



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:27 PM UTC

PDB ID : 2JJB / pdb_00002jjb
Title : Family 37 trehalase from Escherichia coli in complex with casuarine-6- O-alpha-glucopyranose
Authors : Gloster, T.M.; Roberts, S.; Davies, G.J.; Cardona, F.; Parmeggiani, C.; Bonaccini, C.; Gratteri, P.; Sim, L.; Rose, D.R.; Goti, A.
Deposited on : 2008-03-28
Resolution : 1.90 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

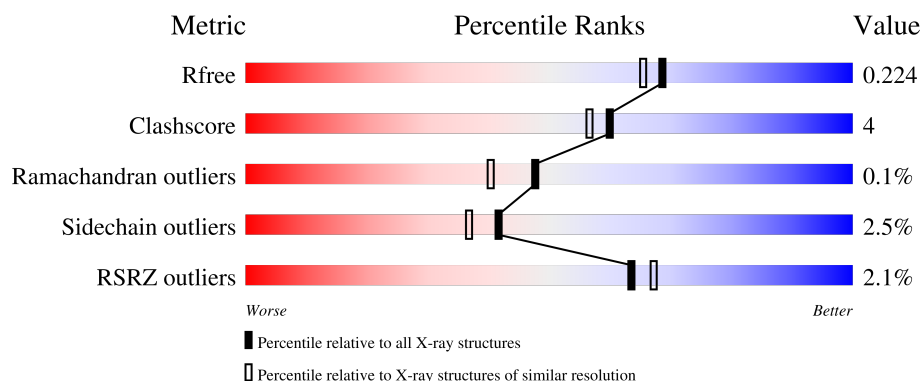
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	535	1% 85% 8% 6%
1	B	535	2% 83% 8% 8%
1	C	535	1% 83% 9% 7%
1	D	535	4% 83% 10% 7%

2 Entry composition [i](#)

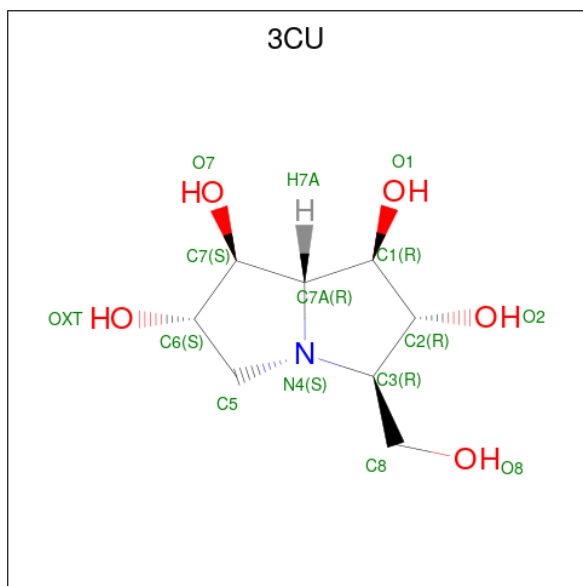
There are 6 unique types of molecules in this entry. The entry contains 18411 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PERIPLASMIC TREHALASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	26	0
			4155	2652	704	781	18			
1	B	493	Total	C	N	O	S	0	21	0
			4045	2575	690	762	18			
1	C	500	Total	C	N	O	S	0	16	0
			4070	2589	693	771	17			
1	D	500	Total	C	N	O	S	0	18	0
			4054	2587	681	768	18			

- Molecule 2 is CASUARINE (CCD ID: 3CU) (formula: $C_8H_{15}NO_5$).



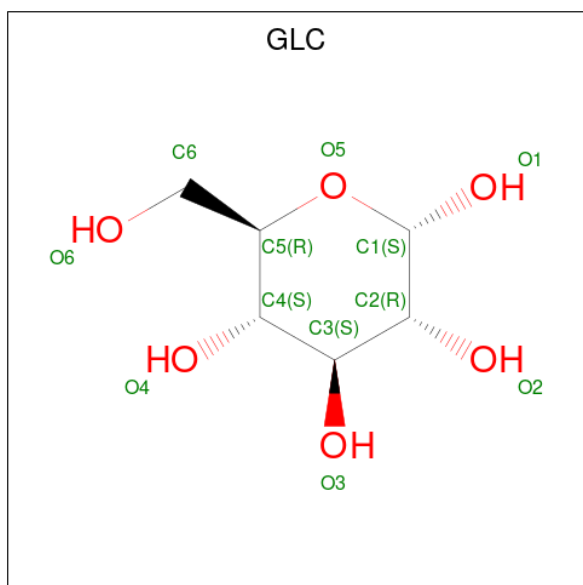
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	8	1	4		
2	B	1	Total	C	N	O	0	0
			13	8	1	4		

Continued on next page...

Continued from previous page...

