



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:24 AM GMT

PDB ID : 3EII
Title : Zinc-bound glycoside hydrolase 61 E from Thielavia terrestris
Authors : Salbo, R.; Welner, D.; Lo Leggio, L.; Harris, P.; McFarland, K.
Deposited on : 2008-09-16
Resolution : 2.25 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

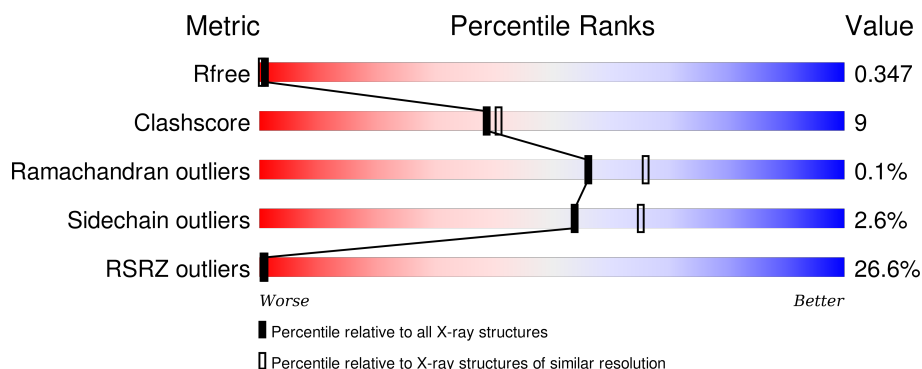
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	208	<div> <div>16%</div> <div>83%</div> <div>17%</div> </div>
1	B	208	<div> <div>26%</div> <div>78%</div> <div>21%</div> </div>
1	C	208	<div> <div>36%</div> <div>84%</div> <div>15%</div> </div>
1	D	208	<div> <div>29%</div> <div>82%</div> <div>18%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	601	-	-	-	X
3	NAG	C	601	-	-	-	X
4	SO4	A	3404	-	-	-	X
4	SO4	B	3403	-	-	-	X
4	SO4	B	4851	-	-	-	X
5	GOL	C	2647	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7221 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 protein GH61E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1599	1025	265	304	5			
1	B	208	Total	C	N	O	S	0	0	0
			1599	1025	265	304	5			
1	C	208	Total	C	N	O	S	0	0	0
			1599	1025	265	304	5			
1	D	208	Total	C	N	O	S	0	0	0
			1599	1025	265	304	5			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



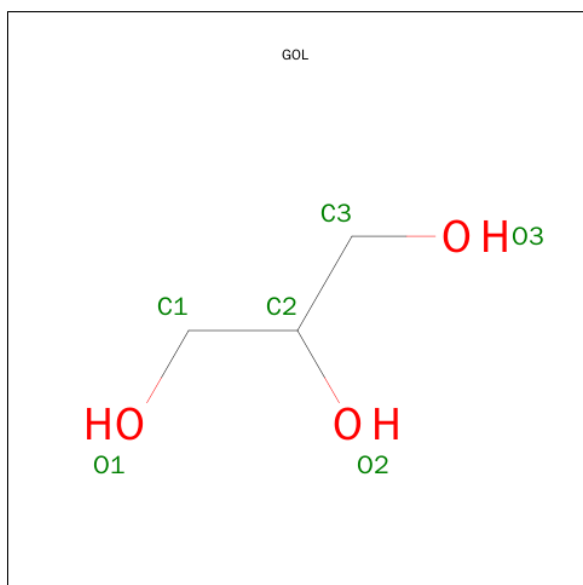
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

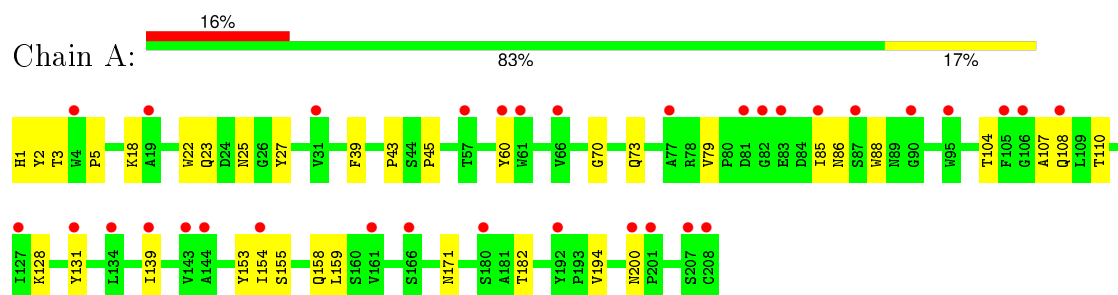
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	183	Total	O	0	0
			183	183		
6	B	151	Total	O	0	0
			151	151		
6	C	192	Total	O	0	0
			192	192		
6	D	170	Total	O	0	0
			170	170		

