



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:33 AM UTC

PDB ID : 4IGB / pdb_00004igb
Title : Crystal structure of the N-terminal domain of the Streptococcus gordonii adhesin Sgo0707
Authors : Nylander, A.; Svensater, G.; Senadheera, D.B.; Cvitkovitch, D.G.; Davies, J.R.; Persson, K.
Deposited on : 2012-12-17
Resolution : 2.09 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

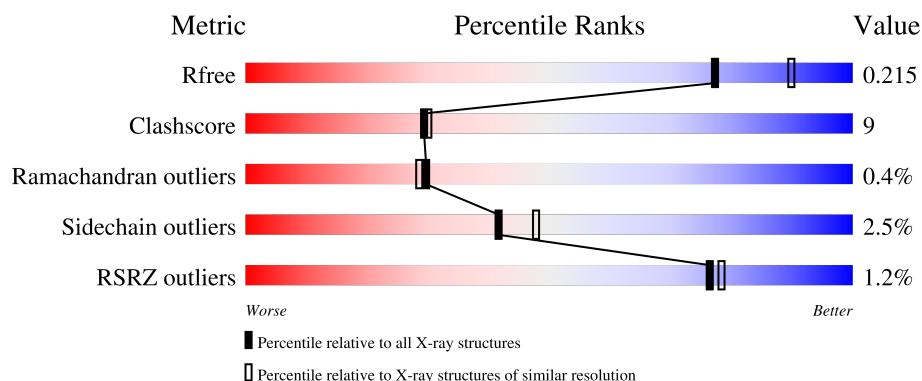
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	430	% 83% 15% ..
2	B	435	% 84% 13% .
3	C	436	% 85% 14% ..
4	D	423	% 80% 17% ..

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
6	GOL	D	503	-	-	X	-
7	ACT	C	504	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14782 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 LPXTG cell wall surface protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3348	2105	547	686	10			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP A8AW49
A	-5	TYR	-	expression tag	UNP A8AW49
A	-4	PHE	-	expression tag	UNP A8AW49
A	-3	GLN	-	expression tag	UNP A8AW49
A	-2	GLY	-	expression tag	UNP A8AW49
A	-1	ALA	-	expression tag	UNP A8AW49
A	0	MET	-	expression tag	UNP A8AW49

- Molecule 2 is a protein called LPXTG cell wall surface protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	435	Total	C	N	O	S	0	0	0
			3417	2146	559	702	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	PRO	-	expression tag	UNP A8AW49
B	-10	THR	-	expression tag	UNP A8AW49
B	-9	THR	-	expression tag	UNP A8AW49
B	-8	GLU	-	expression tag	UNP A8AW49
B	-7	ASN	-	expression tag	UNP A8AW49
B	-6	LEU	-	expression tag	UNP A8AW49
B	-5	TYR	-	expression tag	UNP A8AW49
B	-4	PHE	-	expression tag	UNP A8AW49
B	-3	GLN	-	expression tag	UNP A8AW49

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP A8AW49
B	-1	ALA	-	expression tag	UNP A8AW49
B	0	MET	-	expression tag	UNP A8AW49

- Molecule 3 is a protein called LPXTG cell wall surface protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	433	Total	C	N	O	S	0	0	0
			3395	2132	556	697	10			

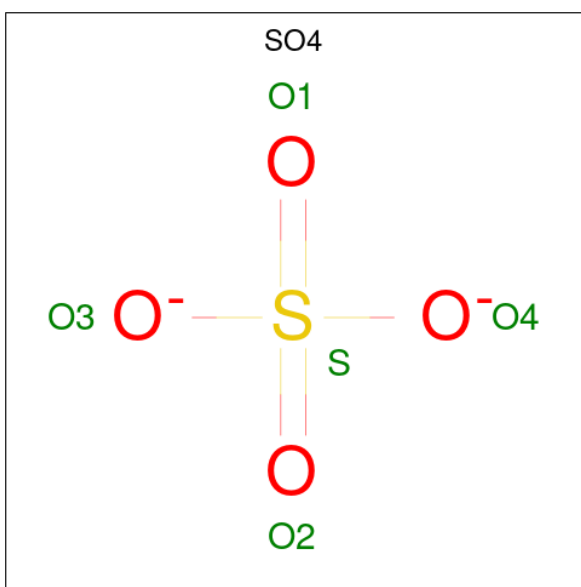
There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	ILE	-	expression tag	UNP A8AW49
C	-11	PRO	-	expression tag	UNP A8AW49
C	-10	THR	-	expression tag	UNP A8AW49
C	-9	THR	-	expression tag	UNP A8AW49
C	-8	GLU	-	expression tag	UNP A8AW49
C	-7	ASN	-	expression tag	UNP A8AW49
C	-6	LEU	-	expression tag	UNP A8AW49
C	-5	TYR	-	expression tag	UNP A8AW49
C	-4	PHE	-	expression tag	UNP A8AW49
C	-3	GLN	-	expression tag	UNP A8AW49
C	-2	GLY	-	expression tag	UNP A8AW49
C	-1	ALA	-	expression tag	UNP A8AW49
C	0	MET	-	expression tag	UNP A8AW49

- Molecule 4 is a protein called LPXTG cell wall surface protein.

