Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2020 – 02:49 am BST

PDB ID	:	4FIN
Title	:	Crystal Structure of EttA (formerly YjjK) - an E. coli ABC-type ATPase
Authors	:	Smith, P.; Yuan, Y.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2012-06-09
Resolution	:	2.40 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:

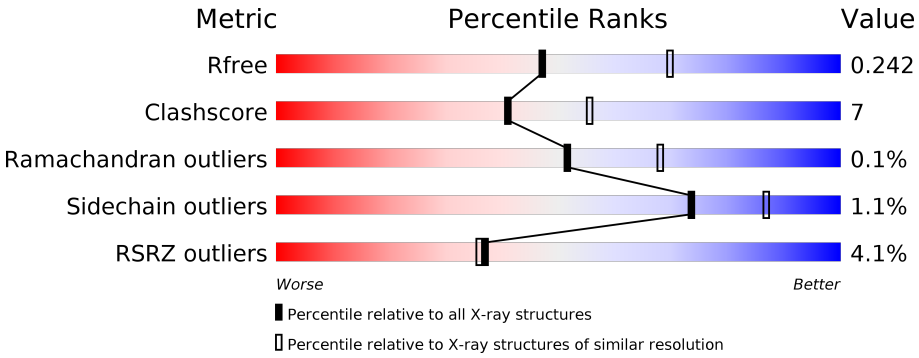
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	555	4% 81% 15%
1	B	555	4% 81% 13% 5%

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
2	SO4	B	604	-	-	X	-
5	GOL	B	608	-	-	X	-
5	GOL	B	609	-	-	X	-

2 Entry composition

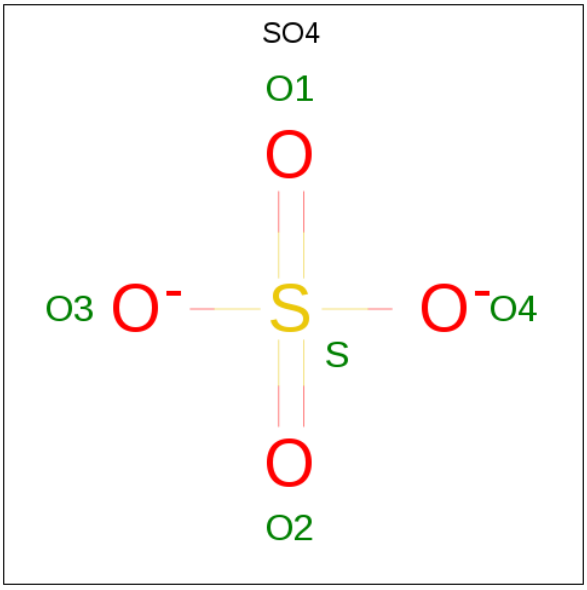
There are 6 unique types of molecules in this entry. The entry contains 8943 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EttA (YjjK) ABCF family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	Se	0	3	0
			4241	2676	738	815	2	10			
1	B	527	Total	C	N	O	S	Se	0	3	0
			4174	2630	733	800	2	9			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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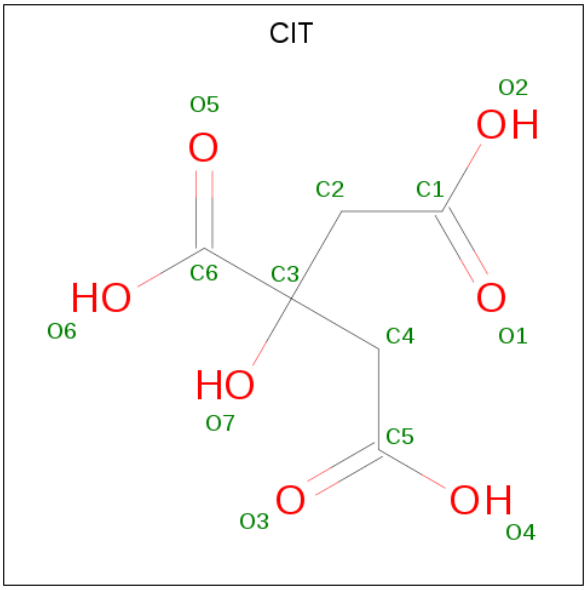
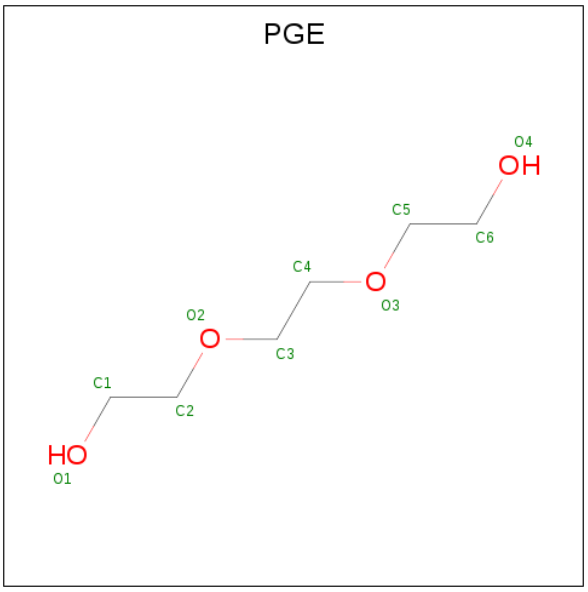
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



