.49
1:A:543:VAL:HG13	1:A:576:LEU:HB3	1.94	0.49
1:A:625:TYR:CZ	1:A:648:PHE:HA	2.46	0.49
1:B:306:PHE:O	1:B:310:VAL:HG23	2.12	0.49
1:A:179:ASP:OD1	1:A:181:THR:HG23	2.12	0.49
1:A:156:MET:HE3	1:A:164:VAL:HG21	1.94	0.49
1:B:317:ASN:ND2	2:B:922:HOH:O	2.36	0.48
1:A:256:ASN:ND2	2:A:921:HOH:O	2.33	0.48
1:B:72:GLU:O	2:B:901:HOH:O	2.20	0.48
1:B:793:ILE:O	1:B:797:GLU:HG2	2.13	0.48
1:B:200:LEU:HD23	1:B:201:LEU:HG	1.95	0.48
1:A:617:HIS:CG	2:A:925:HOH:O	2.66	0.47
1:B:304:ARG:CZ	1:B:315:LEU:HD23	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PRO:HD2	1:B:175:GLN:HB3	1.96	0.47
1:B:752:TYR:HB2	2:B:976:HOH:O	2.14	0.47
1:B:89:MET:CE	1:B:315:LEU:HD21	2.45	0.47
1:A:201:LEU:HB3	1:A:205:ILE:HD12	1.96	0.47
1:A:543:VAL:HG21	1:A:553:ALA:HA	1.97	0.47
1:B:505:MET:HA	1:B:508:ILE:HD12	1.97	0.47
1:B:484:LEU:HD22	1:B:618:GLU:HG2	1.96	0.47
1:B:613:MET:HA	1:B:613:MET:CE	2.40	0.47
1:A:625:TYR:OH	1:A:648:PHE:HA	2.14	0.47
1:B:201:LEU:HB3	1:B:205:ILE:HD12	1.97	0.47
1:B:563:LEU:HD22	1:B:563:LEU:N	2.30	0.47
1:A:625:TYR:CD1	1:A:626:LEU:HD23	2.50	0.46
1:B:357:ARG:O	2:B:903:HOH:O	2.21	0.46
1:B:370:ARG:NH2	2:B:943:HOH:O	2.47	0.46
1:B:626:LEU:HD13	1:B:796:VAL:HG21	1.97	0.46
1:A:508:ILE:HD13	1:A:746:PHE:HB3	1.97	0.46
1:B:105:ARG:NH1	2:B:940:HOH:O	2.44	0.46
1:B:511:SER:HB2	2:B:1187:HOH:O	2.15	0.46
1:A:175:GLN:HA	1:A:260:ASN:OD1	2.16	0.45
1:B:508:ILE:HD13	1:B:746:PHE:HB3	1.97	0.45
1:A:508:ILE:HG13	2:A:1025:HOH:O	2.17	0.45
1:B:434:HIS:HB3	1:B:457:LEU:HD23	1.97	0.45
1:A:154:PHE:CZ	1:A:516:LEU:HD23	2.51	0.45
1:B:163:MET:HE1	1:B:186:LEU:HB2	1.98	0.45
1:B:311:PHE:HB2	1:B:388:MET:HE2	1.98	0.45
1:A:89:MET:CE	1:A:315:LEU:HD11	2.46	0.45
1:A:106:ASN:HA	1:A:282:ARG:CD	2.45	0.45
1:B:87:LEU:HD12	1:B:107:LEU:HG	1.99	0.45
1:A:626:LEU:HA	1:A:686:GLY:HA3	1.99	0.45
1:A:785:LEU:O	2:A:901:HOH:O	2.20	0.45
1:A:235:LYS:NZ	2:A:916:HOH:O	2.31	0.44
1:B:379:TYR:C	1:B:379:TYR:CD1	2.95	0.44
1:B:708:MET:HE2	1:B:726:PHE:CD2	2.51	0.44
1:B:726:PHE:CZ	1:B:730:TYR:HE2	2.35	0.44
1:B:762:LEU:C	1:B:763:ILE:HD12	2.42	0.44
1:A:765:GLU:HG2	1:A:774:THR:O	2.17	0.44
1:B:420:ASN:HA	2:B:902:HOH:O	2.16	0.44
1:B:775:ALA:HA	1:B:779:MET:HE3	2.00	0.44
1:A:549:ASN:HB2	2:A:1243:HOH:O	2.16	0.44
1:A:761:ASN:ND2	2:A:961:HOH:O	2.50	0.44
1:B:314:ALA:HB2	1:B:447:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:ARG:HB3	2:B:1021:HOH:O	2.18	0.44
1:A:156:MET:CE	1:A:164:VAL:HG21	2.48	0.44
1:A:716:VAL:HG13	1:A:717:ALA:N	2.33	0.44
1:A:539:ASN:HB2	1:A:542:SER:OG	2.18	0.44
1:B:89:MET:HE2	1:B:315:LEU:HD21	1.99	0.44
1:B:379:TYR:HD1	1:B:380:GLY:O	2.00	0.44
1:A:229:LEU:C	1:A:229:LEU:HD13	2.43	0.43
1:B:659:ARG:O	1:B:665:VAL:HA	2.18	0.43
1:B:716:VAL:CG1	1:B:717:ALA:N	2.82	0.43
1:B:521:GLN:O	1:B:521:GLN:NE2	2.51	0.43
1:A:448:GLY:HA3	1:A:577:MET:O	2.18	0.43
1:B:505:MET:O	1:B:750:MET:HE1	2.19	0.43
1:A:597:VAL:O	1:A:601:ILE:HG12	2.19	0.43
1:A:306:PHE:O	1:A:310:VAL:HG23	2.18	0.43
1:A:45:TRP:O	1:A:49:THR:OG1	2.33	0.42
1:A:715:VAL:HG13	1:A:716:VAL:O	2.19	0.42
1:B:463:ILE:O	1:B:467:LEU:HD23	2.19	0.42
1:B:328:LEU:O	1:B:334:SER:HB3	2.20	0.42
1:B:235:LYS:HD3	1:B:235:LYS:C	2.44	0.42
1:B:541:ASP:OD1	1:B:541:ASP:O	2.37	0.42
1:B:626:LEU:HA	1:B:626:LEU:HD23	1.88	0.42
1:A:328:LEU:O	1:A:334:SER:HB3	2.19	0.42
1:A:669:LEU:HD11	2:A:1082:HOH:O	2.19	0.42
1:A:20:TYR:HB2	1:A:229:LEU:HD23	2.02	0.42
1:A:108:THR:HG21	1:A:282:ARG:HH21	1.84	0.42
1:A:343:GLN:N	1:A:343:GLN:CD	2.78	0.42
1:B:704:VAL:O	1:B:707:ILE:HG13	2.19	0.42
1:A:296:SER:O	1:A:301:GLN:NE2	2.53	0.42
1:A:709:LYS:O	1:A:713:GLU:HG3	2.20	0.42
1:A:718:ARG:HH11	1:A:718:ARG:HB3	1.84	0.42
1:A:155:GLU:OE2	1:A:748:THR:HG23	2.21	0.41
1:A:526:GLN:HG2	2:A:913:HOH:O	2.20	0.41
1:B:448:GLY:HA3	1:B:577:MET:O	2.20	0.41
1:B:379:TYR:CD1	1:B:380:GLY:O	2.74	0.41
1:B:722:THR:OG1	1:B:724:THR:HG22	2.21	0.41
1:A:156:MET:HE2	1:A:180:PHE:HE1	1.86	0.41
1:A:413:ASN:O	2:A:903:HOH:O	2.21	0.41
1:A:763:ILE:HG23	1:A:774:THR:HG23	2.03	0.41
1:B:718:ARG:NH2	1:B:719:GLU:HG3	2.36	0.41
1:A:314:ALA:HB2	1:A:447:ARG:O	2.21	0.41
1:A:617:HIS:CE1	2:A:902:HOH:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:LEU:HD11	1:A:801:GLN:CB	2.51	0.41
1:A:767:ARG:HA	1:A:773:ILE:HG12	2.02	0.41
1:B:173:THR:OG1	1:B:175:GLN:CG	2.68	0.41
1:B:157:THR:HG23	2:B:1097:HOH:O	2.20	0.40
1:A:715:VAL:HG12	1:A:720:GLN:HG3	2.03	0.40
1:B:173:THR:OG1	1:B:175:GLN:HG2	2.21	0.40
1:B:512:GLN:NE2	2:B:935:HOH:O	2.42	0.40
1:B:529:ARG:HH21	1:B:590:VAL:HG22	1.86	0.40
1:A:304:ARG:CZ	1:A:315:LEU:HD12	2.51	0.40
1:A:504:LYS:NZ	1:A:742:ASN:OD1	2.51	0.40
1:A:735:GLN:HG3	2:A:915:HOH:O	2.22	0.40
1:A:775:ALA:H	1:A:779:MET:HE3	1.87	0.40
1:A:108:THR:HG21	1:A:282:ARG:NH2	2.37	0.40
1:A:734:ILE:HB	2:A:915:HOH:O	2.22	0.40
1:B:16:LEU:HG	1:B:190:LEU:HD23	2.03	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	787/883 (89%)	755 (96%)	32 (4%)	0	100	100
1	B	784/883 (89%)	751 (96%)	33 (4%)	0	100	100
All	All	1571/1766 (89%)	1506 (96%)	65 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	699/777 (90%)	684 (98%)	15 (2%)	47	69
1	B	699/777 (90%)	683 (98%)	16 (2%)	44	66
All	All	1398/1554 (90%)	1367 (98%)	31 (2%)	45	67

