Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2024 – 12:10 PM JST

PDB ID	:	9IMP
Title	:	The complex of PDZ3 and PBM
Authors	:	Huang, S.J.
Deposited on	:	2024-07-04
Resolution	:	2.87 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:

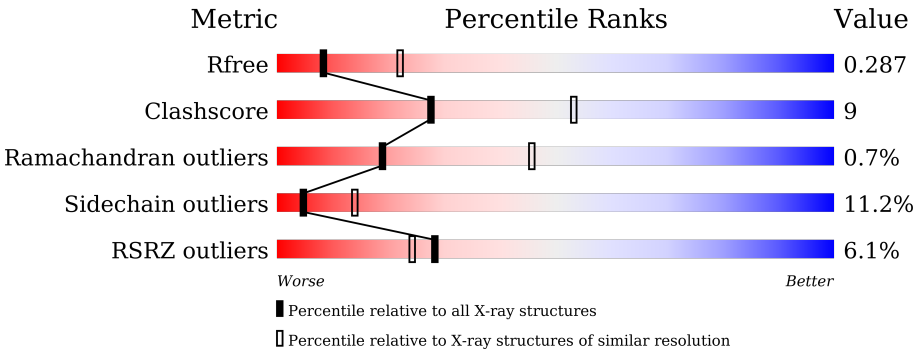
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 2.87 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}	164625	3316 (2.90-2.86)
Clashscore	180529	3609 (2.90-2.86)
Ramachandran outliers	177936	3529 (2.90-2.86)
Sidechain outliers	177891	3532 (2.90-2.86)
RSRZ outliers	164620	3319 (2.90-2.86)

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	112	5% 71% 12% • 15%
1	B	112	5% 71% 8% 6% 14%
1	C	112	4% 72% 12% • 12%
1	D	112	3% 65% 19% • 13%
1	E	112	10% 68% 13% • 15%
1	F	112	5% 59% 17% •• 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	10	30% 40% 30%
2	H	10	30% 30% 40%
2	I	10	30% 20% 50%
2	J	10	60% 10% 30%
2	K	10	30% 40% 30%
2	L	10	30% 10% 60%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4605 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 Partitioning defective 3 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	95	Total	C	N	O	S	0	0	0
			705	436	128	138	3			
1	B	96	Total	C	N	O	S	0	0	0
			719	444	135	137	3			
1	C	99	Total	C	N	O	S	0	0	0
			744	456	140	145	3			
1	D	97	Total	C	N	O	S	0	0	0
			720	443	132	142	3			
1	E	95	Total	C	N	O	S	0	0	0
			714	440	134	137	3			
1	F	88	Total	C	N	O	S	0	0	0
			657	407	122	125	3			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	574	GLY	-	expression tag	UNP Q9Z340
A	575	PRO	-	expression tag	UNP Q9Z340
A	576	GLY	-	expression tag	UNP Q9Z340
A	577	SER	-	expression tag	UNP Q9Z340
A	578	GLU	-	expression tag	UNP Q9Z340
A	579	PHE	-	expression tag	UNP Q9Z340
B	574	GLY	-	expression tag	UNP Q9Z340
B	575	PRO	-	expression tag	UNP Q9Z340
B	576	GLY	-	expression tag	UNP Q9Z340
B	577	SER	-	expression tag	UNP Q9Z340
B	578	GLU	-	expression tag	UNP Q9Z340
B	579	PHE	-	expression tag	UNP Q9Z340
C	574	GLY	-	expression tag	UNP Q9Z340
C	575	PRO	-	expression tag	UNP Q9Z340
C	576	GLY	-	expression tag	UNP Q9Z340
C	577	SER	-	expression tag	UNP Q9Z340
C	578	GLU	-	expression tag	UNP Q9Z340

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	579	PHE	-	expression tag	UNP Q9Z340
D	574	GLY	-	expression tag	UNP Q9Z340
D	575	PRO	-	expression tag	UNP Q9Z340
D	576	GLY	-	expression tag	UNP Q9Z340
D	577	SER	-	expression tag	UNP Q9Z340
D	578	GLU	-	expression tag	UNP Q9Z340
D	579	PHE	-	expression tag	UNP Q9Z340
E	574	GLY	-	expression tag	UNP Q9Z340
E	575	PRO	-	expression tag	UNP Q9Z340
E	576	GLY	-	expression tag	UNP Q9Z340
E	577	SER	-	expression tag	UNP Q9Z340
E	578	GLU	-	expression tag	UNP Q9Z340
E	579	PHE	-	expression tag	UNP Q9Z340
F	574	GLY	-	expression tag	UNP Q9Z340
F	575	PRO	-	expression tag	UNP Q9Z340
F	576	GLY	-	expression tag	UNP Q9Z340
F	577	SER	-	expression tag	UNP Q9Z340
F	578	GLU	-	expression tag	UNP Q9Z340
F	579	PHE	-	expression tag	UNP Q9Z340

