WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 08:43 PM EDT

PDB ID	:	4LXF
Title	:	Crystal structure of M. tuberculosis TreS
Authors	:	Roy, R.; Besra, G.S.; Futterer, K.
Deposited on	:	2013-07-29
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance ⓘ

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.
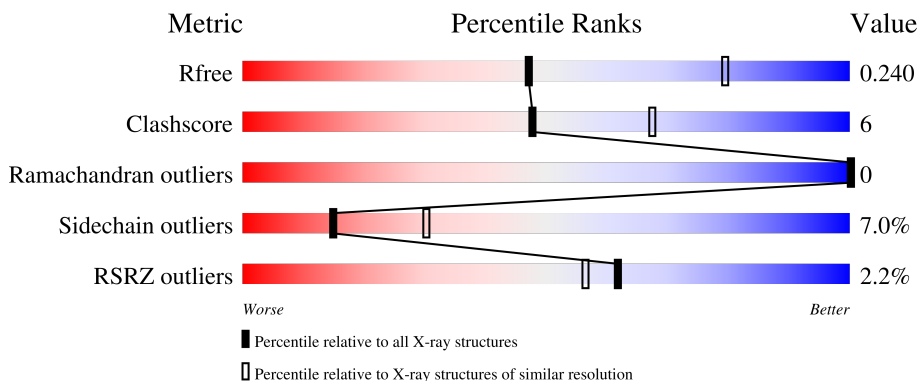
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	620	% 75% 14% • 8%
1	B	620	3% 75% 11% • 12%

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
3	GOL	A	705	-	-	X	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8845 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 Trehalose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total 4472	C 2887	N 750	O 820	S 15	0	0	0
1	B	546	Total 4265	C 2748	N 727	O 778	S 12	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP I6X8K8
A	-17	GLY	-	expression tag	UNP I6X8K8
A	-16	SER	-	expression tag	UNP I6X8K8
A	-15	SER	-	expression tag	UNP I6X8K8
A	-14	HIS	-	expression tag	UNP I6X8K8
A	-13	HIS	-	expression tag	UNP I6X8K8
A	-12	HIS	-	expression tag	UNP I6X8K8
A	-11	HIS	-	expression tag	UNP I6X8K8
A	-10	HIS	-	expression tag	UNP I6X8K8
A	-9	HIS	-	expression tag	UNP I6X8K8
A	-8	SER	-	expression tag	UNP I6X8K8
A	-7	SER	-	expression tag	UNP I6X8K8
A	-6	GLY	-	expression tag	UNP I6X8K8
A	-5	LEU	-	expression tag	UNP I6X8K8
A	-4	VAL	-	expression tag	UNP I6X8K8
A	-3	PRO	-	expression tag	UNP I6X8K8
A	-2	ARG	-	expression tag	UNP I6X8K8
A	-1	GLY	-	expression tag	UNP I6X8K8
A	0	SER	-	expression tag	UNP I6X8K8
B	-18	MET	-	expression tag	UNP I6X8K8
B	-17	GLY	-	expression tag	UNP I6X8K8
B	-16	SER	-	expression tag	UNP I6X8K8
B	-15	SER	-	expression tag	UNP I6X8K8
B	-14	HIS	-	expression tag	UNP I6X8K8
B	-13	HIS	-	expression tag	UNP I6X8K8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP I6X8K8
B	-11	HIS	-	expression tag	UNP I6X8K8
B	-10	HIS	-	expression tag	UNP I6X8K8
B	-9	HIS	-	expression tag	UNP I6X8K8
B	-8	SER	-	expression tag	UNP I6X8K8
B	-7	SER	-	expression tag	UNP I6X8K8
B	-6	GLY	-	expression tag	UNP I6X8K8
B	-5	LEU	-	expression tag	UNP I6X8K8
B	-4	VAL	-	expression tag	UNP I6X8K8
B	-3	PRO	-	expression tag	UNP I6X8K8
B	-2	ARG	-	expression tag	UNP I6X8K8
B	-1	GLY	-	expression tag	UNP I6X8K8
B	0	SER	-	expression tag	UNP I6X8K8

