Full wwPDB X-ray Structure Validation Report (i)

Mar 21, 2016 – 12:17 AM EDT

PDB ID	:	5AYW
Title	:	Structure of a membrane complex
Authors	:	Huang, Y.; Han, L.; Zheng, J.
Deposited on	:	2015-09-14
Resolution	:	3.56 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:

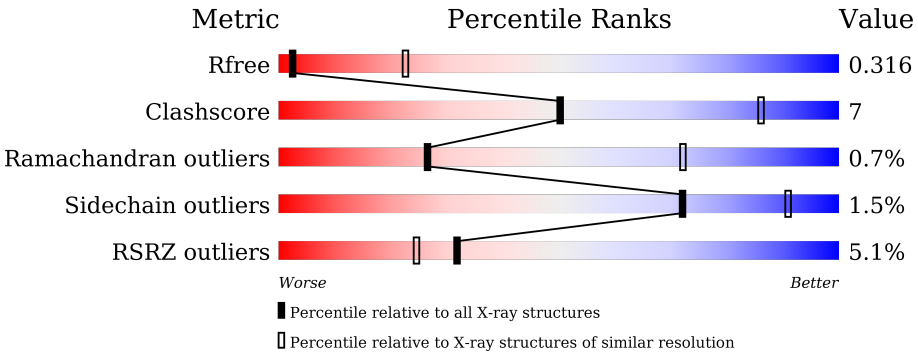
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 3.56 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	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

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 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	789	6% 81% 18% ••
2	B	383	3% 78% 12% • 9%
3	C	56	11% 82% 16% •
4	D	226	% 78% 15% 6%
5	E	102	4% 54% 30% • 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11497 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	785	Total	C	N	O	S	0	0	0
			6133	3864	1034	1219	16			

- Molecule 2 is a protein called Outer membrane protein assembly factor BamB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	348	Total	C	N	O	S	0	0	0
			2600	1633	447	514	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	393	LYS	-	expression tag	UNP P77774
B	394	LEU	-	expression tag	UNP P77774
B	395	TRP	-	expression tag	UNP P77774
B	396	SER	-	expression tag	UNP P77774
B	397	HIS	-	expression tag	UNP P77774
B	398	PRO	-	expression tag	UNP P77774
B	399	GLN	-	expression tag	UNP P77774
B	400	PHE	-	expression tag	UNP P77774
B	401	GLU	-	expression tag	UNP P77774
B	402	LYS	-	expression tag	UNP P77774

- Molecule 3 is a protein called Outer membrane protein assembly factor BamC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	56	Total	C	N	O	S	0	0	0
			391	247	65	78	1			

- Molecule 4 is a protein called Outer membrane protein assembly factor BamD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	212	Total	C	N	O	S	0	0	0
			1701	1069	297	328	7			

- Molecule 5 is a protein called Outer membrane protein assembly factor BamE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	88	Total	C	N	O	S	0	0	0
			672	420	117	133	2			