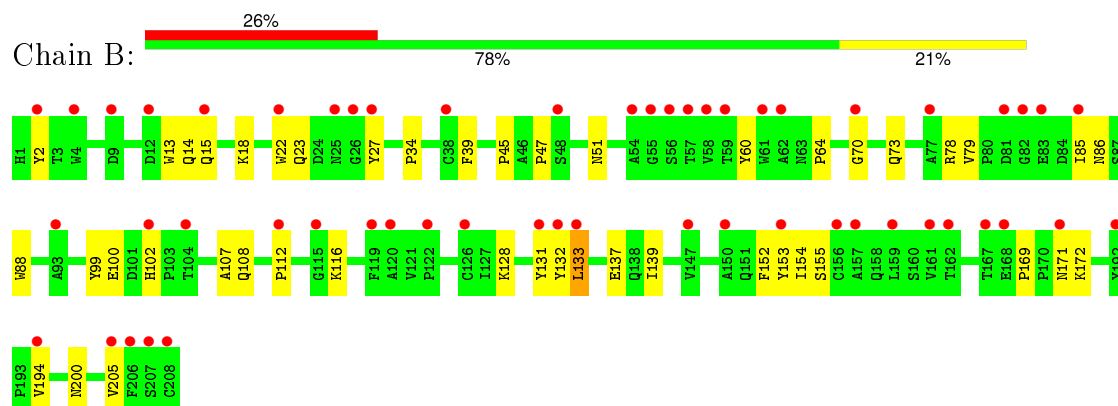
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

