Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:23 pm BST

PDB ID	:	6O38
Title	:	Structure of a chaperone-substrate complex
Authors	:	Urusova, D.V.; Tolia, N.H.
Deposited on	:	2019-02-26
Resolution	:	2.60 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 following versions of software and data (see references ⓘ) were used in the production of this report:

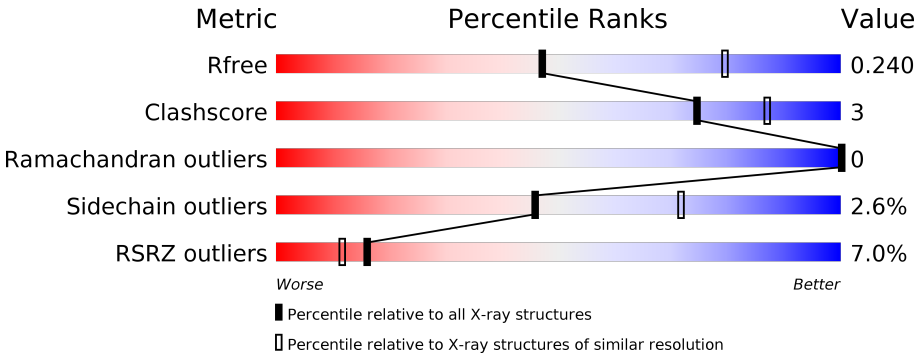
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	578	6% 92% 7%
1	B	578	2% 89% 10%
1	C	578	7% 80% 9% 11%
1	D	578	3% 92% 7%
1	E	578	% 90% 9%
1	F	578	10% 88% 9%

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Mol	Chain	Length	Quality of chain
2	G	178	12% 61% 10% 28%
2	H	178	9% 54% 12% 34%
2	K	178	17% 54% 12% 34%
2	L	178	7% 62% 10% 27%
2	M	178	5% 61% 11% 28%
2	N	178	12% 57% 11% 30%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	D	602	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32308 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 Acinetobacter secreted protease CpaA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	Se	0	0	0
			4399	2771	744	874	2	8			
1	B	573	Total	C	N	O	S	Se	0	0	0
			4398	2771	743	874	2	8			
1	C	514	Total	C	N	O	S	Se	0	0	0
			3949	2496	666	777	2	8			
1	D	573	Total	C	N	O	S	Se	0	0	0
			4399	2771	744	874	2	8			
1	E	573	Total	C	N	O	S	Se	0	0	0
			4399	2771	744	874	2	8			
1	F	561	Total	C	N	O	S	Se	0	0	0
			4308	2715	727	856	2	8			

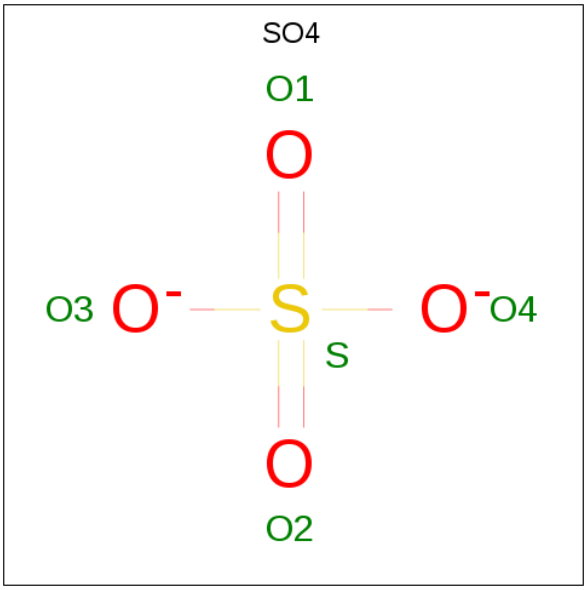
- Molecule 2 is a protein called Type II secretion chaperone CpaB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	128	Total	C	N	O	Se	0	0	0
			1038	654	175	205	4			
2	H	118	Total	C	N	O	Se	0	0	0
			958	607	160	187	4			
2	K	117	Total	C	N	O	Se	0	0	0
			945	595	159	187	4			
2	L	130	Total	C	N	O	Se	0	0	0
			1054	664	178	208	4			
2	M	129	Total	C	N	O	Se	0	0	0
			1046	658	176	208	4			
2	N	124	Total	C	N	O	Se	0	0	0
			1006	635	170	197	4			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0
4	N	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	36	Total O 36 36	0	0
5	B	54	Total O 54 54	0	0
5	C	38	Total O 38 38	0	0

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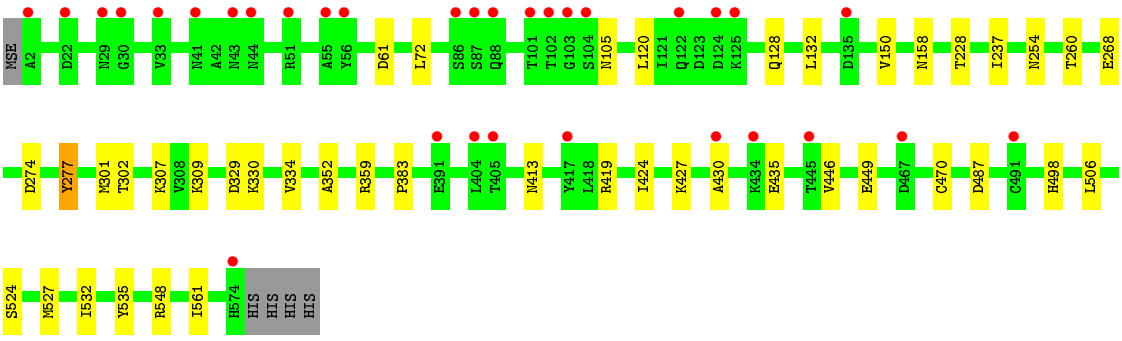
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	49	Total O 49 49	0	0
5	E	56	Total O 56 56	0	0
5	F	46	Total O 46 46	0	0
5	H	3	Total O 3 3	0	0
5	L	5	Total O 5 5	0	0
5	M	3	Total O 3 3	0	0
5	N	3	Total O 3 3	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

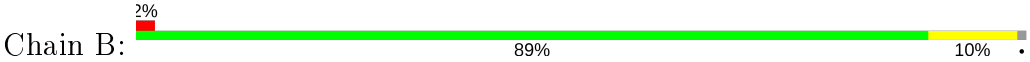
- Molecule 1: Acinetobacter secreted protease CpaA

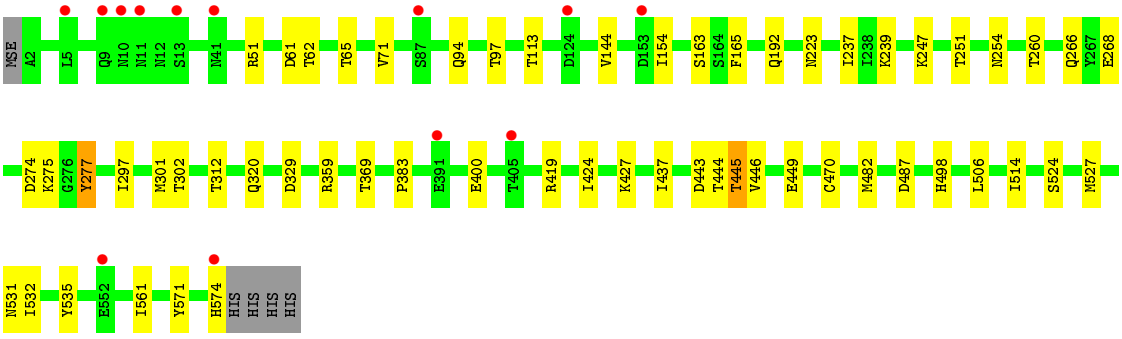
Chain A:



- Molecule 1: Acinetobacter secreted protease CpaA

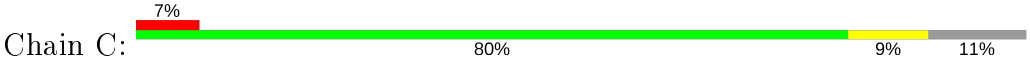
Chain B:

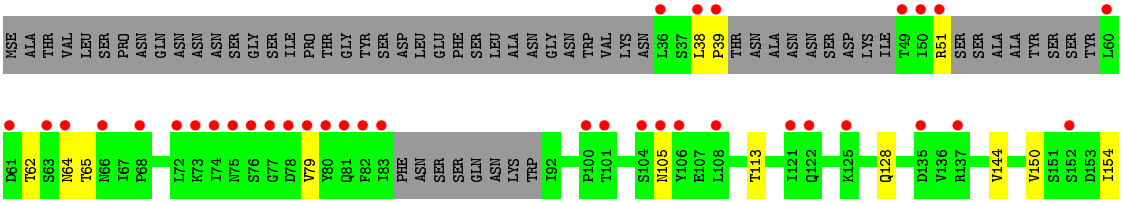


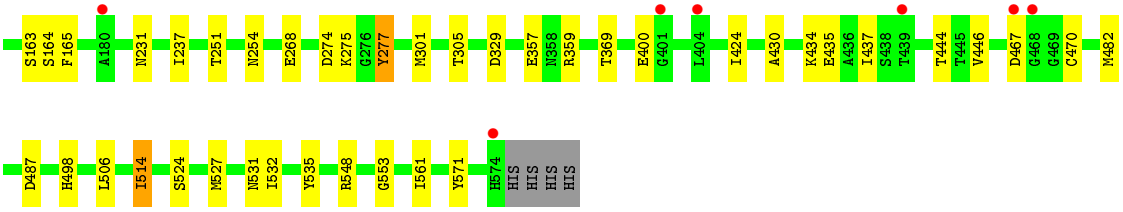


- Molecule 1: Acinetobacter secreted protease CpaA

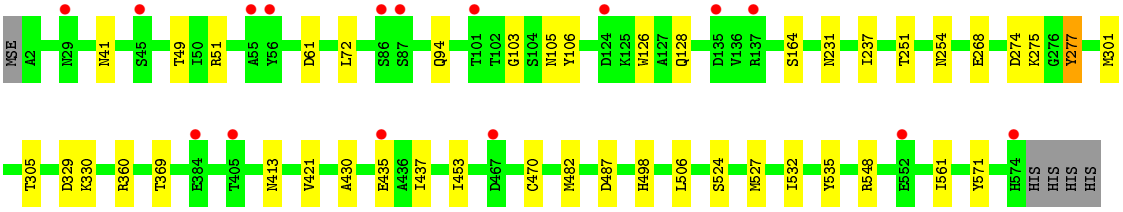
Chain C:



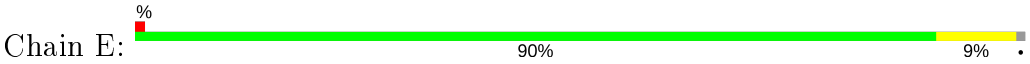


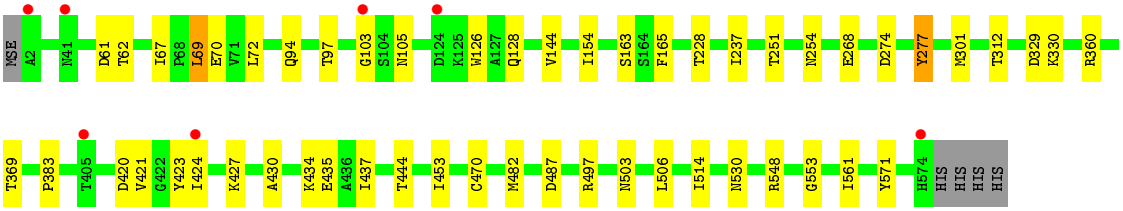


• Molecule 1: Acinetobacter secreted protease CpaA

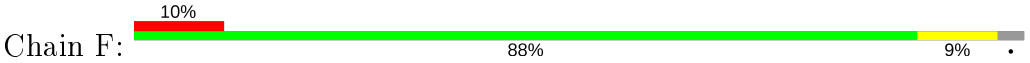


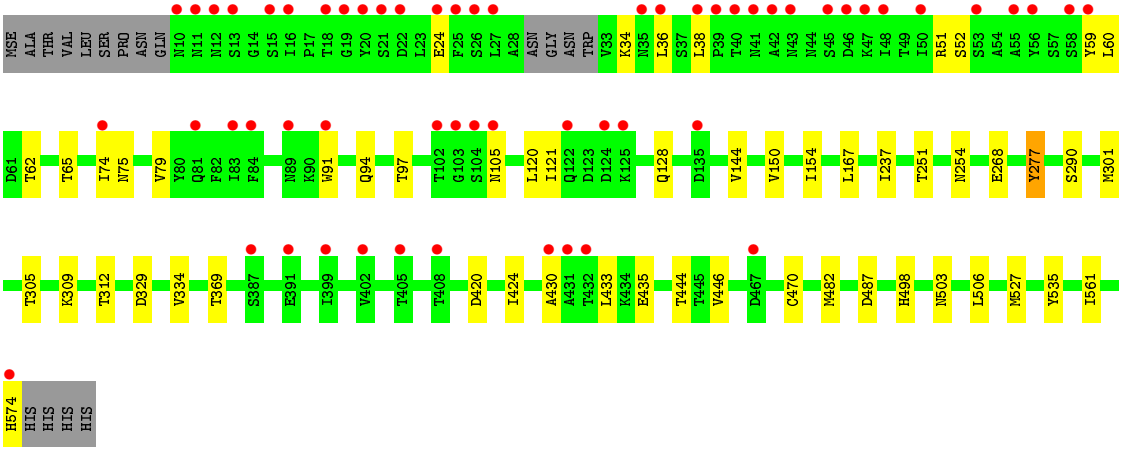
• Molecule 1: Acinetobacter secreted protease CpaA