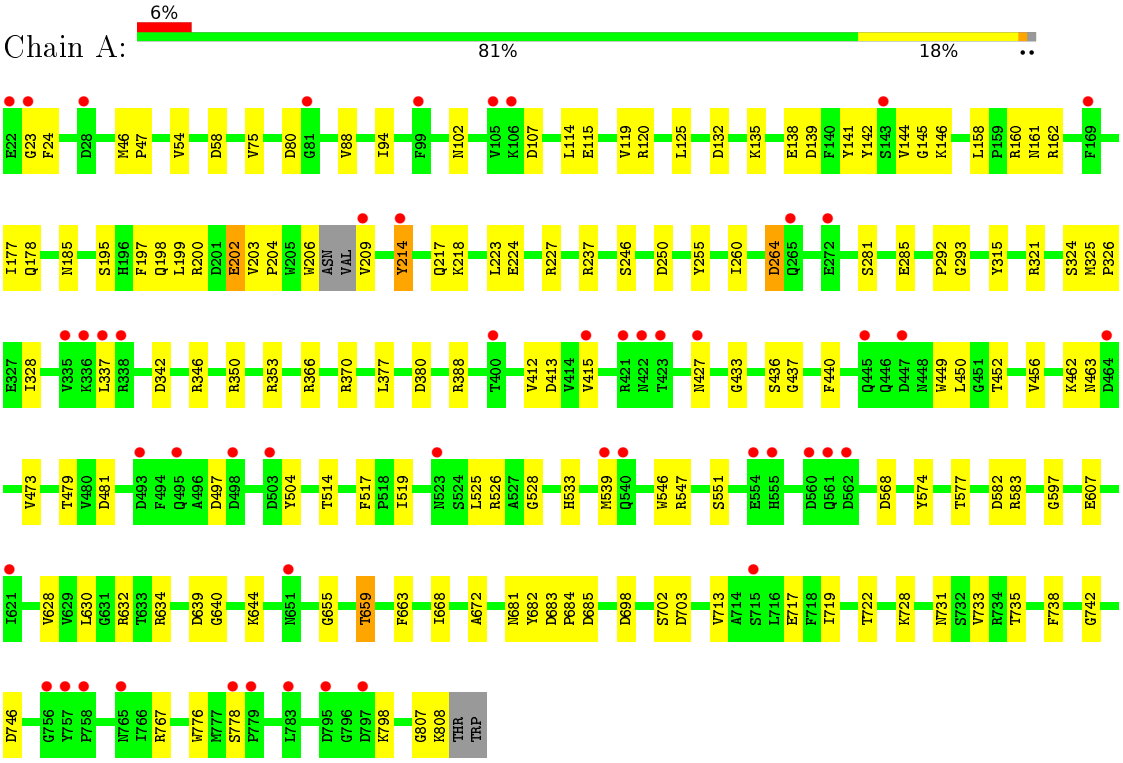
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	114	LYS	-	expression tag	UNP P0A937
E	115	LEU	-	expression tag	UNP P0A937
E	116	HIS	-	expression tag	UNP P0A937
E	117	HIS	-	expression tag	UNP P0A937
E	118	HIS	-	expression tag	UNP P0A937
E	119	HIS	-	expression tag	UNP P0A937
E	120	HIS	-	expression tag	UNP P0A937
E	121	HIS	-	expression tag	UNP P0A937

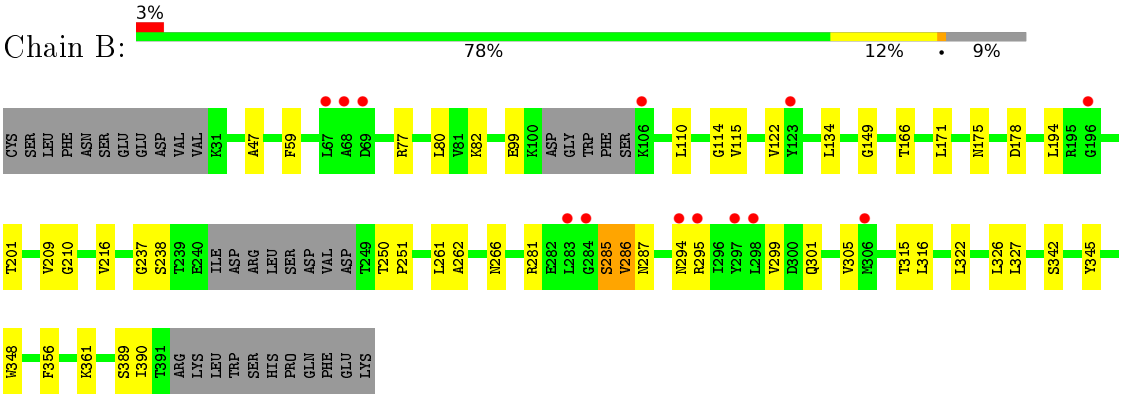
3 Residue-property plots (i)

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.

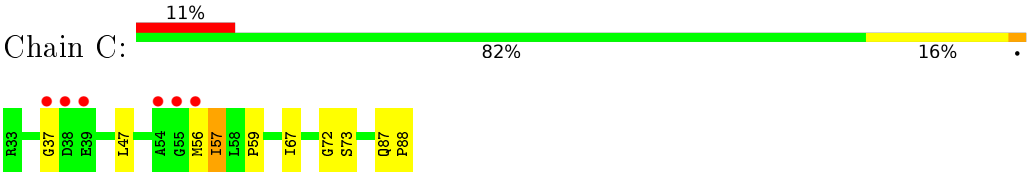
- Molecule 1: Outer membrane protein assembly factor BamA