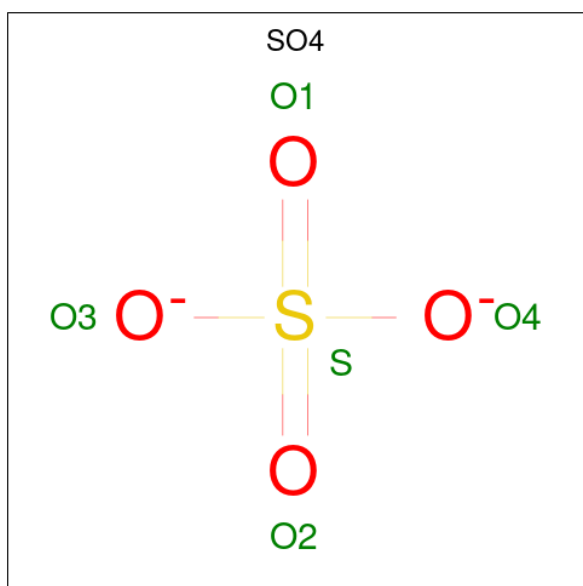- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
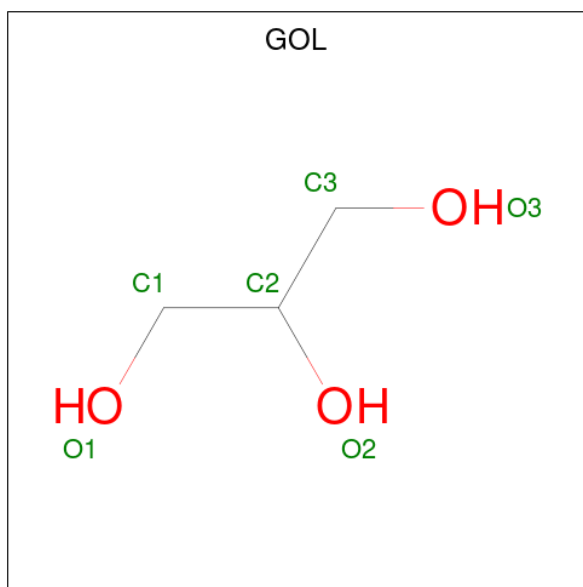
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0

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

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

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total 38	O 38	0	0
5	B	8	Total 8	O 8	0	0