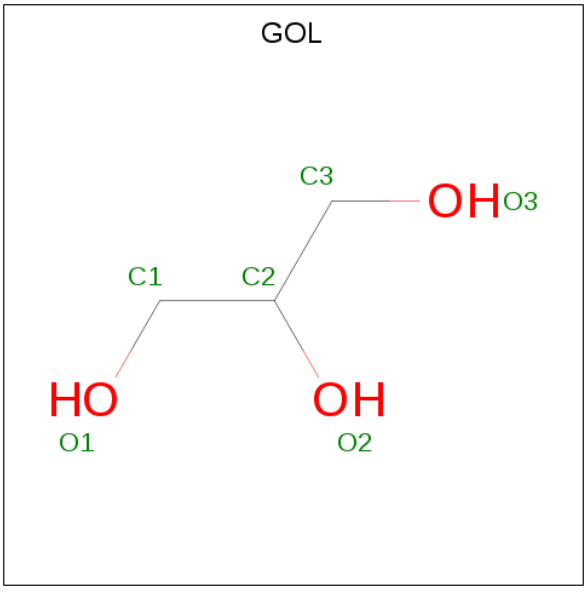
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

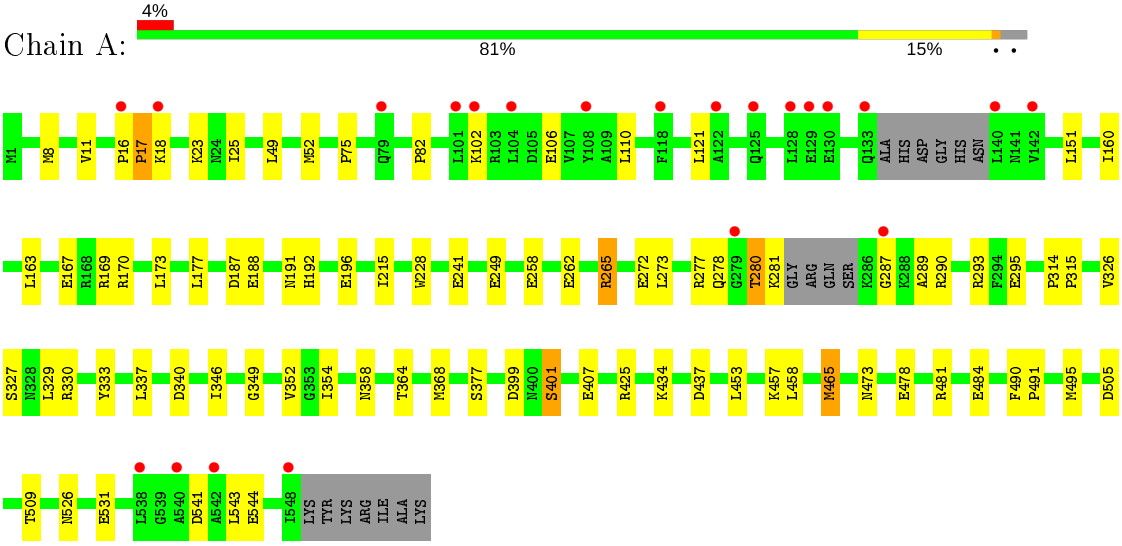
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	200	Total O 200 200	0	0
6	B	196	Total O 196 196	0	0