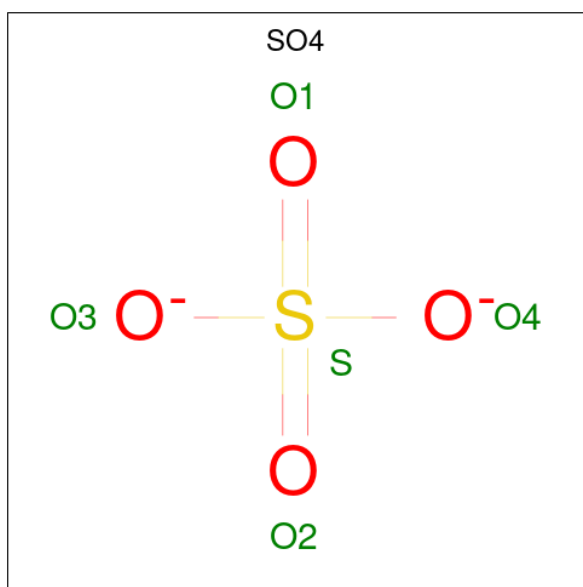
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			13	8	1	4		
2	D	1	Total	C	N	O	0	0
			13	8	1	4		

- Molecule 3 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

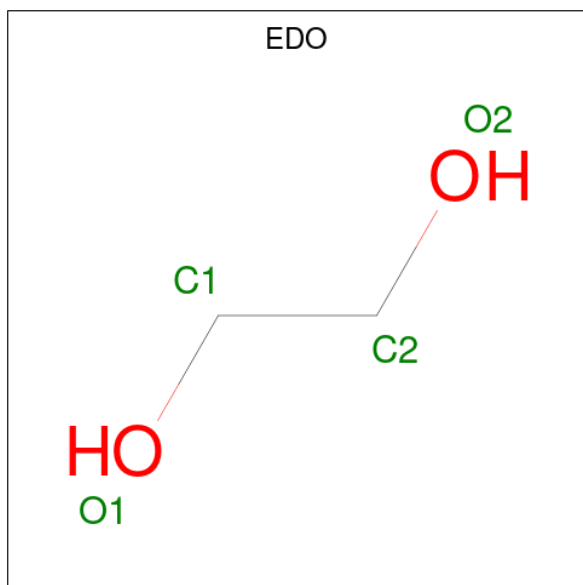
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	517	Total	O	0	26
			523	523		
6	B	460	Total	O	0	1
			461	461		
6	C	454	Total	O	0	6
			458	458		

Continued on next page...

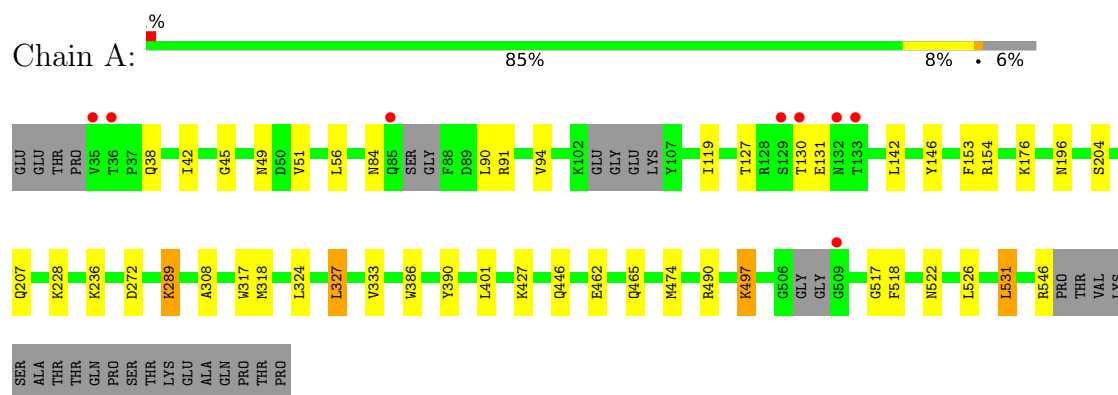
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	339	Total	O	0	4
			343	343		

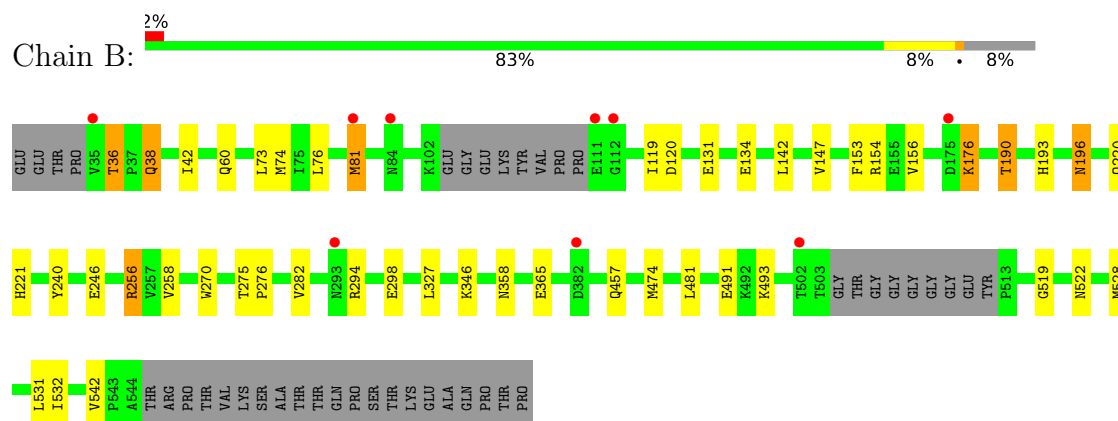
3 Residue-property plots

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.