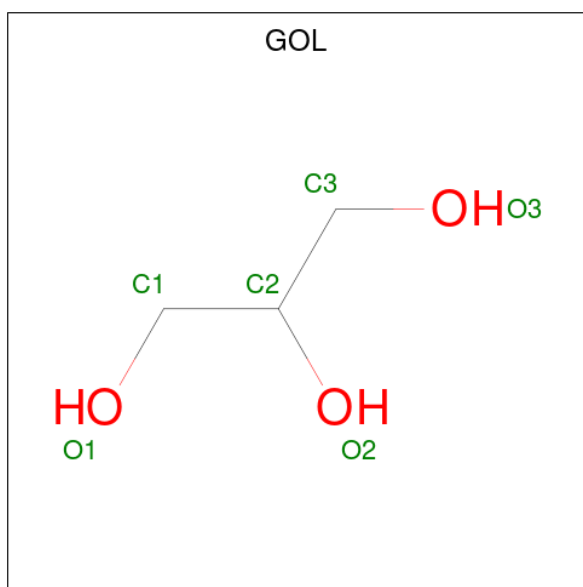
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	416	Total	C	N	O	S	0	0	0
			3264	2049	536	670	9			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



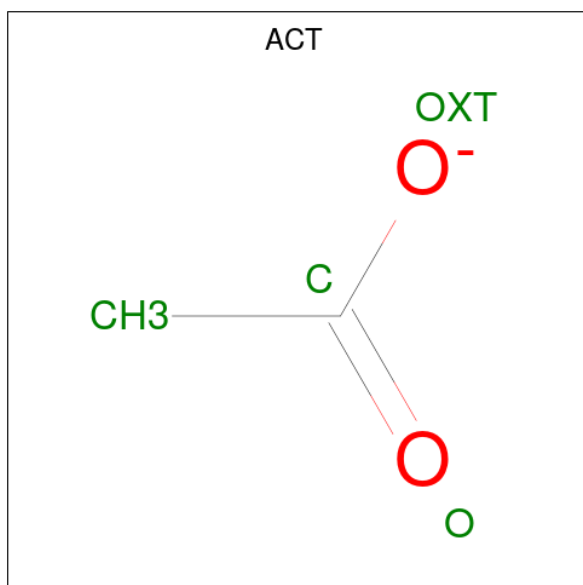
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0
8	B	1	Total Na 1 1	0	0
8	C	1	Total Na 1 1	0	0
8	D	1	Total Na 1 1	0	0

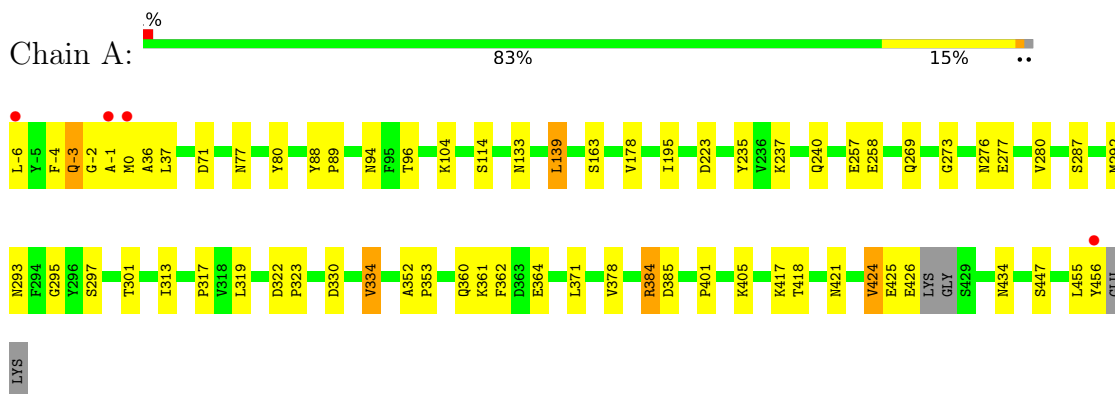
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	408	Total O 408 408	0	0
9	B	352	Total O 352 352	0	0
9	C	267	Total O 267 267	0	0
9	D	255	Total O 255 255	0	0

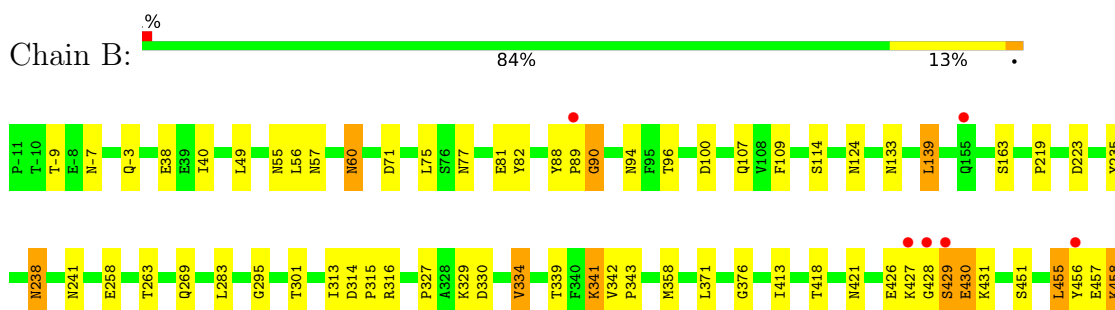
3 Residue-property plots

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.

