Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2024 – 04:09 PM EST

PDB ID	:	9D29
Title	:	Crystal structure of (+)-sabinene synthase from Thuja plicata: condition 2
Authors	:	Gaynes, M.N.; Christianson, D.W.
Deposited on	:	2024-08-08
Resolution	:	2.72 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:

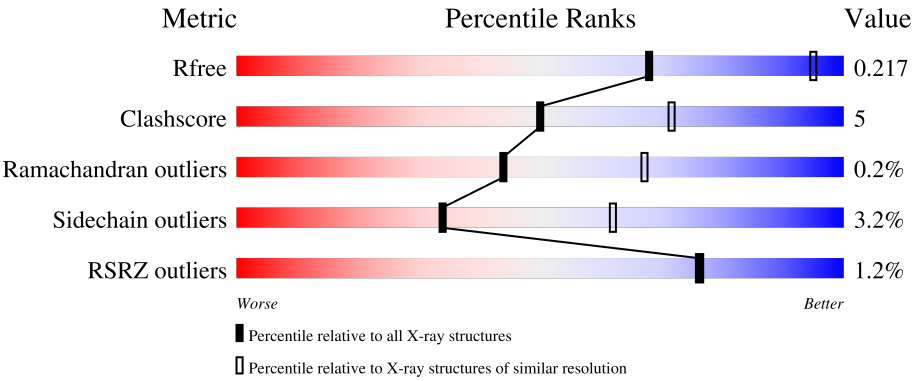
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.72 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}	164625	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

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	554	81% 13% 6%
1	B	554	80% 12% 8%
1	C	554	82% 12% 5%
1	D	554	79% 12% 8%

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	704	-	-	X	-
3	GOL	B	703	-	-	X	-
3	GOL	B	704	-	-	X	-

2 Entry composition

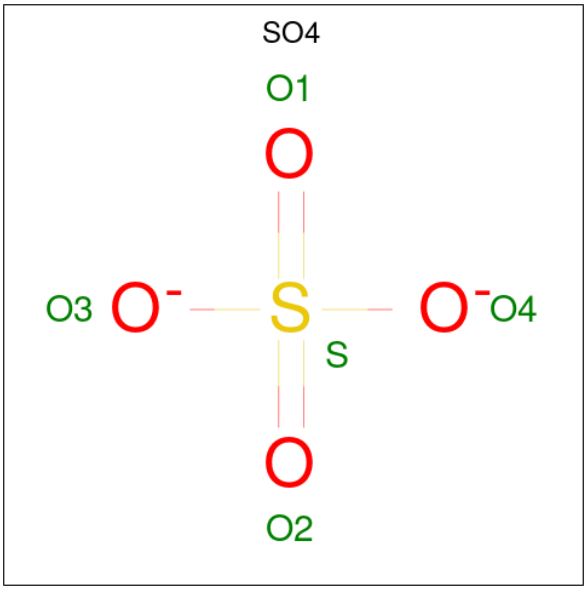
There are 4 unique types of molecules in this entry. The entry contains 16364 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sabinene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			4056	2587	687	762	20			
1	B	512	Total	C	N	O	S	0	0	0
			3970	2537	668	745	20			
1	C	529	Total	C	N	O	S	0	0	0
			4126	2625	700	781	20			
1	D	512	Total	C	N	O	S	0	0	0
			3973	2539	670	744	20			

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



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

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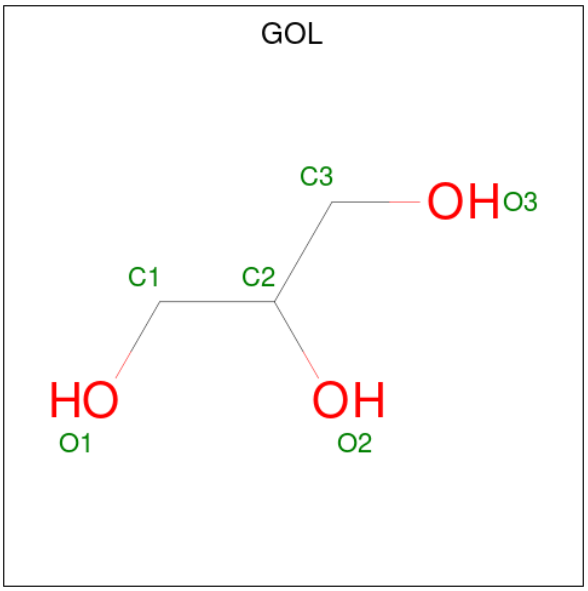
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 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 C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	24	Total O 24 24	0	0
4	B	18	Total O 18 18	0	0
4	C	28	Total O 28 28	0	0