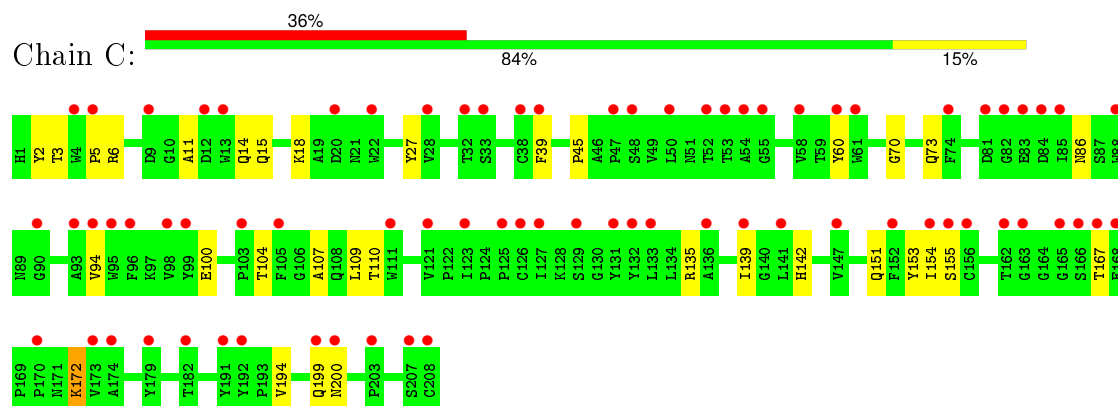
- Molecule 1: protein GH61E



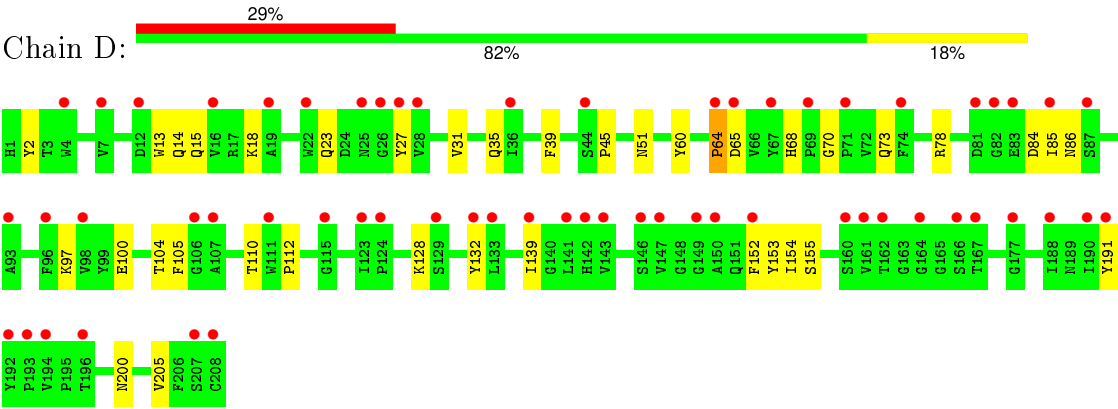
- Molecule 1: protein GH61E



- Molecule 1: protein GH61E



- Molecule 1: protein GH61E



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	220.92Å 220.92Å 220.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 19.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-2.25) 98.8 (19.92-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.251 0.343 , 0.347	Depositor DCC
R_{free} test set	2142 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.4	EDS
Estimated twinning fraction	0.045 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 59168 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	7221	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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 24.85 % 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 3.5412e-03.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, ZN, NAG, 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	0.54	0/1659	0.69	0/2284
1	B	0.52	0/1659	0.68	0/2284
1	C	0.54	0/1659	0.69	0/2284
1	D	0.52	0/1659	0.67	0/2284
All	All	0.53	0/6636	0.68	0/9136

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	64	PRO	Mainchain

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	1599	0	1487	22	1
1	B	1599	0	1487	34	0
1	C	1599	0	1487	25	1
1	D	1599	0	1487	32	1
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	14	0	13	0	0
3	B	14	0	13	1	0
3	C	14	0	13	0	1
3	D	14	0	13	4	0
4	A	15	0	0	0	0
4	B	20	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	C	6	0	8	6	0
5	D	6	0	8	1	0
6	A	183	0	0	5	0
6	B	151	0	0	5	0
6	C	192	0	0	5	3
6	D	170	0	0	10	2
All	All	7221	0	6016	113	5

