Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 03:14 pm GMT

PDB ID	:	8BOU
Title	:	Crystal structure of Blautia producta GH94
Authors	:	Levy, C.W.
Deposited on	:	2022-11-15
Resolution	:	2.32 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 (i) 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 (i)) were used in the production of this report:

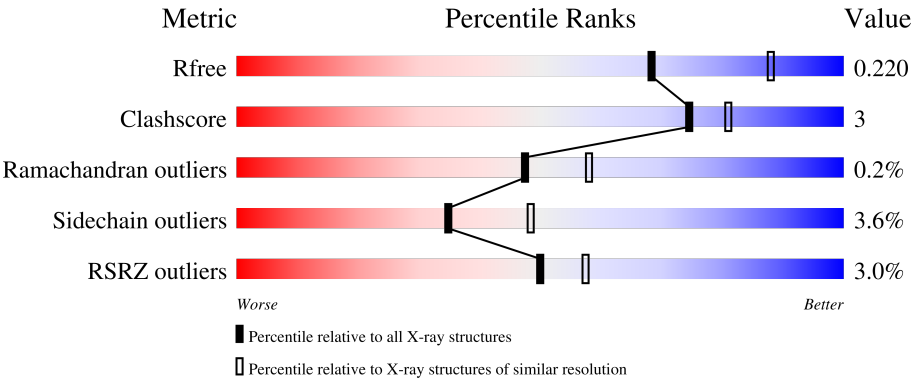
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 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	824	5% 86% 12% ·
1	B	824	88% 9% ·

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
7	EDO	B	903	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 13781 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 N,N'-diacetylchitobiose phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	807	Total	C	N	O	S	0	0	0
			6481	4129	1103	1214	35			
1	B	805	Total	C	N	O	S	0	7	0
			6533	4158	1113	1226	36			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A7G5MNS2
A	2	GLY	-	expression tag	UNP A0A7G5MNS2
A	3	SER	-	expression tag	UNP A0A7G5MNS2
A	4	SER	-	expression tag	UNP A0A7G5MNS2
A	5	HIS	-	expression tag	UNP A0A7G5MNS2
A	6	HIS	-	expression tag	UNP A0A7G5MNS2
A	7	HIS	-	expression tag	UNP A0A7G5MNS2
A	8	HIS	-	expression tag	UNP A0A7G5MNS2
A	9	HIS	-	expression tag	UNP A0A7G5MNS2
A	10	HIS	-	expression tag	UNP A0A7G5MNS2
A	11	SER	-	expression tag	UNP A0A7G5MNS2
A	12	SER	-	expression tag	UNP A0A7G5MNS2
A	13	GLY	-	expression tag	UNP A0A7G5MNS2
A	14	LEU	-	expression tag	UNP A0A7G5MNS2
A	15	VAL	-	expression tag	UNP A0A7G5MNS2
A	16	PRO	-	expression tag	UNP A0A7G5MNS2
A	17	ARG	-	expression tag	UNP A0A7G5MNS2
A	18	GLY	-	expression tag	UNP A0A7G5MNS2
A	19	SER	-	expression tag	UNP A0A7G5MNS2
A	20	HIS	-	expression tag	UNP A0A7G5MNS2
B	1	MET	-	initiating methionine	UNP A0A7G5MNS2
B	2	GLY	-	expression tag	UNP A0A7G5MNS2
B	3	SER	-	expression tag	UNP A0A7G5MNS2
B	4	SER	-	expression tag	UNP A0A7G5MNS2
B	5	HIS	-	expression tag	UNP A0A7G5MNS2

