Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2023 – 10:11 AM EDT

PDB ID	:	7S5U
Title	:	Extended bipolar assembly domain of kinesin-5 minifilament
Authors	:	Nithianantham, S.; Al-Bassam, J.
Deposited on	:	2021-09-12
Resolution	:	4.41 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:

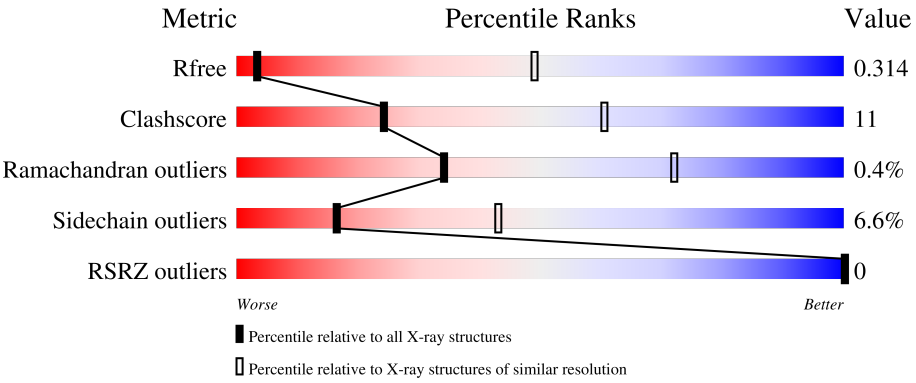
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 4.41 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	1046 (5.04-3.80)
Clashscore	141614	1114 (5.04-3.80)
Ramachandran outliers	138981	1061 (5.04-3.80)
Sidechain outliers	138945	1043 (5.04-3.80)
RSRZ outliers	127900	1096 (5.12-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	248	53% 18% · 28%
1	B	248	50% 21% · 27%
1	C	248	52% 16% · 30%
1	D	248	51% 16% · 31%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5023 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 Kinesin-like protein Klp61F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1273	766	231	269	7			
1	B	180	Total	C	N	O	S	0	0	0
			1290	775	230	279	6			
1	D	170	Total	C	N	O	S	0	0	0
			1233	741	226	259	7			
1	C	173	Total	C	N	O	S	0	0	0
			1227	738	218	264	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	596	MET	-	initiating methionine	UNP P46863
A	836	SER	-	expression tag	UNP P46863
A	837	GLY	-	expression tag	UNP P46863
A	838	HIS	-	expression tag	UNP P46863
A	839	HIS	-	expression tag	UNP P46863
A	840	HIS	-	expression tag	UNP P46863
A	841	HIS	-	expression tag	UNP P46863
A	842	HIS	-	expression tag	UNP P46863
A	843	HIS	-	expression tag	UNP P46863
B	596	MET	-	initiating methionine	UNP P46863
B	836	SER	-	expression tag	UNP P46863
B	837	GLY	-	expression tag	UNP P46863
B	838	HIS	-	expression tag	UNP P46863
B	839	HIS	-	expression tag	UNP P46863
B	840	HIS	-	expression tag	UNP P46863
B	841	HIS	-	expression tag	UNP P46863
B	842	HIS	-	expression tag	UNP P46863
B	843	HIS	-	expression tag	UNP P46863
D	596	MET	-	initiating methionine	UNP P46863
D	836	SER	-	expression tag	UNP P46863
D	837	GLY	-	expression tag	UNP P46863

Continued on next page...

Continued from previous page...