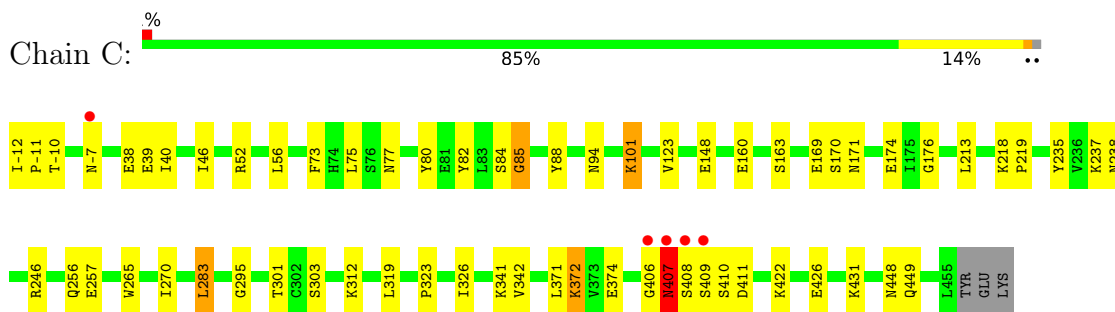
• Molecule 1: LPXTG cell wall surface protein



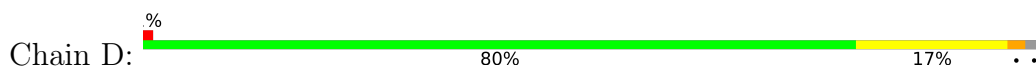
• Molecule 2: LPXTG cell wall surface protein

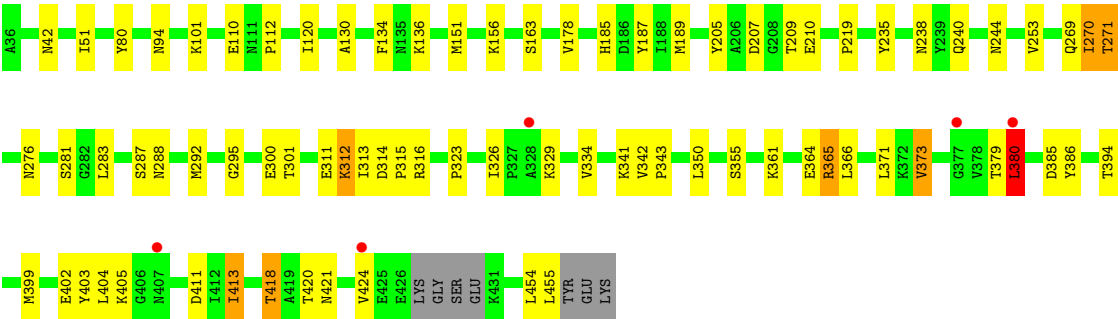


• Molecule 3: LPXTG cell wall surface protein



• Molecule 4: LPXTG cell wall surface protein





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	152.13Å 158.12Å 164.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.07 – 2.09 41.07 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.5 (41.07-2.09) 98.3 (41.07-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.08Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.179 , 0.225 0.171 , 0.215	Depositor DCC
R_{free} test set	5758 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14782	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/3407	0.82	0/4622
2	B	0.45	0/3478	0.76	0/4718
3	C	0.43	0/3455	0.75	0/4689
4	D	0.42	0/3320	0.78	0/4505
All	All	0.45	0/13660	0.78	0/18534

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 [i](#)

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	3348	0	3261	56	0
2	B	3417	0	3330	55	0
3	C	3395	0	3313	51	0
4	D	3264	0	3184	71	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	10	0	0	0	0
5	D	10	0	0	1	0
6	A	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	6	0	8	1	0
6	C	6	0	8	0	0
6	D	6	0	8	5	0
7	A	4	0	3	1	0
7	C	4	0	3	3	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	408	0	0	4	0
9	B	352	0	0	3	0
9	C	267	0	0	2	0
9	D	255	0	0	5	0
All	All	14782	0	13126	230	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 9.

