Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 11:24 PM GMT

PDB ID	:	5EKQ
Title	:	The structure of the BamACDE subcomplex from E. coli
Authors	:	Bakelar, J.; Buchanan, S.K.; Noinaj, N.
Deposited on	:	2015-11-04
Resolution	:	3.39 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:

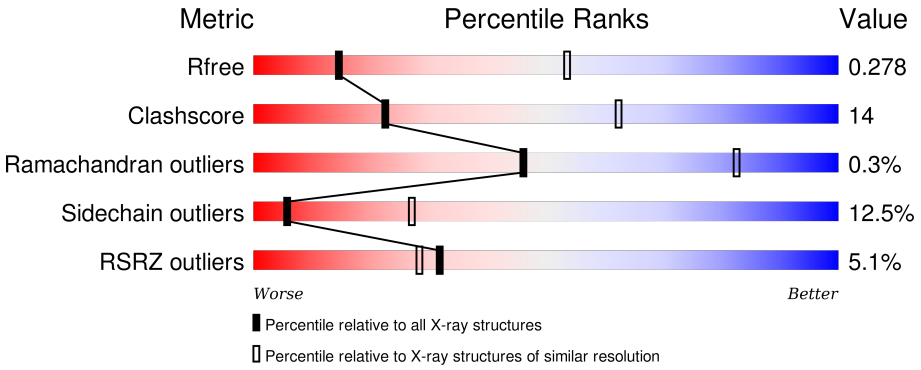
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.39 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	790	5% 61% 32%
2	D	226	5% 64% 29%
3	C	320	4% 43% 11% 44%
4	E	94	2% 53% 35% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9451 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	763	Total	C	N	O	S	0	0	0
			5752	3613	968	1156	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	219	Total	C	N	O	S	0	0	0
			1721	1079	305	330	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	179	Total	C	N	O	S	0	0	0
			1272	788	225	255	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			706	445	122	137	2			

3 Residue-property plots (i)

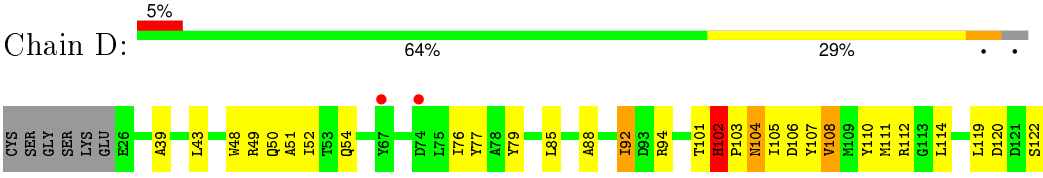
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

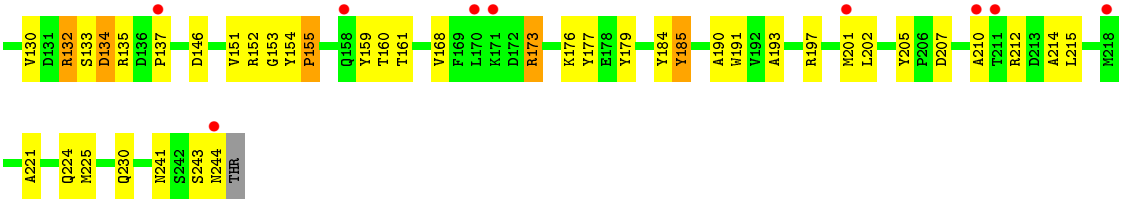
- Molecule 1: Outer membrane protein assembly factor BamA

Chain A:

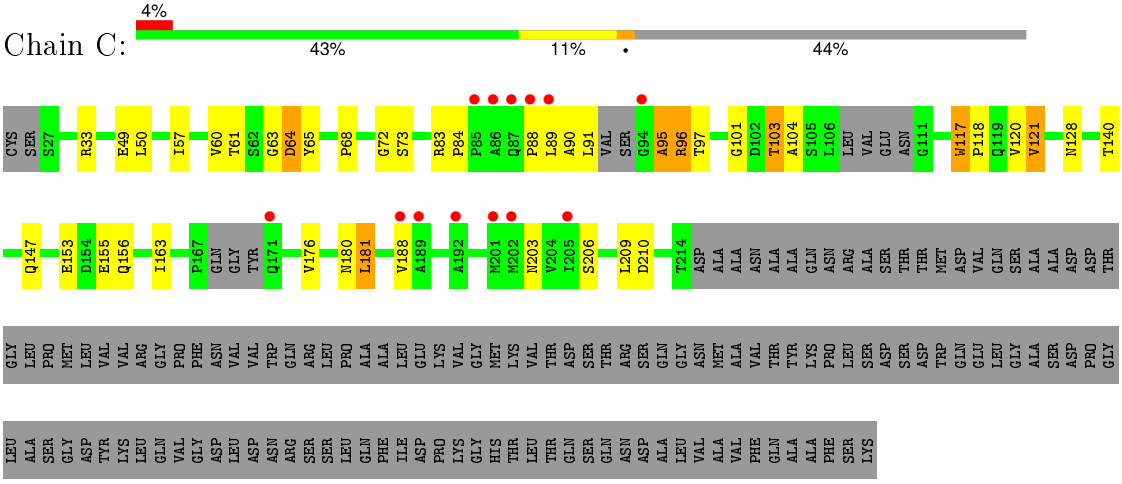
- Molecule 2: Outer membrane protein assembly factor BamD