- Molecule 2 is a protein called INSC spindle orientation adaptor protein.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	G	7	Total C N O S 59 36 8 14 1	0	0	0
2	H	6	Total C N O S 51 32 6 12 1	0	0	0
2	I	5	Total C N O 43 27 5 11	0	0	0
2	J	7	Total C N O S 59 36 8 14 1	0	0	0
2	K	7	Total C N O S 59 36 8 14 1	0	0	0
2	L	4	Total C N O 34 22 4 8	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 3 3	0	0
3	B	4	Total O 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total O 1 1	0	0
3	C	5	Total O 5 5	0	0
3	I	1	Total O 1 1	0	0
3	D	9	Total O 9 9	0	0
3	J	1	Total O 1 1	0	0
3	E	9	Total O 9 9	0	0
3	F	7	Total O 7 7	0	0
3	L	1	Total O 1 1	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: Partitioning defective 3 homolog

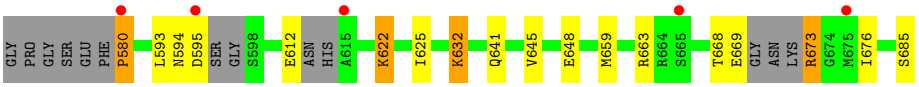
Chain A:

• Molecule 1: Partitioning defective 3 homolog

Chain B:

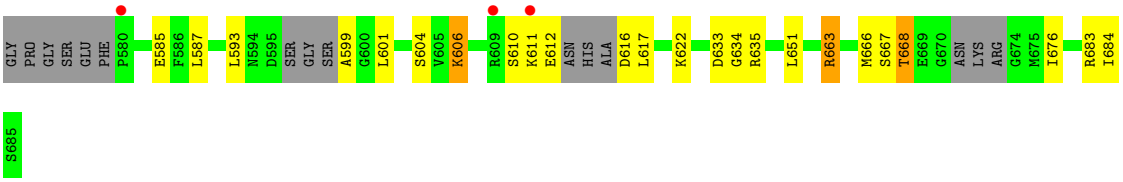
• Molecule 1: Partitioning defective 3 homolog

Chain C:



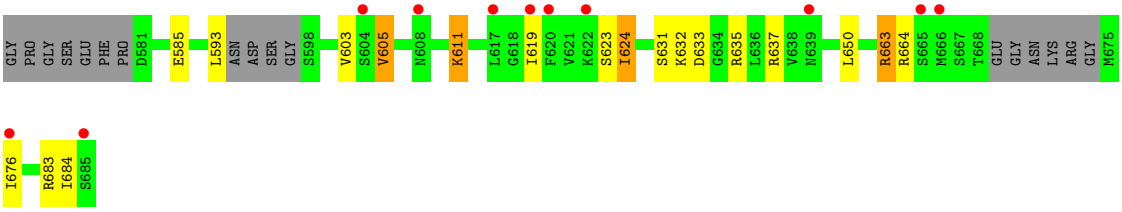
• Molecule 1: Partitioning defective 3 homolog

Chain D:

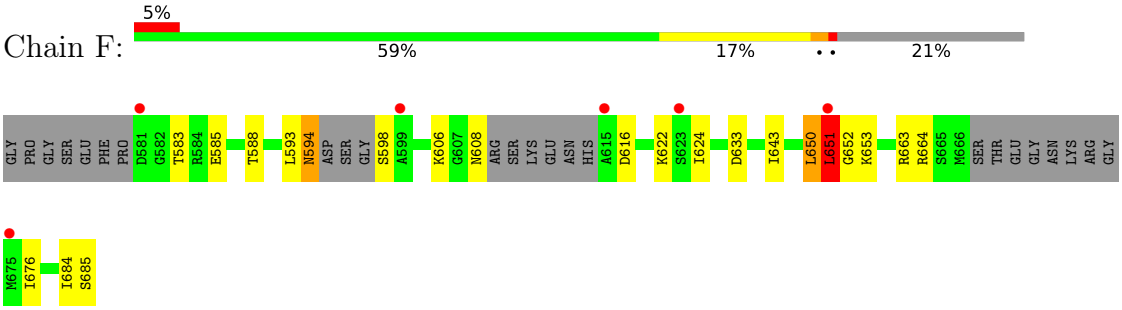


• Molecule 1: Partitioning defective 3 homolog

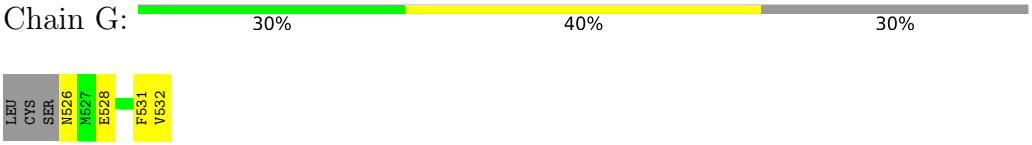
Chain E:



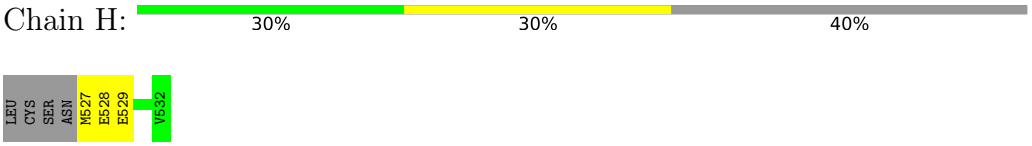
• Molecule 1: Partitioning defective 3 homolog



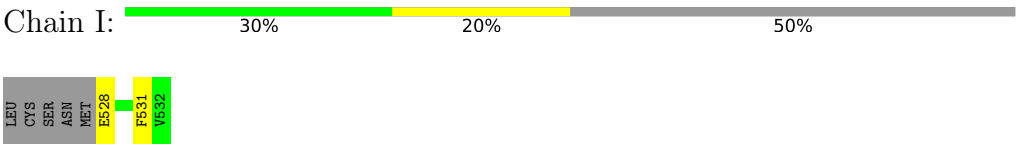
• Molecule 2: INSC spindle orientation adaptor protein



• Molecule 2: INSC spindle orientation adaptor protein



• Molecule 2: INSC spindle orientation adaptor protein



• Molecule 2: INSC spindle orientation adaptor protein

• Molecule 2: INSC spindle orientation adaptor protein

• Molecule 2: INSC spindle orientation adaptor protein

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.39Å 90.38Å 170.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.87 50.00 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.87) 99.9 (50.00-2.87)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.225 , 0.282 0.232 , 0.287	Depositor DCC
R_{free} test set	1113 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	82.5	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 74.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4605	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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	0.44	0/708	0.75	0/946
1	B	0.43	0/722	0.72	0/962
1	C	0.47	0/745	0.75	0/991
1	D	0.41	0/721	0.70	0/960
1	E	0.43	0/716	0.74	0/954
1	F	0.42	0/657	0.70	0/875
2	G	0.52	0/59	0.65	0/76
2	H	0.63	0/51	0.61	0/65
2	I	0.61	0/43	0.69	0/55
2	J	0.44	0/59	0.63	0/76
2	K	0.50	0/59	0.61	0/76
2	L	0.52	0/34	0.67	0/43
All	All	0.44	0/4574	0.72	0/6079

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	705	0	713	13	0
1	B	719	0	743	16	0
1	C	744	0	765	13	0
1	D	720	0	734	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	714	0	737	15	0
1	F	657	0	682	11	0
2	G	59	0	49	2	0
2	H	51	0	43	2	0
2	I	43	0	34	1	0
2	J	59	0	49	1	0
2	K	59	0	49	3	0
2	L	34	0	28	0	0
3	A	3	0	0	0	0
3	B	4	0	0	1	0
3	C	5	0	0	0	0
3	D	9	0	0	1	0
3	E	9	0	0	0	0
3	F	7	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
All	All	4605	0	4626	82	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 9.