All (230) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:GLU:O	2:B:458:LYS:HB2	1.57	1.01
1:A:313:ILE:H	6:A:503:GOL:H12	1.26	0.98
3:C:319:LEU:H	3:C:448:ASN:HD21	1.18	0.92
2:B:38:GLU:OE2	2:B:40:ILE:HD11	1.74	0.87
3:C:-12:ILE:O	3:C:-10:THR:HG23	1.74	0.86
3:C:169:GLU:OE2	9:C:834:HOH:O	1.95	0.85
1:A:237:LYS:NZ	1:A:293:ASN:HD21	1.78	0.82
1:A:-6:LEU:HD23	1:A:-4:PHE:H	1.45	0.81
4:D:314:ASP:OD1	4:D:315:PRO:HA	1.81	0.81
1:A:-1:ALA:O	1:A:0:MET:HG3	1.80	0.81
4:D:334:VAL:O	4:D:418:THR:HG22	1.81	0.79
1:A:421:ASN:O	1:A:424:VAL:HG22	1.82	0.79
4:D:271:THR:HG21	4:D:281:SER:OG	1.84	0.78
2:B:457:GLU:O	2:B:458:LYS:CB	2.32	0.78
2:B:427:LYS:HA	2:B:428:GLY:C	2.08	0.78
3:C:246:ARG:C	3:C:246:ARG:HD2	2.09	0.77
2:B:100:ASP:H	2:B:107:GLN:HE22	1.31	0.77
1:A:37:LEU:HD23	3:C:-7:ASN:ND2	2.00	0.76
4:D:316:ARG:HH22	6:D:503:GOL:H11	1.51	0.76
1:A:313:ILE:H	6:A:503:GOL:C1	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:246:ARG:HH21	3:C:256:GLN:HE22	1.36	0.73
4:D:366:LEU:HD13	4:D:418:THR:HG21	1.71	0.73
1:A:313:ILE:N	6:A:503:GOL:H12	2.04	0.72
3:C:73:PHE:HE1	3:C:75:LEU:HD11	1.58	0.69
2:B:334:VAL:HG22	2:B:418:THR:OG1	1.92	0.69
4:D:420:THR:HB	4:D:424:VAL:HG11	1.75	0.68
3:C:38:GLU:OE2	3:C:40:ILE:HD11	1.94	0.67
4:D:373:VAL:HG22	4:D:380:LEU:HD22	1.76	0.66
4:D:270:ILE:HD13	4:D:271:THR:N	2.11	0.66
4:D:316:ARG:HH22	6:D:503:GOL:C1	2.08	0.66
4:D:210:GLU:CD	4:D:210:GLU:H	2.04	0.65
2:B:371:LEU:HD12	2:B:371:LEU:C	2.22	0.64
2:B:427:LYS:HG2	2:B:429:SER:HB2	1.80	0.64
2:B:429:SER:OG	2:B:430:GLU:HA	1.98	0.63
3:C:56:LEU:H	3:C:171:ASN:HB3	1.64	0.62
1:A:-1:ALA:O	1:A:0:MET:CG	2.47	0.62
4:D:421:ASN:O	4:D:424:VAL:HG22	2.00	0.62
3:C:-7:ASN:HB3	3:C:39:GLU:HB2	1.81	0.62
4:D:379:THR:HG22	4:D:379:THR:O	1.99	0.62
2:B:427:LYS:HA	2:B:428:GLY:O	1.99	0.61
2:B:339:THR:HG23	2:B:413:ILE:CD1	2.31	0.61
2:B:427:LYS:HE2	2:B:429:SER:OG	2.01	0.61
3:C:303:SER:OG	7:C:504:ACT:H3	2.00	0.61
3:C:406:GLY:C	3:C:408:SER:H	2.09	0.61
2:B:426:GLU:O	2:B:428:GLY:HA3	2.01	0.60
3:C:256:GLN:HE21	3:C:265:TRP:HE1	1.49	0.60
3:C:94:ASN:HD22	3:C:163:SER:HB3	1.65	0.60
1:A:287:SER:HB2	1:A:292:MET:HE3	1.84	0.59
2:B:77:ASN:HA	2:B:88:TYR:O	2.02	0.59
3:C:341:LYS:HG2	3:C:411:ASP:OD1	2.03	0.59
3:C:371:LEU:C	3:C:371:LEU:HD12	2.28	0.59
4:D:420:THR:HB	4:D:424:VAL:CG1	2.33	0.59
4:D:373:VAL:CG2	4:D:380:LEU:HD22	2.33	0.58
4:D:402:GLU:O	4:D:405:LYS:HG2	2.03	0.58
2:B:427:LYS:HG2	2:B:429:SER:CB	2.34	0.58
2:B:57:ASN:H	2:B:60:ASN:HD21	1.52	0.58
3:C:301:THR:HG23	3:C:301:THR:O	2.02	0.58
4:D:364:GLU:O	4:D:365:ARG:HB2	2.03	0.58
4:D:402:GLU:HA	4:D:405:LYS:HE3	1.86	0.58
4:D:380:LEU:HD23	4:D:386:TYR:HD2	1.69	0.58
4:D:51:ILE:HA	9:D:831:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD21	1:A:434:ASN:HD22	1.70	0.57
4:D:219:PRO:HD2	4:D:283:LEU:O	2.05	0.57
4:D:207:ASP:HB3	4:D:209:THR:H	1.70	0.56
3:C:246:ARG:HD2	3:C:246:ARG:O	2.05	0.56
1:A:94:ASN:HD22	1:A:163:SER:HB3	1.71	0.56
4:D:244:ASN:HB2	4:D:288:ASN:ND2	2.20	0.56
1:A:114:SER:HB2	1:A:133:ASN:ND2	2.21	0.56
2:B:429:SER:CB	2:B:430:GLU:HA	2.34	0.56
3:C:407:ASN:H	3:C:407:ASN:HD22	1.52	0.56
3:C:270:ILE:HD12	3:C:270:ILE:H	1.70	0.56
1:A:371:LEU:C	1:A:371:LEU:HD12	2.31	0.55
2:B:124:ASN:HA	2:B:316:ARG:HD2	1.88	0.55
2:B:456:TYR:O	2:B:457:GLU:HG3	2.05	0.55
3:C:73:PHE:CE1	3:C:75:LEU:HD11	2.41	0.55
3:C:-11:PRO:HD3	4:D:276:ASN:OD1	2.07	0.55
3:C:256:GLN:NE2	3:C:265:TRP:HE1	2.05	0.55
1:A:77:ASN:HA	1:A:88:TYR:O	2.08	0.54
2:B:55:ASN:C	2:B:56:LEU:HD12	2.33	0.54