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 (113) 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:D:51:ASN:HD22	3:D:601:NAG:H82	1.34	0.93
1:C:135:ARG:HG2	6:C:4615:HOH:O	1.69	0.90
1:C:107:ALA:O	1:C:194:VAL:HG21	1.89	0.72
1:D:35:GLN:HG3	6:D:4228:HOH:O	1.90	0.72
1:B:34:PRO:HD2	6:B:4250:HOH:O	1.92	0.70
1:B:107:ALA:O	1:B:194:VAL:HG21	1.92	0.70
1:D:51:ASN:HD22	3:D:601:NAG:C8	2.05	0.69
1:D:51:ASN:ND2	3:D:601:NAG:C8	2.57	0.68
1:D:51:ASN:ND2	3:D:601:NAG:H82	2.07	0.68
1:B:14:GLN:HG2	1:B:15:GLN:NE2	2.11	0.65
1:A:171:ASN:O	6:A:4341:HOH:O	2.15	0.64
1:D:112:PRO:HG3	6:D:4509:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:THR:OG1	1:C:110:THR:OG1	2.17	0.61
1:C:151:GLN:HE22	5:C:2647:GOL:H31	1.66	0.61
1:B:85:ILE:HD12	1:B:131:TYR:HB3	1.82	0.61
1:A:154:ILE:HG22	1:A:155:SER:N	2.16	0.61
1:A:18:LYS:HE2	1:A:22:TRP:CE2	2.36	0.61
1:B:116:LYS:HD3	6:B:4454:HOH:O	2.01	0.60
1:A:171:ASN:HB2	6:A:4321:HOH:O	2.02	0.60
1:C:199:GLN:HG2	6:D:4486:HOH:O	2.02	0.59
1:D:70:GLY:HA3	1:D:139:ILE:O	2.03	0.58
1:B:171:ASN:HB3	6:B:4410:HOH:O	2.02	0.58
1:A:107:ALA:O	1:A:194:VAL:HG21	2.03	0.58
1:B:70:GLY:HA3	1:B:139:ILE:O	2.03	0.58
1:A:43:PRO:HG3	6:A:4677:HOH:O	2.04	0.57
1:C:70:GLY:HA3	1:C:139:ILE:O	2.03	0.57
1:D:104:THR:OG1	1:D:110:THR:HB	2.05	0.57
1:D:14:GLN:NE2	1:D:15:GLN:HE22	2.02	0.56
1:C:167:THR:HG23	6:C:4577:HOH:O	2.04	0.56
1:B:47:PRO:HG3	6:B:4585:HOH:O	2.04	0.56
1:A:70:GLY:HA3	1:A:139:ILE:O	2.05	0.56
1:A:79:VAL:HG22	1:A:88:TRP:CE3	2.40	0.56
1:B:108:GLN:HG2	6:B:4150:HOH:O	2.06	0.55
1:B:51:ASN:HD22	3:B:601:NAG:H82	1.72	0.55
1:C:142:HIS:NE2	5:C:2647:GOL:H11	2.22	0.53
1:B:100:GLU:HG2	1:B:205:VAL:CG2	2.39	0.53
1:C:151:GLN:HE22	5:C:2647:GOL:C3	2.20	0.53
1:D:100:GLU:HG2	1:D:205:VAL:CG2	2.39	0.53
1:A:1:HIS:CE1	6:A:4281:HOH:O	2.61	0.53
1:D:154:ILE:HG22	1:D:155:SER:N	2.24	0.53
1:C:199:GLN:HB3	6:C:4685:HOH:O	2.08	0.53
1:D:105:PHE:HB3	6:D:4199:HOH:O	2.09	0.52
1:D:100:GLU:HG2	1:D:205:VAL:HG21	1.92	0.52
1:C:154:ILE:CG2	1:C:155:SER:N	2.72	0.52
1:C:151:GLN:HE22	5:C:2647:GOL:H12	1.75	0.51
1:D:14:GLN:NE2	1:D:15:GLN:NE2	2.59	0.51
1:D:31:VAL:HG22	6:D:4039:HOH:O	2.11	0.51
1:B:152:PHE:HB3	1:B:154:ILE:HD11	1.93	0.51
1:D:45:PRO:HB3	1:D:86:ASN:O	2.11	0.51
1:C:142:HIS:NE2	5:C:2647:GOL:C1	2.73	0.51
1:A:3:THR:HG23	1:A:25:ASN:OD1	2.12	0.50
1:D:154:ILE:CG2	1:D:155:SER:N	2.75	0.49
1:A:104:THR:HB	1:A:110:THR:OG1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLN:OE1	1:A:200:ASN:HB3	2.13	0.49
1:A:45:PRO:HB3	1:A:86:ASN:O	2.13	0.49
1:C:94:VAL:C	1:C:172:LYS:HG2	2.33	0.49
1:B:128:LYS:HB2	1:B:128:LYS:NZ	2.28	0.49
1:D:112:PRO:CG	6:D:4509:HOH:O	2.58	0.49
1:B:100:GLU:OE2	1:B:102:HIS:HE1	1.96	0.48
1:B:154:ILE:CG2	1:B:155:SER:N	2.77	0.48
1:B:22:TRP:CZ2	1:B:23:GLN:NE2	2.81	0.48