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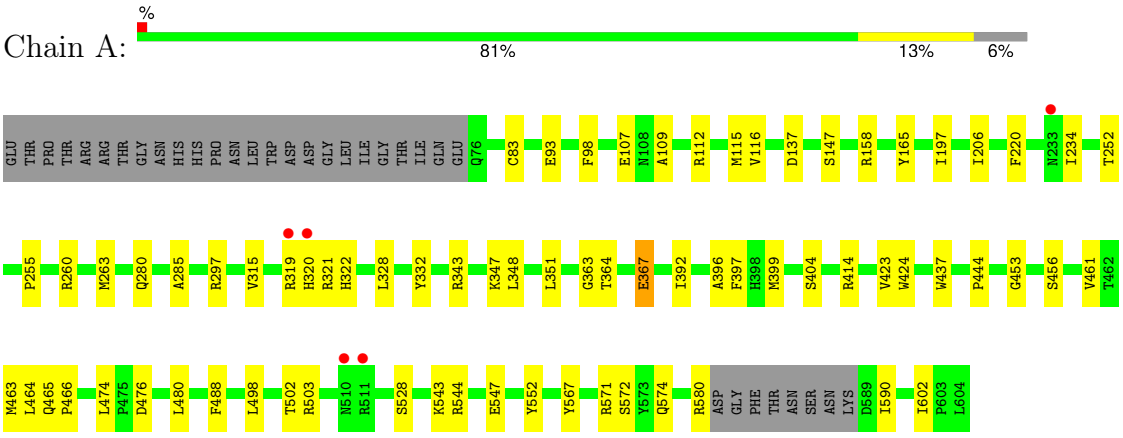
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	30	Total O 30 30	0	0

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.

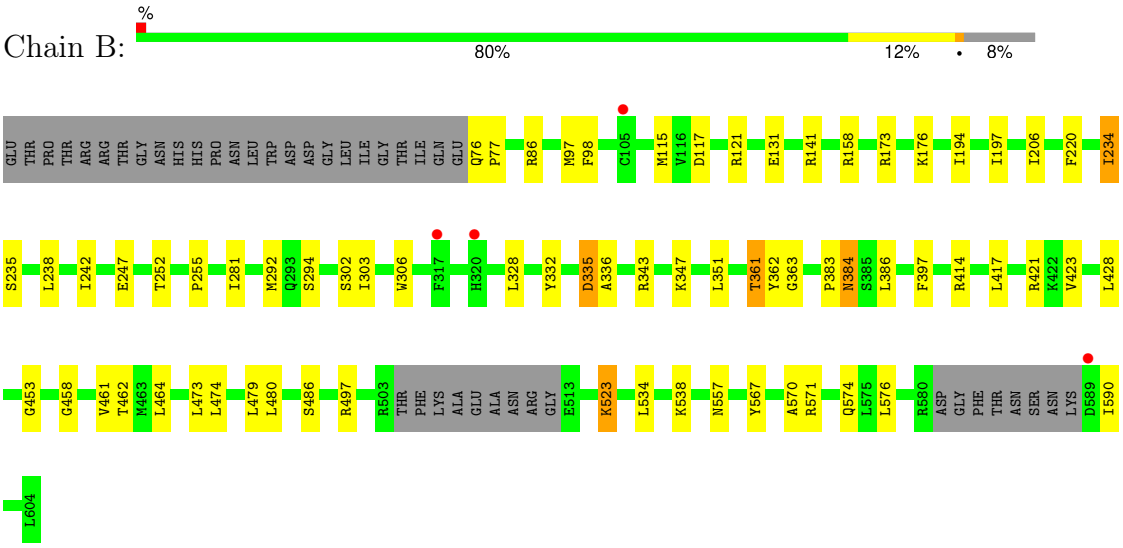
• Molecule 1: Sabinene synthase

Chain A:



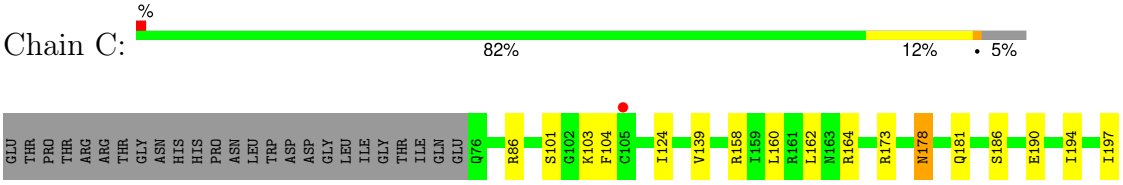
• Molecule 1: Sabinene synthase

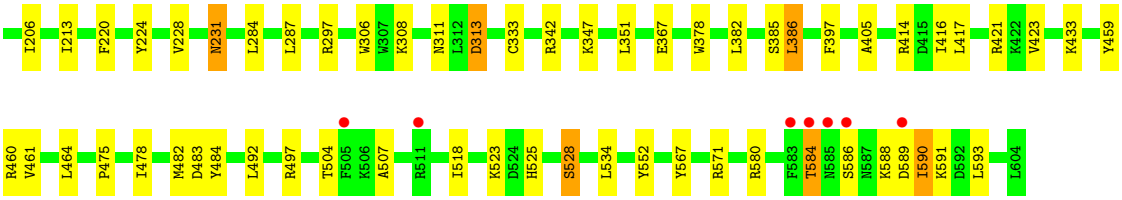
Chain B:



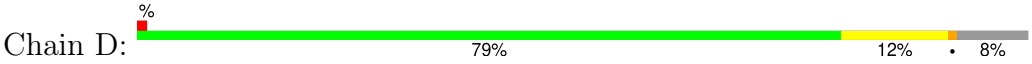
• Molecule 1: Sabinene synthase

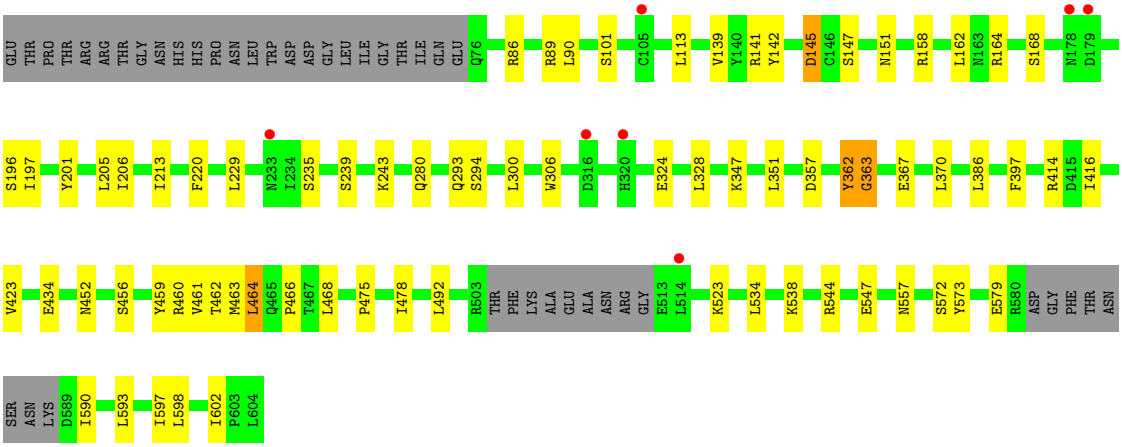
Chain C:





• Molecule 1: Sabinene synthase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	271.99Å 88.42Å 190.65Å 90.00° 134.25° 90.00°	Depositor
Resolution (Å)	29.13 – 2.72 29.13 – 2.72	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.13-2.72) 98.4 (29.13-2.72)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.178 , 0.217 0.178 , 0.217	Depositor DCC
R_{free} test set	85049 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 27.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h+2*l,k,-h-l 0.000 for h,-k,-h-l 0.000 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16364	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2128e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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, 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	0.42	0/4145	0.57	0/5640
1	B	0.42	0/4057	0.57	0/5525
1	C	0.44	0/4217	0.57	0/5737
1	D	0.43	0/4061	0.58	0/5527
All	All	0.43	0/16480	0.57	0/22429

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4056	0	3816	43	0
1	B	3970	0	3726	45	0
1	C	4126	0	3887	42	0
1	D	3973	0	3716	35	0
2	A	15	0	0	0	0
2	B	25	0	0	0	0
2	C	25	0	0	1	0
2	D	20	0	0	2	0
3	A	12	0	16	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	24	10	0
3	C	18	0	24	1	0
3	D	6	0	8	1	0
4	A	24	0	0	0	0
4	B	18	0	0	0	0
4	C	28	0	0	0	0
4	D	30	0	0	0	0
All	All	16364	0	15217	163	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 5.