3 Residue-property plots ⓘ

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: Trehalose synthase
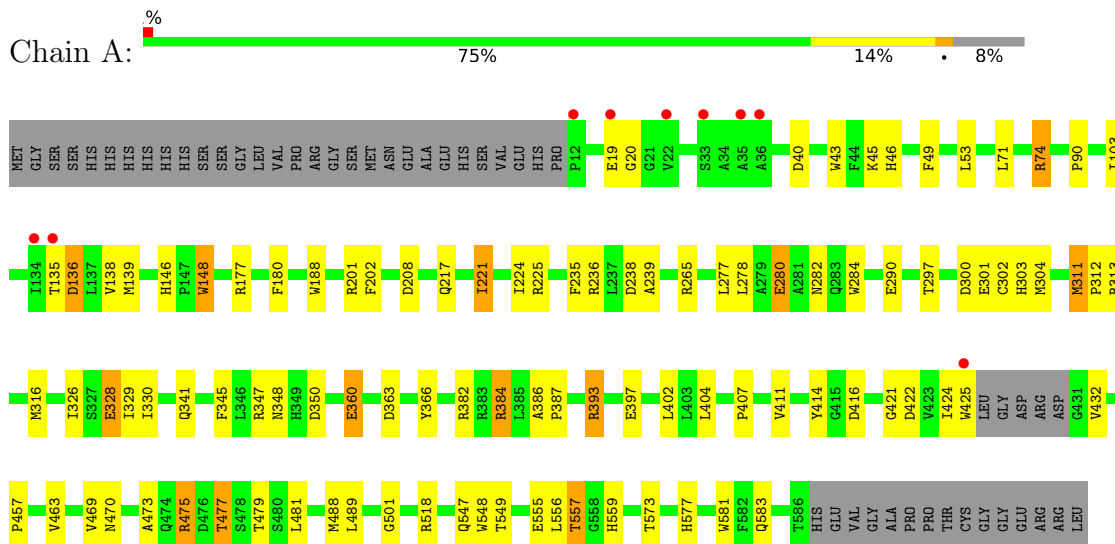
- Molecule 1: Trehalose synthase
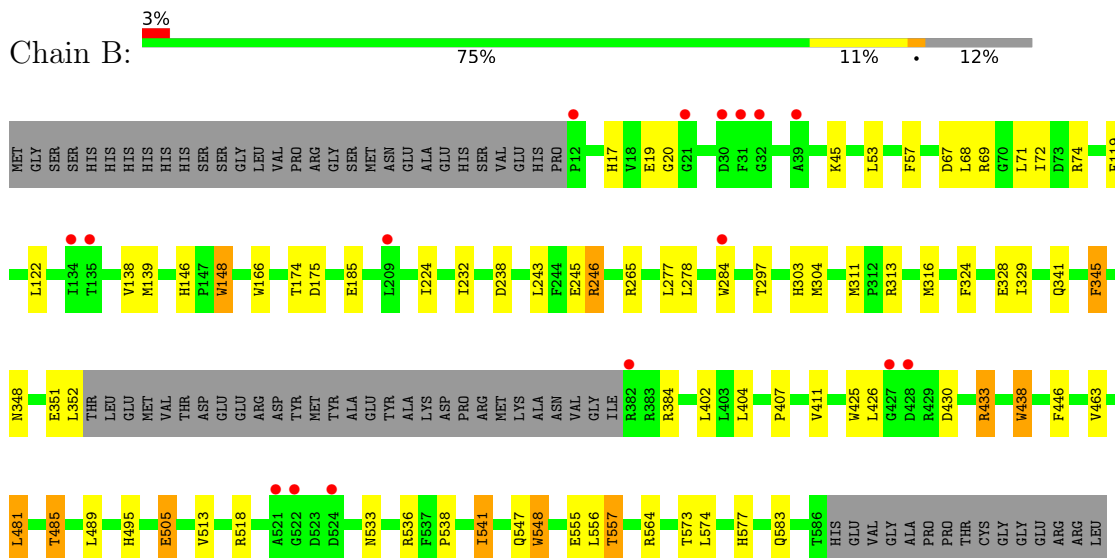
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α, β, γ	161.64Å 161.64Å 139.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.20 – 2.60 29.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.20-2.60) 99.5 (29.16-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.213 , 0.240 0.212 , 0.240	Depositor DCC
R_{free} test set	3601 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	60.2	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.9	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8845	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: SO4, CA, GOL

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	0.50	3/4614 (0.1%)	0.53	0/6315
1	B	0.50	5/4400 (0.1%)	0.53	0/6022
All	All	0.50	8/9014 (0.1%)	0.53	0/12337

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	425	TRP	CD2-CE2	5.84	1.48	1.41
1	B	284	TRP	CD2-CE2	5.35	1.47	1.41
1	B	166	TRP	CD2-CE2	5.30	1.47	1.41
1	A	148	TRP	CD2-CE2	5.23	1.47	1.41
1	B	438	TRP	CD2-CE2	5.13	1.47	1.41
1	A	188	TRP	CD2-CE2	5.10	1.47	1.41
1	B	148	TRP	CD2-CE2	5.03	1.47	1.41
1	B	548	TRP	CD2-CE2	5.01	1.47	1.41

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	4472	0	4113	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4265	0	3915	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	24	0	32	7	0
3	B	6	0	8	1	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
5	A	38	0	0	1	0
5	B	8	0	0	0	0
All	All	8845	0	8068	102	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 6.