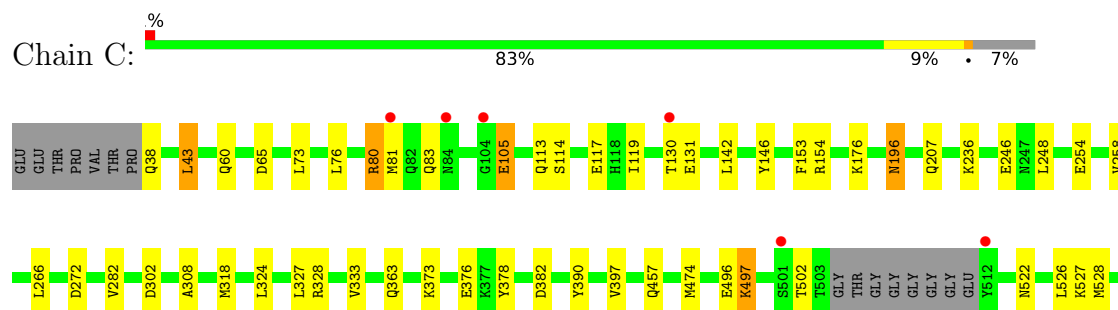
• Molecule 1: PERIPLASMIC TREHALASE

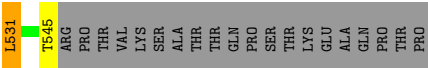


• Molecule 1: PERIPLASMIC TREHALASE

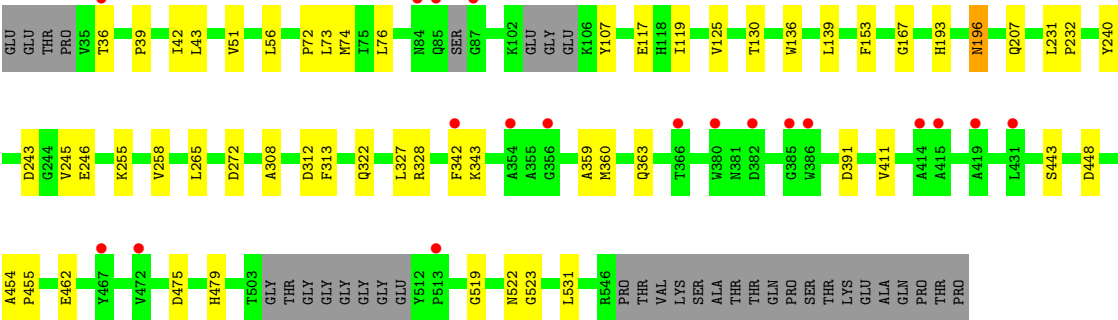
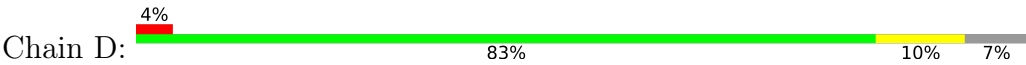


• Molecule 1: PERIPLASMIC TREHALASE





● Molecule 1: PERIPLASMIC TREHALASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.48Å 117.86Å 203.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 1.90 19.92 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.92-1.90) 99.4 (19.92-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.4.0065	Depositor
R, R_{free}	0.177 , 0.224 0.177 , 0.224	Depositor DCC
R_{free} test set	8658 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18411	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: EDO, SO4, 3CU, GLC

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	0.75	0/4340	0.89	2/5912 (0.0%)
1	B	0.71	0/4215	0.86	1/5740 (0.0%)
1	C	0.71	0/4229	0.86	0/5765
1	D	0.65	0/4216	0.86	0/5758
All	All	0.70	0/17000	0.87	3/23175 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	GLY	CA-C-N	6.22	125.90	119.56
1	A	45	GLY	C-N-CA	6.22	125.90	119.56
1	B	358	ASN	N-CA-C	5.18	117.01	111.36

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	4155	0	4037	41	0
1	B	4045	0	3915	30	0
1	C	4070	0	3907	39	0
1	D	4054	0	3847	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	13	0	13	1	0
2	B	13	0	13	1	0
2	C	13	0	13	1	0
2	D	13	0	13	1	0
3	A	12	0	11	0	0
3	B	12	0	11	0	0
3	C	12	0	11	0	0
3	D	12	0	11	0	0
4	A	60	0	0	2	0
4	B	35	0	0	1	0
4	C	55	0	0	1	0
4	D	40	0	0	1	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	4	0	6	0	0
6	A	523	0	0	6	0
6	B	461	0	0	4	0
6	C	458	0	0	8	0
6	D	343	0	0	3	0
All	All	18411	0	15820	138	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 4.

