Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:21 AM GMT

PDB ID	:	3EBB
Title	:	PLAP/P97 complex
Authors	:	Walker, J.R.; Qiu, L.; Akutsu, M.; Slessarev, Y.; Amaya, M.F.; Li, Y.; Bountra, C.; Weigelt, J.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)
Deposited on	:	2008-08-27
Resolution	:	1.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

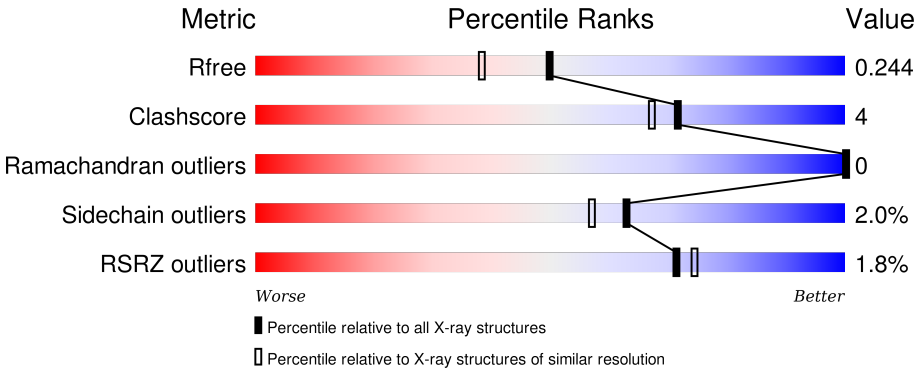
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	304	78% 9% 13%
1	B	304	79% 7% 14%
1	C	304	78% 9% 13%
1	D	304	75% 11% 14%
2	E	10	10% 10% 80%

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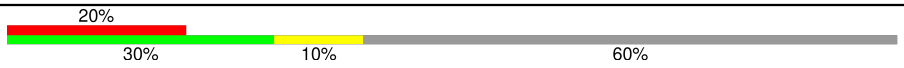
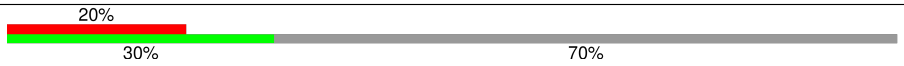
Mol	Chain	Length	Quality of chain
2	F	10	
2	G	10	
2	H	10	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8729 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 PHOSPHOLIPASE A2-ACTIVATING PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	Se	0	2	0
			2038	1297	346	381	10	4			
1	B	262	Total	C	N	O	S	Se	0	9	0
			2068	1314	351	388	11	4			
1	C	265	Total	C	N	O	S	Se	0	3	0
			2047	1304	349	381	9	4			
1	D	261	Total	C	N	O	S	Se	0	1	0
			1994	1268	337	377	9	3			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	492	MSE	-	expression tag	UNP Q9Y263
A	493	GLY	-	expression tag	UNP Q9Y263
A	494	SER	-	expression tag	UNP Q9Y263
A	495	SER	-	expression tag	UNP Q9Y263
A	496	HIS	-	expression tag	UNP Q9Y263
A	497	HIS	-	expression tag	UNP Q9Y263
A	498	HIS	-	expression tag	UNP Q9Y263
A	499	HIS	-	expression tag	UNP Q9Y263
A	500	HIS	-	expression tag	UNP Q9Y263
A	501	HIS	-	expression tag	UNP Q9Y263
A	502	SER	-	expression tag	UNP Q9Y263
A	503	SER	-	expression tag	UNP Q9Y263
A	504	GLY	-	expression tag	UNP Q9Y263
A	505	LEU	-	expression tag	UNP Q9Y263
A	506	VAL	-	expression tag	UNP Q9Y263
A	507	PRO	-	expression tag	UNP Q9Y263
A	508	ARG	-	expression tag	UNP Q9Y263
A	509	GLY	-	expression tag	UNP Q9Y263
A	510	SER	-	expression tag	UNP Q9Y263
A	570	GLU	-	expression tag	UNP Q9Y263
B	492	MSE	-	expression tag	UNP Q9Y263