All (102) 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:B:246:ARG:HH11	1:B:246:ARG:HG2	1.31	0.95
1:B:313:ARG:HG3	1:B:329:ILE:HG12	1.60	0.81
1:A:297:THR:HG21	1:A:300:ASP:HB3	1.63	0.81
1:A:146:HIS:HD2	1:A:148:TRP:H	1.30	0.76
1:B:246:ARG:HG2	1:B:246:ARG:NH1	2.02	0.75
1:B:513:VAL:HG11	1:B:541:ILE:HG12	1.70	0.74
1:A:475:ARG:HH11	1:A:475:ARG:HG3	1.55	0.71
1:A:393:ARG:NH1	1:A:397:GLU:OE1	2.24	0.69
1:A:393:ARG:NH2	1:A:479:THR:O	2.26	0.69
1:B:277:LEU:H	1:B:303:HIS:HD2	1.38	0.69
1:A:407:PRO:HA	1:A:518:ARG:NH2	2.09	0.68
1:A:384:ARG:NH2	1:A:432:VAL:O	2.27	0.67
1:A:46:HIS:HE1	3:A:703:GOL:H2	1.60	0.67
1:B:53:LEU:HD22	1:B:433:ARG:HG2	1.77	0.66
1:B:146:HIS:HD2	1:B:148:TRP:H	1.42	0.66
1:B:555:GLU:OE2	1:B:557:THR:HB	1.95	0.65
1:A:384:ARG:NH1	1:A:414:TYR:O	2.29	0.65
1:B:541:ILE:HD11	1:B:574:LEU:HD12	1.78	0.64
1:A:49:PHE:HB2	1:A:411:VAL:HG22	1.80	0.64
1:A:556:LEU:HD12	1:A:581:TRP:HB3	1.81	0.62
1:A:313:ARG:HH12	1:A:328:GLU:CG	2.13	0.61
1:A:311:MET:HG3	1:A:312:PRO:HD3	1.85	0.58
1:A:238:ASP:HA	1:A:280:GLU:HG2	1.86	0.57
1:A:382:ARG:HG2	3:A:705:GOL:H32	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:HIS:CD2	1:A:148:TRP:H	2.19	0.56
1:A:221:ILE:HD11	1:A:225:ARG:CZ	2.35	0.56
1:A:278:LEU:HG	1:A:304:MET:HB2	1.87	0.56
1:A:313:ARG:HH12	1:A:328:GLU:HG3	1.71	0.55
1:A:277:LEU:H	1:A:303:HIS:HD2	1.55	0.54
1:A:555:GLU:OE2	1:A:557:THR:HB	2.07	0.54
1:B:481:LEU:O	1:B:485:THR:HG23	2.09	0.53
1:A:139:MET:HE3	1:A:224:ILE:HD11	1.89	0.53
1:B:119:PHE:HZ	1:B:232:ILE:HD12	1.73	0.53
1:A:40:ASP:O	1:A:43:TRP:HD1	1.92	0.53
1:A:475:ARG:HG3	1:A:475:ARG:NH1	2.21	0.53
1:A:382:ARG:HA	3:A:705:GOL:H12	1.90	0.53
1:A:457:PRO:HD3	1:B:425:TRP:CG	2.43	0.52
1:A:238:ASP:HA	1:A:280:GLU:CG	2.38	0.52
1:B:74:ARG:HD2	1:B:438:TRP:CH2	2.44	0.52
1:B:277:LEU:H	1:B:303:HIS:CD2	2.24	0.52
1:A:74:ARG:HH11	1:A:74:ARG:HA	1.76	0.51
1:A:312:PRO:HG3	1:A:348:ASN:HB3	1.92	0.51
1:A:180:PHE:HE2	1:A:202:PHE:HD2	1.58	0.51
1:A:135:THR:O	1:A:235:PHE:HA	2.10	0.50
1:A:277:LEU:H	1:A:303:HIS:CD2	2.29	0.50
1:A:386:ALA:HB3	1:A:387:PRO:HD3	1.93	0.50
1:B:538:PRO:HA	1:B:574:LEU:O	2.11	0.50
1:A:559:HIS:CD2	3:A:702:GOL:H2	2.47	0.50
1:A:177:ARG:O	1:A:201:ARG:NH1	2.45	0.50
1:A:470:ASN:ND2	1:A:473:ALA:H	2.09	0.50
1:B:139:MET:HE3	1:B:224:ILE:HD11	1.95	0.49
1:B:138:VAL:HA	1:B:238:ASP:HB2	1.93	0.49
1:A:45:LYS:HA	1:A:341:GLN:HG3	1.95	0.49
1:B:45:LYS:HA	1:B:341:GLN:HG3	1.95	0.48
