Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2023 – 12:36 PM JST

PDB ID	:	8IGL
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:

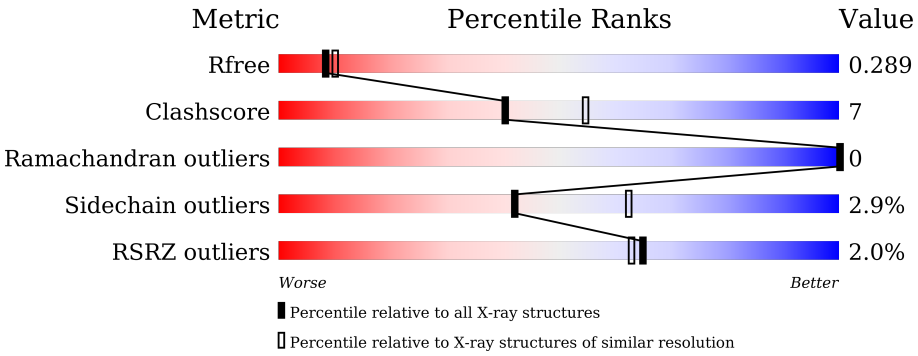
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	2% 76% 13% • 10%
1	B	883	2% 74% 15% 10%

2 Entry composition (i)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.

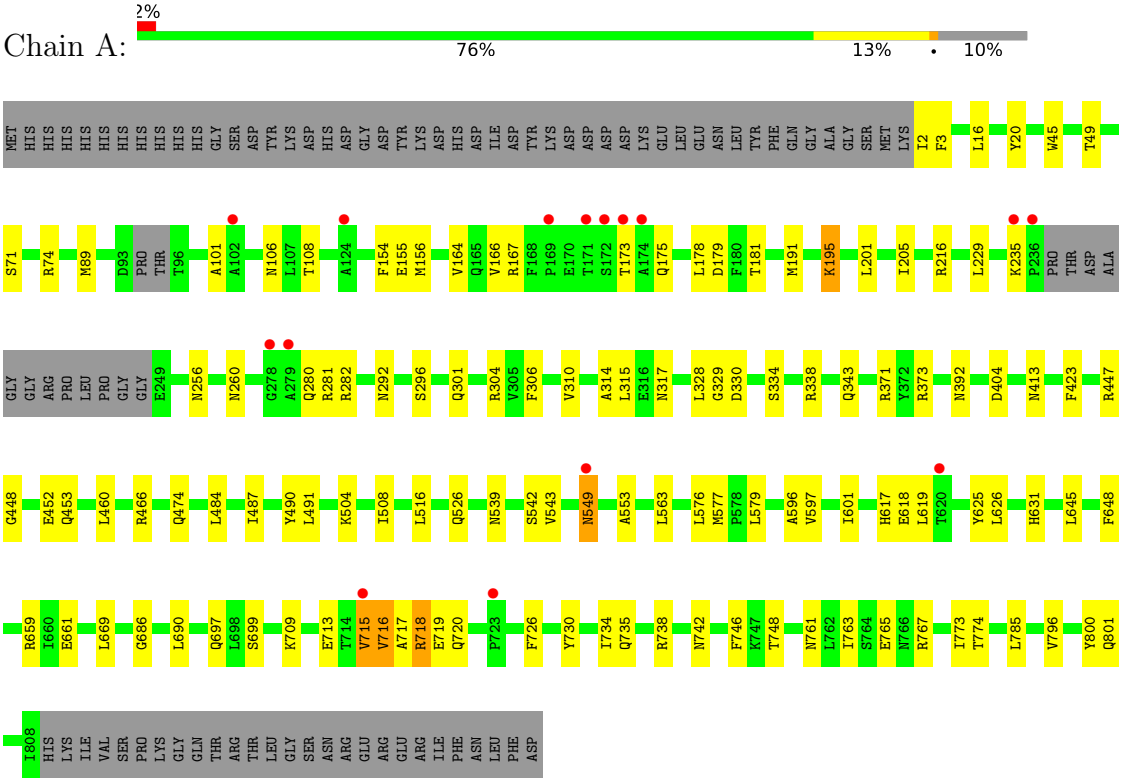
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	370	Total O 370 370	0	0
2	B	355	Total O 355 355	0	0

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.

