Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 06:55 PM JST

PDB ID	:	6LYQ
Title	:	Structure of the BAM complex
Authors	:	Xiao, L.; Huang, Y.
Deposited on	:	2020-02-15
Resolution	:	3.19 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:

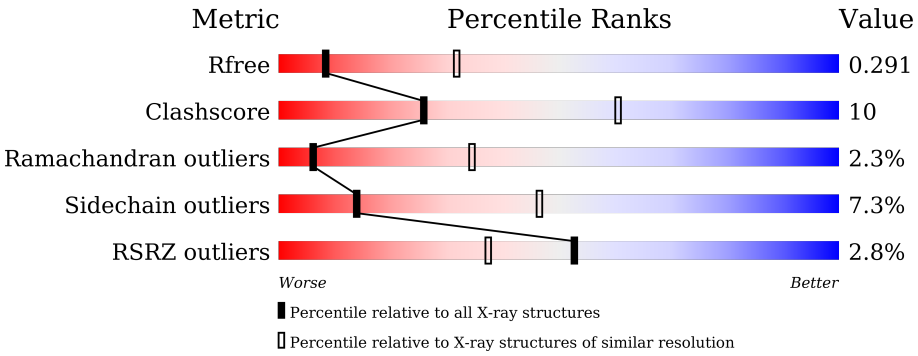
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.19 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	810	3% 74% 20%
2	B	400	4% 65% 22% 11%
3	C	344	13% 84%
4	D	245	% 63% 19% 15%
5	E	119	% 55% 19% 26%
6	O	16	56% 25% 19%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11463 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	787	Total	C	N	O	S	0	0	0
			6078	3825	1024	1213	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	760	TRP	TYR	conflict	UNP P0A940

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	356	Total	C	N	O	S	0	0	0
			2610	1640	444	520	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	393	TRP	-	expression tag	UNP P77774
B	394	SER	-	expression tag	UNP P77774
B	395	HIS	-	expression tag	UNP P77774
B	396	PRO	-	expression tag	UNP P77774
B	397	GLN	-	expression tag	UNP P77774
B	398	PHE	-	expression tag	UNP P77774
B	399	GLU	-	expression tag	UNP P77774
B	400	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
			378	239	63	75	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1642	1035	286	314	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
			657	415	108	132	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	114	HIS	-	expression tag	UNP P0A937
E	115	HIS	-	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

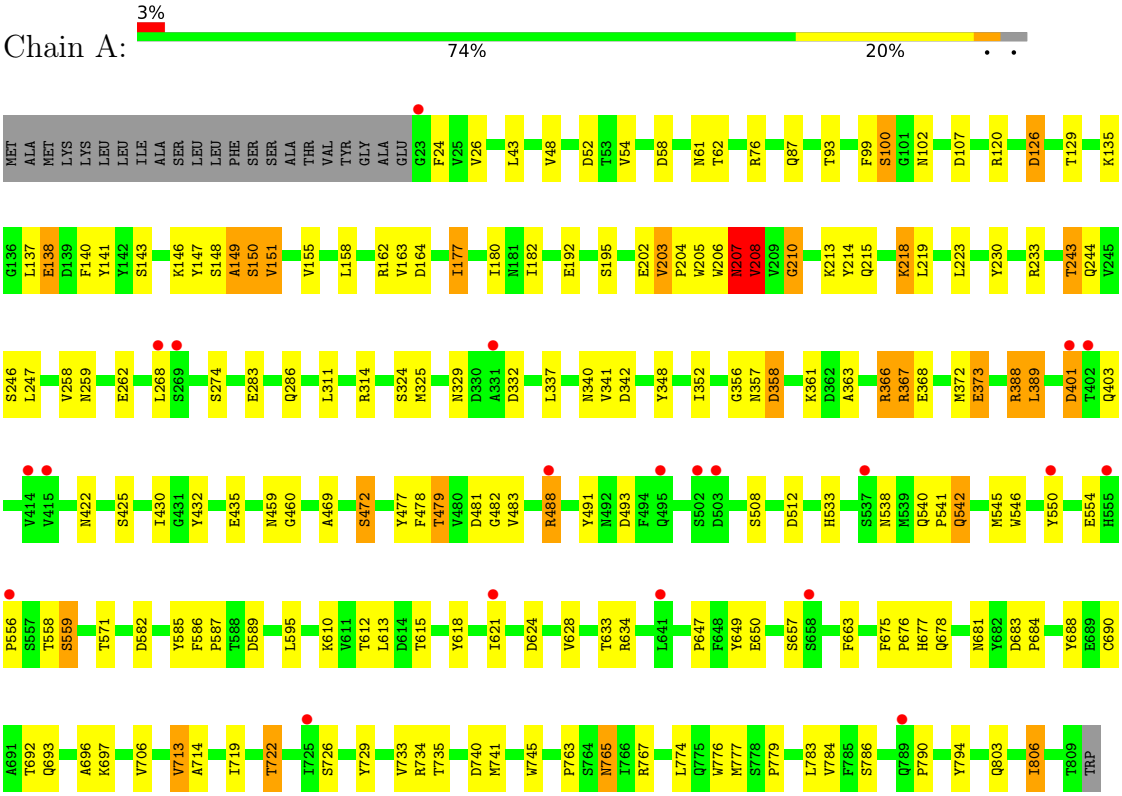
- Molecule 6 is a protein called Peptide from Phospholipase A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	13	Total	C	N	O	S	0	0	0
			98	63	17	17	1			