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Chain	Residue	Modelled	Actual	Comment	Reference
B	493	GLY	-	expression tag	UNP Q9Y263
B	494	SER	-	expression tag	UNP Q9Y263
B	495	SER	-	expression tag	UNP Q9Y263
B	496	HIS	-	expression tag	UNP Q9Y263
B	497	HIS	-	expression tag	UNP Q9Y263
B	498	HIS	-	expression tag	UNP Q9Y263
B	499	HIS	-	expression tag	UNP Q9Y263
B	500	HIS	-	expression tag	UNP Q9Y263
B	501	HIS	-	expression tag	UNP Q9Y263
B	502	SER	-	expression tag	UNP Q9Y263
B	503	SER	-	expression tag	UNP Q9Y263
B	504	GLY	-	expression tag	UNP Q9Y263
B	505	LEU	-	expression tag	UNP Q9Y263
B	506	VAL	-	expression tag	UNP Q9Y263
B	507	PRO	-	expression tag	UNP Q9Y263
B	508	ARG	-	expression tag	UNP Q9Y263
B	509	GLY	-	expression tag	UNP Q9Y263
B	510	SER	-	expression tag	UNP Q9Y263
B	570	GLU	-	expression tag	UNP Q9Y263
C	492	MSE	-	expression tag	UNP Q9Y263
C	493	GLY	-	expression tag	UNP Q9Y263
C	494	SER	-	expression tag	UNP Q9Y263
C	495	SER	-	expression tag	UNP Q9Y263
C	496	HIS	-	expression tag	UNP Q9Y263
C	497	HIS	-	expression tag	UNP Q9Y263
C	498	HIS	-	expression tag	UNP Q9Y263
C	499	HIS	-	expression tag	UNP Q9Y263
C	500	HIS	-	expression tag	UNP Q9Y263
C	501	HIS	-	expression tag	UNP Q9Y263
C	502	SER	-	expression tag	UNP Q9Y263
C	503	SER	-	expression tag	UNP Q9Y263
C	504	GLY	-	expression tag	UNP Q9Y263
C	505	LEU	-	expression tag	UNP Q9Y263
C	506	VAL	-	expression tag	UNP Q9Y263
C	507	PRO	-	expression tag	UNP Q9Y263
C	508	ARG	-	expression tag	UNP Q9Y263
C	509	GLY	-	expression tag	UNP Q9Y263
C	510	SER	-	expression tag	UNP Q9Y263
C	570	GLU	-	expression tag	UNP Q9Y263
D	492	MSE	-	expression tag	UNP Q9Y263
D	493	GLY	-	expression tag	UNP Q9Y263
D	494	SER	-	expression tag	UNP Q9Y263

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Chain	Residue	Modelled	Actual	Comment	Reference
D	495	SER	-	expression tag	UNP Q9Y263
D	496	HIS	-	expression tag	UNP Q9Y263
D	497	HIS	-	expression tag	UNP Q9Y263
D	498	HIS	-	expression tag	UNP Q9Y263
D	499	HIS	-	expression tag	UNP Q9Y263
D	500	HIS	-	expression tag	UNP Q9Y263
D	501	HIS	-	expression tag	UNP Q9Y263
D	502	SER	-	expression tag	UNP Q9Y263
D	503	SER	-	expression tag	UNP Q9Y263
D	504	GLY	-	expression tag	UNP Q9Y263
D	505	LEU	-	expression tag	UNP Q9Y263
D	506	VAL	-	expression tag	UNP Q9Y263
D	507	PRO	-	expression tag	UNP Q9Y263
D	508	ARG	-	expression tag	UNP Q9Y263
D	509	GLY	-	expression tag	UNP Q9Y263
D	510	SER	-	expression tag	UNP Q9Y263
D	570	GLU	-	expression tag	UNP Q9Y263

- Molecule 2 is a protein called TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE (TER ATP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			20	15	2	3			
2	F	4	Total	C	N	O	0	0	0
			32	21	4	7			
2	G	3	Total	C	N	O	0	0	0
			24	17	3	4			
2	H	3	Total	C	N	O	0	0	0
			28	19	3	6			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	1
			140	140		