All (82) 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:E:593:LEU:HD11	1:E:676:ILE:HD13	1.65	0.77
1:A:601:LEU:HD22	1:A:603:VAL:HG12	1.68	0.75
1:C:622:LYS:O	1:C:622:LYS:HE3	1.87	0.75
1:F:593:LEU:HD11	1:F:676:ILE:HD11	1.69	0.74
1:B:645:VAL:HG13	1:B:676:ILE:HD11	1.69	0.74
1:A:646:ASN:HD21	1:A:676:ILE:HD13	1.54	0.72
1:F:593:LEU:HD21	1:F:676:ILE:CD1	2.19	0.72
1:B:591:VAL:HG13	1:B:676:ILE:HG23	1.74	0.70
1:A:646:ASN:ND2	1:A:676:ILE:HD13	2.07	0.69
1:E:611:LYS:HD3	1:E:611:LYS:H	1.59	0.66
1:E:633:ASP:O	1:E:635:ARG:NH1	2.29	0.66
1:B:645:VAL:HG13	1:B:676:ILE:CD1	2.24	0.66
1:D:606:LYS:HD3	1:D:622:LYS:HB2	1.79	0.65
1:F:593:LEU:HD21	1:F:676:ILE:HD11	1.80	0.63
1:B:609:ARG:HG3	1:B:609:ARG:HH11	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LEU:HD22	1:A:603:VAL:CG1	2.29	0.63
1:E:624:ILE:HD11	1:E:631:SER:HA	1.83	0.61
1:E:619:ILE:HD11	1:E:650:LEU:HD13	1.82	0.60
1:F:594:ASN:HA	1:F:598:SER:HB2	1.84	0.60
1:D:616:ASP:HB3	1:D:617:LEU:HD22	1.86	0.57
1:F:606:LYS:HD3	1:F:622:LYS:HB2	1.86	0.57
1:B:593:LEU:HD11	1:B:676:ILE:HG22	1.85	0.57
1:B:611:LYS:H	1:B:611:LYS:CD	2.18	0.56
1:D:666:MET:O	1:D:668:THR:N	2.38	0.55
1:C:580:PRO:HG2	1:C:641:GLN:OE1	2.08	0.53
1:E:593:LEU:HD11	1:E:676:ILE:CD1	2.37	0.53
1:E:611:LYS:H	1:E:611:LYS:CD	2.21	0.53
1:F:664:ARG:O	1:F:664:ARG:NH1	2.40	0.53
1:B:612:GLU:O	1:B:613:ASN:HB2	2.09	0.53
1:C:593:LEU:HD11	1:C:676:ILE:HD11	1.91	0.52
1:B:632:LYS:HA	1:B:632:LYS:HE2	1.91	0.52
1:E:624:ILE:HD11	1:E:631:SER:CA	2.39	0.52
1:C:668:THR:O	1:C:669:GLU:C	2.48	0.52
1:C:685:SER:HB2	1:D:634:GLY:O	2.10	0.51
1:A:606:LYS:HD2	1:A:622:LYS:HB2	1.93	0.51
1:B:611:LYS:N	1:B:611:LYS:HE3	2.26	0.51
1:E:663:ARG:HB2	2:K:531:PHE:HE1	1.76	0.51
1:D:585:GLU:HB3	1:D:684:ILE:HD11	1.92	0.50
1:C:632:LYS:HA	1:C:632:LYS:HE2	1.94	0.49
1:C:594:ASN:O	1:C:595:ASP:C	2.50	0.49
1:D:633:ASP:OD2	1:D:635:ARG:NH1	2.46	0.49
1:E:624:ILE:HD11	1:E:631:SER:CB	2.43	0.48
1:D:593:LEU:HD11	1:D:676:ILE:CD1	2.43	0.48
1:F:650:LEU:O	1:F:652:GLY:N	2.46	0.48
1:E:624:ILE:O	1:E:624:ILE:HD13	2.14	0.48
3:B:703:HOH:O	1:C:673:ARG:HB2	2.14	0.48
1:A:606:LYS:HE2	1:A:608:ASN:HD21	1.79	0.47
2:K:532:VAL:OXT	2:K:532:VAL:HG12	2.14	0.47