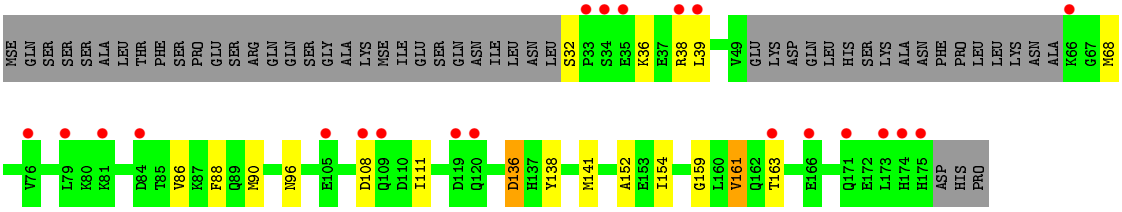


• Molecule 1: Acinetobacter secreted protease CpaA



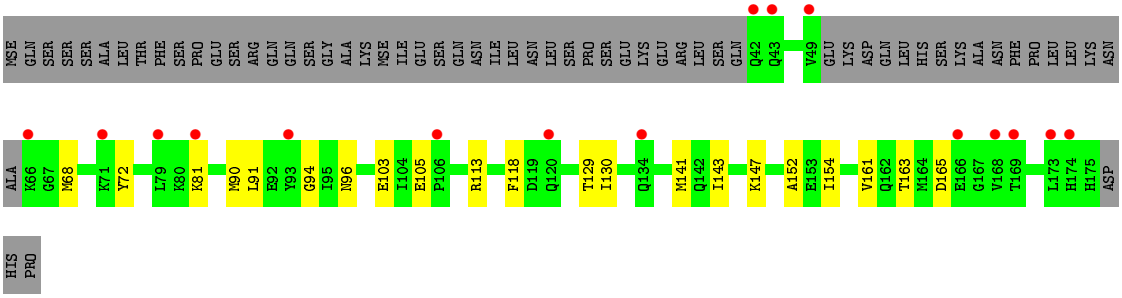


• Molecule 2: Type II secretion chaperone CpaB



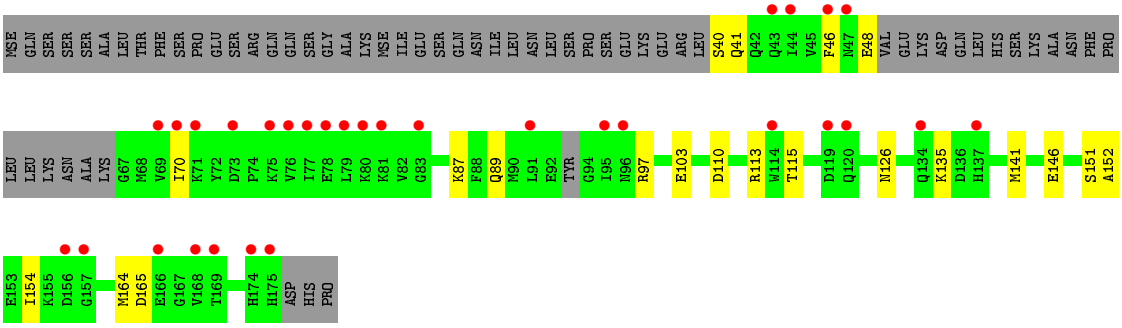
• Molecule 2: Type II secretion chaperone CpaB

Chain H:



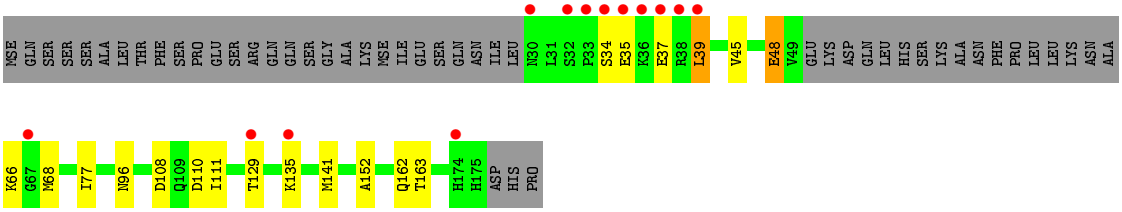
• Molecule 2: Type II secretion chaperone CpaB

Chain K:



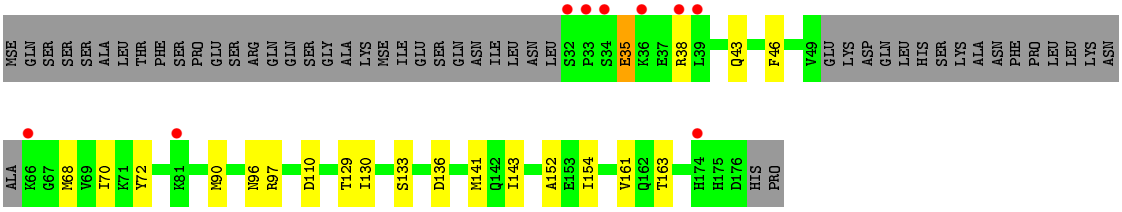
• Molecule 2: Type II secretion chaperone CpaB

Chain L:

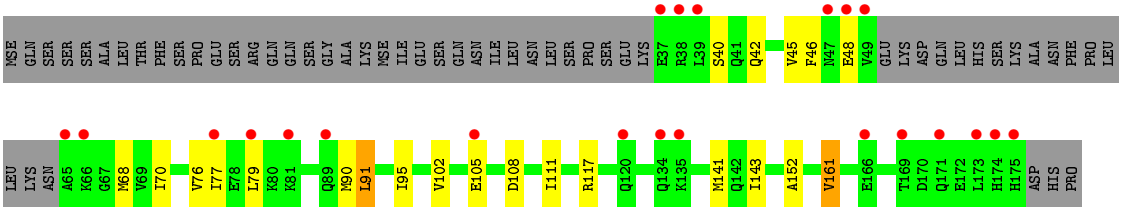


• Molecule 2: Type II secretion chaperone CpaB

Chain M:



- Molecule 2: Type II secretion chaperone CpaB



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	110.75Å 118.49Å 129.58Å 108.94° 103.97° 100.10°	Depositor
Resolution (Å)	35.79 – 2.60 35.79 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.5 (35.79-2.60) 89.5 (35.79-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.225 , 0.240 0.225 , 0.240	Depositor DCC
R_{free} test set	7917 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	45.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 29.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	32308	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4

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	0.24	0/4485	0.43	0/6109
1	B	0.24	0/4484	0.43	0/6107
1	C	0.24	0/4021	0.44	0/5470
1	D	0.24	0/4485	0.43	0/6109
1	E	0.24	0/4485	0.44	0/6109
1	F	0.25	0/4390	0.44	0/5975
2	G	0.25	0/1051	0.46	0/1407
2	H	0.26	0/970	0.45	0/1299
2	K	0.24	0/955	0.44	0/1277
2	L	0.24	0/1067	0.44	0/1429
2	M	0.24	0/1059	0.44	0/1418
2	N	0.24	0/1018	0.46	0/1363
All	All	0.24	0/32470	0.44	0/44072

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	4399	0	4306	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4398	0	4302	29	0
1	C	3949	0	3895	26	0
1	D	4399	0	4306	21	0
1	E	4399	0	4306	25	0
1	F	4308	0	4222	23	0
2	G	1038	0	1017	8	0
2	H	958	0	938	13	0
2	K	945	0	919	12	0
2	L	1054	0	1034	10	0
2	M	1046	0	1021	13	0
2	N	1006	0	986	15	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	15	0	0	1	0
4	B	15	0	0	2	0
4	C	15	0	0	1	0
4	D	5	0	0	2	0
4	E	10	0	0	0	0
4	F	15	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
4	L	10	0	0	0	0
4	M	10	0	0	1	0
4	N	5	0	0	0	0
5	A	36	0	0	1	0
5	B	54	0	0	2	0
5	C	38	0	0	0	0
5	D	49	0	0	0	0
5	E	56	0	0	1	0
5	F	46	0	0	0	0
5	H	3	0	0	0	0
5	L	5	0	0	0	0
5	M	3	0	0	0	0
5	N	3	0	0	0	0
All	All	32308	0	31252	204	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 3.