All (163) 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:423:VAL:HG21	1:A:464:LEU:HD22	1.47	0.93
1:D:423:VAL:HG21	1:D:464:LEU:HD22	1.67	0.76
1:C:423:VAL:HG21	1:C:464:LEU:HD22	1.67	0.76
1:B:158:ARG:HG3	1:B:206:ILE:HD13	1.70	0.72
1:A:503:ARG:HH12	3:A:704:GOL:H12	1.56	0.70
1:B:158:ARG:HE	3:B:704:GOL:H11	1.55	0.70
1:C:584:THR:HG23	1:D:164:ARG:HB2	1.75	0.68
1:D:423:VAL:HG12	1:D:461:VAL:HG12	1.77	0.67
1:B:423:VAL:HG21	1:B:464:LEU:HD22	1.77	0.67
1:C:351:LEU:HD13	1:C:397:PHE:HA	1.76	0.66
1:B:351:LEU:HD13	1:B:397:PHE:HA	1.79	0.64
1:B:384:ASN:N	1:B:384:ASN:OD1	2.30	0.62
1:A:414:ARG:NH2	1:A:474:LEU:O	2.31	0.61
1:B:383:PRO:HG2	1:B:386:LEU:HD13	1.82	0.61
1:D:306:TRP:CE2	1:D:347:LYS:HD3	2.35	0.61
1:D:475:PRO:HD2	1:D:478:ILE:HD12	1.83	0.61
1:B:567:TYR:CE2	1:B:571:ARG:HD2	2.37	0.60
1:A:567:TYR:CE2	1:A:571:ARG:HD2	2.37	0.60
1:D:158:ARG:HD2	1:D:206:ILE:HD13	1.84	0.60
1:C:423:VAL:HG12	1:C:461:VAL:HG12	1.84	0.59
1:B:423:VAL:HG12	1:B:461:VAL:HG12	1.82	0.59
1:A:315:VAL:HG23	1:A:392:ILE:HD11	1.84	0.59
1:A:503:ARG:HH12	3:A:704:GOL:C1	2.15	0.59
1:B:335:ASP:HA	3:B:703:GOL:H2	1.86	0.58
1:C:158:ARG:HG3	1:C:206:ILE:HD13	1.86	0.58
1:B:336:ALA:H	3:B:703:GOL:H2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:TYR:CE2	1:C:571:ARG:HD2	2.39	0.57
1:A:580:ARG:HH21	3:A:704:GOL:H11	1.70	0.57
1:C:518:ILE:HD11	1:C:534:LEU:HD13	1.86	0.56
1:D:300:LEU:HD22	1:D:598:LEU:HD13	1.88	0.56
1:D:573:TYR:CE1	3:D:702:GOL:H11	2.41	0.55
1:C:162:LEU:HD21	1:C:206:ILE:HG12	1.88	0.55
1:B:361:THR:OG1	1:B:362:TYR:N	2.40	0.54
1:C:590:ILE:HG13	1:C:590:ILE:O	2.08	0.54
1:B:336:ALA:H	3:B:703:GOL:H11	1.73	0.53
1:A:351:LEU:HD13	1:A:397:PHE:HA	1.90	0.53
1:D:462:THR:O	1:D:466:PRO:HG2	2.09	0.53
1:C:417:LEU:O	1:C:421:ARG:HG3	2.09	0.53
1:D:351:LEU:HD13	1:D:397:PHE:HA	1.91	0.53
1:A:260:ARG:CZ	1:A:602:ILE:HD12	2.39	0.52
1:C:367:GLU:HG2	1:C:386:LEU:HD23	1.91	0.52
1:C:483:ASP:CG	1:C:484:TYR:H	2.12	0.52
1:A:396:ALA:HA	1:A:399:MET:HE2	1.92	0.52
1:A:348:LEU:HD12	1:A:466:PRO:HD3	1.92	0.51
1:C:224:TYR:O	1:C:228:VAL:HG23	2.10	0.51
1:D:197:ILE:HD12	1:D:220:PHE:HE2	1.75	0.51
1:B:234:ILE:HG13	1:B:238:LEU:HD23	1.92	0.51
1:D:357:ASP:HB3	1:D:362:TYR:HE2	1.74	0.51
1:B:197:ILE:HD12	1:B:220:PHE:HE2	1.75	0.51
1:B:292:MET:SD	3:B:703:GOL:H12	2.51	0.51
1:B:303:ILE:HD11	1:B:343:ARG:HA	1.91	0.51
1:A:263:MET:HE1	1:A:285:ALA:O	2.10	0.50
1:C:475:PRO:HD2	1:C:478:ILE:HG13	1.93	0.50
1:A:158:ARG:HG3	1:A:206:ILE:HD13	1.92	0.50
1:A:476:ASP:O	1:A:480:LEU:HG	2.11	0.50
1:B:328:LEU:HD11	1:B:576:LEU:HD13	1.94	0.50