4:D:334:VAL:HB	4:D:418:THR:CG2	2.37	0.54
4:D:314:ASP:OD1	4:D:315:PRO:CA	2.54	0.54
4:D:287:SER:HB2	4:D:292:MET:HE3	1.90	0.53
1:A:360:GLN:HE21	1:A:361:LYS:H	1.55	0.53
2:B:109:PHE:HE1	2:B:139:LEU:HD22	1.73	0.53
3:C:319:LEU:H	3:C:448:ASN:ND2	1.98	0.53
4:D:253:VAL:HG21	4:D:269:GLN:HG2	1.91	0.53
4:D:94:ASN:HD22	4:D:163:SER:HB3	1.73	0.53
4:D:399:MET:HB2	4:D:404:LEU:HD11	1.91	0.53
1:A:237:LYS:HZ3	1:A:293:ASN:HD21	1.52	0.53
2:B:109:PHE:CE1	2:B:139:LEU:HD22	2.42	0.53
1:A:269:GLN:HG3	9:A:704:HOH:O	2.08	0.53
3:C:323:PRO:HG2	3:C:326:ILE:HG22	1.91	0.53
1:A:237:LYS:HZ2	1:A:293:ASN:HD21	1.53	0.53
4:D:329:LYS:C	4:D:424:VAL:HG21	2.34	0.52
4:D:244:ASN:HB2	4:D:288:ASN:HD22	1.75	0.52
4:D:364:GLU:O	4:D:365:ARG:CB	2.57	0.52
1:A:0:MET:SD	1:A:36:ALA:N	2.82	0.52
2:B:313:ILE:HB	6:B:503:GOL:H2	1.92	0.52
3:C:342:VAL:HG11	3:C:409:SER:HA	1.92	0.52
1:A:114:SER:OG	7:A:504:ACT:H3	2.08	0.52
4:D:120:ILE:HD13	4:D:130:ALA:HB2	1.92	0.52
1:A:258:GLU:HG3	9:C:754:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:GLN:HG2	1:A:362:PHE:CZ	2.45	0.52
1:A:-2:GLY:O	1:A:-1:ALA:C	2.53	0.51
1:A:-6:LEU:HB3	1:A:-3:GLN:HG3	1.91	0.51
4:D:373:VAL:O	4:D:380:LEU:HB3	2.11	0.51
2:B:329:LYS:NZ	2:B:458:LYS:HG2	2.26	0.51
3:C:246:ARG:NH2	3:C:256:GLN:HE22	2.08	0.51
4:D:112:PRO:HD2	4:D:134:PHE:O	2.11	0.51
1:A:257:GLU:HG3	3:C:257:GLU:OE2	2.11	0.51
3:C:77:ASN:HA	3:C:88:TYR:O	2.10	0.51
3:C:408:SER:C	3:C:410:SER:H	2.19	0.51
2:B:223:ASP:HB2	2:B:269:GLN:O	2.11	0.50
4:D:316:ARG:NH1	6:D:503:GOL:O1	2.40	0.50
1:A:384:ARG:HD2	9:A:674:HOH:O	2.11	0.50
4:D:205:TYR:HB3	4:D:207:ASP:HB2	1.94	0.50
4:D:312:LYS:HG3	9:D:821:HOH:O	2.10	0.50
1:A:301:THR:HG23	1:A:301:THR:O	2.11	0.50
2:B:235:TYR:CZ	2:B:295:GLY:HA3	2.46	0.49
4:D:341:LYS:HD2	4:D:411:ASP:OD1	2.12	0.49
1:A:-6:LEU:HD23	1:A:-4:PHE:N	2.22	0.49
2:B:330:ASP:OD1	2:B:421:ASN:HA	2.13	0.49
5:D:501:SO4:O2	9:D:748:HOH:O	2.19	0.49
2:B:81:GLU:HG2	2:B:82:TYR:CD2	2.49	0.48
4:D:311:GLU:O	6:D:503:GOL:H12	2.13	0.48
3:C:246:ARG:HH21	3:C:256:GLN:NE2	2.07	0.48
4:D:316:ARG:NH2	6:D:503:GOL:H11	2.25	0.48
4:D:380:LEU:HD23	4:D:386:TYR:CD2	2.48	0.48
4:D:380:LEU:HD11	4:D:403:TYR:CE1	2.48	0.48
2:B:314:ASP:O	2:B:341:LYS:HE2	2.13	0.48
4:D:326:ILE:HG13	4:D:454:LEU:HD23	1.96	0.48
3:C:80:TYR:OH	7:C:504:ACT:H1	2.14	0.47
1:A:240:GLN:HE22	3:C:-7:ASN:HD22	1.62	0.47
4:D:185:HIS:HA	4:D:187:TYR:CE1	2.49	0.47
4:D:380:LEU:CD2	4:D:386:TYR:HD2	2.25	0.47
3:C:94:ASN:ND2	3:C:160:GLU:OE2	2.37	0.47
1:A:425:GLU:O	1:A:426:GLU:C	2.57	0.47
2:B:57:ASN:H	2:B:60:ASN:ND2	2.12	0.47
4:D:355:SER:HA	4:D:404:LEU:HD21	1.96	0.47
1:A:71:ASP:HB3	1:A:96:THR:OG1	2.13	0.47
1:A:223:ASP:HB2	1:A:269:GLN:O	2.13	0.47
3:C:235:TYR:CZ	3:C:295:GLY:HA3	2.49	0.47
4:D:371:LEU:C	4:D:371:LEU:HD12	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:TYR:CZ	4:D:178:VAL:HG11	2.50	0.47
4:D:156:LYS:HB3	4:D:189:MET:HG2	1.97	0.47
3:C:170:SER:O	3:C:171:ASN:C	2.57	0.46
3:C:123:VAL:HG11	3:C:213:LEU:HD21	1.97	0.46
2:B:458:LYS:HD2	2:B:458:LYS:HA	1.65	0.46
1:A:114:SER:CB	1:A:133:ASN:HD22	2.29	0.46
2:B:327:PRO:HB2	2:B:329:LYS:HD2	1.97	0.46
1:A:114:SER:HB2	1:A:133:ASN:HD22	1.79	0.46
3:C:270:ILE:HD12	3:C:270:ILE:N	2.30	0.46
4:D:334:VAL:HB	4:D:418:THR:HG22	1.98	0.45
1:A:-6:LEU:HB3	1:A:-3:GLN:CG	2.45	0.45
2:B:-3:GLN:HG2	2:B:241:ASN:HD21	1.81	0.45
3:C:406:GLY:C	3:C:408:SER:N	2.72	0.45
3:C:52:ARG:HB2	3:C:312:LYS:HD2	1.99	0.45
4:D:379:THR:O	4:D:380:LEU:O	2.35	0.45
4:D:323:PRO:HG2	4:D:326:ILE:HG22	1.99	0.45
2:B:81:GLU:HG2	2:B:82:TYR:CE2	2.51	0.45