All (204) 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)
2:N:68:MSE:HE1	2:N:90:MSE:HG2	1.63	0.80
2:G:68:MSE:HE1	2:G:90:MSE:HG2	1.64	0.80
2:M:68:MSE:HE1	2:M:90:MSE:HG2	1.66	0.77
2:H:68:MSE:HE1	2:H:90:MSE:HG2	1.69	0.74
1:D:274:ASP:OD2	1:D:548:ARG:NH2	2.25	0.69
2:M:68:MSE:HE3	2:M:70:ILE:HD11	1.75	0.69
1:F:498:HIS:HA	1:F:527:MSE:HE1	1.75	0.68
2:H:94:GLY:O	2:H:147:LYS:NZ	2.24	0.68
1:A:307:LYS:NZ	5:A:701:HOH:O	2.26	0.68
1:D:498:HIS:HA	1:D:527:MSE:HE1	1.76	0.68
1:D:61:ASP:OD1	2:L:96:ASN:ND2	2.26	0.68
1:B:62:THR:OG1	1:B:65:THR:OG1	2.13	0.66
1:B:275:LYS:NZ	4:B:604:SO4:O1	2.25	0.66
1:A:61:ASP:OD1	2:G:96:ASN:ND2	2.29	0.66
1:B:498:HIS:HA	1:B:527:MSE:HE1	1.75	0.66
1:C:498:HIS:HA	1:C:527:MSE:HE1	1.77	0.66
2:L:141:MSE:HB2	2:L:152:ALA:HB3	1.78	0.65
1:A:498:HIS:HA	1:A:527:MSE:HE1	1.77	0.65
1:A:274:ASP:OD2	1:A:548:ARG:NH2	2.31	0.64
1:E:274:ASP:OD2	1:E:548:ARG:NH2	2.29	0.64
1:C:62:THR:OG1	1:C:65:THR:OG1	2.17	0.63
1:F:62:THR:OG1	1:F:65:THR:OG1	2.18	0.62
2:M:35:GLU:O	2:M:38:ARG:NH2	2.33	0.61
1:B:192:GLN:NE2	5:B:701:HOH:O	2.32	0.60
2:G:108:ASP:OD1	2:G:111:ILE:N	2.33	0.60
2:L:66:LYS:N	2:L:162:GLN:OE1	2.35	0.60
2:K:103:GLU:HB3	2:K:115:THR:HB	1.84	0.59
1:C:38:LEU:HB2	1:C:64:ASN:HD21	1.67	0.59
2:L:108:ASP:OD1	2:L:111:ILE:N	2.33	0.59
2:L:45:VAL:HG13	2:L:77:ILE:HD11	1.85	0.59
2:L:34:SER:HB3	2:L:37:GLU:HB2	1.85	0.59
2:N:76:VAL:HG13	2:N:77:ILE:HD12	1.83	0.58
2:H:141:MSE:HB2	2:H:152:ALA:HB3	1.84	0.58
2:N:108:ASP:OD1	2:N:111:ILE:N	2.32	0.58
1:A:419:ARG:NH1	4:A:603:SO4:O4	2.36	0.58
1:D:430:ALA:HB1	1:D:435:GLU:HB3	1.86	0.58
2:M:141:MSE:HB2	2:M:152:ALA:HB3	1.85	0.58
1:F:52:SER:OG	1:F:75:ASN:O	2.20	0.58
1:C:430:ALA:HB1	1:C:435:GLU:HB3	1.86	0.56
1:A:470:CYS:HB2	1:A:487:ASP:OD1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:GLU:OE2	1:F:51:ARG:NH1	2.38	0.55
1:F:51:ARG:HG2	1:F:79:VAL:HG22	1.88	0.55
2:K:87:LYS:HE2	2:K:89:GLN:HE21	1.70	0.55
1:B:71:VAL:HG21	2:H:91:LEU:HA	1.89	0.55
2:N:102:VAL:HG21	2:N:117:ARG:HG3	1.88	0.55
1:E:514:ILE:HD11	1:E:553:GLY:HA2	1.89	0.55
1:F:59:TYR:HB2	2:N:91:LEU:HB2	1.89	0.54
1:B:61:ASP:OD1	2:H:96:ASN:ND2	2.40	0.54
1:E:67:ILE:HG21	1:E:72:LEU:HD21	1.89	0.54
1:D:482:MSE:HE3	1:D:571:TYR:HE2	1.73	0.54
1:D:470:CYS:HB2	1:D:487:ASP:OD1	2.08	0.54
1:B:531:ASN:HB3	2:H:165:ASP:HB3	1.90	0.54
2:N:141:MSE:HB2	2:N:152:ALA:HB3	1.89	0.54
1:F:470:CYS:HB2	1:F:487:ASP:OD1	2.08	0.54
1:B:239:LYS:HG2	1:B:266:GLN:HG3	1.90	0.53
1:C:275:LYS:NZ	4:C:603:SO4:O1	2.41	0.53
1:E:470:CYS:HB2	1:E:487:ASP:OD1	2.08	0.53
2:H:130:ILE:HG12	2:H:141:MSE:HG2	1.90	0.53
1:B:359:ARG:NH1	5:B:705:HOH:O	2.42	0.53
1:E:430:ALA:HB1	1:E:435:GLU:HB3	1.91	0.52
1:B:237:ILE:HG12	1:B:268:GLU:HG3	1.90	0.52
2:N:90:MSE:HB2	2:N:95:ILE:HB	1.92	0.52
1:C:470:CYS:HB2	1:C:487:ASP:OD1	2.10	0.52
1:E:383:PRO:HD2	1:E:427:LYS:HB2	1.92	0.52
1:D:506:LEU:HD11	1:D:561:ILE:HD11	1.91	0.52
1:B:527:MSE:HE3	1:B:535:TYR:HE1	1.75	0.51
1:E:301:MSE:HE2	1:E:329:ASP:HB3	1.92	0.51
1:A:430:ALA:HB1	1:A:435:GLU:HB3	1.93	0.51
1:B:237:ILE:HG21	1:B:239:LYS:HE3	1.92	0.51
1:C:274:ASP:OD2	1:C:548:ARG:NH2	2.29	0.51
1:C:105:ASN:HA	1:C:128:GLN:HB3	1.92	0.51
1:F:301:MSE:HE2	1:F:329:ASP:HB3	1.93	0.51
1:A:424:ILE:HG21	1:A:449:GLU:HG2	1.92	0.51
1:C:506:LEU:HD11	1:C:561:ILE:HD11	1.93	0.51
2:G:141:MSE:HB2	2:G:152:ALA:HB3	1.92	0.51
2:N:45:VAL:HG13	2:N:77:ILE:HD11	1.92	0.51
1:A:309:LYS:HA	1:A:334:VAL:HG22	1.93	0.51
1:A:506:LEU:HD11	1:A:561:ILE:HD11	1.93	0.51
1:B:419:ARG:NH1	4:B:603:SO4:O1	2.36	0.51
1:C:51:ARG:HG2	1:C:79:VAL:HG22	1.92	0.51
1:D:105:ASN:HA	1:D:128:GLN:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:90:MSE:HE1	2:N:143:ILE:HD13	1.93	0.50
1:A:105:ASN:HA	1:A:128:GLN:HB3	1.92	0.50
1:B:482:MSE:HE3	1:B:571:TYR:HE2	1.76	0.50
1:F:506:LEU:HD11	1:F:561:ILE:HD11	1.94	0.50
1:C:527:MSE:HE3	1:C:535:TYR:HE1	1.77	0.50
1:F:105:ASN:HA	1:F:128:GLN:HB3	1.94	0.50
1:E:70:GLU:OE2	2:M:97:ARG:NH2	2.33	0.49
2:K:126:ASN:ND2	2:K:146:GLU:OE1	2.45	0.49
1:D:237:ILE:HG12	1:D:268:GLU:HG3	1.94	0.49
1:B:443:ASP:OD1	1:B:445:THR:HG23	2.13	0.49
1:F:65:THR:HG22	1:F:91:TRP:HB2	1.95	0.49
1:F:527:MSE:HE3	1:F:535:TYR:HE1	1.78	0.49
2:M:46:PHE:HB2	2:M:70:ILE:HG23	1.95	0.49
2:N:91:LEU:HD13	2:N:91:LEU:H	1.78	0.49
1:B:470:CYS:HB2	1:B:487:ASP:OD1	2.11	0.49
2:L:48:GLU:HG2	2:L:68:MSE:HE3	1.94	0.48
1:B:424:ILE:HG21	1:B:449:GLU:HG2	1.96	0.48
1:F:309:LYS:HA	1:F:334:VAL:HG22	1.95	0.48
1:B:506:LEU:HD11	1:B:561:ILE:HD11	1.96	0.47
1:F:38:LEU:HD11	1:F:60:LEU:HD21	1.96	0.47
1:C:531:ASN:HB3	2:K:165:ASP:HB3	1.96	0.47
1:F:430:ALA:HB1	1:F:435:GLU:HB3	1.97	0.47
1:B:301:MSE:HE2	1:B:329:ASP:HB3	1.97	0.47
1:B:254:ASN:HB2	1:B:277:TYR:CD1	2.49	0.47
2:K:46:PHE:CD2	2:K:141:MSE:HE1	2.49	0.47
1:F:290:SER:OG	2:N:105:GLU:OE1	2.25	0.47
1:C:482:MSE:HE3	1:C:571:TYR:HE2	1.80	0.47
1:E:61:ASP:OD1	2:M:96:ASN:ND2	2.47	0.47
1:A:527:MSE:HE3	1:A:535:TYR:HE1	1.80	0.46
1:C:38:LEU:HB2	1:C:39:PRO:HD2	1.98	0.46
1:E:482:MSE:HE3	1:E:571:TYR:HE2	1.80	0.46
1:A:301:MSE:HE2	1:A:329:ASP:HB3	1.97	0.46
1:E:62:THR:OG1	1:E:69:LEU:O	2.27	0.46
1:D:277:TYR:OH	4:D:602:SO4:O1	2.30	0.46
1:A:132:LEU:O	1:A:158:ASN:ND2	2.41	0.46