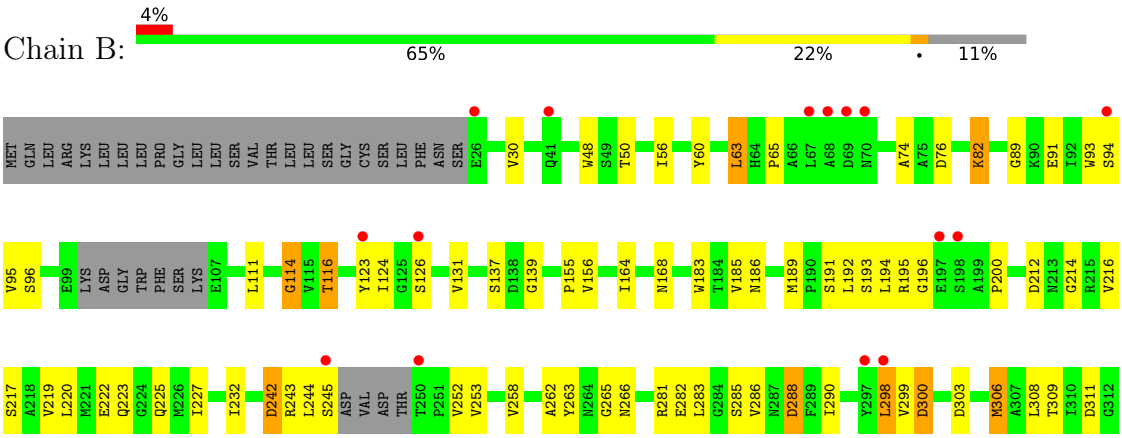
3 Residue-property plots (i)

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: Outer membrane protein assembly factor BamA



• Molecule 2: Outer membrane protein assembly factor BamB

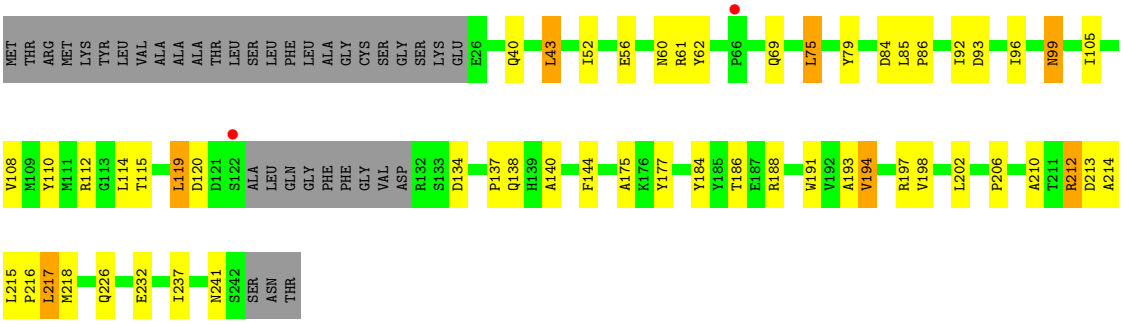


• Molecule 3: Outer membrane protein assembly factor BamC

Chain C:

• Molecule 4: Outer membrane protein assembly factor BamD

Chain D:



• Molecule 5: Outer membrane protein assembly factor BamE

Chain E:

• Molecule 6: Peptide from Phospholipase A1

Chain O:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	117.27Å 117.27Å 429.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 3.19 40.37 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.41-3.19) 98.8 (40.37-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.18Å)	Xtriage
Refinement program	PHENIX 3.1	Depositor
R, R_{free}	0.265 , 0.293 0.259 , 0.291	Depositor DCC
R_{free} test set	2548 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	113.6	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 62.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11463	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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	0.66	0/6216	0.80	2/8453 (0.0%)
2	B	0.69	0/2654	0.80	0/3627
3	C	0.68	0/387	0.76	0/533
4	D	0.65	0/1678	0.75	0/2285
5	E	0.66	0/671	0.81	0/919
6	O	0.79	0/98	1.36	2/131 (1.5%)
All	All	0.67	0/11704	0.80	4/15948 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	O	282	GLY	N-CA-C	-9.79	88.63	113.10
1	A	206	TRP	CB-CA-C	-9.68	91.04	110.40
6	O	283	VAL	N-CA-C	-5.79	95.37	111.00
1	A	207	ASN	N-CA-C	-5.61	95.85	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	550	TYR	Peptide
1	A	722	THR	Peptide

5.2 Too-close contacts (i)

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	6078	0	5676	120	0
2	B	2610	0	2528	62	0
3	C	378	0	362	6	0
4	D	1642	0	1559	53	0
5	E	657	0	615	10	0
6	O	98	0	102	1	0
All	All	11463	0	10842	234	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 10.