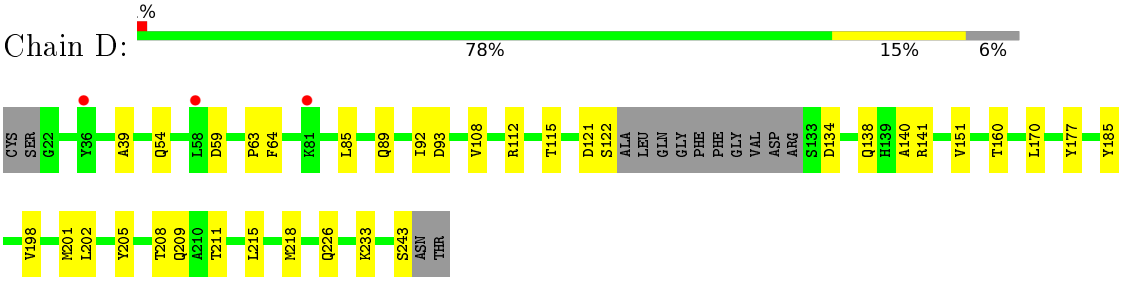
- Molecule 2: Outer membrane protein assembly factor BamB



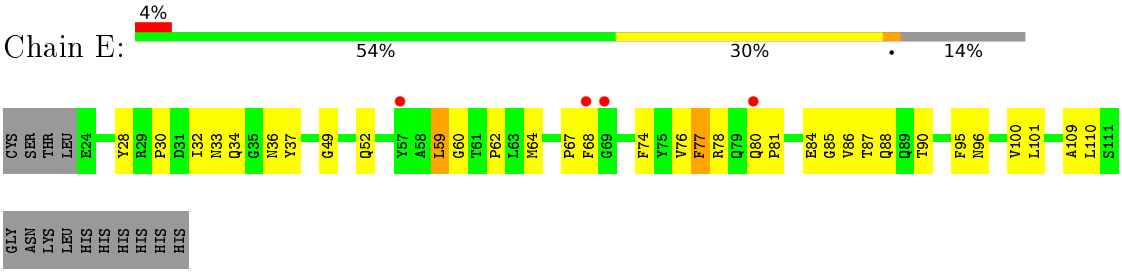
- Molecule 3: Outer membrane protein assembly factor BamC



• Molecule 4: Outer membrane protein assembly factor BamD



• Molecule 5: Outer membrane protein assembly factor BamE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	116.43Å 116.43Å 434.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.57 – 3.56 37.40 – 3.56	Depositor EDS
% Data completeness (in resolution range)	97.8 (34.57-3.56) 98.7 (37.40-3.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 3.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.271 , 0.314 0.277 , 0.316	Depositor DCC
R_{free} test set	2503 reflections (6.90%)	DCC
Wilson B-factor (Å^2)	108.5	Xtriage
Anisotropy	0.833	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 72.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 36626 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	11497	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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

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	0.22	0/6271	0.40	0/8511
2	B	0.21	0/2645	0.41	0/3605
3	C	0.22	0/400	0.43	0/550
4	D	0.20	0/1738	0.36	0/2361
5	E	0.28	0/685	0.55	1/936 (0.1%)
All	All	0.22	0/11739	0.41	1/15963 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	59	LEU	CA-CB-CG	5.71	128.44	115.30