1:C:144:VAL:HG11	1:C:154:ILE:HD11	1.96	0.46
1:A:383:PRO:HD2	1:A:427:LYS:HB2	1.98	0.45
1:C:237:ILE:HG12	1:C:268:GLU:HG3	1.98	0.45
1:E:144:VAL:HG11	1:E:154:ILE:HD11	1.98	0.45
1:F:36:LEU:HD13	1:F:74:ILE:HD12	1.96	0.45
1:F:144:VAL:HG11	1:F:154:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ASN:HB2	1:C:277:TYR:CD1	2.52	0.45
1:E:506:LEU:HD11	1:E:561:ILE:HD11	1.97	0.45
1:D:254:ASN:HB2	1:D:277:TYR:CD1	2.52	0.45
2:M:68:MSE:HE2	2:M:161:VAL:HB	1.98	0.45
1:F:254:ASN:HB2	1:F:277:TYR:CD1	2.52	0.44
1:A:237:ILE:HG12	1:A:268:GLU:HG3	1.99	0.44
1:A:254:ASN:HB2	1:A:277:TYR:CD1	2.53	0.44
1:C:301:MSE:HE2	1:C:329:ASP:HB3	1.99	0.44
1:D:527:MSE:HE3	1:D:535:TYR:HE1	1.82	0.44
2:H:90:MSE:HE1	2:H:143:ILE:HD13	2.00	0.44
2:L:110:ASP:OD1	2:L:135:LYS:HG3	2.18	0.44
2:H:118:PHE:HZ	2:H:143:ILE:HG23	1.82	0.44
2:K:40:SER:OG	2:K:41:GLN:N	2.49	0.44
1:A:330:LYS:NZ	1:A:413:ASN:OD1	2.49	0.43
1:C:39:PRO:HD2	1:C:64:ASN:HD21	1.83	0.43
2:M:90:MSE:HE1	2:M:143:ILE:HD13	2.00	0.43
2:H:103:GLU:HG2	2:H:105:GLU:HG3	2.00	0.43
2:L:34:SER:OG	2:L:35:GLU:N	2.51	0.43
1:F:237:ILE:HG12	1:F:268:GLU:HG3	1.99	0.43
2:K:97:ARG:NH2	2:K:146:GLU:OE2	2.37	0.43
1:D:164:SER:OG	1:D:231:ASN:ND2	2.42	0.42
2:M:72:TYR:CG	2:M:154:ILE:HD13	2.54	0.42
1:B:163:SER:HB2	1:B:165:PHE:CE2	2.55	0.42
2:N:70:ILE:HG13	2:N:161:VAL:CG2	2.49	0.42
1:A:524:SER:O	1:A:532:ILE:HG12	2.20	0.42
1:E:163:SER:HB2	1:E:165:PHE:CE2	2.54	0.42
1:E:254:ASN:HB2	1:E:277:TYR:CD1	2.54	0.42
2:N:152:ALA:HB2	2:N:161:VAL:HG13	2.01	0.42
1:B:223:ASN:HA	1:B:247:LYS:O	2.19	0.42
1:B:400:GLU:OE2	2:H:113:ARG:NH1	2.53	0.42
2:N:40:SER:HB2	2:N:79:LEU:HD12	2.01	0.42
2:H:72:TYR:CG	2:H:154:ILE:HD13	2.55	0.42
1:B:383:PRO:HD2	1:B:427:LYS:HB2	2.01	0.42
2:H:81:LYS:HE3	2:H:81:LYS:HB2	1.93	0.42
2:G:154:ILE:HG12	2:G:159:GLY:HA3	2.01	0.42
1:D:437:ILE:HA	1:D:437:ILE:HD13	1.92	0.41
1:D:524:SER:O	1:D:532:ILE:HG12	2.20	0.41
1:E:423:TYR:OH	5:E:701:HOH:O	2.20	0.41
1:F:482:MSE:SE	1:F:503:ASN:HB3	2.70	0.41
1:A:352:ALA:O	1:A:359:ARG:NH1	2.52	0.41
2:G:152:ALA:HB2	2:G:161:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:46:PHE:HB2	2:N:70:ILE:HG23	2.01	0.41
2:K:110:ASP:OD1	2:K:135:LYS:HG3	2.20	0.41
1:C:524:SER:O	1:C:532:ILE:HG12	2.21	0.41
1:C:514:ILE:HD11	1:C:553:GLY:HA2	2.02	0.41
2:K:151:SER:HB3	2:K:164:MSE:HE2	2.03	0.41
2:L:39:LEU:HA	2:L:39:LEU:HD22	1.89	0.41
2:M:43:GLN:N	4:M:202:SO4:O1	2.51	0.41
1:B:144:VAL:HG11	1:B:154:ILE:HD11	2.03	0.41
1:C:400:GLU:OE2	2:K:113:ARG:NH1	2.54	0.41
1:B:297:ILE:HA	1:B:320:GLN:HB3	2.03	0.41
1:D:103:GLY:HA2	1:D:126:TRP:O	2.21	0.41
1:D:421:VAL:HG23	1:D:453:ILE:HD12	2.03	0.41
1:E:237:ILE:HG12	1:E:268:GLU:HG3	2.02	0.41
1:E:330:LYS:HD3	1:E:360:ARG:HD2	2.03	0.41
1:E:421:VAL:HG23	1:E:453:ILE:HD12	2.02	0.41
2:M:130:ILE:HG12	2:M:141:MSE:HE3	2.03	0.41
1:B:274:ASP:OD1	1:B:275:LYS:HG2	2.21	0.41
1:C:357:GLU:OE2	1:C:359:ARG:HD3	2.21	0.41
1:D:330:LYS:HD3	1:D:360:ARG:HD2	2.03	0.41
1:D:330:LYS:NZ	1:D:413:ASN:OD1	2.53	0.41
1:E:482:MSE:SE	1:E:503:ASN:HB3	2.71	0.41
1:E:67:ILE:HD13	1:E:72:LEU:HD11	2.02	0.41
2:G:88:PHE:HB3	2:G:90:MSE:HE2	2.02	0.41
2:M:110:ASP:OD2	2:M:133:SER:OG	2.25	0.41
1:B:260:THR:HB	1:B:302:THR:O	2.21	0.40
1:C:163:SER:HB2	1:C:165:PHE:CE2	2.55	0.40
1:D:301:MSE:HE2	1:D:329:ASP:HB3	2.02	0.40
2:G:136:ASP:O	2:G:138:TYR:N	2.54	0.40
1:E:497:ARG:NE	1:E:530:ASN:OD1	2.54	0.40
1:F:433:LEU:HD23	1:F:433:LEU:HA	1.92	0.40
2:K:141:MSE:HE2	2:K:154:ILE:HD11	2.02	0.40
2:K:141:MSE:HB2	2:K:152:ALA:HB3	2.02	0.40
1:C:434:LYS:O	1:C:437:ILE:HG22	2.21	0.40
1:E:103:GLY:HA2	1:E:126:TRP:O	2.20	0.40
1:E:105:ASN:O	1:E:128:GLN:HB3	2.21	0.40
1:A:260:THR:HB	1:A:302:THR:O	2.21	0.40
1:B:524:SER:O	1:B:532:ILE:HG12	2.22	0.40
1:C:164:SER:OG	1:C:231:ASN:ND2	2.47	0.40
1:D:275:LYS:NZ	4:D:602:SO4:O2	2.48	0.40
1:E:434:LYS:O	1:E:437:ILE:HG22	2.21	0.40
1:F:121:ILE:HD12	1:F:167:LEU:HD13	2.04	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	571/578 (99%)	563 (99%)	8 (1%)	0	100	100
1	B	571/578 (99%)	563 (99%)	8 (1%)	0	100	100
1	C	506/578 (88%)	498 (98%)	8 (2%)	0	100	100
1	D	571/578 (99%)	563 (99%)	8 (1%)	0	100	100
1	E	571/578 (99%)	563 (99%)	8 (1%)	0	100	100
1	F	557/578 (96%)	549 (99%)	8 (1%)	0	100	100
2	G	124/178 (70%)	121 (98%)	3 (2%)	0	100	100
2	H	114/178 (64%)	113 (99%)	1 (1%)	0	100	100
2	K	111/178 (62%)	110 (99%)	1 (1%)	0	100	100
2	L	126/178 (71%)	117 (93%)	9 (7%)	0	100	100
2	M	125/178 (70%)	123 (98%)	2 (2%)	0	100	100
2	N	120/178 (67%)	118 (98%)	2 (2%)	0	100	100
All	All	4067/4536 (90%)	4001 (98%)	66 (2%)	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	485/481 (101%)	479 (99%)	6 (1%)	71	87
1	B	485/481 (101%)	471 (97%)	14 (3%)	42	68
1	C	434/481 (90%)	423 (98%)	11 (2%)	47	73
1	D	485/481 (101%)	475 (98%)	10 (2%)	53	77
1	E	485/481 (101%)	474 (98%)	11 (2%)	50	75
1	F	475/481 (99%)	460 (97%)	15 (3%)	39	65
2	G	117/156 (75%)	109 (93%)	8 (7%)	16	32
2	H	107/156 (69%)	104 (97%)	3 (3%)	43	69
2	K	106/156 (68%)	104 (98%)	2 (2%)	57	79
2	L	119/156 (76%)	115 (97%)	4 (3%)	37	63
2	M	118/156 (76%)	114 (97%)	4 (3%)	37	63
2	N	112/156 (72%)	108 (96%)	4 (4%)	35	61
All	All	3528/3822 (92%)	3436 (97%)	92 (3%)	46	72