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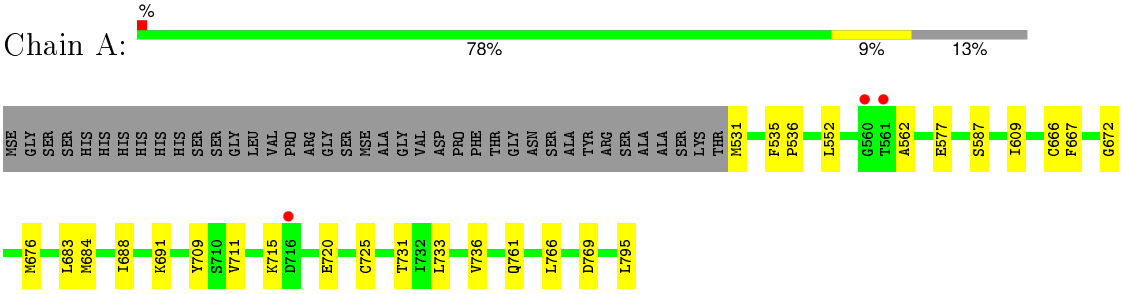
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	147	Total O 153 153	0	6
4	C	99	Total O 100 100	0	1
4	D	81	Total O 82 82	0	1
4	F	1	Total O 1 1	0	0
4	G	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

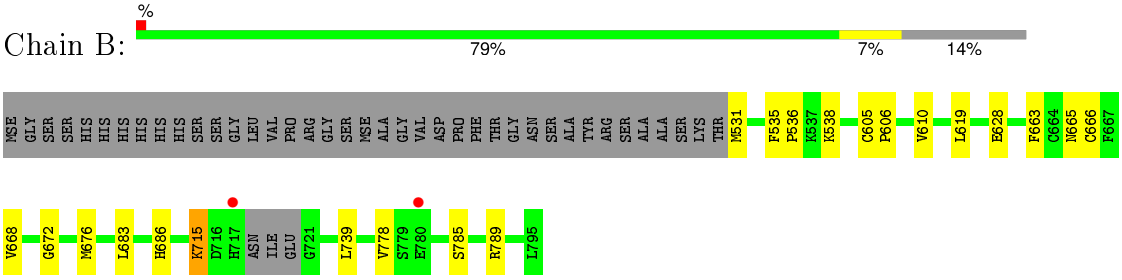
- Molecule 1: PHOSPHOLIPASE A2-ACTIVATING PROTEIN

Chain A:



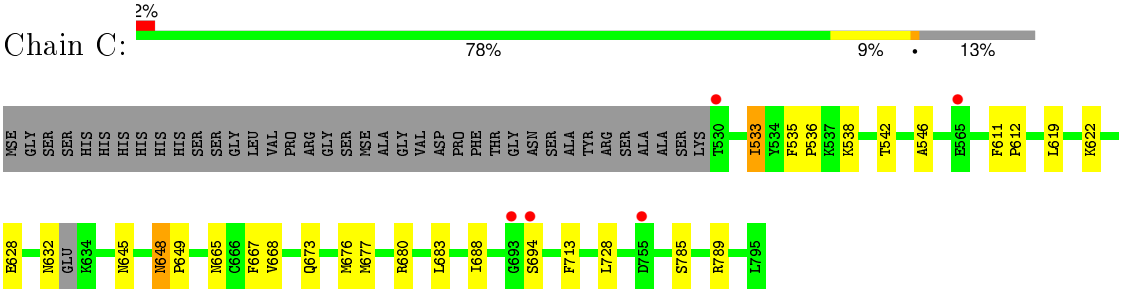
- Molecule 1: PHOSPHOLIPASE A2-ACTIVATING PROTEIN

Chain B:



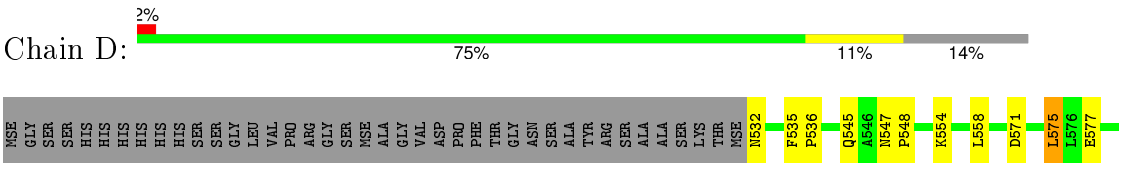
- Molecule 1: PHOSPHOLIPASE A2-ACTIVATING PROTEIN

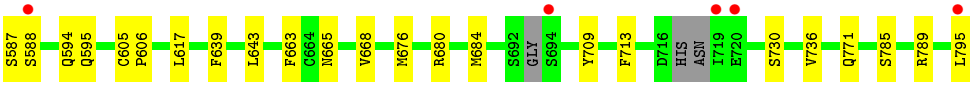
Chain C:



- Molecule 1: PHOSPHOLIPASE A2-ACTIVATING PROTEIN

Chain D:



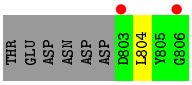


• Molecule 2: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE (TER ATP

Chain E:

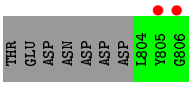
• Molecule 2: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE (TER ATP

Chain F:



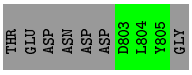
• Molecule 2: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE (TER ATP

Chain G:



• Molecule 2: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE (TER ATP

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.38Å 68.65Å 143.97Å 90.00° 103.45° 90.00°	Depositor
Resolution (Å)	41.49 – 1.90 38.61 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.49-1.90) 98.8 (38.61-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.248 0.188 , 0.244	Depositor DCC
R_{free} test set	3849 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 76563 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8729	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.57	0/2064	0.62	0/2785
1	B	0.58	0/2092	0.62	0/2819
1	C	0.50	0/2072	0.56	0/2794
1	D	0.48	0/2018	0.56	0/2725
2	E	0.52	0/20	0.43	0/26
2	F	0.60	0/32	0.78	0/42
2	G	0.52	0/24	0.41	0/31
2	H	0.50	0/28	0.67	0/37
All	All	0.53	0/8350	0.59	0/11259

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	2038	0	2090	19	0
1	B	2068	0	2121	14	0
1	C	2047	0	2109	22	0
1	D	1994	0	2031	22	0
2	E	20	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	32	0	26	0	0
2	G	24	0	22	0	0
2	H	28	0	23	0	0
3	B	1	0	0	0	0
4	A	140	0	0	0	0
4	B	153	0	0	2	0
4	C	100	0	0	0	0
4	D	82	0	0	2	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
All	All	8729	0	8441	71	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 4.