All (234) 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:208:VAL:CG1	1:A:779:PRO:HD3	1.97	0.94
1:A:208:VAL:HG13	1:A:779:PRO:HD3	1.45	0.94
4:D:217:LEU:HD12	4:D:217:LEU:H	1.30	0.93
4:D:214:ALA:O	4:D:217:LEU:CD1	2.21	0.88
4:D:214:ALA:HA	4:D:217:LEU:HD11	1.56	0.86
1:A:213:LYS:CB	1:A:215:GLN:OE1	2.24	0.86
1:A:678:GLN:HG2	1:A:693:GLN:HE22	1.39	0.85
1:A:208:VAL:HG11	1:A:779:PRO:CD	2.07	0.84
1:A:208:VAL:CG1	1:A:779:PRO:CD	2.60	0.79
1:A:722:THR:HG22	1:A:735:THR:HG23	1.63	0.79
2:B:63:LEU:HA	2:B:114:GLY:HA2	1.67	0.76
2:B:266:ASN:HD22	2:B:282:GLU:HA	1.49	0.76
1:A:329:ASN:ND2	1:A:332:ASP:OD1	2.19	0.74
4:D:61:ARG:HG3	4:D:62:TYR:CZ	2.22	0.73
1:A:247:LEU:HD23	2:B:192:LEU:HD11	1.70	0.72
1:A:692:THR:HA	1:A:696:ALA:HB2	1.72	0.72
1:A:363:ALA:O	1:A:367:ARG:HB3	1.90	0.71
2:B:82:LYS:HZ1	2:B:95:VAL:H	1.39	0.71
1:A:765:ASN:HB3	1:A:794:TYR:CD2	2.26	0.70
4:D:214:ALA:O	4:D:217:LEU:HD12	1.91	0.69
1:A:192:GLU:O	1:A:195:SER:HB3	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:PRO:HB3	1:A:649:TYR:CZ	2.29	0.67
2:B:214:GLY:HA3	2:B:243:ARG:CB	2.24	0.67
1:A:735:THR:HG22	1:A:774:LEU:CD2	2.25	0.66
2:B:308:LEU:CD2	2:B:315:THR:HA	2.26	0.66
4:D:61:ARG:HG3	4:D:62:TYR:CE2	2.30	0.65
4:D:212:ARG:HG3	4:D:213:ASP:H	1.61	0.65
1:A:126:ASP:O	1:A:129:THR:OG1	2.09	0.65
4:D:212:ARG:HG3	4:D:213:ASP:N	2.12	0.65
2:B:214:GLY:CA	2:B:243:ARG:CB	2.75	0.64
4:D:75:LEU:HD22	4:D:79:TYR:CE2	2.32	0.63
1:A:54:VAL:HG23	1:A:58:ASP:HB2	1.81	0.63
1:A:205:TRP:HA	1:A:208:VAL:HG23	1.81	0.62
4:D:214:ALA:O	4:D:217:LEU:HD13	1.97	0.62
4:D:217:LEU:HD12	4:D:217:LEU:N	2.11	0.62
1:A:745:TRP:CE3	1:A:763:PRO:HB3	2.35	0.62
4:D:191:TRP:HA	4:D:194:VAL:CG2	2.30	0.61
4:D:214:ALA:CA	4:D:217:LEU:HD11	2.29	0.61
4:D:40:GLN:HA	4:D:43:LEU:HD22	1.83	0.59
2:B:298:LEU:CD2	2:B:306:MET:HG2	2.33	0.58
5:E:47:ARG:O	5:E:50:MET:HG3	2.03	0.58
4:D:92:ILE:HG23	4:D:108:VAL:HG12	1.85	0.58
5:E:62:PRO:HB3	5:E:75:TYR:CE1	2.38	0.58
4:D:214:ALA:HA	4:D:217:LEU:CD1	2.30	0.58
1:A:205:TRP:HA	1:A:208:VAL:CB	2.35	0.57
1:A:223:LEU:CD2	1:A:243:THR:HG21	2.35	0.57
4:D:214:ALA:C	4:D:217:LEU:CD1	2.72	0.57
2:B:308:LEU:HD22	2:B:315:THR:HA	1.86	0.56
1:A:102:ASN:ND2	1:A:107:ASP:OD1	2.38	0.56
2:B:50:THR:OG1	2:B:89:GLY:O	2.21	0.56
1:A:244:GLN:HE22	2:B:168:ASN:HB3	1.69	0.56
1:A:538:ASN:O	1:A:538:ASN:ND2	2.38	0.56
1:A:722:THR:CG2	1:A:735:THR:HG23	2.35	0.56
5:E:88:GLN:HB3	5:E:110:LEU:HD21	1.88	0.56
2:B:111:LEU:HD13	2:B:124:ILE:HG21	1.87	0.56
1:A:137:LEU:O	1:A:140:PHE:HB3	2.06	0.55
1:A:367:ARG:HD2	1:A:477:TYR:CG	2.41	0.55
1:A:714:ALA:O	1:A:741:MET:HG2	2.07	0.55
1:A:177:ILE:HD11	1:A:180:ILE:CG1	2.36	0.55
1:A:208:VAL:HG11	1:A:779:PRO:HD2	1.89	0.55
1:A:401:ASP:OD2	1:A:403:GLN:NE2	2.36	0.55
1:A:177:ILE:HG22	1:A:214:TYR:O	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ILE:HG13	1:A:373:GLU:HB2	1.89	0.54
4:D:92:ILE:HG21	4:D:112:ARG:HB2	1.90	0.54
1:A:479:THR:HB	1:A:483:VAL:HB	1.90	0.54
4:D:93:ASP:OD1	4:D:112:ARG:NH1	2.40	0.54
4:D:191:TRP:O	4:D:194:VAL:HG23	2.08	0.54
1:A:182:ILE:HG12	1:A:258:VAL:HG22	1.89	0.53
1:A:177:ILE:HD11	1:A:180:ILE:HG13	1.90	0.53
2:B:156:VAL:HG21	2:B:200:PRO:O	2.08	0.52
2:B:266:ASN:ND2	2:B:282:GLU:HA	2.23	0.52
3:C:39:GLU:OE2	3:C:78:LYS:N	2.41	0.52
1:A:247:LEU:CD2	2:B:192:LEU:HD11	2.38	0.52
1:A:719:ILE:HD13	1:A:734:ARG:CZ	2.39	0.52
2:B:131:VAL:HG21	2:B:164:ILE:HG12	1.91	0.52
1:A:472:SER:HB2	1:A:488:ARG:CZ	2.40	0.52
1:A:722:THR:HG22	1:A:735:THR:H	1.75	0.52
2:B:303:ASP:O	2:B:327:LEU:HD12	2.10	0.52
1:A:425:SER:HB2	6:O:284:MET:HA	1.92	0.52
1:A:745:TRP:CD2	1:A:763:PRO:HB3	2.45	0.52
4:D:52:ILE:O	4:D:56:GLU:N	2.40	0.52
4:D:75:LEU:HD22	4:D:79:TYR:CZ	2.45	0.52
4:D:226:GLN:HG3	5:E:110:LEU:HD23	1.92	0.51
1:A:647:PRO:HB3	1:A:649:TYR:CE1	2.45	0.51
1:A:324:SER:HB3	1:A:337:LEU:HD11	1.93	0.51
1:A:585:TYR:O	1:A:587:PRO:HD3	2.12	0.50
1:A:676:PRO:CB	1:A:696:ALA:HB1	2.41	0.50
1:A:678:GLN:CG	1:A:693:GLN:HE22	2.18	0.50
3:C:70:THR:O	3:C:72:GLY:N	2.45	0.50
1:A:244:GLN:NE2	2:B:168:ASN:HB3	2.27	0.50
1:A:205:TRP:HA	1:A:208:VAL:CG2	2.42	0.49
1:A:481:ASP:OD1	4:D:188:ARG:NH2	2.38	0.49
1:A:348:TYR:CE1	5:E:36:ASN:HA	2.47	0.49
1:A:508:SER:HA	1:A:533:HIS:O	2.11	0.49
1:A:678:GLN:HG2	1:A:693:GLN:NE2	2.19	0.49
2:B:212:ASP:OD1	2:B:245:SER:HA	2.12	0.49
1:A:244:GLN:NE2	1:A:259:ASN:OD1	2.44	0.49
1:A:558:THR:HG23	1:A:675:PHE:CD2	2.47	0.49
1:A:663:PHE:CZ	1:A:767:ARG:HB3	2.46	0.49
2:B:116:THR:HG21	2:B:155:PRO:O	2.13	0.49
4:D:193:ALA:O	4:D:197:ARG:HB2	2.13	0.49
2:B:183:TRP:CE3	2:B:185:VAL:HG23	2.48	0.49
1:A:432:TYR:O	1:A:806:ILE:HG12	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:GLY:O	2:B:232:ILE:HG22	2.13	0.48
2:B:281:ARG:NH2	2:B:315:THR:OG1	2.46	0.48
4:D:198:VAL:HG11	4:D:218:MET:HB2	1.95	0.48
4:D:85:LEU:HB2	4:D:86:PRO:HD3	1.95	0.48
4:D:175:ALA:HB1	4:D:210:ALA:HB3	1.94	0.48
1:A:676:PRO:HB2	1:A:696:ALA:HB1	1.96	0.48
2:B:82:LYS:HE3	2:B:94:SER:HA	1.95	0.48
1:A:634:ARG:HB3	1:A:713:VAL:HG22	1.95	0.48
2:B:327:LEU:HA	2:B:340:GLY:O	2.14	0.48
4:D:110:TYR:CE2	4:D:114:LEU:HD11	2.48	0.48
5:E:88:GLN:HB3	5:E:110:LEU:HD11	1.96	0.48
1:A:311:LEU:O	1:A:314:ARG:HB3	2.14	0.47
1:A:582:ASP:OD1	1:A:589:ASP:N	2.44	0.47
1:A:726:SER:HB3	1:A:729:TYR:CE1	2.49	0.47
2:B:243:ARG:O	2:B:263:TYR:N	2.45	0.47
4:D:115:THR:O	4:D:119:LEU:HD12	2.14	0.47
1:A:233:ARG:NH2	1:A:624:ASP:OD1	2.35	0.47