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	120	LEU
1	A	150	VAL
1	A	228	THR
1	A	277	TYR
1	A	446	VAL
1	B	51	ARG
1	B	94	GLN
1	B	97	THR
1	B	113	THR
1	B	251	THR
1	B	277	TYR
1	B	312	THR
1	B	369	THR
1	B	437	ILE
1	B	444	THR
1	B	445	THR
1	B	446	VAL
1	B	514	ILE
1	B	574	HIS
1	C	113	THR
1	C	150	VAL

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Mol	Chain	Res	Type
1	C	251	THR
1	C	277	TYR
1	C	305	THR
1	C	369	THR
1	C	424	ILE
1	C	444	THR
1	C	446	VAL
1	C	467	ASP
1	C	514	ILE
1	D	41	ASN
1	D	49	THR
1	D	51	ARG
1	D	72	LEU
1	D	94	GLN
1	D	106	TYR
1	D	251	THR
1	D	277	TYR
1	D	305	THR
1	D	369	THR
1	E	69	LEU
1	E	94	GLN
1	E	97	THR
1	E	228	THR
1	E	251	THR
1	E	277	TYR
1	E	312	THR
1	E	369	THR
1	E	420	ASP
1	E	424	ILE
1	E	444	THR
1	F	34	LYS
1	F	94	GLN
1	F	97	THR
1	F	120	LEU
1	F	150	VAL
1	F	251	THR
1	F	277	TYR
1	F	305	THR
1	F	312	THR
1	F	369	THR
1	F	420	ASP
1	F	424	ILE