All (138) 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:38[B]:GLN:OE1	6:A:2003[B]:HOH:O	1.57	1.22
1:A:176[B]:LYS:NZ	6:A:2203[B]:HOH:O	1.83	1.11
1:A:38[B]:GLN:CD	6:A:2003[B]:HOH:O	1.95	1.09
1:A:38[B]:GLN:NE2	6:A:2003[B]:HOH:O	1.92	1.02
1:C:382[A]:ASP:OD1	6:C:2335[A]:HOH:O	1.87	0.93
1:C:38:GLN:HB3	1:C:43:LEU:HD13	1.60	0.84
1:A:90[B]:LEU:HD23	1:A:90[B]:LEU:O	1.80	0.82
1:A:84:ASN:HD21	1:C:363[A]:GLN:CD	1.90	0.80
1:A:446[A]:GLN:OE1	1:A:497:LYS:HE3	1.87	0.74
1:B:38:GLN:HG2	1:B:42:ILE:HG21	1.72	0.72
1:C:130:THR:HG23	1:C:130:THR:O	1.90	0.72
1:A:90[B]:LEU:HD23	1:A:90[B]:LEU:C	2.15	0.71
1:D:328[A]:ARG:NH1	1:D:391:ASP:OD2	2.20	0.70
1:B:491:GLU:OE1	1:B:493:LYS:HE2	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130[A]:THR:HG22	1:A:146:TYR:HE2	1.58	0.69
1:A:51:VAL:HG22	1:A:90[B]:LEU:HD21	1.74	0.69
1:B:38:GLN:HG2	1:B:42:ILE:CG2	2.24	0.67
1:D:328[A]:ARG:HH12	1:D:391:ASP:CG	2.05	0.65
1:B:81:MET:HA	1:D:360:MET:HE1	1.79	0.64
1:C:328[A]:ARG:NH1	6:C:2304:HOH:O	2.30	0.64
1:B:221:HIS:HD2	6:B:2083:HOH:O	1.80	0.63
1:C:236:LYS:HE2	6:C:2180:HOH:O	1.97	0.63
1:A:90[B]:LEU:C	1:A:90[B]:LEU:CD2	2.74	0.61
1:A:130[A]:THR:HG22	1:A:146:TYR:CE2	2.36	0.60
1:D:43[A]:LEU:HG	1:D:72:PRO:HG2	1.82	0.60
1:A:56:LEU:HD11	1:A:90[B]:LEU:HD22	1.82	0.60
1:B:346:LYS:NZ	1:B:365:GLU:OE2	2.30	0.60
1:D:117[A]:GLU:OE2	1:D:117[A]:GLU:HA	2.01	0.59
1:D:136:TRP:HH2	6:D:2032:HOH:O	1.84	0.59
1:B:74:MET:HE2	1:B:74:MET:HA	1.84	0.59
1:D:243:ASP:OD2	1:D:255:LYS:HE3	2.04	0.58
1:A:289:LYS:HD3	6:C:2233:HOH:O	2.04	0.57
1:D:207:GLN:HA	1:D:308:ALA:O	2.06	0.55
1:A:462:GLU:OE2	1:A:465[B]:GLN:NE2	2.40	0.55
1:A:272[A]:ASP:OD2	4:A:1551:SO4:O4	2.25	0.54
1:B:36:THR:HG21	1:D:36:THR:OG1	2.08	0.54
1:C:196:ASN:C	1:C:196:ASN:HD22	2.16	0.54
1:D:343:LYS:HB2	1:D:411[B]:VAL:HG13	1.90	0.53
1:C:373[A]:LYS:HE3	6:C:2085:HOH:O	2.08	0.53
1:B:220[A]:GLN:NE2	6:B:2189:HOH:O	2.41	0.53
1:B:153:PHE:CZ	2:B:1545:3CU:H5C2	2.43	0.53
1:D:342:PHE:HD2	1:D:411[B]:VAL:HG12	1.74	0.52
1:B:147:VAL:HG23	1:B:176[A]:LYS:HD2	1.90	0.52
1:A:318:MET:HE3	1:A:324:LEU:HA	1.92	0.52
1:C:114:SER:OG	1:C:117[A]:GLU:HG2	2.10	0.51
1:A:474:MET:HE1	1:A:531:LEU:HD22	1.93	0.50
1:A:90[B]:LEU:HD23	1:A:94[B]:VAL:HG23	1.93	0.50
1:D:119:ILE:HG23	1:D:522:ASN:HB3	1.93	0.49
1:C:378:TYR:O	1:C:397[B]:VAL:HG12	2.12	0.49
1:A:119:ILE:HG23	1:A:522:ASN:HB3	1.95	0.49
1:C:113:GLN:HB3	1:C:117[A]:GLU:HG3	1.95	0.49
1:D:443:SER:OG	1:D:448:ASP:OD2	2.24	0.48
1:B:81:MET:HA	1:D:360:MET:CE	2.43	0.48
1:B:120:ASP:HB3	6:B:2161:HOH:O	2.14	0.48
1:D:73:LEU:HD22	1:D:74:MET:HE2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:GLN:CD	1:C:282[A]:VAL:HG22	2.38	0.48
1:A:207:GLN:HA	1:A:308:ALA:O	2.14	0.47
1:D:196:ASN:HD22	1:D:196:ASN:C	2.22	0.47
1:C:117[B]:GLU:OE1	1:C:117[B]:GLU:HA	2.14	0.47
1:D:475:ASP:O	1:D:479:HIS:CD2	2.66	0.47
1:A:153:PHE:CZ	2:A:1547:3CU:H5C2	2.50	0.47
1:B:131:GLU:HA	1:B:142:LEU:O	2.15	0.46
1:B:481:LEU:HB3	1:B:542:VAL:HG21	1.98	0.46
1:A:131:GLU:HA	1:A:142:LEU:O	2.15	0.46
1:B:154:ARG:HD3	6:B:2141:HOH:O	2.15	0.46
1:D:193:HIS:HB3	1:D:240:TYR:CD1	2.50	0.46
1:B:196:ASN:C	1:B:196:ASN:HD22	2.24	0.46
1:C:333:VAL:HB	1:C:390:TYR:HB3	1.97	0.46
1:A:91:ARG:HA	1:A:94[A]:VAL:HG22	1.97	0.45
1:C:302:ASP:HB3	1:C:327:LEU:HG	1.98	0.45