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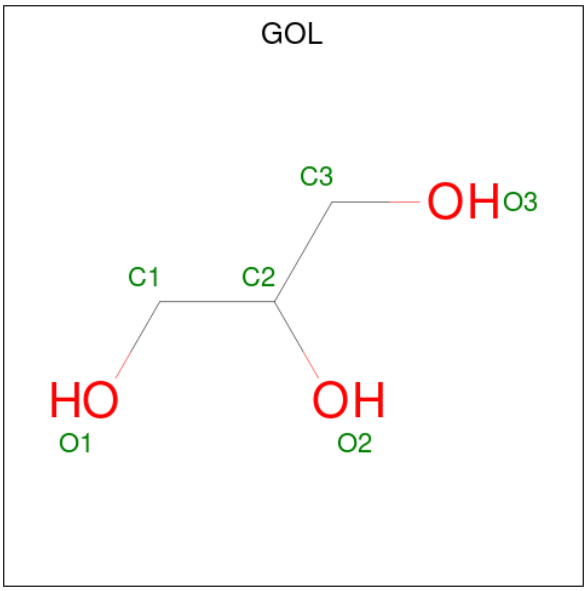
Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	expression tag	UNP A0A7G5MNS2
B	7	HIS	-	expression tag	UNP A0A7G5MNS2
B	8	HIS	-	expression tag	UNP A0A7G5MNS2
B	9	HIS	-	expression tag	UNP A0A7G5MNS2
B	10	HIS	-	expression tag	UNP A0A7G5MNS2
B	11	SER	-	expression tag	UNP A0A7G5MNS2
B	12	SER	-	expression tag	UNP A0A7G5MNS2
B	13	GLY	-	expression tag	UNP A0A7G5MNS2
B	14	LEU	-	expression tag	UNP A0A7G5MNS2
B	15	VAL	-	expression tag	UNP A0A7G5MNS2
B	16	PRO	-	expression tag	UNP A0A7G5MNS2
B	17	ARG	-	expression tag	UNP A0A7G5MNS2
B	18	GLY	-	expression tag	UNP A0A7G5MNS2
B	19	SER	-	expression tag	UNP A0A7G5MNS2
B	20	HIS	-	expression tag	UNP A0A7G5MNS2

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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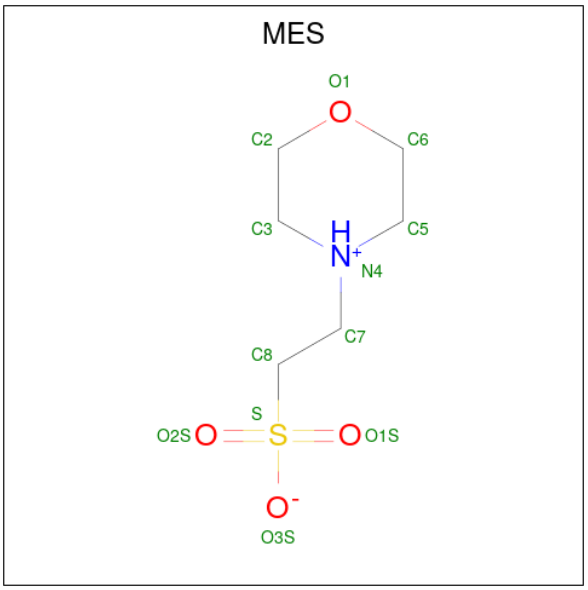
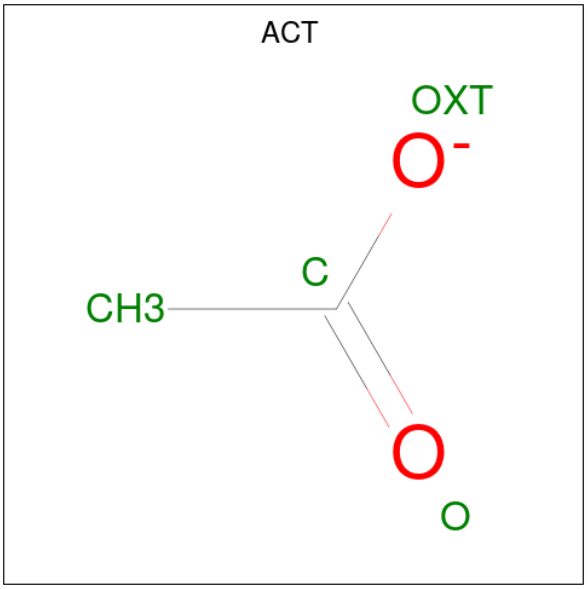
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