1:D:155:SER:HA	6:D:4143:HOH:O	2.14	0.48
1:A:22:TRP:CD2	1:A:23:GLN:HG3	2.48	0.48
1:B:73:GLN:OE1	1:B:200:ASN:HB3	2.14	0.48
1:D:23:GLN:HB2	6:D:4477:HOH:O	2.14	0.47
1:B:45:PRO:HB3	1:B:86:ASN:O	2.14	0.47
1:B:78:ARG:HB2	1:B:132:TYR:CE2	2.49	0.47
1:B:100:GLU:HG2	1:B:205:VAL:HG21	1.97	0.47
1:A:23:GLN:HB2	6:A:4010:HOH:O	2.15	0.46
1:B:128:LYS:HB2	1:B:128:LYS:HZ2	1.81	0.46
1:B:112:PRO:O	1:B:116:LYS:HD2	2.16	0.46
1:C:14:GLN:HG2	1:C:15:GLN:NE2	2.30	0.46
1:B:99:TYR:C	1:B:99:TYR:CD1	2.88	0.45
1:C:154:ILE:HG22	1:C:155:SER:N	2.30	0.45
1:D:18:LYS:HD2	6:D:4654:HOH:O	2.17	0.45
1:A:154:ILE:CG2	1:A:155:SER:N	2.79	0.45
1:D:152:PHE:HB3	1:D:154:ILE:HD11	1.99	0.45
1:A:22:TRP:CE2	1:A:23:GLN:HG3	2.52	0.45
1:B:154:ILE:HG22	1:B:155:SER:N	2.30	0.45
1:D:85:ILE:HG13	1:D:85:ILE:O	2.15	0.45
1:C:45:PRO:HB3	1:C:86:ASN:O	2.17	0.44
1:B:128:LYS:CB	1:B:128:LYS:NZ	2.81	0.44
1:C:109:LEU:HB2	6:C:4125:HOH:O	2.17	0.44
1:D:68:HIS:HE1	5:D:2647:GOL:O2	2.00	0.44
1:C:151:GLN:NE2	5:C:2647:GOL:H31	2.32	0.43
1:B:169:PRO:O	1:B:172:LYS:HD3	2.18	0.43
1:B:133:LEU:HA	1:B:133:LEU:HD12	1.88	0.43
1:B:152:PHE:HB3	1:B:154:ILE:CD1	2.49	0.43
1:A:3:THR:OG1	1:A:5:PRO:HD3	2.17	0.43
1:D:18:LYS:HB2	6:D:4530:HOH:O	2.18	0.43
1:C:6:ARG:HG2	1:C:11:ALA:C	2.38	0.43
1:D:97:LYS:HD3	1:D:100:GLU:HB3	2.01	0.43
1:D:78:ARG:HG3	1:D:132:TYR:CZ	2.53	0.43
1:A:85:ILE:HD12	1:A:131:TYR:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:TYR:HB3	1:C:153:TYR:CE1	2.55	0.42
1:B:99:TYR:CD1	1:B:100:GLU:N	2.88	0.42
1:C:3:THR:OG1	1:C:5:PRO:HD3	2.20	0.42
1:B:13:TRP:CE3	1:B:18:LYS:HA	2.54	0.42
1:B:27:TYR:HB3	1:B:153:TYR:CE1	2.55	0.42
1:B:73:GLN:HB2	1:B:137:GLU:OE1	2.19	0.41
1:D:73:GLN:OE1	1:D:200:ASN:HB3	2.20	0.41
1:A:128:LYS:NZ	1:A:128:LYS:HB2	2.36	0.41
1:D:13:TRP:CG	1:D:18:LYS:HG3	2.55	0.41
1:D:153:TYR:C	1:D:154:ILE:HG13	2.40	0.41
1:A:158:GLN:C	1:A:159:LEU:HD12	2.41	0.41
1:C:73:GLN:OE1	1:C:200:ASN:HB3	2.20	0.41
1:A:27:TYR:HB3	1:A:153:TYR:CE1	2.55	0.41
1:B:79:VAL:HG22	1:B:88:TRP:CE3	2.56	0.41
1:D:27:TYR:HB3	1:D:153:TYR:CE1	2.56	0.41
1:D:64:PRO:O	1:D:65:ASP:HB3	2.21	0.41
1:C:167:THR:CG2	6:C:4577:HOH:O	2.65	0.40
1:B:153:TYR:C	1:B:154:ILE:HG13	2.42	0.40
1:C:18:LYS:HB2	1:C:18:LYS:NZ	2.37	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:TYR:O	6:C:4120:HOH:O[12_665]	1.95	0.25
3:C:601:NAG:O4	6:C:4202:HOH:O[16_556]	2.09	0.11
1:C:172:LYS:O	6:D:4223:HOH:O[6_566]	2.10	0.10
1:A:182:THR:OG1	6:C:4323:HOH:O[45_545]	2.16	0.04
6:D:4287:HOH:O	6:D:4495:HOH:O[12_665]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
1	B	206/208 (99%)	200 (97%)	6 (3%)	0	100	100
1	C	206/208 (99%)	200 (97%)	6 (3%)	0	100	100
1	D	206/208 (99%)	200 (97%)	5 (2%)	1 (0%)	34	34
All	All	824/832 (99%)	798 (97%)	25 (3%)	1 (0%)	56	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	64	PRO