1:A:228:LYS:NZ	6:A:2262:HOH:O	2.39	0.45
1:D:107:TYR:CE1	1:D:125:VAL:HG21	2.50	0.45
1:A:204:SER:HB2	1:A:272[B]:ASP:OD1	2.16	0.45
1:A:127:THR:HG21	1:A:176[A]:LYS:NZ	2.32	0.45
1:A:236:LYS:HG2	1:C:73:LEU:HD12	1.98	0.44
1:C:207:GLN:HA	1:C:308:ALA:O	2.17	0.44
1:C:318:MET:HE3	1:C:324:LEU:HA	1.98	0.44
1:A:49:ASN:ND2	1:C:246:GLU:HG3	2.32	0.44
1:B:176[A]:LYS:HZ2	1:B:176[A]:LYS:HG2	1.52	0.44
1:C:496:GLU:HG3	1:C:497:LYS:HD2	1.99	0.44
1:A:154:ARG:NH1	6:A:2177:HOH:O	2.51	0.44
1:D:359:ALA:O	1:D:363:GLN:HG3	2.18	0.44
1:A:386:TRP:CE2	1:A:401:LEU:HB2	2.53	0.44
1:C:81:MET:HB3	6:C:2064:HOH:O	2.17	0.44
1:D:153:PHE:CZ	2:D:1547:3CU:H5C2	2.52	0.44
1:B:193:HIS:HB3	1:B:240:TYR:CD1	2.53	0.43
1:B:294:ARG:HH21	1:B:298[B]:GLU:HG2	1.82	0.43
1:D:243:ASP:OD2	1:D:255:LYS:CE	2.66	0.43
1:D:39:PRO:HG2	1:D:42:ILE:HG12	2.01	0.43
1:D:130:THR:HG21	1:D:139:LEU:HD21	2.00	0.43
1:C:272[A]:ASP:OD2	4:C:1552:SO4:O2	2.36	0.43
1:C:457:GLN:HB3	1:C:528:MET:HE1	2.00	0.43
1:B:256[A]:ARG:HG3	1:B:270:TRP:HB3	2.01	0.42
1:B:119:ILE:HG23	1:B:522:ASN:HB3	2.02	0.42
1:C:527:LYS:HA	1:C:527:LYS:HD2	1.92	0.42
1:D:454:ALA:N	1:D:455:PRO:HD2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:PHE:CZ	2:C:1546:3CU:H5C2	2.54	0.42
1:D:342:PHE:HD2	1:D:411[B]:VAL:CG1	2.32	0.42
1:B:474:MET:HE1	1:B:532:ILE:HG22	2.01	0.42
1:C:130:THR:O	1:C:130:THR:CG2	2.62	0.42
1:A:91:ARG:O	1:A:94[A]:VAL:HG22	2.19	0.42
1:C:474:MET:HE1	1:C:531:LEU:HD22	2.01	0.42
1:D:272[A]:ASP:OD2	4:D:1552:SO4:O2	2.38	0.42
1:A:176[A]:LYS:HG2	4:A:1552:SO4:O2	2.20	0.42
1:B:73[A]:LEU:CD2	1:B:74:MET:HE3	2.50	0.42
1:C:266:LEU:HD13	1:C:333:VAL:HG11	2.02	0.41
1:D:231:LEU:N	1:D:232:PRO:CD	2.82	0.41
1:B:190[A]:THR:CG2	6:D:2002:HOH:O	2.67	0.41
1:D:167:GLY:HA3	1:D:523:GLY:HA2	2.02	0.41
1:A:90[B]:LEU:CD2	1:A:94[B]:VAL:HG23	2.50	0.41
1:B:275:THR:HB	1:B:276:PRO:HD2	2.02	0.41
1:D:312:ASP:HA	1:D:313:PHE:HA	1.76	0.41
1:C:130:THR:HG22	1:C:146:TYR:HE2	1.85	0.41
1:C:474:MET:HE1	1:C:531:LEU:HD13	2.02	0.41
1:D:462[A]:GLU:OE2	1:D:462[A]:GLU:HA	2.20	0.41
1:A:38[B]:GLN:HB3	1:A:42:ILE:HB	2.02	0.41
1:D:245:VAL:HG23	1:D:265:LEU:HD22	2.03	0.41
1:B:256[A]:ARG:NH1	4:B:1549:SO4:O3	2.53	0.41
1:C:119:ILE:HG23	1:C:522:ASN:HB3	2.02	0.41
1:D:51:VAL:HG13	1:D:56:LEU:HD12	2.02	0.41
1:A:317:TRP:HB2	1:A:327[B]:LEU:HD23	2.02	0.41
1:A:333:VAL:HB	1:A:390:TYR:HB3	2.02	0.41
1:C:131:GLU:HA	1:C:142:LEU:O	2.21	0.41
1:C:248:LEU:HD13	1:C:254:GLU:HG2	2.03	0.41
1:C:80:ARG:NH1	1:C:83:GLN:OE1	2.49	0.41
1:C:376:GLU:HA	1:C:376:GLU:OE1	2.21	0.41
1:A:42:ILE:O	1:C:236:LYS:NZ	2.53	0.40
1:A:517:GLY:HA3	1:A:518:PHE:HA	1.90	0.40
1:B:60:GLN:CD	1:B:282:VAL:HG22	2.46	0.40
1:B:246:GLU:HG2	6:D:2015:HOH:O	2.20	0.40
1:C:105:GLU:HG2	6:C:2091:HOH:O	2.20	0.40
1:D:343:LYS:HB2	1:D:411[B]:VAL:CG1	2.50	0.40
1:C:65:ASP:OD2	1:C:154[A]:ARG:NE	2.55	0.40
1:C:373[B]:LYS:HD2	6:C:2326:HOH:O	2.20	0.40
1:B:457:GLN:HB3	1:B:528:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/535 (98%)	507 (97%)	15 (3%)	0	100	100
1	B	508/535 (95%)	494 (97%)	13 (3%)	1 (0%)	43	36
1	C	512/535 (96%)	499 (98%)	13 (2%)	0	100	100
1	D	510/535 (95%)	495 (97%)	14 (3%)	1 (0%)	43	36
All	All	2052/2140 (96%)	1995 (97%)	55 (3%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	519	GLY
1	B	519	GLY