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	6133	0	5804	86	0
2	B	2600	0	2562	28	0
3	C	391	0	383	6	0
4	D	1701	0	1636	22	0
5	E	672	0	646	23	0
All	All	11497	0	11031	157	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 (157) 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:197:PHE:HA	1:A:198:GLN:HB3	1.59	0.85
1:A:681:ASN:HB2	1:A:683:ASP:H	1.44	0.81
1:A:246:SER:HB2	1:A:255:TYR:HB2	1.65	0.79
2:B:286:VAL:HG22	2:B:287:ASN:HA	1.65	0.79
1:A:479:THR:HG23	1:A:481:ASP:H	1.48	0.78
5:E:85:GLY:HA2	5:E:86:VAL:HG22	1.66	0.76
1:A:681:ASN:N	1:A:682:TYR:HA	2.03	0.73
2:B:326:LEU:HB2	2:B:342:SER:HB3	1.69	0.73
1:A:681:ASN:H	1:A:682:TYR:HA	1.52	0.73
1:A:54:VAL:HG13	1:A:58:ASP:HB2	1.71	0.73
1:A:440:PHE:HB2	1:A:462:LYS:HB3	1.71	0.72
1:A:717:GLU:HB3	1:A:738:PHE:HB3	1.72	0.71
1:A:370:ARG:HE	1:A:388:ARG:HH21	1.40	0.69
1:A:195:SER:O	1:A:731:ASN:ND2	2.26	0.68
1:A:200:ARG:NH1	1:A:728:LYS:O	2.26	0.68
1:A:547:ARG:NH2	1:A:746:ASP:OD2	2.29	0.66
5:E:33:ASN:O	5:E:34:GLN:NE2	2.28	0.66
1:A:141:TYR:HD1	1:A:146:LYS:HG3	1.62	0.65
5:E:32:ILE:H	5:E:81:PRO:HA	1.62	0.65
1:A:504:TYR:HB2	1:A:539:MET:HG2	1.80	0.64
4:D:92:ILE:HG21	4:D:112:ARG:HB2	1.83	0.61
4:D:202:LEU:HD21	4:D:215:LEU:HD21	1.82	0.60
1:A:632:ARG:NH2	1:A:717:GLU:OE1	2.35	0.60
2:B:80:LEU:HD21	2:B:82:LYS:HE3	1.82	0.60
1:A:144:VAL:HG13	1:A:146:LYS:HG2	1.84	0.60
1:A:197:PHE:HB2	1:A:198:GLN:O	2.03	0.59
5:E:85:GLY:HA3	5:E:87:THR:HG23	1.84	0.59
2:B:77:ARG:HH11	2:B:110:LEU:HD23	1.68	0.58
1:A:517:PHE:HB2	1:A:525:LEU:HB2	1.85	0.58
1:A:102:ASN:ND2	1:A:107:ASP:OD1	2.34	0.58
1:A:158:LEU:HB2	1:A:162:ARG:HB2	1.86	0.57
1:A:713:VAL:HG12	1:A:742:GLY:HA3	1.85	0.57
1:A:350:ARG:NH2	1:A:413:ASP:OD2	2.38	0.55
2:B:77:ARG:HG3	2:B:110:LEU:HA	1.88	0.55
1:A:456:VAL:HG12	1:A:473:VAL:HG22	1.88	0.55
5:E:64:MET:HB2	5:E:74:PHE:HB2	1.88	0.55
1:A:250:ASP:OD1	1:A:250:ASP:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:TYR:HB3	1:A:146:LYS:HB2	1.90	0.54
2:B:295:ARG:HH11	2:B:316:LEU:HD13	1.73	0.53
5:E:96:ASN:HD21	5:E:100:VAL:HB	1.74	0.53
2:B:171:LEU:HD22	2:B:209:VAL:HG11	1.91	0.53
2:B:262:ALA:HB3	2:B:266:ASN:H	1.73	0.52
5:E:60:GLY:HA2	5:E:62:PRO:HD3	1.91	0.52
5:E:88:GLN:O	5:E:109:ALA:HB3	2.09	0.52
2:B:175:ASN:ND2	2:B:178:ASP:OD1	2.39	0.51
1:A:324:SER:HB3	1:A:337:LEU:HD11	1.92	0.51
1:A:668:ILE:HG23	1:A:767:ARG:HD3	1.92	0.51
1:A:204:PRO:HG3	1:A:214:TYR:CE2	2.46	0.51
1:A:24:PHE:N	1:A:54:VAL:O	2.44	0.50
4:D:151:VAL:HG12	4:D:160:THR:HG23	1.93	0.50