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Mol	Chain	Res	Type
1	F	444	THR
1	F	446	VAL
1	F	574	HIS
2	G	32	SER
2	G	36	LYS
2	G	38	ARG
2	G	39	LEU
2	G	86	VAL
2	G	136	ASP
2	G	161	VAL
2	G	163	THR
2	H	129	THR
2	H	161	VAL
2	H	163	THR
2	K	48	GLU
2	K	70	ILE
2	L	39	LEU
2	L	48	GLU
2	L	129	THR
2	L	163	THR
2	M	35	GLU
2	M	129	THR
2	M	136	ASP
2	M	163	THR
2	N	42	GLN
2	N	48	GLU
2	N	91	LEU
2	N	161	VAL

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

Mol	Chain	Res	Type
1	C	64	ASN
2	K	89	GLN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	L	202	-	4,4,4	0.15	0	6,6,6	0.04	0
4	SO4	F	602	-	4,4,4	0.15	0	6,6,6	0.04	0
4	SO4	B	604	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	G	201	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	E	602	-	4,4,4	0.13	0	6,6,6	0.05	0
4	SO4	B	603	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	C	603	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	F	604	-	4,4,4	0.13	0	6,6,6	0.05	0
4	SO4	B	602	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	M	202	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	C	602	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	602	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	L	201	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	604	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	F	603	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	D	602	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	N	201	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	H	201	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	M	201	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	E	603	-	4,4,4	0.14	0	6,6,6	0.09	0

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.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	SO4	1	0
4	B	603	SO4	1	0
4	C	603	SO4	1	0
4	M	202	SO4	1	0
4	D	602	SO4	2	0
4	A	603	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	565/578 (97%)	0.30	32 (5%) 23 18	31, 52, 78, 91	0
1	B	565/578 (97%)	0.17	13 (2%) 60 54	28, 43, 67, 80	0
1	C	506/578 (87%)	0.39	43 (8%) 10 7	31, 50, 102, 113	0
1	D	565/578 (97%)	0.25	16 (2%) 53 46	29, 45, 74, 82	0
1	E	565/578 (97%)	0.12	7 (1%) 79 76	28, 41, 64, 74	0
1	F	553/578 (95%)	0.59	58 (10%) 6 4	29, 51, 107, 124	0
2	G	124/178 (69%)	0.96	21 (16%) 1 1	56, 73, 101, 117	0
2	H	114/178 (64%)	0.91	16 (14%) 2 1	54, 68, 81, 94	0
2	K	113/178 (63%)	1.40	31 (27%) 0 0	63, 87, 107, 122	0
2	L	126/178 (70%)	0.64	13 (10%) 6 4	46, 57, 93, 104	0
2	M	125/178 (70%)	0.63	9 (7%) 15 11	45, 58, 96, 117	0
2	N	120/178 (67%)	1.03	22 (18%) 1 0	59, 77, 89, 103	0
All	All	4041/4536 (89%)	0.41	281 (6%) 16 12	28, 51, 89, 124	0