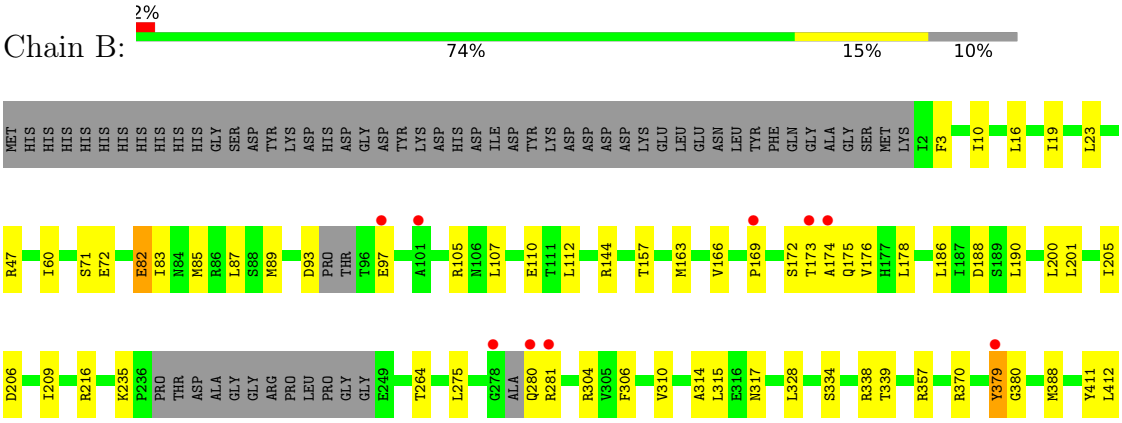
• Molecule 1: CP2475L

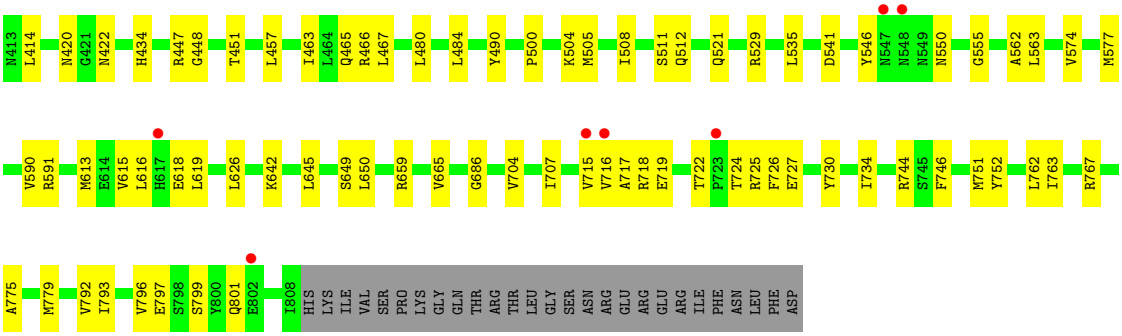
Chain A:



• Molecule 1: CP2475L

Chain B:




N413 L414 N420 G421 N422 H434 R447 G448 T451 L457 I463 L464 Q465 R466 L467 L480 L484 Y490 P500 K504 M505 I508 S511 Q512 Q521 R529 L535 D541 Y546 N547 N548 N549 N550 G555 A562 L563 V574 M577
V590 R591 M613 E614 V615 L616 H617 E618 L619 L626 K642 L645 S649 L650 R659 V665 G686 V704 I707 V715 V716 A717 R718 E719 T722 P723 T724 R725 F726 E727 Y730 I734 R744 S745 F746 M751 Y752 L762 I763 R767
A775 M779 V792 I793 V796 E797 S798 S799 Y800 Q801 E802 I808 HIS LYS ILE VAL SER PRO LYS GLY GLN THR ARG THR LEU GLY SER ASN ARG GLU ARG GLU ARG ILE PHE ASN LEU PHE ASP

4 Data and refinement statistics (i)

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 40.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.1 (32.54-2.40) 92.8 (40.79-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.97 (at 2.29Å)	Xtriage
Refinement program	PHENIX Version 1.20.1-4487	Depositor
R, R_{free}	0.238 , 0.283 0.245 , 0.289	Depositor DCC
R_{free} test set	3287 reflections (5.07%)	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)	0.39 , 16.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
F_o,F_c correlation	0.85	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.33	0/6502	0.59	0/8823
1	B	0.32	0/6496	0.57	0/8813
All	All	0.33	0/12998	0.58	0/17636

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

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	89	0
1	B	6373	6341	6347	96	0
2	A	370	0	0	31	0
2	B	355	0	0	26	0
All	All	13476	12696	12700	184	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 7.