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%)	438 (98%)	11 (2%)	43	38
1	B	436/456 (96%)	420 (96%)	16 (4%)	30	22
1	C	436/456 (96%)	424 (97%)	12 (3%)	38	32
1	D	428/456 (94%)	420 (98%)	8 (2%)	50	47
All	All	1749/1824 (96%)	1702 (97%)	47 (3%)	42	34

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	289	LYS
1	A	327[A]	LEU
1	A	327[B]	LEU
1	A	427	LYS
1	A	490[A]	ARG
1	A	490[B]	ARG
1	A	497	LYS
1	A	526	LEU
1	A	531	LEU
1	A	546	ARG
1	B	36	THR
1	B	38	GLN
1	B	76	LEU
1	B	81	MET
1	B	134	GLU
1	B	156	VAL
1	B	176[A]	LYS
1	B	176[B]	LYS
1	B	190[A]	THR
1	B	190[B]	THR
1	B	196	ASN
1	B	256[A]	ARG
1	B	256[B]	ARG
1	B	258	VAL
1	B	327	LEU
1	B	531	LEU
1	C	43	LEU
1	C	76	LEU
1	C	80	ARG
1	C	105	GLU
1	C	176	LYS
1	C	196	ASN
1	C	258	VAL
1	C	497	LYS
1	C	502	THR
1	C	526	LEU
1	C	531	LEU
1	C	545	THR
1	D	76	LEU
1	D	196	ASN
1	D	246	GLU
1	D	258	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	322[A]	GLN
1	D	322[B]	GLN
1	D	327	LEU
1	D	531	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	235	GLN
1	A	261	GLN
1	A	322	GLN
1	A	384	GLN
1	A	432	GLN
1	B	38	GLN
1	B	113	GLN
1	B	235	GLN
1	B	432	GLN
1	C	38	GLN
1	C	85	GLN
1	C	221	HIS
1	C	235	GLN
1	C	465	GLN
1	D	235	GLN
1	D	249	GLN
1	D	293	ASN
1	D	369	ASN
1	D	412	ASN
1	D	429	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

49 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	$\# Z > 2$
4	SO4	D	1551	-	4,4,4	0.23	0	6,6,6	0.30	0
4	SO4	A	1557	-	4,4,4	0.27	0	6,6,6	0.21	0
5	EDO	A	1561	-	3,3,3	0.45	0	2,2,2	0.54	0
4	SO4	A	1551	-	4,4,4	0.20	0	6,6,6	0.33	0
5	EDO	B	1554	-	3,3,3	0.45	0	2,2,2	0.94	0
4	SO4	C	1554	-	4,4,4	0.23	0	6,6,6	0.15	0
3	GLC	B	1546	2	12,12,12	0.57	0	17,17,17	1.08	1 (5%)
4	SO4	D	1555	-	4,4,4	0.23	0	6,6,6	0.16	0
4	SO4	A	1550	-	4,4,4	0.21	0	6,6,6	0.29	0
4	SO4	A	1549	-	4,4,4	0.28	0	6,6,6	0.33	0
4	SO4	A	1556	-	4,4,4	0.24	0	6,6,6	0.12	0
5	EDO	C	1559	-	3,3,3	0.52	0	2,2,2	0.11	0
3	GLC	D	1548	2	12,12,12	0.72	0	17,17,17	0.98	2 (11%)
4	SO4	B	1550	-	4,4,4	0.21	0	6,6,6	0.26	0
4	SO4	B	1549	-	4,4,4	0.24	0	6,6,6	0.35	0
4	SO4	A	1558[A]	-	4,4,4	0.30	0	6,6,6	0.49	0
4	SO4	C	1558	-	4,4,4	0.24	0	6,6,6	0.17	0
2	3CU	A	1547	3	14,14,15	0.87	0	17,21,23	2.85	6 (35%)
4	SO4	C	1553	-	4,4,4	0.22	0	6,6,6	0.22	0
4	SO4	A	1554	-	4,4,4	0.24	0	6,6,6	0.14	0
4	SO4	C	1548	-	4,4,4	0.27	0	6,6,6	0.44	0
4	SO4	D	1549	-	4,4,4	0.30	0	6,6,6	0.36	0
4	SO4	B	1552	-	4,4,4	0.21	0	6,6,6	0.11	0
4	SO4	A	1552	-	4,4,4	0.28	0	6,6,6	0.16	0
4	SO4	C	1550	-	4,4,4	0.26	0	6,6,6	0.55	0
4	SO4	C	1556	-	4,4,4	0.24	0	6,6,6	0.21	0
4	SO4	D	1552	-	4,4,4	0.27	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	1551	-	4,4,4	0.22	0	6,6,6	0.23	0
4	SO4	C	1555	-	4,4,4	0.22	0	6,6,6	0.30	0
4	SO4	D	1553	-	4,4,4	0.20	0	6,6,6	0.42	0
4	SO4	A	1559	-	4,4,4	0.25	0	6,6,6	0.13	0
2	3CU	B	1545	3	14,14,15	0.87	0	17,21,23	2.95	7 (41%)
4	SO4	A	1553	-	4,4,4	0.27	0	6,6,6	0.26	0
4	SO4	B	1547	-	4,4,4	0.28	0	6,6,6	0.41	0
2	3CU	C	1546	3	14,14,15	0.89	2 (14%)	17,21,23	3.00	8 (47%)
4	SO4	B	1548	-	4,4,4	0.40	0	6,6,6	0.34	0
4	SO4	A	1560	-	4,4,4	0.23	0	6,6,6	0.23	0
3	GLC	A	1548	2	12,12,12	0.65	0	17,17,17	1.05	1 (5%)
4	SO4	D	1556	-	4,4,4	0.24	0	6,6,6	0.19	0
2	3CU	D	1547	3	14,14,15	0.80	0	17,21,23	3.04	7 (41%)
4	SO4	B	1553	-	4,4,4	0.34	0	6,6,6	0.25	0
4	SO4	C	1552	-	4,4,4	0.22	0	6,6,6	0.35	0
4	SO4	D	1554	-	4,4,4	0.25	0	6,6,6	0.13	0
4	SO4	A	1555	-	4,4,4	0.22	0	6,6,6	0.17	0
4	SO4	C	1549	-	4,4,4	0.37	0	6,6,6	0.25	0
4	SO4	C	1557	-	4,4,4	0.23	0	6,6,6	0.13	0
4	SO4	D	1550	-	4,4,4	0.25	0	6,6,6	0.39	0
4	SO4	C	1551	-	4,4,4	0.27	0	6,6,6	0.47	0
3	GLC	C	1547	2	12,12,12	0.62	0	17,17,17	1.06	1 (5%)