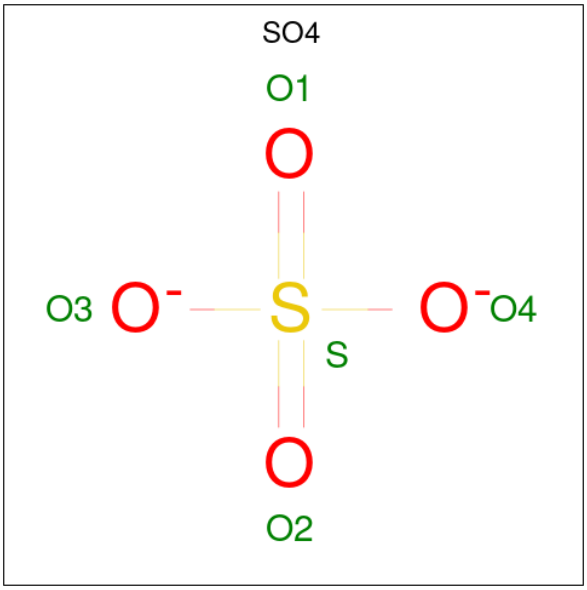


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

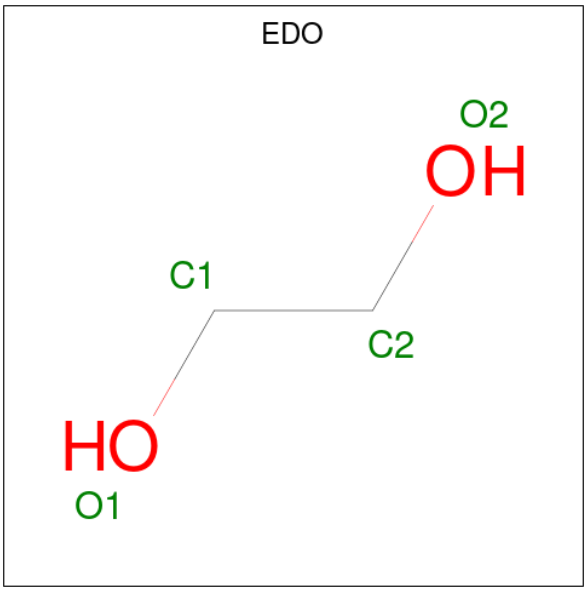
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

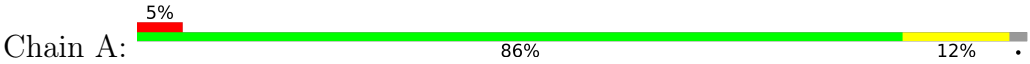
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	274	Total O 274 274	0	0
8	B	431	Total O 431 431	0	0

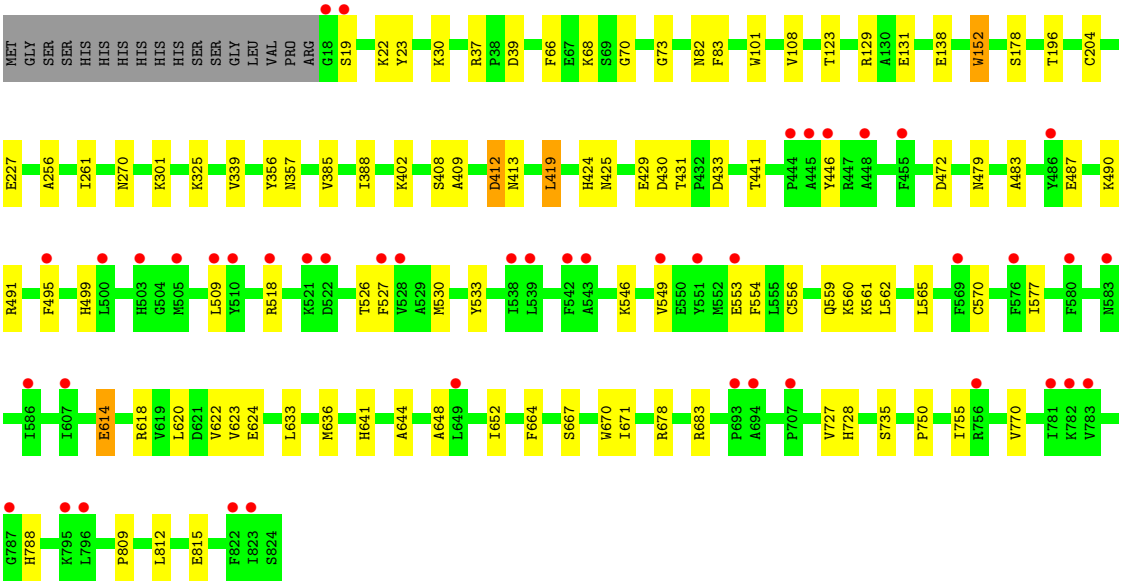
3 Residue-property plots (i)