Chain D:

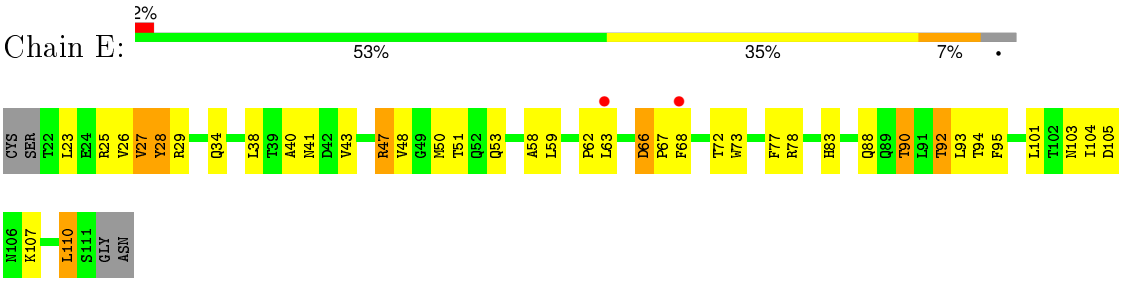




- Molecule 3: Outer membrane protein assembly factor BamC



- Molecule 4: Outer membrane protein assembly factor BamE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	234.85Å 109.23Å 103.99Å 90.00° 95.04° 90.00°	Depositor
Resolution (Å)	29.91 – 3.39 49.49 – 3.39	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.91-3.39) 89.8 (49.49-3.39)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.10_2142: ???)	Depositor
R, R_{free}	0.238 , 0.281 0.237 , 0.278	Depositor DCC
R_{free} test set	1813 reflections (5.54%)	DCC
Wilson B-factor (Å^2)	122.6	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 64.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	4 of 36095 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9451	wwPDB-VP
Average B, all atoms (Å^2)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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	0.27	0/5879	0.56	0/8014
2	D	0.25	0/1759	0.52	1/2395 (0.0%)
3	C	0.26	0/1292	0.52	0/1768
4	E	0.26	0/721	0.60	1/984 (0.1%)
All	All	0.26	0/9651	0.55	2/13161 (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	7
3	C	0	1
4	E	0	2
All	All	0	10

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	102	HIS	C-N-CD	-5.66	108.16	120.60
4	E	110	LEU	CA-CB-CG	5.46	127.85	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	ARG	Peptide
1	A	176	GLU	Peptide
1	A	196	HIS	Peptide
1	A	215	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	A	558	THR	Peptide
1	A	697	LYS	Peptide
1	A	755	SER	Peptide
3	C	95	ALA	Peptide
4	E	58	ALA	Peptide
4	E	66	ASP	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	5752	0	5229	152	0
2	D	1721	0	1621	51	0
3	C	1272	0	1171	31	0
4	E	706	0	689	25	0
All	All	9451	0	8710	249	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 14.