All (71) 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:A:676:MSE:HE1	1:A:683:LEU:CD2	1.83	1.08
1:A:676:MSE:HE1	1:A:683:LEU:HD21	1.48	0.95
1:C:676:MSE:HE1	1:C:683:LEU:CD2	2.02	0.89
1:A:587:SER:HA	1:B:538[A]:LYS:HD3	1.56	0.87
1:C:676:MSE:HE1	1:C:683:LEU:HD21	1.56	0.85
1:A:676:MSE:CE	1:A:683:LEU:CD2	2.62	0.78
1:B:628:GLU:OE1	4:B:935:HOH:O	2.05	0.74
1:B:686:HIS:NE2	4:B:807[B]:HOH:O	2.24	0.69
1:D:676:MSE:HA	1:D:676:MSE:HE2	1.73	0.68
1:D:785:SER:O	1:D:789:ARG:HG3	1.93	0.68
1:A:676:MSE:CE	1:A:683:LEU:HD23	2.25	0.67
1:C:667:PHE:CE2	1:C:676:MSE:HE2	2.31	0.65
1:C:667:PHE:HE2	1:C:676:MSE:HE2	1.62	0.64
1:D:680:ARG:HD2	1:D:713:PHE:HZ	1.63	0.64
1:A:676:MSE:HE1	1:A:683:LEU:HD23	1.76	0.64
1:B:665:ASN:O	1:B:668:VAL:HG22	1.98	0.64
1:C:676:MSE:CE	1:C:683:LEU:CD2	2.77	0.62
1:C:538[A]:LYS:HD3	1:D:587:SER:HA	1.82	0.60
1:C:546:ALA:HB2	1:C:619:LEU:HD21	1.82	0.60
1:D:594:GLN:HG2	1:D:595:GLN:N	2.20	0.57
1:A:552:LEU:HD11	1:A:577:GLU:HG3	1.85	0.57
1:D:535:PHE:HB2	1:D:536:PRO:HA	1.87	0.56
1:B:535:PHE:HB2	1:B:536:PRO:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:785:SER:O	1:C:789:ARG:HG3	2.05	0.55
1:C:533[A]:ILE:CD1	1:D:577:GLU:HG3	2.37	0.54
1:D:532:ASN:N	4:D:271:HOH:O	2.40	0.54
1:A:667:PHE:CE2	1:A:676:MSE:HE2	2.42	0.54
1:B:538[B]:LYS:HD2	1:B:715:LYS:HE3	1.91	0.53
1:C:645:ASN:O	1:C:648:ASN:HB3	2.11	0.51
1:C:688:ILE:HD13	1:C:728:LEU:HG	1.93	0.51
1:D:575:LEU:HD21	1:D:594:GLN:HG3	1.92	0.50
1:B:785:SER:O	1:B:789:ARG:HG3	2.11	0.50
1:A:684:MSE:HE3	1:A:709:TYR:CD2	2.49	0.48
1:C:533[B]:ILE:HD12	1:D:548:PRO:HB2	1.95	0.48
1:C:538[A]:LYS:NZ	1:D:588:SER:H	2.12	0.47
1:D:547:ASN:OD1	1:D:547:ASN:N	2.48	0.47
1:D:605:CYS:HB3	1:D:606:PRO:CD	2.45	0.47
1:D:643:LEU:HB2	1:D:663:PHE:CZ	2.50	0.47
1:A:535:PHE:HB2	1:A:536:PRO:HA	1.96	0.46
1:D:665:ASN:O	1:D:668:VAL:HG22	2.16	0.46
1:A:691:LYS:HD3	1:A:731:THR:HG22	1.96	0.46
1:B:778:VAL:O	1:B:785:SER:HB3	2.15	0.46
1:B:672:GLY:O	1:B:676:MSE:HG2	2.16	0.46
1:B:531:MSE:HG3	1:B:536:PRO:HD2	1.98	0.46
1:A:666[A]:CYS:O	1:A:672:GLY:HA3	2.16	0.45
1:C:628:GLU:O	1:C:632:ASN:HB3	2.16	0.45
1:B:666[A]:CYS:O	1:B:672:GLY:HA3	2.15	0.45
1:A:562:ALA:HB2	1:A:609:ILE:CD1	2.47	0.44
1:C:680:ARG:HD3	1:C:713:PHE:HZ	1.83	0.44
1:A:733:LEU:HA	1:A:736:VAL:HG12	2.00	0.44
1:C:535:PHE:HB2	1:C:536:PRO:HA	2.00	0.44
1:A:769:ASP:OD1	1:A:769:ASP:N	2.51	0.43
1:C:538[A]:LYS:HZ3	1:D:588:SER:H	1.67	0.43
1:C:673:GLN:O	1:C:677:MSE:HG2	2.18	0.43
1:A:676:MSE:HE3	1:A:683:LEU:HD23	2.00	0.43
1:D:676:MSE:HA	1:D:676:MSE:CE	2.48	0.43
1:A:684:MSE:HE1	1:A:725:CYS:SG	2.58	0.42
1:A:711:VAL:O	1:A:715:LYS:HG3	2.20	0.42
1:C:611:PHE:CG	1:C:612:PRO:HD3	2.55	0.42
1:A:676:MSE:HE3	1:A:709:TYR:OH	2.19	0.41
1:C:648:ASN:HA	1:C:649:PRO:HD3	1.80	0.41
1:D:730:SER:OG	1:D:771:GLN:OE1	2.35	0.41
1:D:554:LYS:HE3	1:D:558:LEU:HD11	2.02	0.41
1:D:545:GLN:OE1	4:D:296:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:617:LEU:HD21	1:D:639:PHE:HE1	1.86	0.41
1:C:542:THR:HG21	1:C:668:VAL:HG11	2.03	0.41
1:B:605[B]:CYS:HB2	1:B:606:PRO:CD	2.51	0.41
1:C:622:LYS:HD2	1:C:665:ASN:ND2	2.36	0.41
1:B:610:VAL:HG22	1:B:610:VAL:O	2.21	0.40
1:B:663:PHE:CD2	1:B:683[B]:LEU:HD21	2.57	0.40
1:D:684:MSE:HE3	1:D:709:TYR:CG	2.56	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	265/304 (87%)	261 (98%)	4 (2%)	0	100	100
1	B	267/304 (88%)	262 (98%)	5 (2%)	0	100	100
1	C	264/304 (87%)	260 (98%)	4 (2%)	0	100	100
1	D	256/304 (84%)	256 (100%)	0	0	100	100
2	F	2/10 (20%)	2 (100%)	0	0	100	100
2	G	1/10 (10%)	1 (100%)	0	0	100	100
2	H	1/10 (10%)	1 (100%)	0	0	100	100
All	All	1056/1246 (85%)	1043 (99%)	13 (1%)	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	228/260 (88%)	222 (97%)	6 (3%)	54 45
1	B	234/260 (90%)	231 (99%)	3 (1%)	76 73
1	C	231/260 (89%)	227 (98%)	4 (2%)	68 64
1	D	224/260 (86%)	220 (98%)	4 (2%)	66 61
2	E	2/9 (22%)	1 (50%)	1 (50%)	0 0
2	F	3/9 (33%)	2 (67%)	1 (33%)	0 0
2	G	2/9 (22%)	2 (100%)	0	100 100
2	H	3/9 (33%)	3 (100%)	0	100 100
All	All	927/1076 (86%)	908 (98%)	19 (2%)	63 57