1:D:544:ARG:NH1	1:D:547:GLU:OE2	2.45	0.50
1:B:173:ARG:HH12	1:B:176:LYS:NZ	2.10	0.49
1:D:459:TYR:OH	1:D:492:LEU:HD13	2.12	0.49
1:A:260:ARG:NH1	1:A:602:ILE:HD12	2.28	0.49
1:C:382:LEU:HB3	1:C:386:LEU:HD13	1.96	0.48
1:A:503:ARG:NH1	3:A:704:GOL:H12	2.27	0.48
1:B:255:PRO:HD2	1:B:332:TYR:HB3	1.96	0.48
1:A:423:VAL:HG12	1:A:461:VAL:HG12	1.95	0.48
1:B:158:ARG:NE	3:B:704:GOL:H11	2.28	0.48
1:C:173:ARG:HG2	1:C:213:ILE:HD13	1.96	0.48
1:C:306:TRP:CE2	1:C:347:LYS:HD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LEU:HB2	1:D:139:VAL:HG21	1.96	0.48
1:B:336:ALA:H	3:B:703:GOL:C2	2.27	0.48
1:B:523:LYS:HE3	1:C:173:ARG:O	2.14	0.47
1:C:589:ASP:C	1:C:591:LYS:N	2.67	0.47
1:C:378:TRP:CD2	1:C:421:ARG:HD2	2.49	0.47
1:A:543:LYS:O	1:A:547:GLU:HG3	2.15	0.47
1:C:525:HIS:O	1:C:528:SER:OG	2.32	0.47
1:A:98:PHE:CE1	1:A:115:MET:HG2	2.49	0.47
1:B:576:LEU:HD12	1:B:590:ILE:HD13	1.95	0.47
1:D:145:ASP:N	1:D:145:ASP:OD1	2.47	0.47
1:A:498:LEU:O	1:A:502:THR:HG23	2.14	0.47
1:A:437:TRP:CE3	1:A:444:PRO:HG3	2.51	0.46
1:A:437:TRP:CZ3	1:A:444:PRO:HG3	2.50	0.46
1:D:324:GLU:HG2	1:D:590:ILE:HG13	1.97	0.46
1:B:98:PHE:CG	1:B:131:GLU:HB3	2.50	0.46
1:C:124:ILE:HD12	1:C:284:LEU:HD23	1.98	0.46
1:D:293:GLN:HG3	1:D:597:ILE:O	2.15	0.46
1:A:488:PHE:HE1	1:A:552:TYR:HB2	1.81	0.46
1:A:580:ARG:NH2	3:A:704:GOL:H11	2.30	0.46
1:A:255:PRO:HD2	1:A:332:TYR:HB3	1.97	0.46
1:B:98:PHE:CE1	1:B:115:MET:HG2	2.51	0.46
1:D:141:ARG:HD2	1:D:142:TYR:CE1	2.49	0.46
1:B:194:ILE:HG21	1:B:242:ILE:HD11	1.98	0.45
1:A:197:ILE:HD12	1:A:220:PHE:HE2	1.81	0.45
1:B:117:ASP:O	1:B:121:ARG:HG3	2.15	0.45
1:A:320:HIS:HA	1:A:322:HIS:CE1	2.52	0.45
1:B:121:ARG:HG2	3:B:704:GOL:H32	1.98	0.45
1:B:306:TRP:CE2	1:B:347:LYS:HD2	2.51	0.45
1:B:570:ALA:O	1:B:574:GLN:HG2	2.17	0.45
1:B:158:ARG:HE	3:B:704:GOL:C1	2.27	0.45
1:A:112:ARG:O	1:A:116:VAL:HG23	2.15	0.45
1:B:473:LEU:O	1:B:474:LEU:HD23	2.17	0.45
1:A:107:GLU:OE2	1:A:109:ALA:HB3	2.16	0.45
1:D:328:LEU:HD22	1:D:572:SER:HB2	1.99	0.44
1:D:229:LEU:HD13	1:D:243:LYS:HE2	1.99	0.44
1:C:190:GLU:O	1:C:194:ILE:HG13	2.17	0.44
1:C:580:ARG:O	1:C:586:SER:HA	2.18	0.44
1:B:458:GLY:O	1:B:462:THR:HG23	2.18	0.44
1:B:534:LEU:HG	1:B:538:LYS:HE2	2.00	0.44
1:D:151:ASN:HB2	1:D:196:SER:OG	2.18	0.44
1:C:86:ARG:HD3	1:C:287:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ILE:HG22	2:D:705:SO4:O3	2.18	0.43
1:A:453:GLY:HA2	1:A:456:SER:OG	2.19	0.43
1:C:588:LYS:C	1:C:590:ILE:N	2.70	0.43
1:A:137:ASP:OD1	1:A:165:TYR:OH	2.29	0.43
1:B:336:ALA:H	3:B:703:GOL:C1	2.31	0.43