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	20	TYR	8.6
2	L	33	PRO	6.9
1	F	27	LEU	6.7
1	F	46	ASP	6.6
1	F	13	SER	6.5
1	F	55	ALA	6.5
1	F	41	ASN	6.2
1	F	19	GLY	6.1
1	C	50	ILE	6.0
1	F	22	ASP	5.9
1	C	83	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
2	K	69	VAL	5.7
1	C	76	SER	5.6
1	F	10	ASN	5.6
1	F	25	PHE	5.5
1	F	47	LYS	5.3
1	F	56	TYR	5.3
2	N	38	ARG	5.3
1	F	35	ASN	5.3
1	D	574	HIS	5.2
1	F	84	PHE	5.2
2	H	169	THR	5.1
1	F	12	ASN	5.0
2	N	175	HIS	4.9
1	D	87	SER	4.9
1	C	75	ASN	4.8
1	D	101	THR	4.8
1	C	74	ILE	4.8
1	D	135	ASP	4.8
1	A	87	SER	4.7
1	D	86	SER	4.5
1	F	16	ILE	4.5
2	K	70	ILE	4.5
2	K	114	TRP	4.4
1	A	2	ALA	4.4
1	A	55	ALA	4.4
2	G	174	HIS	4.4
1	A	124	ASP	4.3
1	C	73	LYS	4.3
1	C	61	ASP	4.3
1	A	574	HIS	4.3
1	D	55	ALA	4.2
1	F	53	SER	4.2
1	F	43	ASN	4.1
1	F	431	ALA	4.1
1	C	38	LEU	4.1
2	G	175	HIS	4.1
2	L	39	LEU	4.0
2	K	79	LEU	4.0
2	G	35	GLU	4.0
1	C	51	ARG	3.9
1	D	124	ASP	3.8
1	F	124	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	79	VAL	3.8
1	F	40	THR	3.8
2	K	78	GLU	3.8
2	L	32	SER	3.8
1	C	49	THR	3.8
1	E	103	GLY	3.7
2	H	174	HIS	3.7
2	L	174	HIS	3.7
1	D	56	TYR	3.7
1	C	77	GLY	3.7
2	K	76	VAL	3.6
2	K	47	ASN	3.6
1	F	430	ALA	3.6
2	M	38	ARG	3.6
2	K	44	ILE	3.6
2	K	75	LYS	3.6
1	C	81	GLN	3.6
2	K	174	HIS	3.5
2	H	166	GLU	3.5
1	F	104	SER	3.5
1	A	43	ASN	3.5
2	L	30	ASN	3.4
1	F	83	ILE	3.4
2	K	43	GLN	3.4
1	C	60	LEU	3.4
1	A	56	TYR	3.4
1	A	102	THR	3.4
1	C	101	THR	3.4
2	L	35	GLU	3.4
1	F	50	ILE	3.4
1	F	26	SER	3.3
1	F	135	ASP	3.3
1	F	48	ILE	3.3
2	L	37	GLU	3.3
2	H	66	LYS	3.3
1	F	391	GLU	3.3
1	F	21	SER	3.3
1	F	15	SER	3.3
2	N	49	VAL	3.3
2	N	174	HIS	3.2
1	F	24	GLU	3.2
1	A	391	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	104	SER	3.2
2	N	39	LEU	3.1
1	C	467	ASP	3.1
1	F	74	ILE	3.1
2	L	38	ARG	3.1
1	E	124	ASP	3.1
2	G	105	GLU	3.1
2	K	156	ASP	3.1
2	N	37	GLU	3.1
1	F	105	ASN	3.1
2	K	157	GLY	3.1
2	M	39	LEU	3.0
2	N	79	LEU	3.0
1	C	68	PRO	3.0
2	N	77	ILE	3.0
2	M	66	LYS	3.0
2	N	171	GLN	3.0
1	C	135	ASP	3.0
1	D	45	SER	3.0
2	N	135	LYS	3.0
1	C	36	LEU	3.0
1	B	10	ASN	3.0
2	L	36	LYS	2.9
1	E	41	ASN	2.9
1	A	467	ASP	2.9
1	F	574	HIS	2.9
2	G	84	ASP	2.9
1	C	180	ALA	2.9
1	A	122	GLN	2.9
1	F	432	THR	2.9
1	F	91	TRP	2.9
1	D	137	ARG	2.8
2	H	81	LYS	2.8
1	C	82	PHE	2.8
1	A	135	ASP	2.8
2	H	173	LEU	2.8
1	A	44	ASN	2.8
1	A	29	ASN	2.8
1	B	11	ASN	2.8
1	A	404	LEU	2.8
2	H	43	GLN	2.7
2	N	169	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	G	66	LYS	2.7
1	E	574	HIS	2.7
1	B	552	GLU	2.7
1	A	101	THR	2.7
2	G	171	GLN	2.7
2	H	79	LEU	2.7
2	L	34	SER	2.7
1	E	424	ILE	2.7
2	H	42	GLN	2.7
2	K	134	GLN	2.7
1	A	86	SER	2.6
1	C	104	SER	2.6
1	C	66	ASN	2.6
1	F	18	THR	2.6
1	C	72	LEU	2.6
1	F	38	LEU	2.6
1	A	30	GLY	2.6
1	C	78	ASP	2.5
1	B	391	GLU	2.5
1	F	122	GLN	2.5
2	H	168	VAL	2.5
2	K	168	VAL	2.5
2	H	120	GLN	2.5
2	N	65	ALA	2.5
1	B	574	HIS	2.5
1	C	100	PRO	2.5
1	C	64	ASN	2.5
1	C	121	ILE	2.5
2	K	46	PHE	2.5
2	K	71	LYS	2.5
1	A	445	THR	2.5
2	N	89	GLN	2.5
2	M	34	SER	2.5
1	C	122	GLN	2.4
2	K	91	LEU	2.4
2	K	73	ASP	2.4
2	N	48	GLU	2.4
2	H	71	LYS	2.4
1	C	105	ASN	2.4
2	K	83	GLY	2.4
2	N	47	ASN	2.4
1	A	51	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	106	PRO	2.4
1	F	42	ALA	2.4
2	N	166	GLU	2.4
2	K	80	LYS	2.4
2	M	174	HIS	2.4
1	F	405	THR	2.4
2	G	119	ASP	2.4
2	N	66	LYS	2.4
1	A	88	GLN	2.4
1	A	41	ASN	2.4
2	G	33	PRO	2.4
2	G	163	THR	2.4
1	C	39	PRO	2.4
1	B	13	SER	2.4
1	B	41	ASN	2.4
2	N	120	GLN	2.4
2	M	32	SER	2.4
2	G	38	ARG	2.3
1	F	45	SER	2.3
2	G	39	LEU	2.3
2	K	77	ILE	2.3
1	D	29	ASN	2.3
1	B	9	GLN	2.3
1	F	11	ASN	2.3
2	G	79	LEU	2.3
1	F	89	ASN	2.3
2	K	166	GLU	2.3
2	K	81	LYS	2.3
1	D	467	ASP	2.3
1	F	467	ASP	2.3
1	C	80	TYR	2.3
1	C	574	HIS	2.3
1	A	125	LYS	2.3
2	L	67	GLY	2.3
1	C	63	SER	2.2
2	G	34	SER	2.2
2	L	129	THR	2.2
1	F	36	LEU	2.2
2	K	119	ASP	2.2
2	K	137	HIS	2.2
1	F	387	SER	2.2
1	F	402	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	439	THR	2.2
1	D	435	GLU	2.2
1	D	552	GLU	2.2
1	F	39	PRO	2.2
2	K	120	GLN	2.2
2	H	93	TYR	2.2
1	A	430	ALA	2.2
1	C	468	GLY	2.2
1	C	137	ARG	2.2
1	A	33	VAL	2.2
2	G	81	LYS	2.2
1	C	404	LEU	2.2
1	F	58	SER	2.2
1	E	2	ALA	2.2
1	F	399	ILE	2.2
1	A	491	CYS	2.2
2	H	49	VAL	2.1
2	G	173	LEU	2.1
2	N	81	LYS	2.1
1	B	153	ASP	2.1
1	C	125	LYS	2.1
2	M	81	LYS	2.1
1	B	405	THR	2.1
1	F	81	GLN	2.1
1	B	87	SER	2.1
1	D	384	GLU	2.1
2	N	105	GLU	2.1
1	A	434	LYS	2.1
1	A	405	THR	2.1
2	N	173	LEU	2.1
2	K	175	HIS	2.1
1	F	103	GLY	2.1
2	K	169	THR	2.1
2	K	95	ILE	2.1
2	K	96	ASN	2.1
2	G	120	GLN	2.1
2	N	134	GLN	2.1
1	E	405	THR	2.1
2	M	33	PRO	2.1
1	F	59	TYR	2.1
2	H	134	GLN	2.1
1	F	102	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	G	76	VAL	2.0
1	A	417	TYR	2.0
1	C	152	SER	2.0
1	A	103	GLY	2.0
1	A	22	ASP	2.0
1	B	124	ASP	2.0
2	G	109	GLN	2.0
2	M	36	LYS	2.0
1	B	5	LEU	2.0
2	G	108	ASP	2.0
1	D	405	THR	2.0
1	F	125	LYS	2.0
1	F	408	THR	2.0
1	C	401	GLY	2.0
1	C	108	LEU	2.0
1	C	106	TYR	2.0
2	G	166	GLU	2.0
2	L	135	LYS	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)

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. 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	B-factors(Å^2)	Q<0.9
4	SO4	H	201	5/5	0.83	0.38	95,95,95,95	5
4	SO4	N	201	5/5	0.84	0.22	85,85,85,85	5
4	SO4	F	604	5/5	0.85	0.19	43,43,43,43	5
4	SO4	C	603	5/5	0.87	0.19	40,41,45,48	5
4	SO4	F	602	5/5	0.88	0.24	60,63,71,77	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	E	603	5/5	0.88	0.16	48,48,48,48	5
4	SO4	B	603	5/5	0.90	0.17	51,51,51,51	5
4	SO4	A	603	5/5	0.90	0.15	51,51,51,51	5
4	SO4	L	202	5/5	0.90	0.14	60,63,67,68	5
4	SO4	G	201	5/5	0.91	0.17	74,76,80,83	5
4	SO4	L	201	5/5	0.91	0.18	55,60,70,76	5
4	SO4	A	604	5/5	0.92	0.25	45,45,45,45	5
4	SO4	F	603	5/5	0.93	0.15	51,51,51,51	5
4	SO4	D	602	5/5	0.93	0.21	42,42,42,42	5
4	SO4	B	604	5/5	0.93	0.17	41,41,41,41	5
4	SO4	M	201	5/5	0.94	0.15	57,63,79,83	0
4	SO4	B	602	5/5	0.94	0.14	52,59,64,79	5
4	SO4	C	604	5/5	0.94	0.15	47,49,52,52	5
4	SO4	M	202	5/5	0.95	0.14	54,56,64,70	5
4	SO4	A	602	5/5	0.96	0.28	66,72,77,90	0
4	SO4	E	602	5/5	0.96	0.15	35,35,37,38	5
4	SO4	C	602	5/5	0.97	0.15	53,60,71,80	0
3	ZN	C	601	1/1	0.98	0.10	50,50,50,50	0
3	ZN	E	601	1/1	0.99	0.08	43,43,43,43	0
3	ZN	F	601	1/1	0.99	0.11	55,55,55,55	0
3	ZN	D	601	1/1	0.99	0.12	43,43,43,43	0
3	ZN	A	601	1/1	0.99	0.07	55,55,55,55	0
3	ZN	B	601	1/1	1.00	0.10	45,45,45,45	0

6.5 Other polymers

There are no such residues in this entry.