2:B:299:VAL:HG23	2:B:330:PRO:HD3	1.97	0.47
2:B:288:ASP:OD1	2:B:288:ASP:N	2.46	0.47
1:A:585:TYR:CE2	1:A:586:PHE:CE1	3.02	0.47
1:A:587:PRO:HB2	1:A:618:TYR:CE2	2.48	0.47
2:B:168:ASN:HA	2:B:189:MET:HE1	1.97	0.47
2:B:232:ILE:HG23	2:B:262:ALA:HB2	1.97	0.47
2:B:220:LEU:HD12	2:B:223:GLN:NE2	2.30	0.47
3:C:42:LEU:HD21	3:C:76:VAL:CG1	2.45	0.47
1:A:361:LYS:HG2	4:D:134:ASP:OD2	2.16	0.46
2:B:223:GLN:HE21	2:B:225:GLN:HB3	1.80	0.46
1:A:491:TYR:CE2	1:A:493:ASP:OD1	2.68	0.46
4:D:96:ILE:HG12	4:D:105:ILE:HD11	1.96	0.46
2:B:363:ASP:OD1	2:B:365:SER:HB3	2.15	0.46
1:A:205:TRP:C	1:A:207:ASN:H	2.19	0.46
5:E:56:ALA:O	5:E:60:GLY:N	2.45	0.46
2:B:48:TRP:CE3	2:B:89:GLY:HA3	2.51	0.46
1:A:210:GLY:N	1:A:777:MET:O	2.47	0.46
1:A:150:SER:OG	1:A:151:VAL:N	2.48	0.46
3:C:65:TYR:HA	4:D:144:PHE:CE2	2.50	0.45
4:D:61:ARG:HG3	4:D:62:TYR:CE1	2.51	0.45
1:A:435:GLU:CD	1:A:657:SER:H	2.19	0.45
2:B:223:GLN:HG3	2:B:225:GLN:CB	2.46	0.45
4:D:92:ILE:HG23	4:D:108:VAL:CG1	2.46	0.45
4:D:61:ARG:CG	4:D:62:TYR:CZ	2.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:VAL:HG22	2:B:258:VAL:HG22	1.97	0.45
1:A:207:ASN:ND2	1:A:207:ASN:O	2.49	0.45
1:A:735:THR:HG22	1:A:774:LEU:HD23	1.98	0.45
1:A:663:PHE:CE1	1:A:790:PRO:HB3	2.52	0.45
1:A:158:LEU:HD11	1:A:164:ASP:CG	2.37	0.45
1:A:615:THR:HB	1:A:633:THR:OG1	2.17	0.45
1:A:352:ILE:O	1:A:366:ARG:NH1	2.44	0.45
2:B:308:LEU:HD23	2:B:315:THR:HA	1.97	0.45
1:A:205:TRP:HA	1:A:208:VAL:CA	2.47	0.44
1:A:219:LEU:O	1:A:219:LEU:HD12	2.16	0.44
2:B:156:VAL:HG11	2:B:200:PRO:O	2.17	0.44
2:B:82:LYS:CE	2:B:94:SER:HA	2.47	0.44
1:A:610:LYS:HE3	1:A:650:GLU:O	2.17	0.44
1:A:776:TRP:CZ2	1:A:783:LEU:HD23	2.53	0.44
1:A:595:LEU:HD12	1:A:613:LEU:HD13	2.00	0.44
4:D:237:ILE:O	4:D:241:ASN:ND2	2.49	0.44
4:D:191:TRP:HA	4:D:194:VAL:HG22	2.00	0.44
2:B:194:LEU:HB2	2:B:245:SER:HB3	2.00	0.44
1:A:26:VAL:HG12	1:A:52:ASP:O	2.18	0.44
2:B:309:THR:OG1	2:B:314:VAL:HG22	2.18	0.44
4:D:214:ALA:CA	4:D:217:LEU:CD1	2.94	0.44
2:B:220:LEU:HD23	2:B:220:LEU:HA	1.84	0.43
1:A:48:VAL:HG13	1:A:62:THR:OG1	2.18	0.43
1:A:367:ARG:HA	4:D:184:TYR:OH	2.19	0.43
2:B:283:LEU:HD12	2:B:283:LEU:N	2.33	0.43
5:E:36:ASN:O	5:E:77:PHE:HA	2.18	0.43
4:D:215:LEU:N	4:D:216:PRO:HD2	2.33	0.43
1:A:162:ARG:CD	4:D:60:ASN:O	2.66	0.43
1:A:681:ASN:OD1	1:A:688:TYR:OH	2.36	0.43
1:A:147:TYR:C	1:A:149:ALA:H	2.22	0.43
1:A:554:GLU:C	1:A:556:PRO:HD3	2.38	0.43
2:B:65:PRO:HB3	2:B:74:ALA:HB2	2.00	0.43
2:B:220:LEU:HG	2:B:227:ILE:HD11	1.99	0.43
4:D:137:PRO:HD3	4:D:177:TYR:CE2	2.54	0.43
5:E:27:VAL:HG12	5:E:28:TYR:N	2.34	0.43
2:B:344:GLY:HA3	2:B:363:ASP:O	2.19	0.43
4:D:75:LEU:O	4:D:79:TYR:CD2	2.72	0.43
2:B:93:TRP:CE3	2:B:139:GLY:HA3	2.54	0.43
2:B:193:SER:HB2	2:B:245:SER:HB2	2.00	0.43
1:A:76:ARG:NH2	1:A:87:GLN:OE1	2.47	0.43
1:A:368:GLU:OE1	1:A:388:ARG:HD3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLU:HG2	4:D:193:ALA:HB1	2.00	0.42
1:A:765:ASN:CB	1:A:794:TYR:CD2	2.98	0.42
4:D:202:LEU:O	4:D:206:PRO:HB3	2.19	0.42
1:A:162:ARG:HD2	4:D:60:ASN:O	2.18	0.42
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.91	0.42
2:B:317:TRP:NE1	2:B:351:VAL:O	2.50	0.42
1:A:218:LYS:O	1:A:218:LYS:CG	2.68	0.42
4:D:120:ASP:OD1	4:D:140:ALA:HB2	2.19	0.42
2:B:242:ASP:OD1	2:B:242:ASP:N	2.53	0.42
1:A:722:THR:HG21	1:A:733:VAL:HG13	2.02	0.42
2:B:286:VAL:HG12	2:B:286:VAL:O	2.19	0.42
1:A:147:TYR:CD2	1:A:247:LEU:HD11	2.55	0.42
1:A:478:PHE:HB3	1:A:483:VAL:O	2.20	0.42
2:B:91:GLU:OE2	2:B:94:SER:HB2	2.20	0.42
2:B:319:GLN:NE2	2:B:356:PHE:CE2	2.88	0.42
1:A:219:LEU:HG	1:A:223:LEU:HD11	2.02	0.41
1:A:99:PHE:O	1:A:100:SER:HB3	2.19	0.41
1:A:460:GLY:HA2	1:A:469:ALA:HA	2.03	0.41
2:B:345:TYR:CE1	2:B:361:LYS:HG2	2.55	0.41
4:D:99:ASN:O	4:D:105:ILE:HD13	2.20	0.41
2:B:298:LEU:O	2:B:298:LEU:HD23	2.21	0.41
1:A:203:VAL:HA	1:A:204:PRO:HD3	1.87	0.41
1:A:373:GLU:HG2	4:D:193:ALA:CB	2.50	0.41
2:B:281:ARG:HD2	2:B:313:GLY:O	2.20	0.41
2:B:298:LEU:HD21	2:B:306:MET:SD	2.61	0.41
4:D:79:TYR:O	4:D:84:ASP:N	2.51	0.41
1:A:138:GLU:O	1:A:141:TYR:N	2.53	0.41
1:A:246:SER:HB3	2:B:194:LEU:O	2.21	0.41
1:A:283:GLU:O	1:A:286:GLN:NE2	2.54	0.41
1:A:559:SER:O	1:A:677:HIS:HA	2.21	0.41
1:A:541:PRO:HA	1:A:546:TRP:HE1	1.86	0.41
2:B:116:THR:HG22	2:B:123:TYR:HB2	2.03	0.41
2:B:185:VAL:HG11	2:B:219:VAL:HG11	2.02	0.41
1:A:230:TYR:CE1	1:A:262:GLU:HG2	2.56	0.41
1:A:341:VAL:HG12	1:A:342:ASP:N	2.36	0.41
1:A:356:GLY:O	1:A:358:ASP:N	2.54	0.41
1:A:628:VAL:HB	1:A:719:ILE:HD12	2.02	0.41
3:C:57:ILE:O	5:E:68:PHE:HA	2.21	0.41
1:A:205:TRP:HA	1:A:208:VAL:HB	2.03	0.40
1:A:366:ARG:HG2	4:D:184:TYR:CD2	2.56	0.40
4:D:61:ARG:CG	4:D:62:TYR:CE2	3.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ARG:HD2	1:A:477:TYR:CD1	2.57	0.40
2:B:285:SER:HB2	2:B:300:ASP:HA	2.04	0.40
3:C:38:ASP:OD1	3:C:39:GLU:N	2.54	0.40
1:A:223:LEU:HD22	1:A:243:THR:HG21	2.03	0.40
1:A:274:SER:O	1:A:340:ASN:HA	2.20	0.40
2:B:191:SER:OG	2:B:192:LEU:N	2.53	0.40
1:A:477:TYR:CD2	1:A:482:GLY:HA2	2.56	0.40
1:A:595:LEU:HD23	1:A:595:LEU:O	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	785/810 (97%)	697 (89%)	73 (9%)	15 (2%)	8 39
2	B	350/400 (88%)	305 (87%)	34 (10%)	11 (3%)	4 26
3	C	54/344 (16%)	45 (83%)	7 (13%)	2 (4%)	3 22
4	D	204/245 (83%)	183 (90%)	20 (10%)	1 (0%)	29 67
5	E	86/119 (72%)	69 (80%)	12 (14%)	5 (6%)	1 13
6	O	11/16 (69%)	7 (64%)	4 (36%)	0	100 100
All	All	1490/1934 (77%)	1306 (88%)	150 (10%)	34 (2%)	6 34