All (249) 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)
4:E:77:PHE:O	4:E:88:GLN:HA	1.75	0.86
1:A:195:SER:HB2	1:A:196:HIS:HA	1.59	0.84
3:C:88:PRO:HB2	3:C:89:LEU:HD23	1.65	0.78
1:A:328:ILE:HA	1:A:335:VAL:HG22	1.68	0.75
1:A:509:TYR:HB2	1:A:533:HIS:HB3	1.68	0.75
1:A:755:SER:HB2	1:A:756:GLY:HA3	1.71	0.72
1:A:750:ASP:HB3	1:A:753:GLN:H	1.55	0.71
2:D:105:ILE:O	2:D:108:VAL:N	2.23	0.70
1:A:182:ILE:HG22	1:A:258:VAL:HB	1.73	0.70
4:E:40:ALA:O	4:E:43:VAL:N	2.25	0.69
1:A:600:THR:HG21	1:A:607:GLU:HA	1.73	0.69
1:A:750:ASP:HA	1:A:751:SER:HB2	1.75	0.69
1:A:157:PRO:HA	1:A:163:VAL:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:MET:HB3	1:A:791:PHE:HB2	1.75	0.68
1:A:203:VAL:O	1:A:207:ASN:ND2	2.26	0.68
2:D:152:ARG:N	2:D:153:GLY:HA3	2.08	0.67
3:C:63:GLY:HA2	3:C:65:TYR:H	1.59	0.67
1:A:644:LYS:HB3	1:A:645:GLU:HA	1.77	0.66
3:C:90:ALA:HB2	3:C:97:THR:HG23	1.78	0.66
2:D:102:HIS:HD2	2:D:105:ILE:HG23	1.62	0.65
1:A:533:HIS:ND1	1:A:568:ASP:OD1	2.30	0.65
2:D:39:ALA:O	2:D:43:LEU:HB2	1.96	0.64
1:A:185:ASN:ND2	1:A:188:PHE:O	2.31	0.64
3:C:95:ALA:O	3:C:96:ARG:NH2	2.31	0.64
1:A:130:ILE:HA	1:A:133:ILE:HG22	1.81	0.63
4:E:92:THR:HG23	4:E:105:ASP:HB3	1.79	0.63
1:A:91:ARG:HD2	1:A:126:ASP:HB3	1.81	0.63
1:A:538:ASN:HA	1:A:562:ASP:HA	1.80	0.63
1:A:547:ARG:NH1	1:A:748:ASN:O	2.33	0.62
2:D:102:HIS:CD2	2:D:105:ILE:HG23	2.34	0.62
1:A:446:GLN:HG2	1:A:449:TRP:HA	1.82	0.61
3:C:63:GLY:N	3:C:64:ASP:HB2	2.15	0.61
1:A:653:TYR:HB3	1:A:666:ASN:HA	1.83	0.60
1:A:228:SER:O	1:A:232:ASP:HB2	2.00	0.60
2:D:49:ARG:HA	2:D:52:ILE:HB	1.83	0.60
2:D:125:GLN:N	2:D:126:GLY:HA3	2.17	0.60
3:C:104:ALA:HB3	3:C:176:VAL:H	1.67	0.60
1:A:198:GLN:N	1:A:222:ASP:OD2	2.35	0.59
3:C:57:ILE:O	4:E:68:PHE:HB3	2.03	0.59
1:A:562:ASP:O	1:A:563:ASN:ND2	2.35	0.59
2:D:101:THR:HB	2:D:102:HIS:HA	1.84	0.59
1:A:775:GLN:HG2	1:A:784:VAL:HG22	1.84	0.58
1:A:76:ARG:HB2	1:A:87:GLN:HB2	1.84	0.58
2:D:122:SER:N	2:D:123:ALA:HB2	2.19	0.58
1:A:519:ILE:HG13	1:A:520:ASN:H	1.69	0.57
1:A:750:ASP:HB3	1:A:752:SER:N	2.19	0.57
1:A:504:TYR:HA	1:A:538:ASN:HB2	1.86	0.57
2:D:120:ASP:OD1	2:D:132:ARG:NH2	2.38	0.57
1:A:516:GLY:HA2	1:A:526:ARG:HA	1.87	0.56
4:E:95:PHE:HA	4:E:101:LEU:HA	1.87	0.56
1:A:59:ILE:O	1:A:63:ILE:HB	2.05	0.56
1:A:657:SER:HA	1:A:661:ARG:HG2	1.88	0.56
4:E:101:LEU:HD13	4:E:104:ILE:HD11	1.87	0.56
2:D:102:HIS:HB3	2:D:105:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ASN:O	1:A:584:GLY:N	2.39	0.56
1:A:722:THR:HG21	1:A:733:VAL:HG13	1.87	0.56
4:E:48:VAL:HA	4:E:101:LEU:HD11	1.88	0.55
1:A:668:ILE:O	1:A:671:LYS:NZ	2.39	0.55
1:A:267:LYS:O	1:A:334:THR:HA	2.06	0.55
1:A:790:PRO:HB2	1:A:792:LYS:H	1.72	0.55
1:A:542:GLN:HG3	1:A:545:MET:HB3	1.88	0.55
1:A:622:ASP:OD1	1:A:623:ASP:N	2.39	0.55
1:A:785:PHE:HA	1:A:803:GLN:O	2.07	0.54