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: N,N'-diacetylchitobiose phosphorylase

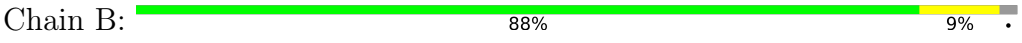
Chain A:

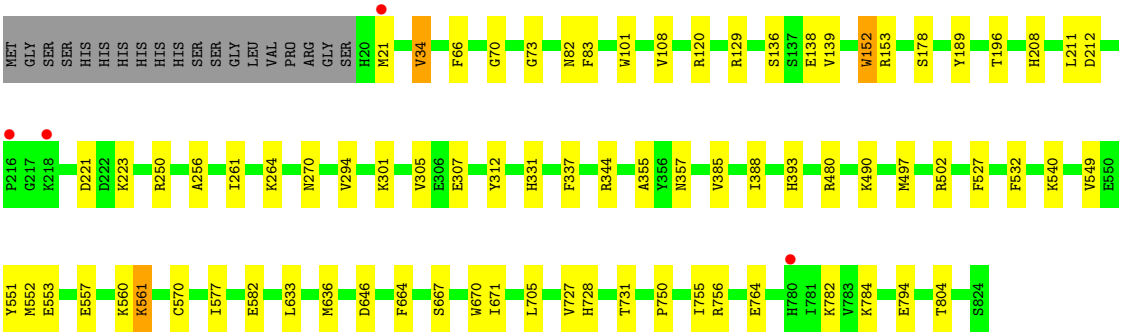




• Molecule 1: N,N'-diacetylchitobiose phosphorylase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.46Å 135.29Å 166.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.56 – 2.32 63.68 – 2.32	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.56-2.32) 89.2 (63.68-2.32)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.72 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.178 , 0.222 0.176 , 0.220	Depositor DCC
R_{free} test set	4886 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	47.7	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13781	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, CL, ACT, EDO, SO4, MES