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	170/170 (100%)	166 (98%)	4 (2%)	57	67
1	B	170/170 (100%)	166 (98%)	4 (2%)	57	67
1	C	170/170 (100%)	165 (97%)	5 (3%)	50	60
1	D	170/170 (100%)	165 (97%)	5 (3%)	50	60
All	All	680/680 (100%)	662 (97%)	18 (3%)	54	65

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TYR
1	A	39	PHE
1	A	60	TYR
1	A	108	GLN
1	B	2	TYR
1	B	39	PHE
1	B	60	TYR
1	B	133	LEU
1	C	2	TYR
1	C	39	PHE

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Mol	Chain	Res	Type
1	C	60	TYR
1	C	100	GLU
1	C	172	LYS
1	D	2	TYR
1	D	39	PHE
1	D	60	TYR
1	D	84	ASP
1	D	128	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	63	ASN
1	A	102	HIS
1	A	108	GLN
1	A	199	GLN
1	B	14	GLN
1	B	108	GLN
1	C	151	GLN
1	C	171	ASN
1	D	14	GLN
1	D	23	GLN
1	D	171	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	SO4	A	3404	-	4,4,4	0.21	0	6,6,6	0.13	0
4	SO4	A	4849	-	4,4,4	1.48	0	6,6,6	1.59	1 (16%)
4	SO4	A	4851	-	4,4,4	1.55	0	6,6,6	1.63	1 (16%)
3	NAG	A	601	1	14,14,15	0.64	0	15,19,21	0.74	1 (6%)
4	SO4	B	3403	-	4,4,4	0.13	0	6,6,6	0.17	0
4	SO4	B	3405	-	4,4,4	0.11	0	6,6,6	0.22	0
4	SO4	B	4849	-	4,4,4	1.55	0	6,6,6	1.63	1 (16%)
4	SO4	B	4851	-	4,4,4	1.59	0	6,6,6	1.61	1 (16%)
3	NAG	B	601	1	14,14,15	1.07	1 (7%)	15,19,21	0.65	0
5	GOL	C	2647	-	5,5,5	0.62	0	5,5,5	2.01	1 (20%)
4	SO4	C	3401	-	4,4,4	0.20	0	6,6,6	0.10	0
4	SO4	C	4849	-	4,4,4	1.63	0	6,6,6	1.62	1 (16%)
3	NAG	C	601	1	14,14,15	0.58	0	15,19,21	0.92	1 (6%)
5	GOL	D	2647	2	5,5,5	0.24	0	5,5,5	0.21	0
4	SO4	D	3402	-	4,4,4	0.16	0	6,6,6	0.09	0
4	SO4	D	4849	-	4,4,4	1.49	0	6,6,6	1.61	1 (16%)
3	NAG	D	601	1	14,14,15	1.07	2 (14%)	15,19,21	1.03	1 (6%)