1:B:426:LEU:HB3	1:B:430:ASP:HB3	1.95	0.48
1:B:69:ARG:HA	1:B:72:ILE:HD12	1.95	0.48
1:A:180:PHE:HE2	1:A:202:PHE:CD2	2.32	0.47
1:A:313:ARG:HG3	1:A:329:ILE:HG12	1.95	0.47
1:A:19:GLU:HA	1:A:20:GLY:HA2	1.69	0.47
1:A:74:ARG:N	1:A:74:ARG:HD2	2.29	0.47
1:A:556:LEU:HD21	1:A:583:GLN:HB2	1.97	0.47
1:A:282:ASN:HD21	1:A:350:ASP:H	1.61	0.46
1:A:138:VAL:HA	1:A:238:ASP:HB2	1.96	0.46
1:A:236:ARG:HA	1:A:278:LEU:HB2	1.97	0.46
1:B:277:LEU:N	1:B:303:HIS:HD2	2.09	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PRO:HD3	1:A:136:ASP:HB2	1.97	0.46
1:B:174:THR:HG22	1:B:175:ASP:H	1.80	0.46
1:A:326:ILE:O	1:A:330:ILE:HG12	2.15	0.46
1:A:387:PRO:CG	1:A:421:GLY:HA2	2.45	0.46
1:A:577:HIS:HD2	5:A:828:HOH:O	2.00	0.46
1:B:278:LEU:HG	1:B:304:MET:HB2	1.98	0.45
1:A:313:ARG:HH12	1:A:328:GLU:HG2	1.79	0.45
1:A:384:ARG:HG2	1:A:416:ASP:OD1	2.16	0.45
1:B:324:PHE:O	1:B:328:GLU:HG3	2.17	0.45
1:A:301:GLU:HB3	1:A:302:CYS:H	1.64	0.45
1:A:479:THR:O	1:A:479:THR:HG22	2.16	0.44
1:A:103:ILE:HD12	1:A:138:VAL:HB	1.99	0.44
1:A:547:GLN:HB3	1:A:548:TRP:CE3	2.52	0.44
1:B:329:ILE:H	1:B:329:ILE:HG13	1.66	0.44
1:B:505:GLU:O	1:B:505:GLU:HG3	2.17	0.44
1:A:284:TRP:CH2	1:A:363:ASP:HB2	2.53	0.44
1:A:347:ARG:HB2	3:A:705:GOL:H11	1.99	0.44
1:B:407:PRO:HA	1:B:518:ARG:NH2	2.32	0.44
1:B:19:GLU:HA	1:B:20:GLY:HA2	1.82	0.43
1:A:217:GLN:O	1:A:221:ILE:HG23	2.18	0.43
1:B:556:LEU:HD21	1:B:583:GLN:HB2	2.00	0.43
1:B:345:PHE:HB3	1:B:411:VAL:HB	2.02	0.42
1:A:501:GLY:O	1:A:518:ARG:NH1	2.52	0.42
1:B:541:ILE:HD11	1:B:574:LEU:CD1	2.48	0.42
1:B:495:HIS:NE2	3:B:702:GOL:H31	2.34	0.42
1:A:473:ALA:O	1:A:477:THR:HG22	2.19	0.42
1:B:45:LYS:HG2	1:B:341:GLN:HG3	2.01	0.42
1:B:53:LEU:HD22	1:B:433:ARG:CG	2.47	0.42
1:A:360:GLU:HG2	1:A:366:TYR:CZ	2.55	0.42
1:B:45:LYS:HG2	1:B:341:GLN:CG	2.49	0.41
1:A:382:ARG:HG2	3:A:705:GOL:H12	2.03	0.41
1:A:559:HIS:NE2	3:A:702:GOL:H2	2.35	0.41
1:B:351:GLU:HA	1:B:352:LEU:C	2.41	0.41
1:B:533:ASN:O	1:B:577:HIS:HA	2.21	0.41
1:A:239:ALA:H	1:A:280:GLU:CG	2.34	0.40
1:B:146:HIS:CD2	1:B:148:TRP:H	2.29	0.40
1:B:547:GLN:HB3	1:B:548:TRP:CE3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	566/620 (91%)	549 (97%)	17 (3%)	0	100	100
1	B	542/620 (87%)	525 (97%)	17 (3%)	0	100	100
All	All	1108/1240 (89%)	1074 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	447/531 (84%)	417 (93%)	30 (7%)	16	33
1	B	423/531 (80%)	392 (93%)	31 (7%)	14	28
All	All	870/1062 (82%)	809 (93%)	61 (7%)	15	30