1:B:557:ASN:OD1	1:B:557:ASN:N	2.48	0.43
1:D:434:GLU:HG3	1:D:452:ASN:ND2	2.33	0.43
1:B:453:GLY:HA2	1:B:497:ARG:HH21	1.83	0.43
1:C:405:ALA:HA	1:C:416:ILE:HD11	2.00	0.43
1:D:201:TYR:O	1:D:205:LEU:HG	2.18	0.43
1:D:423:VAL:HG22	1:D:460:ARG:NH2	2.34	0.43
1:C:173:ARG:HD2	2:C:701:SO4:O1	2.19	0.42
1:A:343:ARG:O	1:A:347:LYS:HG3	2.20	0.42
1:B:428:LEU:HD23	1:B:428:LEU:HA	1.79	0.42
1:C:333:CYS:O	1:C:342:ARG:HD3	2.20	0.42
1:D:363:GLY:HA2	1:D:367:GLU:OE1	2.18	0.42
1:A:234:ILE:HD13	1:A:234:ILE:HG21	1.81	0.42
1:D:534:LEU:HD22	1:D:538:LYS:HE3	2.01	0.42
1:C:504:THR:HA	1:C:507:ALA:HB2	2.01	0.42
1:D:239:SER:O	1:D:243:LYS:HG3	2.19	0.42
1:A:252:THR:HG22	1:A:574:GLN:HB3	2.01	0.42
1:C:497:ARG:HH12	3:C:705:GOL:H2	1.84	0.42
1:A:158:ARG:HE	3:A:703:GOL:HO2	1.62	0.42
1:A:93:GLU:OE1	1:A:280:GLN:NE2	2.46	0.42
1:B:97:MET:HE1	1:B:281:ILE:HD11	2.02	0.42
1:C:164:ARG:NH1	1:C:552:TYR:O	2.53	0.42
1:B:76:GLN:HA	1:B:77:PRO:HD2	1.96	0.41
1:C:433:LYS:HE2	1:C:433:LYS:HB3	1.71	0.41
1:C:459:TYR:OH	1:C:492:LEU:HD13	2.19	0.41
1:A:404:SER:HB3	1:A:465:GLN:NE2	2.36	0.41
1:B:417:LEU:O	1:B:421:ARG:HG3	2.19	0.41
1:D:229:LEU:HD11	1:D:243:LYS:HG2	2.01	0.41
1:B:252:THR:HG22	1:B:574:GLN:HB3	2.02	0.41
1:C:423:VAL:HG22	1:C:460:ARG:NH2	2.35	0.41
1:A:544:ARG:NH1	1:A:547:GLU:OE2	2.53	0.41
1:C:231:ASN:O	1:C:231:ASN:ND2	2.52	0.41
1:A:328:LEU:HD22	1:A:572:SER:HB2	2.02	0.41
1:A:397:PHE:HE2	1:A:424:TRP:CE3	2.38	0.41
1:C:534:LEU:HD12	1:C:534:LEU:HA	1.89	0.41
1:B:480:LEU:O	1:B:486:SER:HB3	2.21	0.41
1:C:103:LYS:O	1:C:104:PHE:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ASN:O	1:C:181:GLN:HG2	2.20	0.41
1:C:139:VAL:HG12	1:C:160:LEU:HD11	2.03	0.41
1:B:335:ASP:OD1	1:B:335:ASP:N	2.53	0.41
1:C:308:LYS:HA	1:C:313:ASP:OD2	2.20	0.41
1:D:90:LEU:HD22	1:D:280:GLN:HB3	2.03	0.41
1:D:162:LEU:HD21	1:D:206:ILE:HG12	2.03	0.41
1:C:197:ILE:HD12	1:C:220:PHE:HE2	1.85	0.41
1:A:364:THR:H	1:A:367:GLU:CD	2.24	0.40
1:B:414:ARG:NH2	1:B:474:LEU:O	2.50	0.40
1:A:319:ARG:C	1:A:321:ARG:H	2.24	0.40
1:A:590:ILE:HD12	1:A:590:ILE:HA	1.87	0.40
1:D:89:ARG:NH2	2:D:701:SO4:O1	2.54	0.40
1:D:416:ILE:HD13	1:D:468:LEU:HD13	2.03	0.40
1:D:598:LEU:HA	1:D:598:LEU:HD23	1.90	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	517/554 (93%)	496 (96%)	20 (4%)	1 (0%)	44	67
1	B	506/554 (91%)	485 (96%)	20 (4%)	1 (0%)	44	67
1	C	527/554 (95%)	504 (96%)	22 (4%)	1 (0%)	44	67
1	D	506/554 (91%)	482 (95%)	22 (4%)	2 (0%)	30	53
All	All	2056/2216 (93%)	1967 (96%)	84 (4%)	5 (0%)	44	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	363	GLY