All (184) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ASP:HB3	1:B:209:ILE:HD12	1.54	0.90
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: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:89:MET:HE2	1:B:315:LEU:HD21	1.74	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: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: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: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:A:329:GLY:N	2:A:919:HOH:O	2.32	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:A:453:GLN:HA	2:A:1120:HOH:O	2.04	0.57
1:B:163:MET:HE1	1:B:186:LEU:HB2	1.86	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:MET:HE3	1:B:613:MET:HA	1.88	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
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:447:ARG:C	1:A:579:LEU:HD21	2.28	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:451:THR:OG1	1:B:574:VAL:O	2.22	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:B:613:MET:HA	1:B:613:MET:CE	2.40	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: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:A:315:LEU:HD22	1:A:315:LEU:O	2.10	0.50
1:A:235:LYS:NZ	2:A:916:HOH:O	2.31	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:89:MET:HE2	1:B:535:LEU:HD13	1.95	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
1:B:169:PRO:HD2	1:B:175:GLN:HB3	1.96	0.47
1:B:775:ALA:HA	1:B:779:MET:HE3	1.97	0.47
1:B:752:TYR:HB2	2:B:976:HOH:O	2.14	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: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:B:562:ALA:C	1:B:563:LEU:HD22	2.37	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:PHE:CZ	1:B:730:TYR:HE2	2.35	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: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
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:163:MET:CE	1:B:186:LEU:HD22	2.48	0.44
1:B:379:TYR:HD1	1:B:380:GLY:O	2.00	0.44
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: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: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: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:B:89:MET:CE	1:B:315:LEU:HD21	2.45	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: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: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:45:TRP:O	1:A:49:THR:OG1	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:379:TYR:CD1	1:B:379:TYR:C	2.95	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:B:613:MET:CE	1:B:616:LEU:HD23	2.51	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
1:B:762:LEU:C	1:B:763:ILE:HD12	2.42	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	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 (i)

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%)	680 (97%)	19 (3%)	44 65
1	B	699/777 (90%)	678 (97%)	21 (3%)	41 61
All	All	1398/1554 (90%)	1358 (97%)	40 (3%)	42 62

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	71	SER
1	A	167	ARG
1	A	173	THR
1	A	195	LYS
1	A	216	ARG
1	A	338	ARG
1	A	343	GLN
1	A	466	ARG
1	A	549	ASN
1	A	659	ARG
1	A	690	LEU
1	A	697	GLN
1	A	699	SER
1	A	715	VAL
1	A	716	VAL
1	A	718	ARG
1	A	726	PHE
1	A	800	TYR
1	B	3	PHE
1	B	71	SER
1	B	82	GLU
1	B	93	ASP
1	B	144	ARG
1	B	176	VAL
1	B	188	ASP
1	B	280	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	281	ARG
1	B	338	ARG
1	B	379	TYR
1	B	490	TYR
1	B	504	LYS
1	B	546	TYR
1	B	619	LEU
1	B	642	LYS
1	B	649	SER
1	B	715	VAL
1	B	727	GLU
1	B	767	ARG
1	B	799	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	161	ASN
1	A	211	GLN
1	A	280	GLN
1	A	635	ASN
1	A	656	HIS
1	B	175	GLN
1	B	368	ASN
1	B	425	GLN
1	B	662	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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%)	-0.18	15 (1%)	66	64	3, 13, 32, 52	0
1	B	792/883 (89%)	-0.13	16 (2%)	65	63	3, 15, 34, 63	0
All	All	1585/1766 (89%)	-0.15	31 (1%)	65	63	3, 14, 34, 63	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	GLN	4.7
1	B	173	THR	4.5
1	A	723	PRO	4.1
1	A	279	ALA	4.0
1	B	716	VAL	3.6
1	B	547	ASN	3.5
1	A	172	SER	3.5
1	A	173	THR	3.3
1	B	548	ASN	3.2
1	B	174	ALA	3.2
1	B	281	ARG	3.2
1	B	97	GLU	3.2
1	A	174	ALA	3.1
1	A	278	GLY	3.0
1	B	802	GLU	2.8
1	A	549	ASN	2.7
1	A	235	LYS	2.6
1	A	236	PRO	2.5
1	B	169	PRO	2.4
1	B	379	TYR	2.3
1	B	278	GLY	2.3
1	B	723	PRO	2.3
1	A	169	PRO	2.3
1	B	715	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	101	ALA	2.2
1	A	171	THR	2.2
1	A	124	ALA	2.2
1	A	715	VAL	2.1
1	B	617	HIS	2.1
1	A	620	THR	2.1
1	A	102	ALA	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 monosaccharides 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.