1:A:114:LEU:HB3	1:A:119:VAL:HG13	1.93	0.50
1:A:185:ASN:HB3	1:A:260:ILE:HD11	1.92	0.50
1:A:514:THR:HA	1:A:528:GLY:HA3	1.94	0.49
4:D:208:THR:OG1	4:D:211:THR:OG1	2.30	0.49
4:D:93:ASP:OD1	4:D:112:ARG:NH1	2.45	0.49
1:A:628:VAL:HB	1:A:719:ILE:HD12	1.93	0.49
4:D:140:ALA:HB1	4:D:170:LEU:HD22	1.95	0.49
5:E:80:GLN:NE2	5:E:88:GLN:OE1	2.45	0.49
2:B:294:ASN:N	2:B:294:ASN:OD1	2.44	0.49
1:A:533:HIS:ND1	1:A:568:ASP:OD1	2.31	0.49
1:A:722:THR:HG22	1:A:735:THR:HG23	1.93	0.49
4:D:92:ILE:HG23	4:D:108:VAL:HG12	1.95	0.48
4:D:63:PRO:HG2	4:D:64:PHE:CD2	2.48	0.48
1:A:370:ARG:NH2	5:E:28:TYR:OH	2.46	0.48
1:A:315:TYR:O	1:A:346:ARG:NH2	2.46	0.48
1:A:449:TRP:HA	1:A:450:LEU:HA	1.61	0.48
1:A:94:ILE:HG12	1:A:125:LEU:HD23	1.96	0.48
3:C:47:LEU:HD11	3:C:67:ILE:HD12	1.95	0.48
1:A:139:ASP:HA	1:A:142:TYR:HD2	1.79	0.48
2:B:122:VAL:HB	2:B:134:LEU:HB2	1.95	0.48
1:A:634:ARG:HB3	1:A:713:VAL:HG22	1.96	0.48
1:A:526:ARG:NH2	1:A:577:THR:OG1	2.45	0.47
1:A:574:TYR:CZ	1:A:597:GLY:HA3	2.49	0.47
1:A:717:GLU:HA	1:A:738:PHE:HA	1.96	0.47
1:A:115:GLU:HG2	1:A:120:ARG:HB3	1.95	0.47
4:D:121:ASP:O	4:D:122:SER:HB3	2.14	0.47
3:C:59:PRO:HG3	5:E:67:PRO:HG2	1.96	0.47
5:E:76:VAL:HG13	5:E:90:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLY:O	1:A:437:GLY:N	2.43	0.46
2:B:261:LEU:HD11	2:B:285:SER:N	2.30	0.46
4:D:138:GLN:HA	4:D:141:ARG:HB3	1.96	0.46
1:A:204:PRO:HG3	1:A:214:TYR:CZ	2.51	0.46
4:D:89:GLN:HG3	4:D:115:THR:HG21	1.97	0.46
1:A:224:GLU:HA	1:A:227:ARG:HB2	1.97	0.46
1:A:582:ASP:OD1	1:A:583:ARG:N	2.49	0.46
2:B:285:SER:HB2	2:B:301:GLN:N	2.30	0.46
1:A:497:ASP:OD1	1:A:497:ASP:N	2.47	0.46
5:E:34:GLN:HB2	5:E:78:ARG:CB	2.46	0.46
5:E:95:PHE:HD1	5:E:101:LEU:HA	1.81	0.46
4:D:134:ASP:HA	4:D:177:TYR:HD2	1.80	0.45
1:A:217:GLN:HG2	1:A:218:LYS:H	1.80	0.45
1:A:162:ARG:NH2	4:D:59:ASP:O	2.49	0.45
1:A:325:MET:HA	1:A:326:PRO:HD3	1.85	0.45
4:D:209:GLN:OE1	4:D:243:SER:OG	2.32	0.45
1:A:427:ASN:OD1	1:A:427:ASN:N	2.50	0.45
3:C:72:GLY:HA3	3:C:73:SER:HA	1.57	0.45
5:E:49:GLY:H	5:E:101:LEU:HB3	1.81	0.45
5:E:67:PRO:HA	5:E:68:PHE:HA	1.54	0.45
2:B:149:GLY:H	2:B:166:THR:HG21	1.80	0.45
5:E:37:TYR:HA	5:E:77:PHE:HD1	1.80	0.45
5:E:85:GLY:CA	5:E:86:VAL:HG22	2.43	0.45
5:E:86:VAL:O	5:E:86:VAL:HG23	2.16	0.45
1:A:292:PRO:HA	1:A:293:GLY:HA2	1.48	0.45
2:B:114:GLY:HA3	2:B:115:VAL:HA	1.74	0.44
1:A:23:GLY:HA2	1:A:24:PHE:HA	1.67	0.44
1:A:138:GLU:O	1:A:141:TYR:N	2.46	0.44
1:A:722:THR:HG21	1:A:733:VAL:HG22	2.00	0.44
2:B:299:VAL:HG22	2:B:305:VAL:HG22	1.99	0.44