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Mol	Chain	Res	Type
1	D	464	LEU
1	A	363	GLY
1	C	584	THR
1	B	363	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	406/487 (83%)	400 (98%)	6 (2%)	60	82
1	B	397/487 (82%)	385 (97%)	12 (3%)	36	64
1	C	417/487 (86%)	402 (96%)	15 (4%)	30	57
1	D	394/487 (81%)	376 (95%)	18 (5%)	23	47
All	All	1614/1948 (83%)	1563 (97%)	51 (3%)	34	62

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	CYS
1	A	147	SER
1	A	297	ARG
1	A	367	GLU
1	A	463	MET
1	A	528	SER
1	B	86	ARG
1	B	141	ARG
1	B	234	ILE
1	B	235	SER
1	B	247	GLU
1	B	294	SER
1	B	302	SER
1	B	335	ASP
1	B	361	THR
1	B	384	ASN
1	B	479	LEU

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Mol	Chain	Res	Type
1	B	523	LYS
1	C	101	SER
1	C	178	ASN
1	C	186	SER
1	C	231	ASN
1	C	297	ARG
1	C	311	ASN
1	C	313	ASP
1	C	385	SER
1	C	386	LEU
1	C	414	ARG
1	C	482	MET
1	C	523	LYS
1	C	528	SER
1	C	590	ILE
1	C	593	LEU
1	D	86	ARG
1	D	101	SER
1	D	145	ASP
1	D	147	SER
1	D	168	SER
1	D	235	SER
1	D	294	SER
1	D	362	TYR
1	D	370	LEU
1	D	386	LEU
1	D	414	ARG
1	D	456	SER
1	D	463	MET
1	D	523	LYS
1	D	557	ASN
1	D	579	GLU
1	D	593	LEU
1	D	602	ILE

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

Mol	Chain	Res	Type
1	A	398	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

26 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	$\#\|Z\| > 2$
2	SO4	D	705	-	4,4,4	0.78	0	6,6,6	0.50	0
3	GOL	B	704	-	5,5,5	0.59	0	5,5,5	0.27	0
3	GOL	A	704	-	5,5,5	0.62	0	5,5,5	0.40	0
2	SO4	B	706	-	4,4,4	0.94	0	6,6,6	0.67	0
3	GOL	C	703	-	5,5,5	0.50	0	5,5,5	0.59	0
2	SO4	A	705	-	4,4,4	0.94	0	6,6,6	0.66	0
2	SO4	C	702	-	4,4,4	0.92	0	6,6,6	0.49	0
3	GOL	D	702	-	5,5,5	0.49	0	5,5,5	0.51	0
3	GOL	A	703	-	5,5,5	0.66	0	5,5,5	0.67	0
2	SO4	A	702	-	4,4,4	0.87	0	6,6,6	0.54	0
3	GOL	C	705	-	5,5,5	0.58	0	5,5,5	0.36	0
3	GOL	B	703	-	5,5,5	0.61	0	5,5,5	0.38	0
2	SO4	B	701	-	4,4,4	0.86	0	6,6,6	0.58	0
3	GOL	C	704	-	5,5,5	0.48	0	5,5,5	0.40	0
2	SO4	C	701	-	4,4,4	0.89	0	6,6,6	0.56	0
2	SO4	D	701	-	4,4,4	0.78	0	6,6,6	0.58	0
2	SO4	A	701	-	4,4,4	0.94	0	6,6,6	0.61	0
2	SO4	C	708	-	4,4,4	0.91	0	6,6,6	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	705	-	4,4,4	1.15	0	6,6,6	0.61	0
2	SO4	D	704	-	4,4,4	0.80	0	6,6,6	0.54	0
3	GOL	B	702	-	5,5,5	0.49	0	5,5,5	0.44	0
2	SO4	C	706	-	4,4,4	0.91	0	6,6,6	0.53	0
2	SO4	B	707	-	4,4,4	0.96	0	6,6,6	0.47	0
2	SO4	B	708	-	4,4,4	0.79	0	6,6,6	0.54	0
2	SO4	C	707	-	4,4,4	0.89	0	6,6,6	0.56	0
2	SO4	D	703	-	4,4,4	0.94	0	6,6,6	0.48	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	703	-	-	3/4/4/4	-
3	GOL	B	704	-	-	2/4/4/4	-
3	GOL	B	703	-	-	4/4/4/4	-
3	GOL	C	705	-	-	4/4/4/4	-
3	GOL	A	704	-	-	2/4/4/4	-
3	GOL	C	703	-	-	2/4/4/4	-
3	GOL	B	702	-	-	0/4/4/4	-
3	GOL	C	704	-	-	4/4/4/4	-
3	GOL	D	702	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