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	71	LEU
1	A	74	ARG
1	A	136	ASP
1	A	208	ASP
1	A	221	ILE
1	A	265	ARG
1	A	280	GLU

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Mol	Chain	Res	Type
1	A	290	GLU
1	A	311	MET
1	A	316	MET
1	A	328	GLU
1	A	345	PHE
1	A	360	GLU
1	A	384	ARG
1	A	393	ARG
1	A	402	LEU
1	A	404	LEU
1	A	422	ASP
1	A	424	ILE
1	A	463	VAL
1	A	469	VAL
1	A	475	ARG
1	A	477	THR
1	A	481	LEU
1	A	488	MET
1	A	489	LEU
1	A	549	THR
1	A	557	THR
1	A	573	THR
1	B	17	HIS
1	B	57	PHE
1	B	67	ASP
1	B	68	LEU
1	B	71	LEU
1	B	122	LEU
1	B	185	GLU
1	B	243	LEU
1	B	245	GLU
1	B	246	ARG
1	B	265	ARG
1	B	297	THR
1	B	311	MET
1	B	316	MET
1	B	345	PHE
1	B	348	ASN
1	B	384	ARG
1	B	402	LEU
1	B	404	LEU
1	B	433	ARG

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Mol	Chain	Res	Type
1	B	446	PHE
1	B	463	VAL
1	B	481	LEU
1	B	485	THR
1	B	489	LEU
1	B	505	GLU
1	B	536	ARG
1	B	541	ILE
1	B	557	THR
1	B	564	ARG
1	B	573	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	127	HIS
1	A	146	HIS
1	A	210	ASN
1	A	217	GLN
1	A	282	ASN
1	A	283	GLN
1	A	303	HIS
1	A	332	GLN
1	A	394	ASN
1	A	395	GLN
1	A	470	ASN
1	A	474	GLN
1	B	146	HIS
1	B	217	GLN
1	B	303	HIS
1	B	395	GLN
1	B	470	ASN
1	B	474	GLN
1	B	519	GLN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	B	703	-	4,4,4	0.33	0	6,6,6	0.08	0
3	GOL	A	705	-	5,5,5	0.40	0	5,5,5	0.65	0
3	GOL	A	702	-	5,5,5	0.23	0	5,5,5	0.50	0
4	SO4	B	704	-	4,4,4	0.33	0	6,6,6	0.07	0
3	GOL	A	703	-	5,5,5	0.26	0	5,5,5	0.40	0
3	GOL	A	704	-	5,5,5	0.39	0	5,5,5	0.30	0
3	GOL	B	702	-	5,5,5	0.19	0	5,5,5	0.39	0
4	SO4	A	707	-	4,4,4	0.34	0	6,6,6	0.04	0
4	SO4	A	708	-	4,4,4	0.31	0	6,6,6	0.20	0
4	SO4	B	705	-	4,4,4	0.33	0	6,6,6	0.06	0
4	SO4	A	706	-	4,4,4	0.34	0	6,6,6	0.06	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
3	GOL	A	705	-	-	2/4/4/4	-
3	GOL	A	702	-	-	3/4/4/4	-
3	GOL	A	703	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	704	-	-	2/4/4/4	-
3	GOL	B	702	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	GOL	C1-C2-C3-O3