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	VAL
1	A	357	ASN
1	A	684	PRO
1	A	697	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	137	SER
2	B	326	LEU
3	C	71	ASN
1	A	210	GLY
2	B	60	TYR
2	B	196	GLY
2	B	265	GLY
2	B	311	ASP
5	E	45	LYS
2	B	63	LEU
2	B	186	ASN
4	D	138	GLN
5	E	81	PRO
1	A	148	SER
1	A	149	ALA
1	A	150	SER
1	A	218	LYS
5	E	83	HIS
2	B	371	PRO
3	C	87	GLN
5	E	31	ASP
1	A	24	PHE
1	A	401	ASP
1	A	542	GLN
1	A	683	ASP
5	E	30	PRO
2	B	372	VAL
1	A	208	VAL
1	A	784	VAL
2	B	114	GLY

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	639/688 (93%)	590 (92%)	49 (8%)	13 44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	274/329 (83%)	253 (92%)	21 (8%)	13 44
3	C	36/276 (13%)	35 (97%)	1 (3%)	43 74
4	D	166/204 (81%)	156 (94%)	10 (6%)	19 54
5	E	71/101 (70%)	66 (93%)	5 (7%)	15 48
6	O	11/14 (79%)	10 (91%)	1 (9%)	9 34
All	All	1197/1612 (74%)	1110 (93%)	87 (7%)	14 46