3 Residue-property plots (i)

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

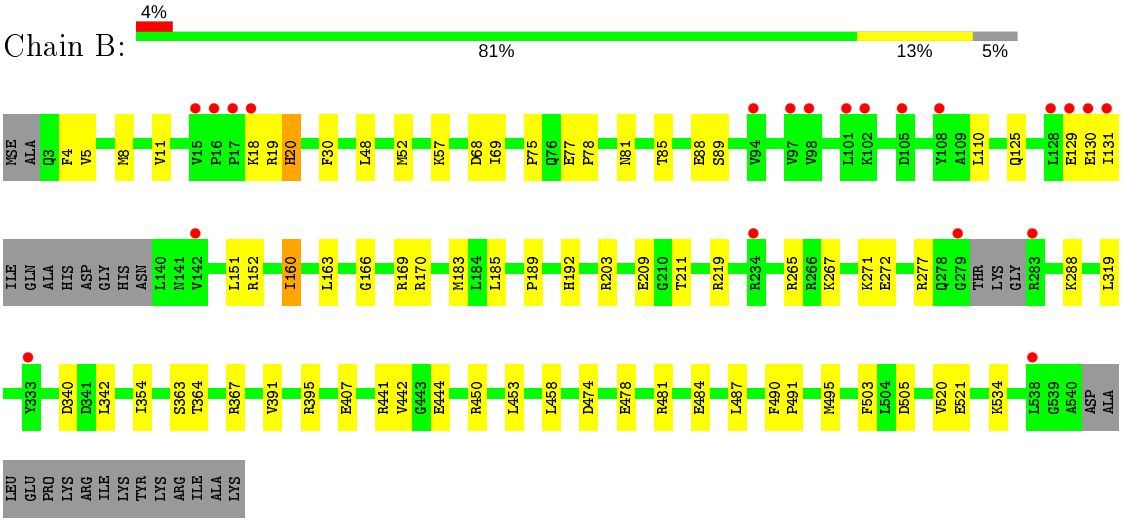
- Molecule 1: EttA (YjjK) ABCF family protein

Chain A:



- Molecule 1: EttA (YjjK) ABCF family protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.36Å 233.47Å 54.09Å 90.00° 91.29° 90.00°	Depositor
Resolution (Å)	49.07 – 2.40 49.07 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.0 (49.07-2.40) 92.3 (49.07-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.183 , 0.243 0.181 , 0.242	Depositor DCC
R_{free} test set	2077 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.078 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8943	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: GOL, PGE, SO4, CIT

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	0.34	0/4317	0.53	0/5814
1	B	0.34	0/4249	0.51	0/5720
All	All	0.34	0/8566	0.52	0/11534