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
4	SO4	A	3404	-	-	0/0/0/0	0/0/0/0
4	SO4	A	4849	-	-	0/0/0/0	0/0/0/0
4	SO4	A	4851	-	-	0/0/0/0	0/0/0/0
3	NAG	A	601	1	-	1/6/23/26	0/1/1/1
4	SO4	B	3403	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	B	3405	-	-	0/0/0/0	0/0/0/0
4	SO4	B	4849	-	-	0/0/0/0	0/0/0/0
4	SO4	B	4851	-	-	0/0/0/0	0/0/0/0
3	NAG	B	601	1	-	1/6/23/26	0/1/1/1
5	GOL	C	2647	-	-	0/4/4/4	0/0/0/0
4	SO4	C	3401	-	-	0/0/0/0	0/0/0/0
4	SO4	C	4849	-	-	0/0/0/0	0/0/0/0
3	NAG	C	601	1	-	2/6/23/26	0/1/1/1
5	GOL	D	2647	2	-	0/4/4/4	0/0/0/0
4	SO4	D	3402	-	-	0/0/0/0	0/0/0/0
4	SO4	D	4849	-	-	0/0/0/0	0/0/0/0
3	NAG	D	601	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	NAG	C8-C7	-2.08	1.46	1.50
3	D	601	NAG	C8-C7	2.15	1.54	1.50
3	D	601	NAG	C1-C2	2.92	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2647	GOL	C3-C2-C1	-3.41	97.76	111.12
3	D	601	NAG	C2-N2-C7	-3.21	118.92	123.04
3	A	601	NAG	C2-N2-C7	-2.46	119.88	123.04
3	C	601	NAG	C2-N2-C7	-2.34	120.04	123.04
4	A	4849	SO4	O4-S-O3	3.71	124.07	108.98
4	D	4849	SO4	O4-S-O3	3.76	124.29	108.98
4	B	4851	SO4	O4-S-O3	3.77	124.30	108.98
4	C	4849	SO4	O4-S-O3	3.78	124.35	108.98
4	A	4851	SO4	O4-S-O3	3.81	124.49	108.98
4	B	4849	SO4	O4-S-O3	3.82	124.52	108.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	NAG	O7-C7-N2-C2
3	C	601	NAG	C8-C7-N2-C2
3	B	601	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	C	601	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	NAG	1	0
5	C	2647	GOL	6	0
3	C	601	NAG	0	1
5	D	2647	GOL	1	0
3	D	601	NAG	4	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	208/208 (100%)	1.34	33 (15%) 3 3	7, 17, 30, 42	0
1	B	208/208 (100%)	1.59	54 (25%) 1 1	8, 20, 33, 44	0
1	C	208/208 (100%)	1.75	74 (35%) 0 0	8, 16, 30, 43	0
1	D	208/208 (100%)	1.73	60 (28%) 1 0	8, 18, 31, 43	0
All	All	832/832 (100%)	1.60	221 (26%) 1 1	7, 18, 31, 44	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	CYS	11.1
1	C	208	CYS	8.1
1	D	82	GLY	7.3
1	D	208	CYS	7.0
1	C	163	GLY	6.4
1	C	166	SER	6.4
1	A	208	CYS	5.9
1	C	82	GLY	5.5
1	D	81	ASP	5.1
1	A	207	SER	5.1
1	B	82	GLY	4.5
1	D	83	GLU	4.5
1	B	26	GLY	4.2
1	D	115	GLY	4.2
1	D	85	ILE	4.0
1	D	164	GLY	4.0
1	D	207	SER	3.7
1	B	207	SER	3.7
1	D	167	THR	3.7
1	D	106	GLY	3.6
1	D	44	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	147	VAL	3.6
1	C	162	THR	3.5
1	C	132	TYR	3.5
1	C	173	VAL	3.5
1	D	65	ASP	3.4
1	B	167	THR	3.4
1	B	93	ALA	3.3
1	C	165	GLY	3.3
1	A	108	GLN	3.3
1	C	99	TYR	3.3
1	B	25	ASN	3.3
1	B	132	TYR	3.2
1	C	168	GLU	3.2
1	D	143	VAL	3.2
1	B	12	ASP	3.2
1	B	83	GLU	3.2
1	A	82	GLY	3.2
1	B	171	ASN	3.2
1	D	146	SER	3.1
1	B	56	SER	3.1
1	D	93	ALA	3.1
1	B	104	THR	3.1
1	B	194	VAL	3.1
1	C	125	PRO	3.1
1	D	142	HIS	3.1
1	D	27	TYR	3.0
1	B	157	ALA	3.0
1	C	5	PRO	3.0
1	C	28	VAL	3.0
1	D	16	VAL	3.0
1	C	95	TRP	2.9
1	D	191	TYR	2.9
1	B	156	CYS	2.9
1	C	136	ALA	2.9
1	C	83	GLU	2.9
1	C	94	VAL	2.9
1	B	161	VAL	2.9
1	D	36	ILE	2.9
1	D	96	PHE	2.9
1	C	48	SER	2.9
1	B	131	TYR	2.9
1	B	120	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	154	ILE	2.8
1	C	207	SER	2.8
1	C	90	GLY	2.8
1	D	28	VAL	2.8
1	A	81	ASP	2.8
1	D	4	TRP	2.8
1	D	190	ILE	2.8
1	B	61	TRP	2.8
1	C	61	TRP	2.8
1	B	192	TYR	2.8
1	B	54	ALA	2.8
1	A	161	VAL	2.8
1	B	15	GLN	2.8
1	C	20	ASP	2.8
1	C	126	CYS	2.7
1	C	96	PHE	2.7
1	D	188	ILE	2.7
1	A	201	PRO	2.7
1	A	77	ALA	2.7
1	B	112	PRO	2.7
1	D	98	VAL	2.7
1	A	87	SER	2.7
1	B	122	PRO	2.7
1	B	168	GLU	2.6
1	A	61	TRP	2.6
1	A	106	GLY	2.6