3	A	705	GOL	C1-C2-C3-O3
3	B	702	GOL	O1-C1-C2-C3
3	A	702	GOL	C1-C2-C3-O3
3	A	704	GOL	O1-C1-C2-C3
3	B	702	GOL	C1-C2-C3-O3
3	A	704	GOL	O1-C1-C2-O2
3	B	702	GOL	O1-C1-C2-O2
3	A	702	GOL	O2-C2-C3-O3
3	A	703	GOL	O2-C2-C3-O3
3	A	705	GOL	O2-C2-C3-O3
3	B	702	GOL	O2-C2-C3-O3
3	A	703	GOL	O1-C1-C2-C3
3	A	702	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	705	GOL	4	0
3	A	702	GOL	2	0
3	A	703	GOL	1	0
3	B	702	GOL	1	0

5.7 Other polymers (i)

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, 95th 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(Å²)	Q<0.9
1	A	570/620 (91%)	-0.43	9 (1%)	72	68	36, 62, 92, 124	0
1	B	546/620 (88%)	-0.18	16 (2%)	51	45	42, 76, 108, 131	0
All	All	1116/1240 (90%)	-0.31	25 (2%)	62	56	36, 69, 103, 131	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	ASP	4.5
1	B	30	ASP	3.6
1	A	33	SER	3.6
1	A	35	ALA	3.3
1	B	12	PRO	3.0
1	A	19	GLU	3.0
1	B	522	GLY	2.9
1	B	32	GLY	2.8
1	B	382	ARG	2.7
1	A	12	PRO	2.7
1	B	21	GLY	2.7
1	B	31	PHE	2.6
1	B	135	THR	2.5
1	A	425	TRP	2.4
1	A	134	ILE	2.3
1	A	135	THR	2.3
1	B	134	ILE	2.2
1	B	284	TRP	2.2
1	B	521	ALA	2.1
1	B	524	ASP	2.1
1	A	22	VAL	2.1
1	A	36	ALA	2.1
1	B	209	LEU	2.0
1	B	39	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	427	GLY	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 monosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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
3	GOL	A	705	6/6	0.61	0.47	75,84,84,89	0
3	GOL	A	704	6/6	0.79	0.37	74,77,78,81	0
3	GOL	A	702	6/6	0.89	0.20	62,64,67,69	0
4	SO4	A	706	5/5	0.89	0.38	118,118,120,123	0
4	SO4	A	707	5/5	0.89	0.22	129,130,131,132	0
3	GOL	B	702	6/6	0.93	0.13	65,66,67,73	0
4	SO4	B	704	5/5	0.93	0.31	120,122,123,126	0
3	GOL	A	703	6/6	0.95	0.28	71,73,76,79	0
4	SO4	B	705	5/5	0.95	0.23	113,116,117,117	0
2	CA	B	701	1/1	0.96	0.13	82,82,82,82	0
4	SO4	B	703	5/5	0.96	0.11	93,95,97,98	0
2	CA	A	701	1/1	0.97	0.10	51,51,51,51	0
4	SO4	A	708	5/5	0.98	0.12	61,62,65,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.