1:A:48:VAL:HG12	1:A:50:THR:H	1.72	0.54
1:A:478:PHE:N	1:A:483:VAL:O	2.39	0.54
1:A:614:ASP:N	1:A:614:ASP:OD1	2.40	0.54
1:A:670:PRO:HG2	1:A:708:GLY:N	2.22	0.54
2:D:212:ARG:HH21	2:D:243:SER:HA	1.73	0.53
1:A:783:LEU:HD23	1:A:806:ILE:HG21	1.90	0.53
2:D:202:LEU:HD21	2:D:215:LEU:HD21	1.89	0.53
2:D:133:SER:HB3	2:D:176:LYS:HB3	1.91	0.53
4:E:28:TYR:CG	4:E:29:ARG:N	2.77	0.53
3:C:33:ARG:HG2	3:C:83:ARG:HH21	1.73	0.53
1:A:750:ASP:CB	1:A:753:GLN:H	2.22	0.53
1:A:504:TYR:HB2	1:A:539:MET:H	1.73	0.53
1:A:359:THR:O	2:D:135:ARG:NH1	2.42	0.53
4:E:88:GLN:HB3	4:E:110:LEU:HD11	1.91	0.52
1:A:693:GLN:H	1:A:695:GLY:HA2	1.72	0.52
2:D:76:ILE:HG12	2:D:92:ILE:HG22	1.90	0.52
2:D:179:TYR:HB2	2:D:210:ALA:HB1	1.92	0.52
1:A:531:TYR:HE1	1:A:568:ASP:HB3	1.75	0.51
1:A:452:THR:OG1	1:A:453:GLY:N	2.44	0.51
2:D:88:ALA:O	2:D:92:ILE:HG23	2.11	0.51
1:A:460:GLY:HA2	1:A:468:TYR:O	2.11	0.51
2:D:79:TYR:HB3	2:D:88:ALA:HB2	1.93	0.51
1:A:623:ASP:O	1:A:625:HIS:ND1	2.43	0.51
3:C:101:GLY:HA3	3:C:103:THR:N	2.26	0.51
1:A:240:ILE:HA	1:A:260:ILE:HG23	1.93	0.51
1:A:575:GLY:HA2	1:A:595:LEU:O	2.11	0.51
4:E:90:THR:HG23	4:E:107:LYS:HG3	1.93	0.51
1:A:324:SER:HB2	1:A:337:LEU:HD11	1.92	0.50
1:A:628:VAL:O	1:A:719:ILE:HB	2.11	0.50
1:A:559:SER:HB2	1:A:676:PRO:O	2.12	0.50
2:D:190:ALA:O	2:D:193:ALA:N	2.45	0.50
1:A:227:ARG:HA	1:A:238:PHE:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:GLU:HG3	1:A:388:ARG:HB3	1.94	0.50
1:A:427:ASN:OD1	1:A:441:GLN:NE2	2.38	0.50
1:A:380:ASP:HA	1:A:383:ASP:HB2	1.93	0.49
1:A:793:LYS:N	1:A:794:TYR:HB2	2.27	0.49
2:D:152:ARG:HH11	3:C:68:PRO:HD3	1.76	0.49
4:E:94:THR:HB	4:E:103:ASN:HB3	1.94	0.49
2:D:230:GLN:NE2	4:E:66:ASP:OD1	2.43	0.49
1:A:526:ARG:NH1	1:A:577:THR:OG1	2.45	0.49
2:D:48:TRP:O	2:D:51:ALA:N	2.34	0.49
2:D:39:ALA:HB2	2:D:54:GLN:HB2	1.95	0.49
1:A:280:HIS:CG	1:A:281:SER:N	2.81	0.49
1:A:782:PRO:O	1:A:806:ILE:HG22	2.12	0.49
1:A:266:TYR:HB3	1:A:335:VAL:HG23	1.95	0.49
2:D:110:TYR:O	2:D:114:LEU:HB2	2.13	0.49
1:A:628:VAL:HG13	1:A:719:ILE:HB	1.93	0.48
3:C:117:TRP:N	3:C:118:PRO:HD2	2.28	0.48
1:A:238:PHE:CE1	1:A:260:ILE:HG21	2.48	0.48
1:A:244:GLN:O	1:A:256:VAL:HA	2.13	0.48
1:A:508:SER:HA	1:A:533:HIS:O	2.14	0.48
1:A:608:TYR:HA	1:A:640:GLY:HA2	1.96	0.48
1:A:348:TYR:HA	1:A:376:TRP:HA	1.96	0.47
1:A:374:GLY:HA2	4:E:63:LEU:HD23	1.95	0.47
1:A:404:ARG:HG2	1:A:405:VAL:H	1.78	0.47
1:A:662:GLY:H	1:A:803:GLN:HE22	1.61	0.47
2:D:134:ASP:HA	2:D:177:TYR:HD1	1.79	0.47
1:A:280:HIS:CG	1:A:281:SER:H	2.33	0.47
1:A:755:SER:HB2	1:A:756:GLY:CA	2.41	0.47
3:C:120:VAL:HG22	3:C:209:LEU:HD11	1.97	0.46
4:E:29:ARG:HB2	4:E:83:HIS:CE1	2.49	0.46
1:A:154:VAL:O	1:A:165:LEU:HA	2.16	0.46
1:A:196:HIS:ND1	1:A:198:GLN:O	2.48	0.46
3:C:49:GLU:HG2	3:C:50:LEU:H	1.80	0.46
1:A:424:GLY:HA2	1:A:445:GLN:O	2.16	0.46