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	0.26	0/6659	0.49	0/9023
1	B	0.26	0/6712	0.50	1/9094 (0.0%)
All	All	0.26	0/13371	0.49	1/18117 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	21	MET	CA-CB-CG	5.15	122.05	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6481	0	6183	51	0
1	B	6533	0	6215	31	0
2	A	12	0	16	0	0
2	B	18	0	24	0	0
3	A	12	0	12	0	0
4	A	4	0	3	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	B	4	0	6	3	0
8	A	274	0	0	4	0
8	B	431	0	0	3	0
All	All	13781	0	12459	81	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 (81) 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:472:ASP:OD1	1:A:546:LYS:NZ	2.14	0.76
1:A:19:SER:HA	1:A:22:LYS:HG2	1.70	0.72
1:A:412:ASP:HB2	1:A:479:ASN:HD21	1.56	0.70
1:A:491:ARG:NH1	8:A:1002:HOH:O	2.26	0.67
1:A:129:ARG:HG2	1:A:138:GLU:HG2	1.77	0.67
1:A:624:GLU:OE1	1:A:683:ARG:NE	2.32	0.63
1:A:431:THR:OG1	1:A:446:TYR:OH	2.18	0.62
1:A:809:PRO:HG2	1:A:812:LEU:HG	1.81	0.62
1:A:652:ILE:HA	1:B:211:LEU:HD21	1.83	0.61
1:A:750:PRO:HA	1:A:755:ILE:HA	1.83	0.60
1:B:355:ALA:HB2	7:B:903:EDO:H21	1.83	0.59
1:B:750:PRO:HA	1:B:755:ILE:HA	1.85	0.58
1:A:385:VAL:HA	1:A:388:ILE:HD12	1.88	0.56
1:A:419:LEU:HD22	1:A:441:THR:HB	1.88	0.56
1:A:431:THR:HG23	1:A:433:ASP:H	1.72	0.55
1:A:633:LEU:HD13	1:A:671:ILE:HG21	1.89	0.53
1:B:497:MET:HG3	1:B:532:PHE:HZ	1.74	0.53
1:A:561:LYS:O	1:A:565:LEU:HD12	2.08	0.53
1:A:526:THR:O	1:A:530:MET:HG2	2.10	0.51
1:B:73:GLY:HA2	1:B:178:SER:HB3	1.92	0.51
1:B:129:ARG:HG2	1:B:138:GLU:HG2	1.92	0.51
1:A:483:ALA:HB1	1:A:487:GLU:HB3	1.93	0.50
1:B:208:HIS:NE2	1:B:223:LYS:HD3	2.28	0.49
1:B:337:PHE:HB3	7:B:903:EDO:H12	1.94	0.49
1:A:68:LYS:NZ	8:A:1007:HOH:O	2.43	0.49
1:B:794:GLU:OE1	8:B:1001:HOH:O	2.20	0.48
1:A:614:GLU:O	1:A:618:ARG:HG3	2.14	0.48
1:A:556:CYS:O	1:A:560:LYS:HD3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:VAL:O	1:A:553:GLU:HG3	2.14	0.47
1:A:620:LEU:HA	1:A:623:VAL:HG22	1.95	0.47
1:B:294:VAL:HG21	1:B:312:TYR:HB3	1.94	0.47
1:A:37:ARG:HG2	1:A:39:ASP:OD1	2.14	0.47
1:A:618:ARG:NH2	8:A:1006:HOH:O	2.43	0.47
1:B:570:CYS:HA	1:B:577:ILE:HG12	1.97	0.47
1:B:633:LEU:HD13	1:B:671:ILE:HG21	1.98	0.46
1:A:667:SER:HA	1:A:670:TRP:CE3	2.51	0.46