2:B:219:PRO:HD2	2:B:283:LEU:O	2.17	0.45
2:B:314:ASP:HA	2:B:315:PRO:C	2.41	0.45
3:C:246:ARG:C	3:C:246:ARG:CD	2.88	0.44
3:C:372:LYS:HE2	3:C:374:GLU:CD	2.42	0.44
4:D:235:TYR:CZ	4:D:295:GLY:HA3	2.51	0.44
4:D:413:ILE:HD12	9:D:720:HOH:O	2.17	0.44
2:B:94:ASN:HD22	2:B:163:SER:HB3	1.83	0.44
1:A:104:LYS:HE3	9:A:897:HOH:O	2.17	0.44
1:A:235:TYR:CZ	1:A:295:GLY:HA3	2.53	0.44
2:B:258:GLU:HG2	2:B:263:THR:OG1	2.18	0.44
1:A:273:GLY:O	1:A:277:GLU:HG3	2.18	0.43
3:C:101:LYS:H	3:C:101:LYS:HG2	1.53	0.43
1:A:195:ILE:O	1:A:297:SER:HA	2.18	0.43
1:A:322:ASP:HA	1:A:323:PRO:HA	1.87	0.43
4:D:373:VAL:HA	4:D:413:ILE:O	2.17	0.43
4:D:379:THR:O	4:D:380:LEU:C	2.61	0.43
4:D:94:ASN:ND2	4:D:163:SER:HB3	2.33	0.43
4:D:238:ASN:OD1	4:D:240:GLN:NE2	2.52	0.43
1:A:-6:LEU:HD22	1:A:-3:GLN:HG2	2.00	0.43
1:A:139:LEU:HD12	1:A:195:ILE:HG22	1.99	0.42
4:D:301:THR:HG23	4:D:301:THR:O	2.19	0.42
3:C:341:LYS:HG2	3:C:411:ASP:CG	2.44	0.42
1:A:317:PRO:HB2	1:A:447:SER:HB3	2.00	0.42
2:B:358:MET:SD	2:B:358:MET:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:364:GLU:HG2	9:D:760:HOH:O	2.19	0.42
3:C:219:PRO:HD2	3:C:283:LEU:O	2.20	0.42
1:A:80:TYR:CZ	1:A:178:VAL:HG11	2.55	0.42
2:B:427:LYS:CE	2:B:429:SER:OG	2.66	0.42
2:B:455:LEU:HD12	2:B:455:LEU:HA	1.85	0.42
1:A:360:GLN:HE21	1:A:361:LYS:N	2.17	0.42
1:A:360:GLN:CG	1:A:362:PHE:CZ	3.02	0.42
1:A:401:PRO:O	1:A:405:LYS:HG3	2.20	0.42
2:B:376:GLY:HA2	9:B:734:HOH:O	2.20	0.42
3:C:82:TYR:O	3:C:85:GLY:N	2.53	0.42
2:B:89:PRO:HA	2:B:90:GLY:HA2	1.69	0.42
4:D:42:ASN:OD1	4:D:42:ASN:C	2.62	0.42
4:D:101:LYS:HE2	4:D:151:MET:O	2.20	0.42
1:A:334:VAL:HG22	1:A:418:THR:OG1	2.19	0.42
2:B:71:ASP:HB3	2:B:96:THR:OG1	2.20	0.41
2:B:430:GLU:CD	2:B:431:LYS:N	2.78	0.41
4:D:361:LYS:HD3	4:D:394:THR:OG1	2.19	0.41
1:A:417:LYS:HD2	9:A:842:HOH:O	2.19	0.41
1:A:88:TYR:HA	1:A:89:PRO:HD3	1.80	0.41
2:B:316:ARG:CZ	9:B:833:HOH:O	2.68	0.41
1:A:384:ARG:HG2	1:A:385:ASP:CG	2.46	0.41
1:A:455:LEU:O	1:A:456:TYR:HB2	2.21	0.41
3:C:176:GLY:HA3	3:C:303:SER:HB3	2.03	0.41
1:A:276:ASN:O	1:A:280:VAL:HB	2.21	0.41
1:A:352:ALA:HA	1:A:353:PRO:HD3	1.90	0.41
4:D:365:ARG:O	4:D:420:THR:HA	2.21	0.41
4:D:300:GLU:HG3	4:D:301:THR:HG22	2.01	0.41
2:B:-9:THR:HG22	9:B:867:HOH:O	2.21	0.41
2:B:301:THR:HG23	2:B:301:THR:O	2.20	0.41
2:B:315:PRO:HD2	2:B:341:LYS:HG3	2.03	0.41
1:A:330:ASP:OD1	1:A:421:ASN:HA	2.22	0.41
2:B:114:SER:HB2	2:B:133:ASN:OD1	2.20	0.41
4:D:313:ILE:HB	4:D:316:ARG:NH1	2.35	0.41
2:B:329:LYS:HZ3	2:B:458:LYS:HG2	1.86	0.40
3:C:46:ILE:HG22	3:C:218:LYS:HD2	2.03	0.40
4:D:342:VAL:HA	4:D:343:PRO:HD3	1.93	0.40
4:D:380:LEU:HD21	4:D:385:ASP:HB3	2.03	0.40
2:B:238:ASN:HD22	2:B:238:ASN:HA	1.69	0.40
3:C:237:LYS:HB3	3:C:237:LYS:HE2	1.90	0.40
4:D:110:GLU:OE2	4:D:136:LYS:HE2	2.22	0.40
2:B:371:LEU:C	2:B:371:LEU:CD1	2.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:TYR:OH	7:C:504:ACT:CH3	2.69	0.40
4:D:207:ASP:HB3	4:D:209:THR:HG23	2.02	0.40
2:B:235:TYR:CE2	2:B:295:GLY:HA3	2.57	0.40
2:B:342:VAL:HA	2:B:343:PRO:HD3	1.97	0.40
3:C:174:GLU:OE2	3:C:303:SER:OG	2.26	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	422/430 (98%)	403 (96%)	18 (4%)	1 (0%)	43	44
2	B	433/435 (100%)	413 (95%)	19 (4%)	1 (0%)	43	44
3	C	431/436 (99%)	407 (94%)	21 (5%)	3 (1%)	18	15
4	D	412/423 (97%)	389 (94%)	21 (5%)	2 (0%)	24	22
All	All	1698/1724 (98%)	1612 (95%)	79 (5%)	7 (0%)	30	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	365	ARG
4	D	380	LEU
3	C	407	ASN
3	C	426	GLU
1	A	364	GLU
3	C	85	GLY
2	B	90	GLY