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	3CU	B	1545	3	-	0/2/31/34	0/2/2/2
5	EDO	A	1561	-	-	0/1/1/1	-
2	3CU	C	1546	3	-	0/2/31/34	0/2/2/2
5	EDO	B	1554	-	-	0/1/1/1	-
3	GLC	A	1548	2	-	0/2/22/22	0/1/1/1
2	3CU	A	1547	3	-	0/2/31/34	0/2/2/2
3	GLC	B	1546	2	-	0/2/22/22	0/1/1/1
5	EDO	C	1559	-	-	1/1/1/1	-
2	3CU	D	1547	3	-	0/2/31/34	0/2/2/2
3	GLC	C	1547	2	-	0/2/22/22	0/1/1/1
3	GLC	D	1548	2	-	0/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1546	3CU	C7A-N4	-2.07	1.44	1.49
2	C	1546	3CU	C5-N4	-2.05	1.44	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1546	3CU	C7A-N4-C3	6.60	119.67	106.53
2	B	1545	3CU	C7A-N4-C3	6.53	119.54	106.53
2	D	1547	3CU	C7A-N4-C3	6.34	119.16	106.53
2	A	1547	3CU	C7A-N4-C3	5.99	118.47	106.53
2	B	1545	3CU	C5-N4-C7A	5.68	116.03	106.06
2	D	1547	3CU	C5-N4-C3	5.63	125.53	114.98
2	A	1547	3CU	C5-N4-C3	5.26	124.85	114.98
2	D	1547	3CU	C2-C3-N4	-4.83	97.19	104.58
2	C	1546	3CU	C5-N4-C3	4.64	123.69	114.98
2	C	1546	3CU	C2-C3-N4	-4.55	97.62	104.58
2	C	1546	3CU	C5-N4-C7A	4.32	113.63	106.06
2	B	1545	3CU	C7-C7A-N4	-4.21	97.91	104.72
2	C	1546	3CU	C7-C7A-N4	-4.21	97.91	104.72
2	A	1547	3CU	C5-N4-C7A	4.17	113.38	106.06
2	D	1547	3CU	C7-C7A-N4	-4.06	98.16	104.72
2	B	1545	3CU	C2-C3-N4	-4.04	98.40	104.58
2	A	1547	3CU	C2-C3-N4	-4.03	98.41	104.58
2	D	1547	3CU	C6-C7-C7A	3.98	107.79	102.80
2	D	1547	3CU	C5-N4-C7A	3.83	112.77	106.06
2	A	1547	3CU	C7-C7A-N4	-3.77	98.62	104.72
2	C	1546	3CU	C6-C7-C7A	3.49	107.17	102.80
2	B	1545	3CU	C5-N4-C3	3.45	121.45	114.98
2	A	1547	3CU	C6-C7-C7A	3.45	107.12	102.80
2	B	1545	3CU	C6-C7-C7A	3.41	107.07	102.80
3	A	1548	GLC	C1-O5-C5	3.28	119.99	113.65
3	B	1546	GLC	C1-O5-C5	3.07	119.60	113.65
3	C	1547	GLC	C1-O5-C5	3.03	119.52	113.65
2	B	1545	3CU	C8-C3-C2	2.83	118.07	113.46
3	D	1548	GLC	C4-C3-C2	-2.35	106.70	110.83
3	D	1548	GLC	C1-O5-C5	2.28	118.06	113.65
2	D	1547	3CU	C8-C3-C2	2.27	117.16	113.46
2	C	1546	3CU	C8-C3-C2	2.27	117.16	113.46
2	C	1546	3CU	O7-C7-C6	-2.01	106.71	111.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1559	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1551	SO4	1	0
4	B	1549	SO4	1	0
2	A	1547	3CU	1	0
4	A	1552	SO4	1	0
4	D	1552	SO4	1	0
2	B	1545	3CU	1	0
2	C	1546	3CU	1	0
2	D	1547	3CU	1	0
4	C	1552	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, 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(Å ²)	Q<0.9
1	A	504/535 (94%)	-0.36	8 (1%) 70 74	11, 22, 36, 46	26 (5%)
1	B	493/535 (92%)	-0.25	9 (1%) 67 71	10, 24, 39, 52	21 (4%)
1	C	500/535 (93%)	-0.28	6 (1%) 76 79	12, 25, 40, 47	16 (3%)
1	D	500/535 (93%)	0.22	19 (3%) 44 47	14, 31, 48, 54	18 (3%)
All	All	1997/2140 (93%)	-0.17	42 (2%) 63 67	10, 25, 43, 54	81 (4%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	GLY	3.8
1	B	112	GLY	3.5
1	D	419	ALA	3.4
1	D	356	GLY	3.2
1	A	36	THR	3.1
1	D	380	TRP	3.1
1	A	35	VAL	2.9
1	D	386	TRP	2.9
1	A	130[A]	THR	2.9
1	D	84	ASN	2.8