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	61	ASN
1	A	93	THR
1	A	100	SER
1	A	120	ARG
1	A	126	ASP
1	A	135	LYS
1	A	138	GLU
1	A	143	SER
1	A	146	LYS
1	A	155	VAL
1	A	163	VAL
1	A	177	ILE
1	A	202	GLU
1	A	203	VAL
1	A	207	ASN
1	A	208	VAL
1	A	243	THR
1	A	268	LEU
1	A	325	MET
1	A	358	ASP
1	A	366	ARG
1	A	367	ARG
1	A	372	MET
1	A	373	GLU
1	A	388	ARG
1	A	389	LEU
1	A	422	ASN
1	A	430	ILE
1	A	459	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	472	SER
1	A	479	THR
1	A	488	ARG
1	A	512	ASP
1	A	540	GLN
1	A	542	GLN
1	A	545	MET
1	A	559	SER
1	A	571	THR
1	A	612	THR
1	A	621	ILE
1	A	690	CYS
1	A	706	VAL
1	A	713	VAL
1	A	740	ASP
1	A	765	ASN
1	A	786	SER
1	A	803	GLN
1	A	806	ILE
2	B	30	VAL
2	B	56	ILE
2	B	76	ASP
2	B	82	LYS
2	B	96	SER
2	B	116	THR
2	B	126	SER
2	B	195	ARG
2	B	216	VAL
2	B	217	SER
2	B	222	GLU
2	B	242	ASP
2	B	244	LEU
2	B	252	VAL
2	B	288	ASP
2	B	290	ILE
2	B	298	LEU
2	B	300	ASP
2	B	306	MET
2	B	320	SER
2	B	331	VAL
3	C	76	VAL
4	D	43	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	69	GLN
4	D	75	LEU
4	D	99	ASN
4	D	119	LEU
4	D	186	THR
4	D	194	VAL
4	D	212	ARG
4	D	217	LEU
4	D	232	GLU
5	E	37	TYR
5	E	63	LEU
5	E	94	THR
5	E	102	THR
5	E	106	ASN
6	O	287	ASP