3:C:89:LEU:HG	3:C:203:ASN:OD1	2.15	0.46
2:D:152:ARG:HG2	3:C:68:PRO:HG3	1.96	0.46
1:A:260:ILE:HA	1:A:261:THR:HB	1.97	0.46
1:A:154:VAL:HB	1:A:166:LYS:O	2.15	0.46
1:A:248:THR:HG22	1:A:250:ASP:H	1.80	0.46
2:D:122:SER:HB3	2:D:123:ALA:HA	1.98	0.46
1:A:396:GLU:HA	1:A:397:THR:HA	1.55	0.46
1:A:94:ILE:HD11	1:A:96:SER:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ILE:HG13	1:A:196:HIS:CE1	2.51	0.46
2:D:151:VAL:C	2:D:153:GLY:HA3	2.36	0.46
1:A:546:TRP:HA	1:A:549:LEU:HB2	1.97	0.46
4:E:34:GLN:O	4:E:78:ARG:HB3	2.16	0.46
1:A:727:ASP:C	1:A:729:TYR:H	2.20	0.46
1:A:208:VAL:HG12	1:A:209:VAL:H	1.81	0.46
1:A:117:SER:N	1:A:118:GLY:HA3	2.30	0.46
1:A:599:VAL:HG22	1:A:609:TYR:HB2	1.98	0.45
1:A:190:THR:O	1:A:194:ILE:HG22	2.16	0.45
3:C:63:GLY:CA	3:C:65:TYR:H	2.25	0.45
1:A:91:ARG:HG2	1:A:124:SER:HA	1.98	0.45
1:A:396:GLU:OE2	1:A:731:ASN:ND2	2.50	0.45
1:A:94:ILE:HD12	1:A:164:ASP:HA	1.98	0.45
1:A:699:LEU:O	1:A:757:TYR:OH	2.35	0.45
1:A:236:ALA:HB3	1:A:266:TYR:HD2	1.80	0.45
1:A:793:LYS:H	1:A:794:TYR:HB2	1.82	0.45
1:A:214:TYR:H	1:A:218:LYS:HG3	1.81	0.45
1:A:127:ARG:O	1:A:130:ILE:HG12	2.16	0.45
1:A:277:LEU:HD13	1:A:278:ALA:H	1.81	0.45
1:A:466:GLN:HG3	1:A:494:PHE:HB3	1.98	0.45
3:C:72:GLY:HA3	3:C:73:SER:HA	1.65	0.45
1:A:232:ASP:O	1:A:297:ASN:HA	2.17	0.44
3:C:163:ILE:HG12	3:C:176:VAL:HG22	1.99	0.44
1:A:499:ALA:N	1:A:500:ASP:HA	2.32	0.44
2:D:225:MET:HB3	2:D:225:MET:HE2	1.78	0.44
3:C:206:SER:O	3:C:210:ASP:HB2	2.17	0.44
1:A:279:GLY:N	1:A:280:HIS:HA	2.32	0.44
1:A:474:THR:HA	1:A:486:GLY:HA3	1.99	0.44
1:A:51:GLY:HA2	1:A:52:ASP:HB2	1.98	0.44
1:A:373:GLU:O	2:D:193:ALA:HB2	2.18	0.44
2:D:197:ARG:O	2:D:201:MET:HG3	2.18	0.44
1:A:43:LEU:HD12	1:A:48:VAL:HG21	1.99	0.44
3:C:60:VAL:HA	3:C:61:THR:HA	1.81	0.44
3:C:90:ALA:C	3:C:95:ALA:HB1	2.38	0.44
1:A:541:PRO:HA	1:A:546:TRP:CE2	2.53	0.44
2:D:191:TRP:HB3	2:D:221:ALA:HB1	2.00	0.44
1:A:91:ARG:HG3	1:A:92:PRO:HD2	1.98	0.44
1:A:110:LEU:H	1:A:110:LEU:HG	1.65	0.44
1:A:488:ARG:HB2	1:A:512:ASP:OD2	2.18	0.44
1:A:468:TYR:OH	1:A:470:GLU:OE1	2.35	0.43
2:D:106:ASP:HB3	2:D:154:TYR:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:PRO:HA	2:D:160:THR:HG21	1.99	0.43
3:C:128:ASN:ND2	3:C:128:ASN:O	2.51	0.43
2:D:77:TYR:CG	3:C:84:PRO:HD3	2.53	0.43
1:A:379:SER:C	1:A:381:LEU:H	2.21	0.43
4:E:59:LEU:HA	4:E:59:LEU:HD23	1.90	0.43
1:A:350:ARG:HH11	1:A:351:LYS:HD2	1.84	0.43
1:A:31:PHE:O	1:A:32:GLU:HB3	2.19	0.43
1:A:775:GLN:HA	1:A:783:LEU:O	2.18	0.43
1:A:81:GLY:HA3	1:A:82:ASP:C	2.39	0.43
2:D:191:TRP:CZ2	2:D:224:GLN:HG2	2.54	0.43
1:A:632:ARG:HG3	1:A:715:SER:HB2	2.01	0.43
2:D:210:ALA:O	2:D:214:ALA:HB2	2.19	0.43
1:A:669:GLY:HA3	1:A:744:VAL:O	2.18	0.43
2:D:94:ARG:HB3	2:D:94:ARG:HE	1.62	0.43
1:A:518:PRO:HA	1:A:524:SER:HA	2.01	0.43
3:C:89:LEU:HD12	3:C:206:SER:HB3	2.01	0.42