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	4241	0	4203	62	1
1	B	4174	0	4136	61	1
2	A	25	0	0	1	0
2	B	30	0	0	4	0
3	A	13	0	5	0	0
4	A	10	0	14	2	0
5	A	24	0	32	1	0
5	B	30	0	40	13	0
6	A	200	0	0	9	0
6	B	196	0	0	11	0
All	All	8943	0	8430	121	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (121) 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:75:PRO:O	1:A:169:ARG:NH1	2.09	0.84
1:A:287:GLY:HA3	1:A:509:THR:HG22	1.59	0.84
1:B:81:ASN:HB3	5:B:611:GOL:H11	1.61	0.81
1:B:152:ARG:NH1	6:B:882:HOH:O	2.18	0.77
1:B:169[B]:ARG:NH1	6:B:889:HOH:O	2.19	0.73
1:A:191[B]:ASN:ND2	6:A:886:HOH:O	2.21	0.73
1:A:280:THR:HB	1:A:281:LYS:HA	1.71	0.72
1:A:364:THR:HG22	1:A:368:MSE:HE2	1.74	0.70
2:A:603:SO4:O1	6:A:702:HOH:O	2.09	0.70
1:A:265:ARG:HH22	1:A:478:GLU:HB2	1.57	0.69
1:B:478:GLU:OE1	6:B:844:HOH:O	2.10	0.69
1:A:280:THR:HB	1:A:281:LYS:HG2	1.76	0.67
1:A:110:LEU:HB3	1:A:121:LEU:HD21	1.77	0.66
1:A:249[A]:GLU:OE1	1:B:277:ARG:NH2	2.27	0.66
1:A:169:ARG:NH2	1:A:187:ASP:O	2.28	0.65
1:A:484:GLU:OE2	1:B:219:ARG:NH2	2.25	0.65
1:A:437:ASP:OD2	6:A:838:HOH:O	2.13	0.65
1:A:425:ARG:HB2	4:A:607:PGE:H1	1.79	0.65
1:A:262:GLU:OE2	6:A:872:HOH:O	2.14	0.65
1:A:16:PRO:O	6:A:882:HOH:O	2.13	0.64
1:A:544:GLU:OE1	1:B:203:ARG:NH1	2.32	0.62
1:B:364:THR:OG1	5:B:608:GOL:H31	2.01	0.61
1:B:395:ARG:NH1	6:B:850:HOH:O	2.33	0.61
1:A:18:LYS:NZ	1:B:18:LYS:O	2.30	0.60
1:B:169[A]:ARG:NH2	1:B:189:PRO:HA	2.17	0.60
1:B:391:VAL:HG13	1:B:458:LEU:HD12	1.83	0.60
2:B:604:SO4:O1	6:B:848:HOH:O	2.16	0.60
1:B:534:LYS:NZ	6:B:810:HOH:O	2.34	0.60
1:A:272:GLU:OE1	1:A:481:ARG:HD3	2.02	0.58
1:B:505:ASP:O	6:B:890:HOH:O	2.17	0.58
1:A:280:THR:CB	1:A:281:LYS:HA	2.33	0.58
1:A:273:LEU:O	1:A:277:ARG:HG2	2.03	0.58
1:B:354:ILE:HD11	1:B:495:MSE:HE2	1.86	0.58
1:A:277:ARG:N	1:A:278:GLN:HA	2.19	0.57
1:B:267:LYS:HE2	1:B:271:LYS:HE3	1.86	0.57
1:B:183:MSE:HE3	1:B:185:LEU:HD21	1.87	0.57
1:A:18:LYS:HB3	1:B:20:HIS:HE1	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169[A]:ARG:HH22	1:B:189:PRO:HA	1.70	0.56
1:B:367:ARG:NH2	6:B:886:HOH:O	2.38	0.56
1:A:151:LEU:O	1:A:170:ARG:HD2	2.07	0.55
1:B:272:GLU:OE1	1:B:481:ARG:HD3	2.07	0.54
2:B:603:SO4:O2	5:B:608:GOL:O3	2.06	0.54
1:A:465:MSE:HE1	1:A:495:MSE:HG3	1.90	0.54
1:B:75:PRO:O	1:B:169[A]:ARG:NH1	2.40	0.54
1:A:293:ARG:NH2	6:A:822:HOH:O	2.21	0.54
1:A:265:ARG:HH22	1:A:478:GLU:CB	2.21	0.54
2:B:604:SO4:O3	6:B:833:HOH:O	2.17	0.53
1:A:277:ARG:HH11	1:A:277:ARG:HG3	1.73	0.53
1:B:521:GLU:HA	5:B:610:GOL:H31	1.90	0.53
1:A:170:ARG:NH1	1:A:192:HIS:O	2.41	0.52
1:B:169[B]:ARG:HH21	5:B:609:GOL:H12	1.75	0.52
1:B:169[B]:ARG:HD2	5:B:609:GOL:O1	2.10	0.52
1:B:265:ARG:NH1	1:B:478:GLU:OE1	2.42	0.52
1:B:85:THR:CG2	1:B:88:GLU:H	2.23	0.52
1:B:442:VAL:HG12	1:B:450:ARG:HH21	1.75	0.51
1:A:289:ALA:O	1:A:293:ARG:HG2	2.11	0.51
1:B:85:THR:HG23	1:B:88:GLU:H	1.77	0.50