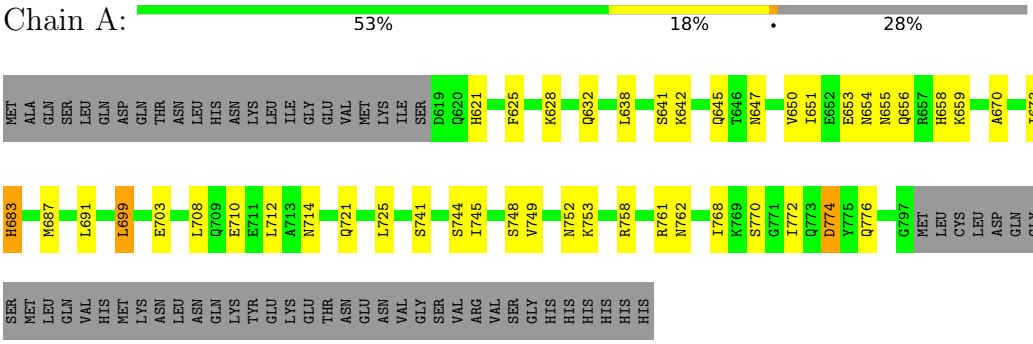
Chain	Residue	Modelled	Actual	Comment	Reference
D	838	HIS	-	expression tag	UNP P46863
D	839	HIS	-	expression tag	UNP P46863
D	840	HIS	-	expression tag	UNP P46863
D	841	HIS	-	expression tag	UNP P46863
D	842	HIS	-	expression tag	UNP P46863
D	843	HIS	-	expression tag	UNP P46863
C	596	MET	-	initiating methionine	UNP P46863
C	836	SER	-	expression tag	UNP P46863
C	837	GLY	-	expression tag	UNP P46863
C	838	HIS	-	expression tag	UNP P46863
C	839	HIS	-	expression tag	UNP P46863
C	840	HIS	-	expression tag	UNP P46863
C	841	HIS	-	expression tag	UNP P46863
C	842	HIS	-	expression tag	UNP P46863
C	843	HIS	-	expression tag	UNP P46863

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.

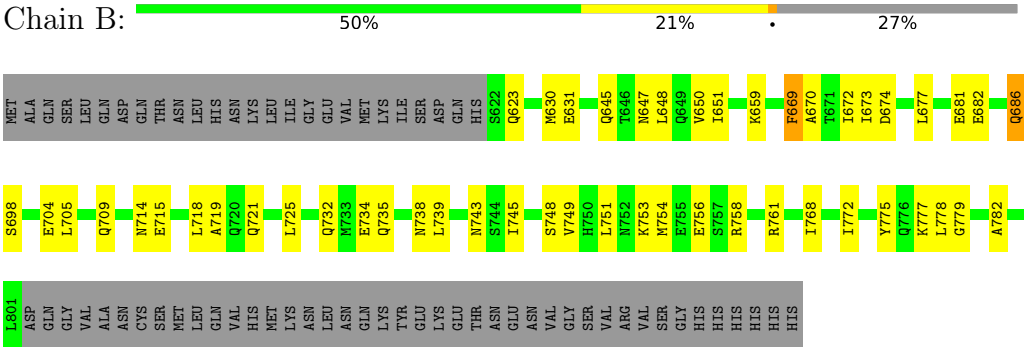
• Molecule 1: Kinesin-like protein Klp61F

Chain A:



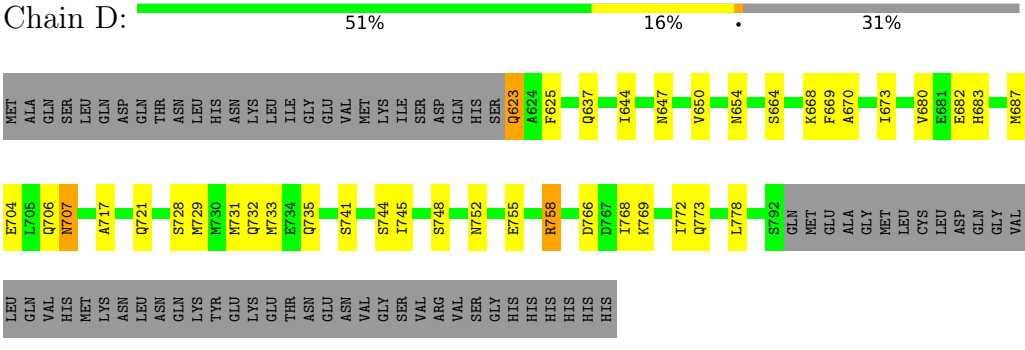
• Molecule 1: Kinesin-like protein Klp61F

Chain B:



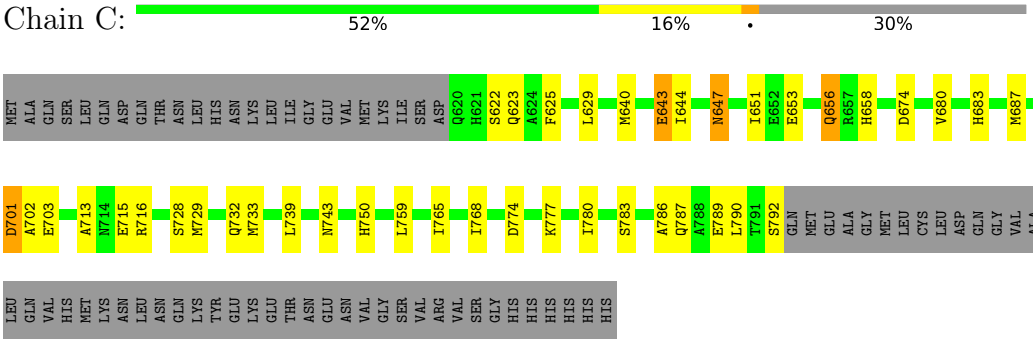
• Molecule 1: Kinesin-like protein Klp61F

Chain D:



• Molecule 1: Kinesin-like protein Klp61F

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	253.18Å 84.89Å 96.77Å 90.00° 91.44° 90.00°	Depositor
Resolution (Å)	96.73 – 4.41 96.74 – 4.41	Depositor EDS
% Data completeness (in resolution range)	79.6 (96.73-4.41) 79.6 (96.74-4.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	6.29 (at 4.47Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.274 , 0.310 0.278 , 0.314	Depositor DCC
R_{free} test set	546 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	96.2	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 86.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
Reported twinning fraction	0.010 for -h,-k,l	Depositor
Outliers	4 of 10515 reflections (0.038%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5023	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.02% 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	0.24	0/1278	0.39	0/1726
1	B	0.24	0/1294	0.37	0/1747
1	C	0.24	0/1233	0.39	0/1668
1	D	0.24	0/1238	0.38	0/1668
All	All	0.24	0/5043	0.38	0/6809

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	1273	0	1143	28	0
1	B	1290	0	1153	39	0
1	C	1227	0	1073	27	0
1	D	1233	0	1125	22	0
All	All	5023	0	4494	105	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 11.