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	531	MSE
1	A	688	ILE
1	A	720	GLU
1	A	761	GLN
1	A	766	LEU
1	A	795	LEU
1	B	619	LEU
1	B	715	LYS
1	B	739	LEU
1	C	533[A]	ILE
1	C	533[B]	ILE
1	C	648	ASN
1	C	694	SER
1	D	571	ASP
1	D	575	LEU
1	D	736	VAL
1	D	795	LEU
2	E	804	LEU
2	F	804	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	623	HIS
1	A	645	ASN
1	B	645	ASN
1	C	793	ASN
1	D	655	ASN
1	D	758	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	261/304 (85%)	-0.07	3 (1%) 82 84	11, 21, 45, 63	0
1	B	258/304 (84%)	-0.12	2 (0%) 87 88	10, 20, 37, 51	0
1	C	261/304 (85%)	-0.01	5 (1%) 70 73	15, 28, 50, 71	0
1	D	258/304 (84%)	0.10	5 (1%) 70 73	14, 29, 54, 119	0
2	E	2/10 (20%)	0.44	0 100 100	35, 35, 35, 39	0
2	F	4/10 (40%)	2.46	2 (50%) 0 0	37, 42, 44, 48	0
2	G	3/10 (30%)	4.05	2 (66%) 0 0	44, 44, 44, 48	0
2	H	3/10 (30%)	1.66	0 100 100	57, 57, 60, 63	0
All	All	1050/1256 (83%)	0.00	19 (1%) 71 74	10, 24, 49, 119	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	719	ILE	9.5
2	G	806	GLY	7.7
2	F	806	GLY	5.6
1	D	720	GLU	4.2
1	A	716	ASP	3.6
1	C	530	THR	3.4
1	B	780	GLU	3.2
1	C	565	GLU	3.1
1	B	717	HIS	3.0
1	C	694	SER	2.8
1	D	694	SER	2.8
2	G	805	TYR	2.6
1	A	561	THR	2.6
2	F	803	ASP	2.5
1	C	755	ASP	2.4
1	D	795	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	560	GLY	2.3
1	C	693	GLY	2.3
1	D	588	SER	2.1

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	B	1	1/1	0.98	0.06	-1.75	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.