1:A:346:ILE:HD12	1:A:352:VAL:HG21	1.93	0.49
1:B:367:ARG:HH12	5:B:608:GOL:H2	1.76	0.49
1:A:457:LYS:HB3	1:A:458:LEU:HD12	1.94	0.49
1:B:183:MSE:HG3	1:B:211:THR:HB	1.95	0.48
1:A:16:PRO:HA	1:A:17:PRO:C	2.34	0.48
1:B:5:VAL:HG13	1:B:69:ILE:HD13	1.96	0.48
1:B:474:ASP:N	1:B:474:ASP:OD1	2.45	0.48
1:A:295:GLU:H	1:A:295:GLU:CD	2.15	0.48
1:B:151:LEU:O	1:B:170:ARG:HD2	2.14	0.48
1:B:484:GLU:HG3	1:B:503:PHE:CD1	2.48	0.48
1:A:102:LYS:NZ	1:A:106:GLU:OE2	2.38	0.48
1:B:367:ARG:HH22	5:B:608:GOL:H2	1.79	0.48
1:B:166:GLY:HA2	5:B:609:GOL:H11	1.96	0.47
1:A:11:VAL:HB	1:A:25:ILE:HB	1.96	0.47
1:A:163:LEU:HG	1:A:167:GLU:HB3	1.96	0.47
1:B:407:GLU:HG2	1:B:453:LEU:HD21	1.96	0.47
1:A:399:ASP:OD1	1:A:401:SER:HB3	2.15	0.47
1:B:8:MSE:HE2	1:B:11:VAL:HG11	1.98	0.46
1:A:228:TRP:CH2	1:A:241:GLU:HB2	2.51	0.46
1:B:441:ARG:HB2	1:B:444:GLU:HG3	1.97	0.46
1:B:4:PHE:CE1	1:B:30:PHE:HE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HG	1:A:215:ILE:HD11	1.98	0.46
1:B:85:THR:HG21	6:B:859:HOH:O	2.16	0.45
1:A:169:ARG:NH2	1:A:188:GLU:O	2.48	0.45
1:A:18:LYS:HZ2	1:A:18:LYS:HG3	1.58	0.45
1:A:407:GLU:HG2	1:A:453:LEU:HD21	2.00	0.44
1:A:531:GLU:OE1	1:A:543:LEU:HD22	2.18	0.44
1:A:290:ARG:NE	1:A:349:GLY:O	2.45	0.44
1:B:130:GLU:N	1:B:131:ILE:HA	2.32	0.44
1:A:337:LEU:HD21	1:A:340:ASP:HB2	2.00	0.44
1:A:473:ASN:HD21	1:B:192:HIS:H	1.66	0.43
1:B:340:ASP:OD2	6:B:778:HOH:O	2.21	0.43
4:A:607:PGE:H3	6:A:898:HOH:O	2.19	0.43
1:B:342:LEU:HD13	1:B:520:VAL:HB	2.01	0.43
1:B:125:GLN:O	1:B:129:GLU:HG2	2.19	0.43
1:A:258:GLU:HG2	6:A:872:HOH:O	2.19	0.43
1:A:280:THR:HB	1:A:281:LYS:CA	2.43	0.42
1:A:8:MSE:HE3	1:A:52:MSE:HG2	2.01	0.42
1:B:160:ILE:HA	1:B:163:LEU:HG	2.01	0.42
1:B:288:LYS:HB2	1:B:288:LYS:HE2	1.71	0.42
1:A:358:ASN:ND2	2:B:605:SO4:O3	2.53	0.42
1:B:363:SER:HB2	5:B:608:GOL:C2	2.50	0.42
1:B:8:MSE:HE2	1:B:11:VAL:HG21	2.01	0.42
1:B:490:PHE:HA	1:B:491:PRO:HD3	1.85	0.42
1:A:434:LYS:HA	1:A:434:LYS:HD3	1.80	0.42
1:A:490:PHE:HA	1:A:491:PRO:HD3	1.74	0.42
1:A:314:PRO:HA	1:A:315:PRO:HD3	1.86	0.41
1:A:505:ASP:HA	1:A:526:ASN:HB2	2.01	0.41
1:A:326:VAL:CG1	1:A:329:LEU:HB2	2.50	0.41
1:B:89:SER:HA	5:B:611:GOL:O2	2.21	0.41
1:A:23:LYS:NZ	1:B:19:ARG:HG2	2.35	0.41
1:B:77:GLU:HA	1:B:78:PRO:HD3	1.95	0.41
1:A:173:LEU:O	1:A:177:LEU:HG	2.20	0.41
1:A:354:ILE:HD11	1:A:495:MSE:HE2	2.02	0.41
1:B:48:LEU:O	1:B:52:MSE:HG3	2.21	0.41
1:A:330:ARG:HB3	1:A:377:SER:HB3	2.03	0.41
1:B:110:LEU:HA	1:B:110:LEU:HD12	1.79	0.41
1:B:169[B]:ARG:HH21	5:B:609:GOL:C1	2.34	0.40
1:B:192:HIS:HB2	5:B:609:GOL:O1	2.21	0.40
1:B:487:LEU:HA	1:B:487:LEU:HD23	1.97	0.40
1:A:196:GLU:OE1	6:A:756:HOH:O	2.22	0.40
1:B:130:GLU:HB2	1:B:131:ILE:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:SER:O	5:A:611:GOL:H11	2.22	0.40
1:A:82:PRO:HA	1:A:160:ILE:HB	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:TYR:OH	1:B:209:GLU:OE2[1_655]	2.01	0.19