1	D	415	ALA	2.8
1	D	382	ASP	2.6
1	D	354	ALA	2.5
1	B	382	ASP	2.5
1	D	472	VAL	2.5
1	B	111	GLU	2.4
1	D	513	PRO	2.4
1	C	84	ASN	2.4
1	A	132	ASN	2.4
1	B	35	VAL	2.4
1	C	130	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	85	GLN	2.3
1	C	501[A]	SER	2.3
1	C	81	MET	2.3
1	D	385	GLY	2.3
1	C	512	TYR	2.3
1	D	87	GLY	2.2
1	B	81	MET	2.2
1	A	129	SER	2.2
1	D	85	GLN	2.2
1	B	175	ASP	2.2
1	D	414	ALA	2.2
1	D	342	PHE	2.2
1	B	502	THR	2.1
1	D	36	THR	2.1
1	A	133	THR	2.1
1	C	104	GLY	2.1
1	D	467	TYR	2.1
1	D	431	LEU	2.1
1	D	366[A]	THR	2.0
1	B	293[A]	ASN	2.0
1	B	84	ASN	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 oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
4	SO4	A	1556	5/5	0.68	0.18	85,85,86,86	0
4	SO4	A	1557	5/5	0.69	0.15	70,71,71,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	D	1554	5/5	0.70	0.15	92,92,93,93	0
4	SO4	A	1560	5/5	0.73	0.16	88,89,89,89	0
4	SO4	C	1557	5/5	0.76	0.12	87,88,88,88	0
4	SO4	A	1554	5/5	0.78	0.11	64,64,65,65	0
4	SO4	C	1558	5/5	0.81	0.12	88,88,88,88	0
4	SO4	C	1556	5/5	0.81	0.11	64,64,65,65	0
4	SO4	A	1555	5/5	0.83	0.10	71,71,72,72	0
4	SO4	A	1559	5/5	0.84	0.11	84,85,85,85	0
4	SO4	A	1558[A]	5/5	0.84	0.18	26,27,32,32	5
4	SO4	D	1551	5/5	0.85	0.13	49,50,51,52	0
4	SO4	B	1553	5/5	0.87	0.17	53,55,56,56	0
4	SO4	B	1551	5/5	0.87	0.12	66,66,67,67	0
4	SO4	D	1553	5/5	0.88	0.15	53,53,55,55	0
4	SO4	D	1555	5/5	0.88	0.09	77,77,78,78	0
4	SO4	C	1554	5/5	0.89	0.09	72,72,73,73	0
4	SO4	A	1553	5/5	0.89	0.10	57,58,59,60	0
4	SO4	A	1551	5/5	0.89	0.13	36,40,41,44	0
4	SO4	C	1553	5/5	0.89	0.10	69,70,70,71	0
5	EDO	B	1554	4/4	0.89	0.09	27,28,29,33	0
4	SO4	C	1555	5/5	0.91	0.12	55,56,57,58	0
4	SO4	B	1552	5/5	0.91	0.08	63,63,64,64	0
4	SO4	B	1550	5/5	0.91	0.09	67,67,67,68	0
4	SO4	D	1550	5/5	0.92	0.08	53,53,55,56	0
5	EDO	A	1561	4/4	0.93	0.09	26,30,32,33	0
4	SO4	C	1552	5/5	0.93	0.09	38,38,40,40	0
4	SO4	B	1549	5/5	0.94	0.10	37,38,38,39	0
4	SO4	D	1556	5/5	0.95	0.07	61,61,63,63	0
4	SO4	D	1552	5/5	0.95	0.08	43,44,45,46	0
4	SO4	C	1551	5/5	0.95	0.07	41,42,43,46	0
4	SO4	B	1547	5/5	0.96	0.08	29,31,33,35	0
4	SO4	A	1552	5/5	0.96	0.07	44,45,45,46	0
4	SO4	C	1548	5/5	0.96	0.09	30,32,33,35	0
2	3CU	D	1547	13/14	0.96	0.06	18,20,22,22	0
2	3CU	A	1547	13/14	0.96	0.05	12,15,16,16	0
2	3CU	C	1546	13/14	0.97	0.04	15,17,19,19	0
2	3CU	B	1545	13/14	0.97	0.05	16,19,21,21	0
4	SO4	C	1549	5/5	0.97	0.07	31,32,33,35	0
3	GLC	B	1546	12/12	0.97	0.05	16,19,20,23	0
5	EDO	C	1559	4/4	0.97	0.06	23,25,25,26	0
3	GLC	D	1548	12/12	0.98	0.04	18,19,20,20	0
4	SO4	A	1550	5/5	0.98	0.05	26,29,32,33	0
3	GLC	A	1548	12/12	0.98	0.04	12,15,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	C	1547	12/12	0.98	0.04	16,18,20,22	0
4	SO4	D	1549	5/5	0.98	0.07	29,32,33,33	0
4	SO4	A	1549	5/5	0.99	0.04	23,25,25,27	0
4	SO4	C	1550	5/5	0.99	0.06	20,21,22,23	0
4	SO4	B	1548	5/5	0.99	0.07	26,27,28,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.