2:D:48:TRP:O	2:D:50:GLN:N	2.52	0.42
3:C:83:ARG:NH1	3:C:153:GLU:OE1	2.52	0.42
1:A:615:THR:O	1:A:632:ARG:HA	2.19	0.42
3:C:181:LEU:HD13	3:C:181:LEU:HA	1.85	0.42
1:A:787:TYR:HA	1:A:801:GLN:O	2.20	0.42
1:A:624:ASP:OD1	1:A:624:ASP:N	2.52	0.42
1:A:367:ARG:HA	2:D:184:TYR:OH	2.20	0.42
2:D:243:SER:HA	2:D:244:ASN:HA	1.78	0.42
1:A:689:GLU:H	1:A:689:GLU:HG2	1.66	0.42
1:A:620:PRO:HG3	1:A:624:ASP:HA	2.01	0.42
2:D:135:ARG:HA	2:D:135:ARG:HD3	1.81	0.42
1:A:227:ARG:HA	1:A:238:PHE:CE2	2.55	0.42
4:E:101:LEU:HD12	4:E:101:LEU:O	2.20	0.42
2:D:92:ILE:HD11	2:D:112:ARG:HB2	2.02	0.42
1:A:395:PHE:HB3	1:A:420:GLU:H	1.84	0.42
4:E:62:PRO:HG3	4:E:73:TRP:CD2	2.54	0.42
2:D:122:SER:H	2:D:132:ARG:HH11	1.66	0.41
3:C:206:SER:O	3:C:210:ASP:CB	2.68	0.41
1:A:504:TYR:HA	1:A:537:SER:O	2.20	0.41
1:A:348:TYR:HB3	4:E:63:LEU:HD21	2.02	0.41
1:A:396:GLU:OE1	1:A:583:ARG:HD2	2.20	0.41
2:D:103:PRO:CB	2:D:104:ASN:HA	2.49	0.41
3:C:140:THR:HA	3:C:163:ILE:O	2.20	0.41
2:D:185:TYR:HB3	2:D:190:ALA:HB3	2.01	0.41
4:E:26:VAL:O	4:E:27:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:SER:OG	1:A:124:SER:O	2.31	0.41
4:E:51:THR:C	4:E:53:GLN:H	2.24	0.41
2:D:137:PRO:HB3	2:D:173:ARG:NH2	2.35	0.41
1:A:803:GLN:HE21	1:A:803:GLN:HB2	1.56	0.41
1:A:706:VAL:HG13	1:A:707:GLY:H	1.85	0.41
4:E:47:ARG:O	4:E:50:MET:HG2	2.20	0.41
1:A:387:GLU:HG2	1:A:391:ARG:HH21	1.85	0.41
2:D:107:TYR:O	2:D:111:MET:HG2	2.21	0.41
1:A:196:HIS:N	1:A:198:GLN:O	2.52	0.41
1:A:276:ASN:HB3	1:A:277:LEU:CB	2.50	0.41
3:C:88:PRO:HB2	3:C:89:LEU:HA	2.03	0.41
4:E:67:PRO:HA	4:E:68:PHE:HA	1.86	0.41
1:A:260:ILE:HA	1:A:261:THR:CB	2.49	0.41
3:C:118:PRO:HA	3:C:121:VAL:HG13	2.03	0.41
1:A:402:THR:HG23	1:A:412:VAL:HG11	2.03	0.41
1:A:300:LYS:HD3	1:A:300:LYS:HA	1.97	0.41
1:A:807:GLY:HA2	1:A:808:LYS:C	2.41	0.41
4:E:72:THR:HA	4:E:93:LEU:O	2.21	0.41
1:A:750:ASP:HA	1:A:751:SER:CB	2.47	0.41
1:A:536:LEU:HD13	1:A:539:MET:HE1	2.03	0.41
1:A:404:ARG:HA	1:A:412:VAL:HG22	2.03	0.41
1:A:97:ILE:HA	1:A:165:LEU:HG	2.02	0.41
2:D:123:ALA:HB1	2:D:125:GLN:H	1.85	0.40
2:D:112:ARG:NH2	2:D:146:ASP:OD1	2.53	0.40
3:C:155:GLU:O	3:C:156:GLN:HB2	2.21	0.40
4:E:95:PHE:CE2	4:E:101:LEU:HB3	2.56	0.40
1:A:671:LYS:HA	1:A:705:ALA:HA	2.04	0.40
1:A:92:PRO:HG2	1:A:125:LEU:O	2.20	0.40
1:A:789:GLN:HA	1:A:790:PRO:HA	1.88	0.40
1:A:350:ARG:HB2	1:A:411:GLN:HB3	2.03	0.40
1:A:490:PHE:HB3	1:A:510:GLY:HA3	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	755/790 (96%)	632 (84%)	119 (16%)	4 (0%)	34 75
2	D	217/226 (96%)	194 (89%)	23 (11%)	0	100 100
3	C	171/320 (53%)	144 (84%)	27 (16%)	0	100 100
4	E	88/94 (94%)	77 (88%)	11 (12%)	0	100 100
All	All	1231/1430 (86%)	1047 (85%)	180 (15%)	4 (0%)	46 82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	ASP
1	A	563	ASN
1	A	209	VAL
1	A	159	PRO