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	535/555 (96%)	525 (98%)	9 (2%)	1 (0%)	47 62
1	B	524/555 (94%)	516 (98%)	8 (2%)	0	100 100
All	All	1059/1110 (95%)	1041 (98%)	17 (2%)	1 (0%)	51 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	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	449/456 (98%)	444 (99%)	5 (1%)	73 87
1	B	443/456 (97%)	438 (99%)	5 (1%)	73 87
All	All	892/912 (98%)	882 (99%)	10 (1%)	73 87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	ARG
1	A	280	THR
1	A	401	SER
1	A	465	MSE
1	A	541	ASP
1	B	20	HIS
1	B	57	LYS
1	B	68	ASP
1	B	160	ILE
1	B	319	LEU

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

Mol	Chain	Res	Type
1	A	358	ASN
1	A	473	ASN
1	A	499	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

22 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
5	GOL	B	611	-	5,5,5	0.40	0	5,5,5	0.58	0
2	SO4	B	601	-	4,4,4	0.17	0	6,6,6	0.24	0
2	SO4	B	602	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	B	606	-	4,4,4	0.14	0	6,6,6	0.08	0
4	PGE	A	607	-	9,9,9	0.57	0	8,8,8	0.68	0
2	SO4	A	602	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	B	604	-	4,4,4	0.16	0	6,6,6	0.26	0
5	GOL	B	609	-	5,5,5	0.29	0	5,5,5	0.41	0
3	CIT	A	606	-	3,12,12	1.26	0	3,17,17	0.96	0
2	SO4	A	603	-	4,4,4	0.11	0	6,6,6	0.16	0
5	GOL	B	608	-	5,5,5	0.38	0	5,5,5	0.41	0
5	GOL	A	610	-	5,5,5	0.29	0	5,5,5	0.36	0
2	SO4	A	601	-	4,4,4	0.11	0	6,6,6	0.12	0
5	GOL	B	607	-	5,5,5	0.36	0	5,5,5	0.21	0
2	SO4	A	605	-	4,4,4	0.15	0	6,6,6	0.19	0
2	SO4	B	605	-	4,4,4	0.15	0	6,6,6	0.15	0
5	GOL	B	610	-	5,5,5	0.38	0	5,5,5	0.36	0
2	SO4	B	603	-	4,4,4	0.16	0	6,6,6	0.19	0
5	GOL	A	611	-	5,5,5	0.34	0	5,5,5	0.39	0
2	SO4	A	604	-	4,4,4	0.19	0	6,6,6	0.15	0
5	GOL	A	609	-	5,5,5	0.35	0	5,5,5	0.48	0
5	GOL	A	608	-	5,5,5	0.31	0	5,5,5	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	609	-	-	4/4/4/4	-
5	GOL	B	611	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	611	-	-	2/4/4/4	-
5	GOL	B	607	-	-	4/4/4/4	-
5	GOL	B	610	-	-	0/4/4/4	-
3	CIT	A	606	-	-	0/6/16/16	-
5	GOL	A	609	-	-	2/4/4/4	-
4	PGE	A	607	-	-	2/7/7/7	-
5	GOL	B	608	-	-	0/4/4/4	-
5	GOL	A	610	-	-	2/4/4/4	-
5	GOL	A	608	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	609	GOL	O1-C1-C2-C3
5	A	610	GOL	O1-C1-C2-C3
5	A	609	GOL	O1-C1-C2-C3
5	A	608	GOL	O1-C1-C2-C3
5	B	609	GOL	O1-C1-C2-O2
5	A	609	GOL	O1-C1-C2-O2
5	B	611	GOL	O1-C1-C2-C3
5	B	611	GOL	C1-C2-C3-O3
5	B	609	GOL	C1-C2-C3-O3
5	B	607	GOL	O1-C1-C2-C3
5	B	607	GOL	C1-C2-C3-O3
5	A	611	GOL	O1-C1-C2-C3
5	B	611	GOL	O1-C1-C2-O2
5	B	609	GOL	O2-C2-C3-O3
5	A	610	GOL	O1-C1-C2-O2
5	B	607	GOL	O2-C2-C3-O3
5	A	611	GOL	O1-C1-C2-O2
5	A	608	GOL	O1-C1-C2-O2
5	A	608	GOL	C1-C2-C3-O3
5	B	607	GOL	O1-C1-C2-O2
4	A	607	PGE	O2-C3-C4-O3
4	A	607	PGE	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	611	GOL	2	0
4	A	607	PGE	2	0
2	B	604	SO4	2	0
5	B	609	GOL	5	0
2	A	603	SO4	1	0
5	B	608	GOL	5	0
2	B	605	SO4	1	0
5	B	610	GOL	1	0
2	B	603	SO4	1	0
5	A	611	GOL	1	0