1	C	123	ILE	2.6
1	B	9	ASP	2.6
1	C	9	ASP	2.6
1	D	12	ASP	2.6
1	D	133	LEU	2.6
1	B	81	ASP	2.6
1	A	105	PHE	2.6
1	D	132	TYR	2.6
1	D	107	ALA	2.6
1	C	4	TRP	2.6
1	A	139	ILE	2.6
1	D	123	ILE	2.6
1	D	196	THR	2.6
1	D	152	PHE	2.6
1	D	26	GLY	2.6
1	C	200	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	59	THR	2.5
1	C	139	ILE	2.5
1	D	150	ALA	2.5
1	C	147	VAL	2.5
1	B	70	GLY	2.5
1	C	39	PHE	2.5
1	C	152	PHE	2.5
1	C	47	PRO	2.5
1	C	85	ILE	2.5
1	B	22	TRP	2.5
1	A	154	ILE	2.5
1	B	133	LEU	2.5
1	C	12	ASP	2.5
1	C	167	THR	2.4
1	D	193	PRO	2.4
1	B	55	GLY	2.4
1	C	129	SER	2.4
1	D	166	SER	2.4
1	D	192	TYR	2.4
1	C	13	TRP	2.4
1	B	205	VAL	2.4
1	C	38	CYS	2.4
1	C	53	THR	2.4
1	B	2	TYR	2.4
1	A	66	VAL	2.4
1	B	102	HIS	2.4
1	C	203	PRO	2.4
1	C	192	TYR	2.4
1	A	127	ILE	2.4
1	C	105	PHE	2.4
1	D	69	PRO	2.4
1	D	139	ILE	2.3
1	B	119	PHE	2.3
1	C	74	PHE	2.3
1	A	4	TRP	2.3
1	A	90	GLY	2.3
1	B	85	ILE	2.3
1	D	67	TYR	2.3
1	B	77	ALA	2.3
1	C	55	GLY	2.3
1	D	111	TRP	2.3
1	C	50	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	180	SER	2.3
1	B	58	VAL	2.3
1	D	64	PRO	2.3
1	D	124	PRO	2.3
1	C	54	ALA	2.3
1	D	87	SER	2.3
1	D	129	SER	2.3
1	A	95	TRP	2.3
1	A	134	LEU	2.3
1	B	162	THR	2.3
1	C	52	THR	2.3
1	C	98	VAL	2.3
1	A	166	SER	2.3
1	B	48	SER	2.3
1	D	149	GLY	2.2
1	A	143	VAL	2.2
1	C	121	VAL	2.2
1	A	60	TYR	2.2
1	B	115	GLY	2.2
1	C	182	THR	2.2
1	C	127	ILE	2.2
1	D	141	LEU	2.2
1	C	170	PRO	2.2
1	D	160	SER	2.2
1	D	7	VAL	2.2
1	B	38	CYS	2.2
1	D	71	PRO	2.2
1	D	25	ASN	2.2
1	C	111	TRP	2.2
1	D	161	VAL	2.2
1	A	131	TYR	2.2
1	B	27	TYR	2.2
1	C	131	TYR	2.2
1	C	32	THR	2.2
1	C	155	SER	2.2
1	A	31	VAL	2.2
1	B	147	VAL	2.2
1	B	153	TYR	2.2
1	C	60	TYR	2.2
1	C	199	GLN	2.2
1	C	22	TRP	2.1
1	B	206	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	33	SER	2.1
1	A	144	ALA	2.1
1	B	62	ALA	2.1
1	B	4	TRP	2.1
1	D	74	PHE	2.1
1	A	19	ALA	2.1
1	D	194	VAL	2.1
1	A	83	GLU	2.1
1	C	58	VAL	2.1
1	A	57	THR	2.1
1	C	179	TYR	2.1
1	B	150	ALA	2.1
1	C	174	ALA	2.1
1	D	19	ALA	2.1
1	D	162	THR	2.1
1	C	93	ALA	2.1
1	D	22	TRP	2.1
1	C	84	ASP	2.1
1	C	103	PRO	2.1
1	C	156	CYS	2.0
1	A	192	TYR	2.0
1	C	81	ASP	2.0
1	C	191	TYR	2.0
1	A	200	ASN	2.0
1	D	177	GLY	2.0
1	C	141	LEU	2.0
1	C	88	TRP	2.0
1	A	85	ILE	2.0
1	B	57	THR	2.0
1	B	159	LEU	2.0
1	C	133	LEU	2.0
1	B	126	CYS	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 carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	C	601	14/15	0.46	0.59	15.70	48,52,53,54	0
5	GOL	C	2647	6/6	0.58	0.33	4.95	43,44,46,46	0
4	SO4	B	3403	5/5	0.58	0.48	4.52	78,78,78,79	0
3	NAG	A	601	14/15	0.54	0.29	3.15	37,39,45,45	0
4	SO4	B	4851	5/5	0.82	0.43	2.78	62,63,63,63	0
4	SO4	A	3404	5/5	0.64	0.25	2.03	59,60,60,60	0
5	GOL	D	2647	6/6	0.71	0.30	1.63	42,42,44,44	0
4	SO4	C	4849	5/5	0.83	0.24	-0.52	70,70,71,71	0
4	SO4	A	4851	5/5	0.84	0.18	-0.65	52,53,53,54	0
4	SO4	C	3401	5/5	0.81	0.18	-0.95	38,38,39,40	0
3	NAG	B	601	14/15	0.59	0.45	-	46,50,52,53	0
2	ZN	D	301	1/1	0.71	0.16	-	27,27,27,27	0
3	NAG	D	601	14/15	0.55	0.44	-	49,53,57,58	0
4	SO4	B	3405	5/5	0.81	0.33	-	61,61,62,62	0
2	ZN	B	301	1/1	0.76	0.13	-	26,26,26,26	0
4	SO4	A	4849	5/5	0.81	0.26	-	51,53,53,54	0
2	ZN	B	352	1/1	0.67	0.15	-	61,61,61,61	0
4	SO4	D	3402	5/5	0.55	0.29	-	58,59,59,59	0
4	SO4	D	4849	5/5	0.71	0.28	-	53,55,56,56	0
4	SO4	B	4849	5/5	0.94	0.19	-	63,64,65,65	0
2	ZN	C	351	1/1	0.81	0.16	-	54,54,54,54	0
2	ZN	A	301	1/1	0.91	0.10	-	18,18,18,18	0
2	ZN	C	301	1/1	0.83	0.12	-	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.