1:D:593:LEU:HD11	1:D:676:ILE:HD11	1.97	0.47
1:F:643:ILE:HG23	1:F:651:LEU:HD22	1.97	0.47
1:B:612:GLU:O	1:B:613:ASN:CB	2.63	0.46
1:D:599:ALA:HB1	3:D:705:HOH:O	2.15	0.46
1:C:673:ARG:CZ	1:C:673:ARG:HB3	2.44	0.46
1:A:601:LEU:CD1	1:A:666:MET:CE	2.93	0.46
2:H:528:GLU:O	2:H:529:GLU:C	2.53	0.46
1:B:580:PRO:O	1:B:683:ARG:HD2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:PRO:HD2	1:F:588:THR:HG23	1.97	0.46
1:A:601:LEU:HD12	1:A:666:MET:HE3	1.97	0.46
1:D:604:SER:HB3	2:J:531:PHE:CE1	2.52	0.45
1:A:601:LEU:HD23	1:A:601:LEU:O	2.17	0.45
1:B:593:LEU:HD13	1:B:674:GLY:HA2	1.97	0.45
1:C:593:LEU:HD11	1:C:676:ILE:CD1	2.47	0.45
1:B:609:ARG:HH11	1:B:609:ARG:CG	2.27	0.45
2:G:531:PHE:O	2:G:532:VAL:OXT	2.36	0.44
1:A:601:LEU:HA	1:A:629:ALA:HB3	2.00	0.43
1:B:611:LYS:H	1:B:611:LYS:HD3	1.83	0.43
1:F:651:LEU:HD12	1:F:651:LEU:HA	1.75	0.43
1:D:610:SER:O	1:D:612:GLU:N	2.52	0.43
1:A:601:LEU:CD1	1:A:666:MET:HE3	2.49	0.42
1:E:585:GLU:HB2	1:E:684:ILE:HD11	2.01	0.42
1:C:625:ILE:HD11	2:I:531:PHE:CE2	2.54	0.42
1:D:663:ARG:HE	1:D:663:ARG:HB2	1.75	0.42
1:A:584:ARG:O	1:D:587:LEU:HA	2.19	0.42
1:B:635:ARG:HD3	1:F:583:THR:OG1	2.19	0.42
1:E:603:VAL:HG23	1:E:605:VAL:HG12	2.02	0.42
1:E:611:LYS:HD3	1:E:611:LYS:N	2.30	0.41
1:E:663:ARG:HB2	2:K:531:PHE:CE1	2.55	0.41
1:B:625:ILE:N	1:B:625:ILE:CD1	2.83	0.41
1:C:659:MET:O	1:C:663:ARG:HG3	2.21	0.41
1:D:601:LEU:HG	1:D:676:ILE:CD1	2.51	0.40
2:H:527:MET:O	2:H:527:MET:HG2	2.21	0.40
1:A:622:LYS:HE3	2:G:528:GLU:OE1	2.21	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	89/112 (80%)	84 (94%)	5 (6%)	0	100 100
1	B	90/112 (80%)	86 (96%)	3 (3%)	1 (1%)	12 34
1	C	91/112 (81%)	86 (94%)	5 (6%)	0	100 100
1	D	89/112 (80%)	82 (92%)	5 (6%)	2 (2%)	5 19
1	E	89/112 (80%)	85 (96%)	4 (4%)	0	100 100
1	F	80/112 (71%)	74 (92%)	5 (6%)	1 (1%)	10 30
2	G	5/10 (50%)	5 (100%)	0	0	100 100
2	H	4/10 (40%)	2 (50%)	2 (50%)	0	100 100
2	I	3/10 (30%)	3 (100%)	0	0	100 100
2	J	5/10 (50%)	5 (100%)	0	0	100 100
2	K	5/10 (50%)	4 (80%)	1 (20%)	0	100 100
2	L	2/10 (20%)	2 (100%)	0	0	100 100
All	All	552/732 (75%)	518 (94%)	30 (5%)	4 (1%)	19 46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	651	LEU
1	D	611	LYS
1	D	667	SER
1	B	613	ASN