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	528/555 (95%)	-0.10	22 (4%)	36	35	12, 31, 71, 108	0
1	B	518/555 (93%)	-0.19	21 (4%)	37	36	12, 30, 68, 94	0
All	All	1046/1110 (94%)	-0.14	43 (4%)	37	36	12, 30, 70, 108	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	GLU	6.6
1	B	17	PRO	5.5
1	A	548	ILE	5.4
1	A	18	LYS	4.9
1	B	131	ILE	4.3
1	A	16	PRO	4.3
1	B	16	PRO	4.2
1	A	542	ALA	4.0
1	B	142	VAL	4.0
1	A	129	GLU	4.0
1	A	142	VAL	3.7
1	A	540	ALA	3.4
1	A	108	TYR	3.4
1	A	287	GLY	3.4
1	A	140	LEU	3.4
1	B	279	GLY	3.4
1	A	122	ALA	3.3
1	B	98	VAL	3.1
1	B	130	GLU	3.1
1	A	101	LEU	3.0
1	A	79	GLN	3.0
1	B	97	VAL	3.0
1	A	128	LEU	2.9
1	A	118	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	538	LEU	2.9
1	B	234	ARG	2.8
1	B	129	GLU	2.6
1	A	133	GLN	2.6
1	A	279	GLY	2.6
1	B	94	VAL	2.6
1	A	125	GLN	2.5
1	B	333	TYR	2.5
1	A	102	LYS	2.5
1	B	108	TYR	2.4
1	B	18	LYS	2.4
1	B	15	VAL	2.4
1	B	101	LEU	2.2
1	B	105	ASP	2.1
1	B	283	ARG	2.1
1	B	102	LYS	2.1
1	A	104	LEU	2.1
1	B	128	LEU	2.1
1	B	538	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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
5	GOL	A	611	6/6	0.76	0.27	57,60,60,62	0
5	GOL	B	607	6/6	0.80	0.23	47,49,50,52	0
5	GOL	B	610	6/6	0.82	0.20	64,65,66,66	0
2	SO4	B	606	5/5	0.83	0.29	65,65,66,66	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CIT	A	606	13/13	0.83	0.23	50,53,57,58	0
5	GOL	B	608	6/6	0.83	0.28	51,58,59,61	0
5	GOL	A	609	6/6	0.86	0.21	55,55,58,59	0
5	GOL	B	611	6/6	0.87	0.34	40,46,48,49	0
4	PGE	A	607	10/10	0.88	0.31	38,50,55,56	0
2	SO4	A	604	5/5	0.89	0.14	64,67,67,68	0
5	GOL	B	609	6/6	0.89	0.24	54,57,58,59	0
5	GOL	A	608	6/6	0.93	0.14	29,34,36,36	0
2	SO4	B	605	5/5	0.95	0.13	92,93,93,93	0
5	GOL	A	610	6/6	0.95	0.14	37,38,40,41	0
2	SO4	B	604	5/5	0.95	0.12	58,59,59,59	0
2	SO4	A	602	5/5	0.97	0.18	56,56,57,58	0
2	SO4	A	605	5/5	0.97	0.09	52,53,54,54	0
2	SO4	B	602	5/5	0.98	0.11	28,36,37,38	0
2	SO4	A	603	5/5	0.99	0.09	24,26,29,30	0
2	SO4	A	601	5/5	0.99	0.08	20,22,24,25	0
2	SO4	B	601	5/5	0.99	0.09	19,20,22,22	0
2	SO4	B	603	5/5	0.99	0.10	30,31,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.