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	SER
1	A	167	ARG
1	A	173	THR
1	A	343	GLN
1	A	378	ASP
1	A	412	LEU
1	A	466	ARG
1	A	549	ASN
1	A	690	LEU
1	A	699	SER
1	A	715	VAL
1	A	716	VAL
1	A	718	ARG
1	A	724	THR
1	A	726	PHE
1	B	71	SER
1	B	82	GLU
1	B	93	ASP
1	B	159	SER
1	B	176	VAL
1	B	188	ASP
1	B	233	LEU
1	B	280	GLN
1	B	281	ARG
1	B	546	TYR
1	B	619	LEU
1	B	642	LYS
1	B	706	LEU
1	B	715	VAL
1	B	727	GLU
1	B	799	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	142	ASN
1	A	161	ASN
1	A	204	HIS
1	A	211	GLN
1	A	280	GLN
1	A	292	ASN
1	A	367	ASN
1	A	416	ASN
1	A	494	ASN
1	A	526	GLN
1	A	540	ASN
1	A	560	GLN
1	A	631	HIS
1	B	106	ASN
1	B	161	ASN
1	B	165	GLN
1	B	204	HIS
1	B	274	GLN
1	B	383	ASN
1	B	416	ASN
1	B	425	GLN
1	B	641	ASN
1	B	656	HIS
1	B	662	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 [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	793/883 (89%)	-1.47	0 100 100	3, 15, 35, 56	0
1	B	792/883 (89%)	-1.46	0 100 100	3, 16, 37, 71	0
All	All	1585/1766 (89%)	-1.46	0 100 100	3, 16, 36, 71	0

There are no RSRZ outliers to report.

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.