1:A:218:LYS:HA	1:A:218:LYS:HE2	1.99	0.44
2:B:210:GLY:HA2	2:B:216:VAL:HA	2.00	0.44
2:B:281:ARG:NH2	2:B:315:THR:OG1	2.51	0.44
2:B:47:ALA:HB3	2:B:389:SER:HB3	1.99	0.43
2:B:322:LEU:HG	2:B:356:PHE:HZ	1.83	0.43
2:B:322:LEU:HD13	2:B:327:LEU:HD21	1.99	0.43
2:B:348:TRP:HZ2	2:B:390:ILE:HG21	1.83	0.43
4:D:85:LEU:HD22	4:D:115:THR:HG23	2.00	0.43
5:E:52:GLN:HG2	5:E:95:PHE:CE2	2.53	0.43
1:A:237:ARG:HH21	1:A:328:ILE:HG21	1.83	0.43
4:D:198:VAL:HG11	4:D:218:MET:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLU:HG2	1:A:203:VAL:HG23	1.99	0.43
1:A:639:ASP:OD1	1:A:640:GLY:N	2.49	0.43
1:A:144:VAL:HG22	1:A:145:GLY:H	1.83	0.43
2:B:345:TYR:CZ	2:B:361:LYS:HD3	2.54	0.43
1:A:206:TRP:O	1:A:209:VAL:HA	2.18	0.43
4:D:92:ILE:HD13	4:D:112:ARG:HA	2.00	0.43
1:A:281:SER:O	1:A:285:GLU:HG2	2.19	0.42
4:D:39:ALA:HB2	4:D:54:GLN:HB3	2.01	0.42
1:A:178:GLN:HG2	2:B:59:PHE:CE2	2.54	0.42
1:A:75:VAL:HG13	1:A:88:VAL:HG12	2.00	0.42
1:A:132:ASP:HA	1:A:135:LYS:HG2	2.02	0.42
1:A:655:GLY:N	1:A:659:THR:OG1	2.52	0.42
2:B:201:THR:HG22	2:B:251:PRO:HG2	2.01	0.42
3:C:56:MET:HE1	4:D:233:LYS:HA	2.01	0.42
4:D:226:GLN:HG3	5:E:110:LEU:HG	2.00	0.42
2:B:99:GLU:N	2:B:99:GLU:OE2	2.53	0.41
1:A:380:ASP:OD1	1:A:380:ASP:N	2.52	0.41
2:B:237:GLY:HA2	2:B:238:SER:HA	1.50	0.41
5:E:84:GLU:HA	5:E:85:GLY:HA2	1.91	0.41
1:A:160:ARG:O	1:A:162:ARG:N	2.53	0.41
1:A:366:ARG:HD3	4:D:185:TYR:CZ	2.55	0.41
1:A:46:MET:HA	1:A:47:PRO:HD3	1.86	0.41
1:A:663:PHE:CZ	1:A:767:ARG:HB3	2.56	0.41
1:A:353:ARG:HB2	1:A:415:VAL:HG22	2.02	0.41
1:A:672:ALA:O	1:A:702:SER:OG	2.32	0.41
1:A:209:VAL:HG11	1:A:776:TRP:CD2	2.56	0.41
1:A:321:ARG:NH2	1:A:342:ASP:OD2	2.53	0.41
1:A:607:GLU:OE1	1:A:644:LYS:NZ	2.53	0.41
1:A:703:ASP:HB3	1:A:798:LYS:HE3	2.03	0.40
1:A:198:GLN:HA	1:A:199:LEU:HA	1.86	0.40
1:A:551:SER:HB2	1:A:644:LYS:HA	2.03	0.40
2:B:250:THR:HA	2:B:251:PRO:HD3	1.91	0.40
3:C:57:ILE:HG23	5:E:68:PHE:CB	2.52	0.40
3:C:87:GLN:HA	3:C:88:PRO:HA	1.82	0.40
1:A:436:SER:HB3	1:A:463:ASN:OD1	2.21	0.40
1:A:630:LEU:HB3	1:A:717:GLU:HG3	2.04	0.40
4:D:201:MET:HE2	4:D:211:THR:HA	2.04	0.40
1:A:377:LEU:HD22	1:A:412:VAL:HG21	2.03	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	781/789 (99%)	715 (92%)	60 (8%)	6 (1%)	24 69
2	B	342/383 (89%)	312 (91%)	29 (8%)	1 (0%)	46 83
3	C	54/56 (96%)	50 (93%)	3 (6%)	1 (2%)	10 53
4	D	208/226 (92%)	197 (95%)	11 (5%)	0	100 100
5	E	86/102 (84%)	70 (81%)	14 (16%)	2 (2%)	8 50
All	All	1471/1556 (94%)	1344 (91%)	117 (8%)	10 (1%)	26 72