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	583/672 (87%)	502 (86%)	81 (14%)	4 23
2	D	172/190 (90%)	153 (89%)	19 (11%)	8 34
3	C	120/258 (46%)	110 (92%)	10 (8%)	14 49
4	E	79/82 (96%)	70 (89%)	9 (11%)	7 31
All	All	954/1202 (79%)	835 (88%)	119 (12%)	6 27

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	34	LEU
1	A	44	LEU
1	A	53	THR

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Mol	Chain	Res	Type
1	A	54	VAL
1	A	63	ILE
1	A	80	ASP
1	A	91	ARG
1	A	96	SER
1	A	110	LEU
1	A	125	LEU
1	A	134	GLU
1	A	144	VAL
1	A	158	LEU
1	A	164	ASP
1	A	183	VAL
1	A	192	GLU
1	A	196	HIS
1	A	208	VAL
1	A	214	TYR
1	A	215	GLN
1	A	219	LEU
1	A	222	ASP
1	A	230	TYR
1	A	232	ASP
1	A	233	ARG
1	A	243	THR
1	A	260	ILE
1	A	277	LEU
1	A	306	ASP
1	A	325	MET
1	A	338	ARG
1	A	370	ARG
1	A	377	LEU
1	A	395	PHE
1	A	398	VAL
1	A	423	THR
1	A	426	PHE
1	A	464	ASP
1	A	467	THR
1	A	471	LEU
1	A	480	VAL
1	A	485	LEU
1	A	512	ASP
1	A	514	THR
1	A	532	VAL