1:A:101:TRP:HA	1:A:108:VAL:HG11	1.98	0.46
1:A:256:ALA:HB1	1:A:261:ILE:HD11	1.98	0.45
1:B:393:HIS:NE2	7:B:903:EDO:H22	2.32	0.45
1:A:644:ALA:HB1	1:A:648:ALA:HB3	1.98	0.45
1:B:82:ASN:HB3	1:B:83:PHE:H	1.61	0.45
1:B:301:LYS:O	1:B:305:VAL:HG23	2.16	0.45
1:A:618:ARG:O	1:A:622:VAL:HG12	2.17	0.45
1:B:667:SER:HA	1:B:670:TRP:CE3	2.52	0.45
1:A:413:ASN:O	1:A:495:PHE:HB2	2.18	0.44
1:A:570:CYS:HA	1:A:577:ILE:HG12	1.98	0.44
1:A:73:GLY:HA2	1:A:178:SER:HB3	2.00	0.43
1:A:562:LEU:HA	1:A:565:LEU:HD12	2.00	0.43
1:A:152:TRP:N	1:A:152:TRP:CD1	2.86	0.43
1:A:22:LYS:HB3	1:A:23:TYR:CD2	2.54	0.43
1:B:490:LYS:HG2	1:B:551:TYR:CZ	2.53	0.43
1:B:764:GLU:HG2	8:B:1002:HOH:O	2.19	0.43
1:A:518:ARG:HD3	1:A:518:ARG:HA	1.74	0.43
1:A:533:TYR:CE2	1:A:559:GLN:HG3	2.54	0.43
1:B:152:TRP:CD1	1:B:152:TRP:N	2.87	0.42
1:B:212:ASP:N	1:B:212:ASP:OD1	2.52	0.42
1:B:385:VAL:HA	1:B:388:ILE:HD12	2.02	0.42
1:A:409:ALA:HA	1:A:424:HIS:CE1	2.55	0.42
1:A:487:GLU:OE2	1:A:491:ARG:NH2	2.39	0.42
1:B:66:PHE:CG	1:B:70:GLY:HA2	2.55	0.42
1:A:499:HIS:HB3	1:A:509:LEU:HD11	2.02	0.42
1:A:533:TYR:HD2	1:A:562:LEU:HD12	1.84	0.42
1:B:502:ARG:NH2	1:B:582:GLU:O	2.51	0.41
1:A:66:PHE:CG	1:A:70:GLY:HA2	2.55	0.41
1:A:425:ASN:O	1:A:429:GLU:HG2	2.20	0.41
1:A:82:ASN:HB3	1:A:83:PHE:H	1.64	0.41
1:B:549:VAL:O	1:B:553:GLU:HG2	2.20	0.41
1:B:756[B]:ARG:NH1	8:B:1017:HOH:O	2.47	0.41
1:A:22:LYS:HG3	8:A:1244:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:VAL:HB	1:B:120:ARG:HG2	2.02	0.41
1:B:256:ALA:HB1	1:B:261:ILE:HD11	2.02	0.41
1:B:561:LYS:HD2	1:B:561:LYS:HA	1.81	0.41
1:A:123:THR:HA	1:A:356:TYR:CZ	2.56	0.41
1:B:101:TRP:HA	1:B:108:VAL:HG11	2.03	0.41
1:A:204:CYS:SG	1:A:227:GLU:HG2	2.61	0.40
1:B:221:ASP:O	1:B:223:LYS:HG3	2.22	0.40
1:A:487:GLU:OE1	1:A:490:LYS:HD3	2.21	0.40
1:B:139:VAL:HA	1:B:153:ARG:O	2.21	0.40
1:A:325:LYS:HB3	1:A:325:LYS:HE2	1.90	0.40
1:A:339:VAL:HG12	1:A:770:VAL:HG22	2.02	0.40
1:A:678:ARG:HD2	1:A:678:ARG:HA	1.87	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	805/824 (98%)	767 (95%)	36 (4%)	2 (0%)	47	58
1	B	810/824 (98%)	779 (96%)	30 (4%)	1 (0%)	51	63
All	All	1615/1648 (98%)	1546 (96%)	66 (4%)	3 (0%)	47	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	641	HIS
1	A	727	VAL
1	B	727	VAL