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	377/380 (99%)	371 (98%)	6 (2%)	55	64
2	B	385/385 (100%)	372 (97%)	13 (3%)	32	35
3	C	383/386 (99%)	373 (97%)	10 (3%)	40	46
4	D	369/375 (98%)	360 (98%)	9 (2%)	43	49
All	All	1514/1526 (99%)	1476 (98%)	38 (2%)	42	48

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	GLN
1	A	139	LEU
1	A	334	VAL
1	A	378	VAL
1	A	384	ARG
1	A	424	VAL
2	B	-7	ASN
2	B	49	LEU
2	B	60	ASN
2	B	75	LEU
2	B	139	LEU
2	B	238	ASN
2	B	334	VAL
2	B	341	LYS
2	B	429	SER
2	B	430	GLU
2	B	451	SER
2	B	455	LEU
2	B	458	LYS
3	C	84	SER
3	C	101	LYS
3	C	148	GLU
3	C	238	ASN
3	C	283	LEU

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Mol	Chain	Res	Type
3	C	372	LYS
3	C	407	ASN
3	C	422	LYS
3	C	431	LYS
3	C	449	GLN
4	D	270	ILE
4	D	271	THR
4	D	312	LYS
4	D	350	LEU
4	D	373	VAL
4	D	380	LEU
4	D	413	ILE
4	D	418	THR
4	D	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	111	ASN
1	A	133	ASN
1	A	293	ASN
1	A	360	GLN
1	A	407	ASN
1	A	434	ASN
2	B	60	ASN
2	B	94	ASN
2	B	107	GLN
2	B	152	ASN
2	B	185	HIS
2	B	238	ASN
2	B	241	ASN
3	C	-7	ASN
3	C	59	ASN
3	C	94	ASN
3	C	105	GLN
3	C	238	ASN
3	C	250	ASN
3	C	256	GLN
3	C	293	ASN
3	C	381	GLN
3	C	407	ASN