All (105) 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:735:GLN:HA	1:B:738:ASN:HD22	1.54	0.72
1:D:758:ARG:HD2	1:C:702:ALA:HB2	1.79	0.64
1:A:699:LEU:O	1:A:703:GLU:N	2.31	0.63
1:D:729:MET:O	1:D:733:MET:HB2	2.00	0.62
1:C:713:ALA:HA	1:C:716:ARG:HB2	1.82	0.61
1:B:714:ASN:OD1	1:B:715:GLU:N	2.36	0.59
1:A:650:VAL:HA	1:A:653:GLU:HB2	1.86	0.57
1:B:782:ALA:O	1:B:786:ALA:N	2.37	0.57
1:B:777:LYS:HD3	1:B:778:LEU:N	2.20	0.56
1:C:786:ALA:O	1:C:790:LEU:N	2.35	0.56
1:A:621:HIS:O	1:A:625:PHE:N	2.38	0.56
1:D:717:ALA:O	1:D:721:GLN:N	2.37	0.56
1:B:739:LEU:O	1:B:743:ASN:N	2.35	0.56
1:C:640:MET:O	1:C:643:GLU:HG3	2.06	0.56
1:B:768:ILE:HG22	1:B:772:ILE:HD11	1.88	0.55
1:C:680:VAL:O	1:C:683:HIS:ND1	2.29	0.55
1:C:687:MET:O	1:C:691:LEU:N	2.32	0.54
1:C:625:PHE:O	1:C:629:LEU:N	2.37	0.54
1:B:645:GLN:HE22	1:D:644:ILE:HG21	1.74	0.53
1:D:680:VAL:O	1:D:683:HIS:ND1	2.37	0.53
1:B:647:ASN:OD1	1:B:648:LEU:N	2.41	0.53
1:B:758:ARG:HA	1:B:761:ARG:HB3	1.91	0.53
1:B:647:ASN:O	1:B:650:VAL:HG12	2.10	0.52
1:A:638:LEU:HA	1:A:641:SER:HB3	1.92	0.52
1:D:647:ASN:O	1:D:650:VAL:HG12	2.09	0.51
1:B:715:GLU:O	1:B:719:ALA:N	2.36	0.51
1:D:664:SER:O	1:D:668:LYS:N	2.34	0.51
1:A:647:ASN:HA	1:A:650:VAL:HG12	1.93	0.51
1:C:699:LEU:O	1:C:703:GLU:N	2.40	0.51
1:B:753:LYS:HA	1:B:756:GLU:HG3	1.93	0.50
1:A:758:ARG:HA	1:A:761:ARG:HB3	1.92	0.50
1:B:704:GLU:OE2	1:C:750:HIS:ND1	2.43	0.50
1:A:628:LYS:O	1:A:632:GLN:HG2	2.11	0.50
1:C:739:LEU:O	1:C:743:ASN:N	2.26	0.50
1:A:651:ILE:HA	1:A:654:ASN:HD22	1.77	0.50
1:B:748:SER:OG	1:B:749:VAL:N	2.45	0.49
1:D:752:ASN:HA	1:D:755:GLU:HB3	1.94	0.49
1:B:647:ASN:O	1:B:651:ILE:HG23	2.13	0.49
1:C:622:SER:OG	1:C:623:GLN:N	2.45	0.49
1:B:725:LEU:HD21	1:C:732:GLN:HG2	1.95	0.49
1:A:655:ASN:O	1:A:659:LYS:HB2	2.12	0.49
1:D:706:GLN:OE1	1:D:707:ASN:ND2	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:PHE:O	1:B:673:ILE:HG23	2.13	0.49
1:D:769:LYS:O	1:D:773:GLN:HG2	2.12	0.48
1:A:741:SER:O	1:A:745:ILE:HG12	2.12	0.48
1:C:729:MET:O	1:C:733:MET:HG2	2.13	0.48
1:A:744:SER:O	1:A:748:SER:N	2.46	0.48
1:B:751:LEU:O	1:B:754:MET:N	2.47	0.48
1:B:698:SER:OG	1:B:698:SER:O	2.30	0.48
1:B:777:LYS:HD3	1:B:777:LYS:C	2.34	0.48
1:A:647:ASN:O	1:A:651:ILE:HG12	2.14	0.48
1:D:700:PRO:O	1:D:704:GLU:HG2	2.14	0.48
1:D:741:SER:O	1:D:745:ILE:HG12	2.15	0.47
1:D:744:SER:O	1:D:748:SER:N	2.43	0.47
1:A:680:VAL:O	1:A:683:HIS:ND1	2.47	0.47
1:A:708:LEU:O	1:A:712:LEU:HG	2.15	0.47
1:B:623:GLN:NE2	1:D:623:GLN:OE1	2.46	0.47
1:B:786:ALA:O	1:B:790:LEU:N	2.48	0.47
1:A:725:LEU:HD21	1:D:732:GLN:HG3	1.97	0.47
1:D:650:VAL:O	1:D:654:ASN:N	2.47	0.47
1:C:789:GLU:O	1:C:792:SER:OG	2.27	0.46
1:A:768:ILE:O	1:A:772:ILE:HG12	2.15	0.46
1:B:734:GLU:O	1:B:738:ASN:ND2	2.48	0.46
1:B:718:LEU:HA	1:B:721:GLN:HB3	1.98	0.45
1:A:748:SER:OG	1:A:749:VAL:N	2.49	0.45
1:A:752:ASN:OD1	1:A:753:LYS:N	2.49	0.45
1:C:653:GLU:O	1:C:656:GLN:HG3	2.16	0.45
1:A:762:ASN:OD1	1:B:698:SER:OG	2.28	0.45
1:B:743:ASN:OD1	1:C:715:GLU:HB2	2.17	0.45
1:B:630:MET:HG3	1:B:631:GLU:N	2.31	0.45
1:D:731:MET:O	1:D:735:GLN:HB2	2.17	0.45
1:B:705:LEU:O	1:B:709:GLN:HB2	2.18	0.44
1:D:670:ALA:O	1:D:673:ILE:HG22	2.16	0.44
1:A:659:LYS:HE2	1:A:659:LYS:HB3	1.86	0.44
1:B:648:LEU:O	1:B:651:ILE:HG12	2.18	0.44
1:B:677:LEU:O	1:B:681:GLU:HG2	2.18	0.44
1:C:777:LYS:O	1:C:780:ILE:HG12	2.18	0.44
1:A:776:GLN:O	1:A:776:GLN:NE2	2.50	0.44
1:C:699:LEU:HD23	1:C:699:LEU:HA	1.75	0.44
1:B:721:GLN:NE2	1:B:725:LEU:HD22	2.34	0.43
1:C:701:ASP:OD1	1:C:701:ASP:N	2.52	0.43
1:B:670:ALA:O	1:B:673:ILE:HG12	2.19	0.43
1:A:687:MET:O	1:A:691:LEU:HG	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:GLN:O	1:A:725:LEU:HB2	2.19	0.42
1:A:710:GLU:O	1:A:714:ASN:ND2	2.51	0.42
1:C:647:ASN:O	1:C:651:ILE:HG12	2.20	0.42
1:B:745:ILE:O	1:B:749:VAL:HG22	2.20	0.42
1:B:758:ARG:HG3	1:C:701:ASP:OD2	2.20	0.42
1:C:700:PRO:HA	1:C:703:GLU:HB3	2.01	0.42
1:B:775:TYR:O	1:B:779:GLY:N	2.52	0.42
1:C:643:GLU:OE2	1:C:644:ILE:HG13	2.20	0.41
1:D:623:GLN:O	1:D:625:PHE:N	2.53	0.41
1:B:725:LEU:HD23	1:C:733:MET:SD	2.60	0.41
1:C:759:LEU:HD12	1:C:759:LEU:HA	1.95	0.41
1:C:765:ILE:O	1:C:768:ILE:HG13	2.21	0.41
1:D:755:GLU:HA	1:D:758:ARG:HB3	2.02	0.41
1:D:768:ILE:O	1:D:772:ILE:HG12	2.20	0.41
1:C:783:SER:O	1:C:787:GLN:HG2	2.21	0.41
1:B:669:PHE:O	1:B:672:ILE:HG22	2.20	0.41
1:A:770:SER:O	1:A:774:ASP:HB2	2.20	0.41
1:A:638:LEU:HA	1:A:638:LEU:HD23	1.93	0.40
1:A:642:LYS:O	1:A:645:GLN:HG2	2.21	0.40
1:A:670:ALA:O	1:A:673:ILE:HG22	2.21	0.40
1:B:645:GLN:OE1	1:D:644:ILE:HD13	2.21	0.40
1:B:682:GLU:O	1:B:686:GLN:HB2	2.22	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	177/248 (71%)	167 (94%)	9 (5%)	1 (1%)	25 65
1	B	178/248 (72%)	170 (96%)	8 (4%)	0	100 100
1	C	171/248 (69%)	165 (96%)	5 (3%)	1 (1%)	25 65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	168/248 (68%)	163 (97%)	4 (2%)	1 (1%)	25 65
All	All	694/992 (70%)	665 (96%)	26 (4%)	3 (0%)	34 72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	699	LEU
1	C	699	LEU
1	D	699	LEU