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

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

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	705	SO4	1	0
3	B	704	GOL	4	0
3	A	704	GOL	5	0
3	D	702	GOL	1	0
3	A	703	GOL	1	0
3	C	705	GOL	1	0
3	B	703	GOL	6	0
2	C	701	SO4	1	0
2	D	701	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, 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	521/554 (94%)	-0.39	5 (0%)	79	79	37, 56, 87, 100	0
1	B	512/554 (92%)	-0.44	4 (0%)	82	82	40, 56, 80, 93	0
1	C	529/554 (95%)	-0.42	8 (1%)	71	71	36, 53, 79, 106	0
1	D	512/554 (92%)	-0.38	7 (1%)	73	73	38, 56, 83, 100	0
All	All	2074/2216 (93%)	-0.41	24 (1%)	76	76	36, 55, 82, 106	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	589	ASP	3.8
1	C	583	PHE	3.8
1	C	105	CYS	3.7
1	C	584	THR	3.7
1	D	233	ASN	3.2
1	D	105	CYS	3.2
1	A	511	ARG	3.0
1	D	316	ASP	3.0
1	A	510	ASN	2.8
1	A	320	HIS	2.8
1	B	105	CYS	2.7
1	C	505	PHE	2.6
1	D	320	HIS	2.6
1	C	586	SER	2.5
1	B	317	PHE	2.5
1	D	514	LEU	2.5
1	A	319	ARG	2.4
1	D	178	ASN	2.3
1	A	233	ASN	2.2
1	B	589	ASP	2.2
1	B	320	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	511	ARG	2.2
1	D	179	ASP	2.1
1	C	585	ASN	2.1

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	SO4	C	708	5/5	0.63	0.13	75,80,91,96	5
3	GOL	C	705	6/6	0.65	0.19	68,76,79,81	0
3	GOL	A	704	6/6	0.70	0.11	71,81,84,85	0
2	SO4	B	708	5/5	0.76	0.20	70,73,75,82	5
2	SO4	B	705	5/5	0.77	0.15	58,61,70,97	5
2	SO4	D	703	5/5	0.80	0.17	54,60,65,69	5
2	SO4	C	707	5/5	0.80	0.15	61,62,68,68	5
2	SO4	A	701	5/5	0.80	0.15	63,68,76,86	5
2	SO4	D	705	5/5	0.81	0.12	77,79,86,90	5
3	GOL	B	703	6/6	0.84	0.30	56,63,66,67	0
2	SO4	C	701	5/5	0.84	0.12	62,71,78,80	5
2	SO4	A	705	5/5	0.85	0.14	61,62,73,84	5
3	GOL	B	702	6/6	0.85	0.19	62,70,79,81	0
2	SO4	A	702	5/5	0.85	0.10	60,64,71,71	5
3	GOL	B	704	6/6	0.85	0.24	60,65,68,69	0
2	SO4	B	706	5/5	0.85	0.10	65,69,76,81	5
3	GOL	A	703	6/6	0.86	0.20	47,59,62,62	0
3	GOL	C	703	6/6	0.87	0.15	55,58,64,65	0
2	SO4	B	707	5/5	0.89	0.13	59,64,70,78	5
2	SO4	C	702	5/5	0.89	0.10	60,70,75,79	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	701	5/5	0.89	0.10	57,64,70,78	5
3	GOL	D	702	6/6	0.89	0.14	61,72,72,78	0
2	SO4	D	704	5/5	0.91	0.12	48,56,63,64	5
2	SO4	C	706	5/5	0.92	0.09	63,74,81,86	5
3	GOL	C	704	6/6	0.92	0.12	58,63,70,70	0
2	SO4	B	701	5/5	0.93	0.10	57,62,71,72	5

6.5 Other polymers (i)

There are no such residues in this entry.