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	680/695 (98%)	659 (97%)	21 (3%)	40	55
1	B	686/695 (99%)	658 (96%)	28 (4%)	30	43
All	All	1366/1390 (98%)	1317 (96%)	49 (4%)	35	48

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	131	GLU
1	A	152	TRP
1	A	196	THR
1	A	270	ASN
1	A	301	LYS
1	A	357	ASN
1	A	402	LYS
1	A	408	SER
1	A	412	ASP
1	A	419	LEU
1	A	430	ASP
1	A	527	PHE
1	A	554	PHE
1	A	614	GLU
1	A	636	MET
1	A	664	PHE
1	A	728	HIS
1	A	735	SER
1	A	788	HIS
1	A	815	GLU
1	B	34	VAL
1	B	136	SER
1	B	152	TRP
1	B	189	TYR
1	B	196	THR
1	B	250	ARG

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Mol	Chain	Res	Type
1	B	264	LYS
1	B	270	ASN
1	B	307	GLU
1	B	331	HIS
1	B	344	ARG
1	B	357	ASN
1	B	480	ARG
1	B	527	PHE
1	B	540	LYS
1	B	552	MET
1	B	557	GLU
1	B	560	LYS
1	B	561	LYS
1	B	636	MET
1	B	646	ASP
1	B	664	PHE
1	B	705	LEU
1	B	728	HIS
1	B	731	THR
1	B	782	LYS
1	B	784	LYS
1	B	804	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	780	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
6	SO4	B	906	-	4,4,4	0.14	0	6,6,6	0.12	0
2	GOL	A	901	-	5,5,5	0.88	0	5,5,5	0.99	0
2	GOL	B	902	-	5,5,5	0.88	0	5,5,5	1.01	0
4	ACT	A	904	-	3,3,3	1.34	0	3,3,3	1.54	0
3	MES	A	903	-	12,12,12	2.32	1 (8%)	14,16,16	2.42	6 (42%)
2	GOL	B	904	-	5,5,5	0.96	0	5,5,5	0.94	0
2	GOL	A	902	-	5,5,5	0.89	0	5,5,5	1.00	0
7	EDO	B	903	-	3,3,3	0.44	0	2,2,2	0.19	0
2	GOL	B	901	-	5,5,5	0.98	0	5,5,5	0.96	0
6	SO4	A	906	-	4,4,4	0.13	0	6,6,6	0.07	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
2	GOL	A	901	-	-	0/4/4/4	-
2	GOL	B	902	-	-	0/4/4/4	-
3	MES	A	903	-	-	1/6/14/14	0/1/1/1
2	GOL	B	904	-	-	0/4/4/4	-
2	GOL	A	902	-	-	0/4/4/4	-
7	EDO	B	903	-	-	0/1/1/1	-
2	GOL	B	901	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	MES	C8-S	-7.76	1.66	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	903	MES	C5-N4-C3	5.17	120.48	108.83
3	A	903	MES	C2-C3-N4	-3.28	105.13	110.10
3	A	903	MES	C7-N4-C3	3.04	119.01	111.23
3	A	903	MES	C7-N4-C5	2.96	118.80	111.23
3	A	903	MES	C6-C5-N4	-2.88	105.74	110.10
3	A	903	MES	O2S-S-C8	2.48	109.91	106.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	GOL	C1-C2-C3-O3
2	B	901	GOL	O2-C2-C3-O3
3	A	903	MES	C8-C7-N4-C3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	903	EDO	3	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	807/824 (97%)	0.35	45 (5%) 24 31	47, 67, 99, 132	0
1	B	805/824 (97%)	-0.17	4 (0%) 91 94	43, 54, 75, 124	0
All	All	1612/1648 (97%)	0.09	49 (3%) 50 57	43, 58, 94, 132	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	MET	4.2
1	A	551	TYR	3.7
1	A	783	VAL	3.2
1	A	543	ALA	3.2
1	A	569	PHE	3.2
1	A	580	PHE	3.1
1	A	19	SER	2.9
1	A	542	PHE	2.9
1	A	510	TYR	2.9
1	A	448	ALA	2.9
1	A	518	ARG	2.8
1	A	495	PHE	2.8
1	A	539	LEU	2.8
1	A	823	ILE	2.6
1	A	528	VAL	2.6
1	A	787	GLY	2.6
1	A	586	ILE	2.6
1	A	796	LEU	2.5
1	A	446	TYR	2.5
1	A	486	TYR	2.5
1	A	509	LEU	2.4
1	A	649	LEU	2.4
1	A	781	ILE	2.4
1	A	694	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	795	LYS	2.4
1	B	216	PRO	2.3
1	B	780	HIS	2.3
1	A	455	PHE	2.3
1	A	693	PRO	2.3
1	A	505	MET	2.2
1	A	444	PRO	2.2
1	A	707	PRO	2.2
1	A	822	PHE	2.2
1	A	503	HIS	2.2
1	B	218	LYS	2.2
1	A	553	GLU	2.2
1	A	18	GLY	2.2
1	A	756	ARG	2.1
1	A	576	PHE	2.1
1	A	538	ILE	2.1
1	A	500	LEU	2.1
1	A	445	ALA	2.1
1	A	549	VAL	2.1
1	A	607	ILE	2.1
1	A	527	PHE	2.1
1	A	521	LYS	2.1
1	A	782	LYS	2.1
1	A	583	ASN	2.0
1	A	522	ASP	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)

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
2	GOL	B	904	6/6	0.79	0.34	60,78,80,87	0
7	EDO	B	903	4/4	0.80	0.62	41,41,52,53	4
2	GOL	A	901	6/6	0.84	0.23	70,73,80,89	0
2	GOL	B	901	6/6	0.86	0.21	58,68,74,85	0
2	GOL	A	902	6/6	0.87	0.46	59,78,81,88	0
6	SO4	A	906	5/5	0.88	0.22	87,95,104,127	0
4	ACT	A	904	4/4	0.89	0.21	56,69,73,80	0
6	SO4	B	906	5/5	0.90	0.13	66,67,78,111	0
3	MES	A	903	12/12	0.91	0.24	67,74,83,86	12
2	GOL	B	902	6/6	0.94	0.39	57,72,84,85	0
5	CL	A	905	1/1	0.97	0.07	64,64,64,64	0
5	CL	B	905	1/1	0.99	0.08	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.