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	121/223 (54%)	116 (96%)	5 (4%)	30 56
1	B	125/223 (56%)	117 (94%)	8 (6%)	17 44
1	C	116/223 (52%)	108 (93%)	8 (7%)	15 42
1	D	121/223 (54%)	110 (91%)	11 (9%)	9 32
All	All	483/892 (54%)	451 (93%)	32 (7%)	16 43

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	656	GLN
1	A	658	HIS
1	A	682	GLU
1	A	683	HIS
1	A	774	ASP
1	B	659	LYS
1	B	669	PHE
1	B	674	ASP
1	B	686	GLN
1	B	691	LEU
1	B	693	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	732	GLN
1	B	787	GLN
1	D	623	GLN
1	D	637	GLN
1	D	669	PHE
1	D	682	GLU
1	D	687	MET
1	D	701	ASP
1	D	707	ASN
1	D	728	SER
1	D	758	ARG
1	D	766	ASP
1	D	778	LEU
1	C	643	GLU
1	C	647	ASN
1	C	656	GLN
1	C	658	HIS
1	C	674	ASP
1	C	701	ASP
1	C	728	SER
1	C	774	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	654	ASN
1	A	714	ASN
1	B	738	ASN
1	D	693	GLN
1	D	732	GLN

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 (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	179/248 (72%)	-0.62	0	100	100	54, 110, 182, 224	0
1	B	180/248 (72%)	-0.70	0	100	100	44, 118, 178, 190	0
1	C	173/248 (69%)	-0.70	0	100	100	38, 107, 150, 180	0
1	D	170/248 (68%)	-0.65	0	100	100	51, 109, 151, 176	0
All	All	702/992 (70%)	-0.67	0	100	100	38, 110, 167, 224	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.