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Mol	Chain	Res	Type
1	A	540	GLN
1	A	563	ASN
1	A	567	THR
1	A	569	ASP
1	A	573	ASN
1	A	582	ASP
1	A	585	TYR
1	A	588	THR
1	A	612	THR
1	A	613	LEU
1	A	614	ASP
1	A	621	ILE
1	A	624	ASP
1	A	625	HIS
1	A	630	LEU
1	A	639	ASP
1	A	659	THR
1	A	667	THR
1	A	687	ASP
1	A	689	GLU
1	A	690	CYS
1	A	694	ASP
1	A	700	CYS
1	A	702	SER
1	A	706	VAL
1	A	720	THR
1	A	748	ASN
1	A	754	TYR
1	A	762	ASP
1	A	767	ARG
1	A	768	MET
1	A	774	LEU
1	A	785	PHE
1	A	803	GLN
1	A	809	THR
2	D	85	LEU
2	D	92	ILE
2	D	102	HIS
2	D	104	ASN
2	D	108	VAL
2	D	119	LEU
2	D	124	LEU

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Mol	Chain	Res	Type
2	D	130	VAL
2	D	132	ARG
2	D	134	ASP
2	D	155	PRO
2	D	159	TYR
2	D	161	THR
2	D	168	VAL
2	D	173	ARG
2	D	185	TYR
2	D	205	TYR
2	D	207	ASP
2	D	241	ASN
3	C	64	ASP
3	C	91	LEU
3	C	96	ARG
3	C	103	THR
3	C	117	TRP
3	C	121	VAL
3	C	147	GLN
3	C	180	ASN
3	C	181	LEU
3	C	188	VAL
4	E	23	LEU
4	E	25	ARG
4	E	27	VAL
4	E	28	TYR
4	E	38	LEU
4	E	41	ASN
4	E	47	ARG
4	E	90	THR
4	E	92	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	563	ASN
1	A	803	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	763/790 (96%)	0.06	38 (4%)	32	29	75, 153, 219, 277	0
2	D	219/226 (96%)	0.27	11 (5%)	32	29	86, 132, 204, 234	0
3	C	179/320 (55%)	0.05	13 (7%)	18	17	109, 175, 233, 285	0
4	E	90/94 (95%)	0.07	2 (2%)	65	60	84, 121, 157, 197	0
All	All	1251/1430 (87%)	0.10	64 (5%)	32	28	75, 149, 218, 285	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	88	PRO	6.4
1	A	77	VAL	6.1
1	A	78	LEU	5.4
1	A	84	LEU	5.2
3	C	86	ALA	5.0
1	A	31	PHE	4.9
1	A	270	GLY	4.8
3	C	89	LEU	4.6
3	C	189	ALA	4.1
1	A	255	TYR	4.1
1	A	119	VAL	3.9
1	A	180	ILE	3.9
1	A	200	ARG	3.7
1	A	29	ILE	3.4
3	C	205	ILE	3.3
3	C	188	VAL	3.3
1	A	153	ALA	3.3
1	A	85	LEU	3.2
1	A	652	PHE	3.2
1	A	79	ARG	3.2
4	E	63	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	175	ALA	3.1
2	D	67	TYR	3.1
3	C	87	GLN	3.1
1	A	536	LEU	3.1
3	C	201	MET	2.9
1	A	271	VAL	2.9
2	D	218	MET	2.9
1	A	637	TYR	2.9
2	D	158	GLN	2.8
1	A	539	MET	2.8
1	A	30	HIS	2.8
1	A	256	VAL	2.6
1	A	199	LEU	2.6
1	A	540	GLN	2.5
4	E	68	PHE	2.5
3	C	192	ALA	2.4
1	A	268	LEU	2.3
1	A	308	ILE	2.3
2	D	210	ALA	2.3
1	A	504	TYR	2.3
2	D	137	PRO	2.3
1	A	211	ASP	2.3
1	A	214	TYR	2.3
1	A	659	THR	2.3
3	C	85	PRO	2.3
1	A	648	PHE	2.3
1	A	125	LEU	2.3
3	C	202	MET	2.2
1	A	320	PRO	2.2
1	A	565	PHE	2.2
2	D	244	ASN	2.2
2	D	171	LYS	2.2
1	A	97	ILE	2.2
3	C	171	GLN	2.1
1	A	564	SER	2.1
2	D	211	THR	2.1
1	A	48	VAL	2.1
1	A	193	LEU	2.1
2	D	201	MET	2.1
2	D	74	ASP	2.0
3	C	94	GLY	2.0
1	A	534	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	170	LEU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.