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Mol	Chain	Res	Type
3	C	448	ASN
3	C	449	GLN
4	D	94	ASN
4	D	229	ASN
4	D	288	ASN
4	D	381	GLN
4	D	393	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\# Z > 2$
5	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.14	0
6	GOL	A	503	-	5,5,5	0.39	0	5,5,5	0.59	0
6	GOL	B	503	-	5,5,5	0.32	0	5,5,5	0.68	0
5	SO4	B	501	-	4,4,4	0.20	0	6,6,6	0.20	0
7	ACT	C	504	-	3,3,3	0.87	0	3,3,3	0.81	0
5	SO4	A	502	8	4,4,4	0.22	0	6,6,6	0.15	0
5	SO4	C	502	8	4,4,4	0.24	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	C	503	-	5,5,5	0.31	0	5,5,5	0.68	0
5	SO4	A	501	-	4,4,4	0.20	0	6,6,6	0.15	0
7	ACT	A	504	-	3,3,3	0.92	0	3,3,3	1.46	0
5	SO4	D	502	-	4,4,4	0.36	0	6,6,6	0.27	0
5	SO4	B	502	8	4,4,4	0.24	0	6,6,6	0.14	0
6	GOL	D	503	-	5,5,5	0.30	0	5,5,5	0.67	0
5	SO4	D	501	-	4,4,4	0.18	0	6,6,6	0.19	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
6	GOL	C	503	-	-	2/4/4/4	-
6	GOL	D	503	-	-	2/4/4/4	-
6	GOL	A	503	-	-	2/4/4/4	-
6	GOL	B	503	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	503	GOL	O1-C1-C2-C3
6	B	503	GOL	O1-C1-C2-O2
6	B	503	GOL	O1-C1-C2-C3
6	B	503	GOL	C1-C2-C3-O3
6	C	503	GOL	O1-C1-C2-C3
6	D	503	GOL	O1-C1-C2-C3
6	A	503	GOL	O1-C1-C2-O2
6	B	503	GOL	O2-C2-C3-O3
6	C	503	GOL	O1-C1-C2-O2
6	D	503	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	503	GOL	3	0
6	B	503	GOL	1	0
7	C	504	ACT	3	0
7	A	504	ACT	1	0
6	D	503	GOL	5	0
5	D	501	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	426/430 (99%)	-0.38	4 (0%) 81 83	12, 25, 45, 89	0
2	B	435/435 (100%)	-0.32	6 (1%) 73 75	14, 26, 48, 112	0
3	C	433/436 (99%)	-0.30	5 (1%) 76 78	14, 28, 49, 89	0
4	D	416/423 (98%)	-0.11	5 (1%) 76 78	16, 29, 53, 88	0
All	All	1710/1724 (99%)	-0.28	20 (1%) 76 78	12, 27, 49, 112	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	428	GLY	6.0
1	A	456	TYR	5.1
2	B	456	TYR	5.0
4	D	424	VAL	4.6
2	B	427	LYS	3.9
1	A	0	MET	3.8
2	B	429	SER	3.8
2	B	89	PRO	3.1
3	C	406	GLY	3.0
3	C	408	SER	2.9
4	D	377	GLY	2.6
1	A	-1	ALA	2.6
4	D	328	ALA	2.5
1	A	-6	LEU	2.5
3	C	407	ASN	2.4
4	D	380	LEU	2.3
3	C	409	SER	2.3
4	D	407	ASN	2.1
3	C	-7	ASN	2.1
2	B	155	GLN	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
8	NA	C	505	1/1	0.65	0.25	40,40,40,40	1
8	NA	D	504	1/1	0.66	0.29	49,49,49,49	0
5	SO4	C	502	5/5	0.81	0.12	54,60,74,75	5
7	ACT	C	504	4/4	0.81	0.14	25,37,52,55	0
6	GOL	C	503	6/6	0.82	0.17	45,51,63,75	0
5	SO4	D	502	5/5	0.83	0.15	43,60,74,78	5
6	GOL	D	503	6/6	0.84	0.16	33,47,52,58	6
7	ACT	A	504	4/4	0.86	0.14	28,30,37,55	4
5	SO4	B	501	5/5	0.87	0.14	38,48,55,79	5
5	SO4	B	502	5/5	0.89	0.14	29,42,53,57	5
5	SO4	C	501	5/5	0.89	0.12	35,38,45,47	5
6	GOL	A	503	6/6	0.89	0.14	20,28,30,32	6
5	SO4	D	501	5/5	0.91	0.15	35,36,47,61	5
6	GOL	B	503	6/6	0.93	0.10	20,27,32,33	6
5	SO4	A	502	5/5	0.95	0.08	23,28,36,44	5
8	NA	A	505	1/1	0.95	0.05	29,29,29,29	0
5	SO4	A	501	5/5	0.96	0.07	27,27,36,42	5
8	NA	B	504	1/1	0.97	0.07	31,31,31,31	1

6.5 Other polymers [i](#)

There are no such residues in this entry.