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	75/89 (84%)	66 (88%)	9 (12%)	4 11
1	B	77/89 (86%)	69 (90%)	8 (10%)	5 16
1	C	80/89 (90%)	73 (91%)	7 (9%)	8 24
1	D	77/89 (86%)	72 (94%)	5 (6%)	14 37
1	E	77/89 (86%)	68 (88%)	9 (12%)	4 12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	70/89 (79%)	58 (83%)	12 (17%)	1 4
2	G	7/10 (70%)	6 (86%)	1 (14%)	2 7
2	H	6/10 (60%)	6 (100%)	0	100 100
2	I	5/10 (50%)	4 (80%)	1 (20%)	1 2
2	J	7/10 (70%)	7 (100%)	0	100 100
2	K	7/10 (70%)	5 (71%)	2 (29%)	0 1
2	L	4/10 (40%)	3 (75%)	1 (25%)	0 1
All	All	492/594 (83%)	437 (89%)	55 (11%)	5 14

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	606	LYS
1	A	611	LYS
1	A	614	HIS
1	A	642	LEU
1	A	656	GLN
1	A	657	GLU
1	A	660	GLU
1	A	666	MET
1	A	676	ILE
2	G	526	ASN
1	B	591	VAL
1	B	609	ARG
1	B	611	LYS
1	B	625	ILE
1	B	632	LYS
1	B	650	LEU
1	B	675	MET
1	B	676	ILE
1	C	580	PRO
1	C	612	GLU
1	C	622	LYS
1	C	632	LYS
1	C	645	VAL
1	C	648	GLU
1	C	673	ARG
2	I	528	GLU
1	D	606	LYS
1	D	651	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	663	ARG
1	D	668	THR
1	D	683	ARG
1	E	605	VAL
1	E	611	LYS
1	E	623	SER
1	E	624	ILE
1	E	632	LYS
1	E	637	ARG
1	E	663	ARG
1	E	664	ARG
1	E	683	ARG
2	K	526	ASN
2	K	527	MET
1	F	585	GLU
1	F	594	ASN
1	F	608	ASN
1	F	616	ASP
1	F	624	ILE
1	F	633	ASP
1	F	650	LEU
1	F	651	LEU
1	F	653	LYS
1	F	663	ARG
1	F	684	ILE
1	F	685	SER
2	L	529	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	608	ASN
1	A	613	ASN
1	A	639	ASN
2	G	526	ASN
1	B	639	ASN
1	C	594	ASN
1	C	655	ASN
1	E	677	GLN
1	F	656	GLN

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, 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	95/112 (84%)	0.64	6 (6%) 27 23	49, 87, 135, 160	0
1	B	96/112 (85%)	0.47	6 (6%) 27 23	52, 82, 125, 158	0
1	C	99/112 (88%)	0.27	5 (5%) 34 30	50, 75, 146, 164	0
1	D	97/112 (86%)	0.45	3 (3%) 51 46	54, 88, 147, 170	0
1	E	95/112 (84%)	0.79	11 (11%) 11 10	61, 98, 136, 160	0
1	F	88/112 (78%)	0.67	6 (6%) 25 21	65, 105, 150, 169	0
2	G	7/10 (70%)	1.06	0 100 100	89, 97, 131, 135	0
2	H	6/10 (60%)	0.77	0 100 100	75, 88, 127, 129	0
2	I	5/10 (50%)	0.34	0 100 100	81, 94, 127, 142	0
2	J	7/10 (70%)	0.76	0 100 100	90, 98, 159, 179	0
2	K	7/10 (70%)	0.85	0 100 100	86, 94, 113, 116	0
2	L	4/10 (40%)	1.05	0 100 100	130, 131, 141, 153	0
All	All	606/732 (82%)	0.56	37 (6%) 28 24	49, 91, 143, 179	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	580	PRO	6.4
1	E	685	SER	3.9
1	A	580	PRO	3.6
1	F	615	ALA	3.6
1	F	599	ALA	3.4
1	E	620	PHE	3.4
1	C	580	PRO	3.4
1	C	615	ALA	3.2
1	E	617	LEU	3.2
1	A	665	SER	3.1
1	E	622	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	604	SER	3.0
1	A	601	LEU	2.9
1	E	666	MET	2.7
1	A	667	SER	2.7
1	B	675	MET	2.6
1	A	663	ARG	2.6
1	F	581	ASP	2.6
1	B	593	LEU	2.6
1	F	675	MET	2.6
1	D	580	PRO	2.5
1	B	592	PRO	2.4
1	D	609	ARG	2.4
1	E	665	SER	2.4
1	E	676	ILE	2.4
1	E	608	ASN	2.3
1	F	623	SER	2.3
1	C	595	ASP	2.3
1	B	591	VAL	2.2
1	E	639	ASN	2.2
1	F	651	LEU	2.2
1	D	611	LYS	2.2
1	C	675	MET	2.1
1	B	676	ILE	2.0
1	C	665	SER	2.0
1	E	619	ILE	2.0
1	A	664	ARG	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.