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	30	PRO
1	A	264	ASP
1	A	161	ASN
1	A	659	THR
1	A	684	PRO
2	B	285	SER
3	C	37	GLY
1	A	202	GLU
1	A	807	GLY
5	E	77	PHE

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	653/672 (97%)	641 (98%)	12 (2%)	66 89
2	B	279/314 (89%)	277 (99%)	2 (1%)	88 96
3	C	39/40 (98%)	38 (97%)	1 (3%)	54 83
4	D	177/190 (93%)	176 (99%)	1 (1%)	90 97
5	E	74/90 (82%)	72 (97%)	2 (3%)	52 83
All	All	1222/1306 (94%)	1204 (98%)	18 (2%)	72 91

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASP
1	A	177	ILE
1	A	214	TYR
1	A	223	LEU
1	A	264	ASP
1	A	452	THR
1	A	519	ILE
1	A	546	TRP
1	A	685	ASP
1	A	698	ASP
1	A	778	SER
1	A	808	LYS
2	B	194	LEU
2	B	286	VAL
3	C	57	ILE
4	D	205	TYR
5	E	36	ASN
5	E	59	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	523	ASN
2	B	62	ASN
5	E	80	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 carbohydrates 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	785/789 (99%)	0.19	50 (6%) 23 17	97, 137, 173, 217	0
2	B	348/383 (90%)	0.10	13 (3%) 45 36	98, 138, 176, 212	0
3	C	56/56 (100%)	0.38	6 (10%) 8 7	112, 148, 190, 205	0
4	D	212/226 (93%)	-0.05	3 (1%) 78 69	108, 136, 183, 202	0
5	E	88/102 (86%)	0.23	4 (4%) 37 29	109, 149, 201, 227	0
All	All	1489/1556 (95%)	0.14	76 (5%) 32 24	97, 138, 179, 227	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	38	ASP	8.3
1	A	555	HIS	4.7
1	A	797	ASP	4.6
1	A	495	GLN	4.6
3	C	56	MET	4.4
1	A	523	ASN	4.2
1	A	795	ASP	4.2
1	A	23	GLY	4.1
5	E	69	GLY	4.0
1	A	539	MET	3.9
1	A	22	GLU	3.9
1	A	337	LEU	3.7
1	A	561	GLN	3.7
1	A	560	ASP	3.7
1	A	757	TYR	3.5
3	C	55	GLY	3.5
1	A	758	PRO	3.4
2	B	284	GLY	3.4
3	C	39	GLU	3.4
1	A	421	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	272	GLU	3.3
2	B	67	LEU	3.3
1	A	503	ASP	3.3
1	A	143	SER	3.2
1	A	336	LYS	3.2
1	A	778	SER	3.2
1	A	498	ASP	3.1
3	C	37	GLY	3.0
1	A	422	ASN	3.0
3	C	54	ALA	3.0
1	A	540	GLN	3.0
4	D	81	LYS	3.0
1	A	81	GLY	2.9
2	B	297	TYR	2.9
1	A	493	ASP	2.8
1	A	447	ASP	2.8
2	B	196	GLY	2.7
2	B	295	ARG	2.7
1	A	209	VAL	2.7
1	A	400	THR	2.7
1	A	28	ASP	2.7
1	A	423	THR	2.7
2	B	283	LEU	2.6
1	A	415	VAL	2.6
2	B	106	LYS	2.5
5	E	57	TYR	2.5
1	A	651	ASN	2.4
1	A	335	VAL	2.4
4	D	36	TYR	2.4
1	A	105	VAL	2.4
1	A	554	GLU	2.4
1	A	99	PHE	2.4
2	B	294	ASN	2.4
1	A	562	ASP	2.3
1	A	214	TYR	2.3
1	A	106	LYS	2.3
1	A	169	PHE	2.3
2	B	306	MET	2.3
4	D	58	LEU	2.2
1	A	464	ASP	2.2
1	A	765	ASN	2.2
2	B	68	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	68	PHE	2.2
1	A	621	ILE	2.2
1	A	779	PRO	2.2
2	B	69	ASP	2.2
1	A	338	ARG	2.1
1	A	756	GLY	2.1
1	A	427	ASN	2.1
2	B	298	LEU	2.0
5	E	80	GLN	2.0
2	B	123	TYR	2.0
1	A	265	GLN	2.0
1	A	715	SER	2.0
1	A	445	GLN	2.0
1	A	783	LEU	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 carbohydrates 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.