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	244	GLN
1	A	259	ASN
1	A	323	GLN
1	A	540	GLN
1	A	677	HIS
2	B	165	HIS
2	B	223	GLN
4	D	41	GLN
6	O	286	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	787/810 (97%)	-0.13	21 (2%) 54 39	91, 125, 156, 201	0
2	B	356/400 (89%)	0.00	17 (4%) 30 18	96, 126, 156, 204	0
3	C	56/344 (16%)	0.04	1 (1%) 68 55	113, 136, 165, 193	0
4	D	208/245 (84%)	-0.16	2 (0%) 82 72	100, 125, 168, 199	0
5	E	88/119 (73%)	-0.06	1 (1%) 80 69	100, 132, 166, 194	0
6	O	13/16 (81%)	0.56	0 100 100	142, 161, 181, 182	0
All	All	1508/1934 (77%)	-0.08	42 (2%) 53 37	91, 126, 161, 204	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	69	ASP	5.3
2	B	68	ALA	5.0
1	A	555	HIS	4.1
1	A	503	ASP	3.9
1	A	414	VAL	3.8
2	B	198	SER	3.7
2	B	298	LEU	3.6
2	B	316	LEU	3.6
2	B	297	TYR	3.5
1	A	269	SER	3.5
1	A	550	TYR	3.4
2	B	375	ASP	3.3
2	B	67	LEU	3.2
2	B	26	GLU	3.2
1	A	488	ARG	3.2
1	A	556	PRO	3.1
5	E	85	GLY	3.0
4	D	122	SER	3.0
1	A	331	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	789	GLN	2.7
2	B	123	TYR	2.7
1	A	415	VAL	2.7
1	A	268	LEU	2.7
1	A	621	ILE	2.5
1	A	495	GLN	2.5
2	B	245	SER	2.5
1	A	641	LEU	2.4
1	A	725	ILE	2.4
2	B	41	GLN	2.4
1	A	402	THR	2.4
2	B	250	THR	2.4
1	A	23	GLY	2.3
1	A	502	SER	2.2
2	B	126	SER	2.2
1	A	537	SER	2.1
2	B	94	SER	2.1
3	C	55	GLY	2.1
2	B	70	ASN	2.1
1	A	401	ASP	2.1
4	D	66	PRO	2.1
2	B	197	GLU	2.0
1	A	658	SER	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.