Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:34 PM GMT

PDB ID	:	1G87
Title	:	THE CRYSTAL STRUCTURE OF ENDOGLUCANASE 9G FROM CLOSTRIDIUM CELLULOLYTICUM
Authors	:	Mandelman, D.; Belaich, A.; Belaich, J.P.; Aghajari, N.; Driguez, H.; Haser, R.
Deposited on	:	2000-11-16
Resolution	:	1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

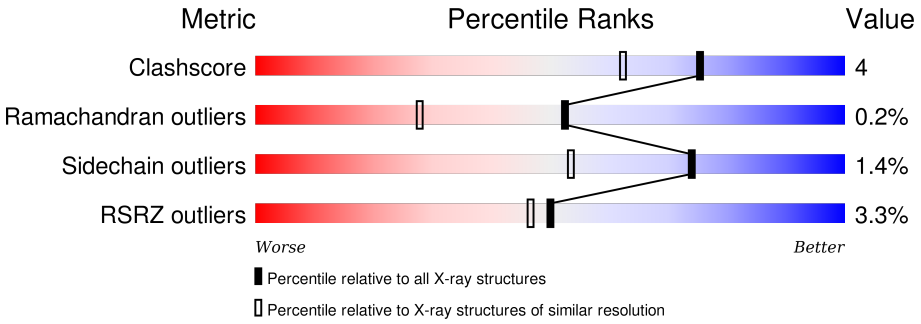
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	614	4% 90% 10%
1	B	614	3% 92% 7%

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
4	EDO	A	620	-	-	-	X
4	EDO	B	622	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	623	-	-	-	X
4	EDO	B	625	-	-	-	X
4	EDO	B	627	-	-	-	X
4	EDO	B	628	-	-	-	X
5	GOL	A	625	-	-	-	X
5	GOL	A	626	-	-	-	X
5	GOL	B	630	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10380 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 ENDOCELLULASE 9G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	4	0
			4812	3061	791	941	19			
1	B	613	Total	C	N	O	S	0	2	0
			4808	3057	790	942	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	574	THR	ARG	CONFLICT	UNP P37700
A	575	THR	ARG	CONFLICT	UNP P37700
B	574	THR	ARG	CONFLICT	UNP P37700
B	575	THR	ARG	CONFLICT	UNP P37700

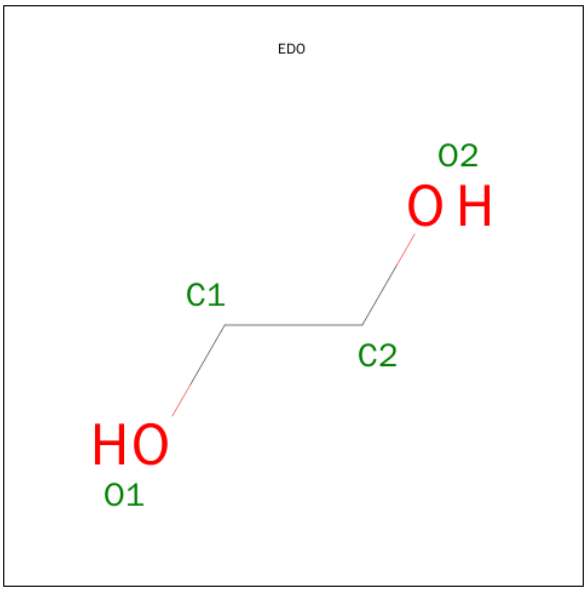
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

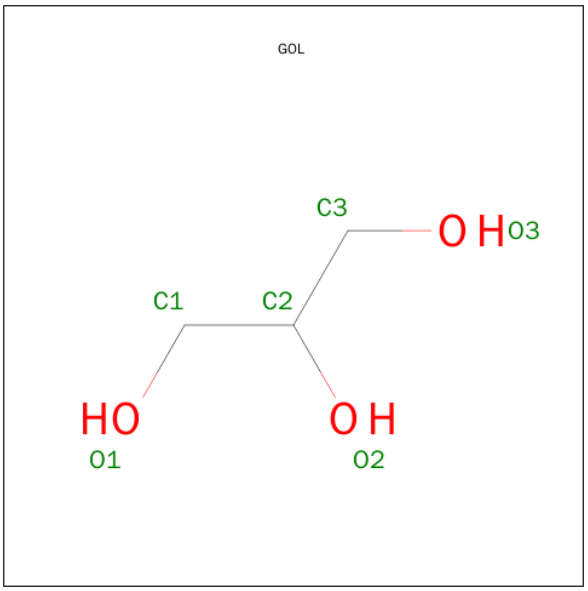
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Mg	0	0
			4	4		
3	A	3	Total	Mg	0	0
			3	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

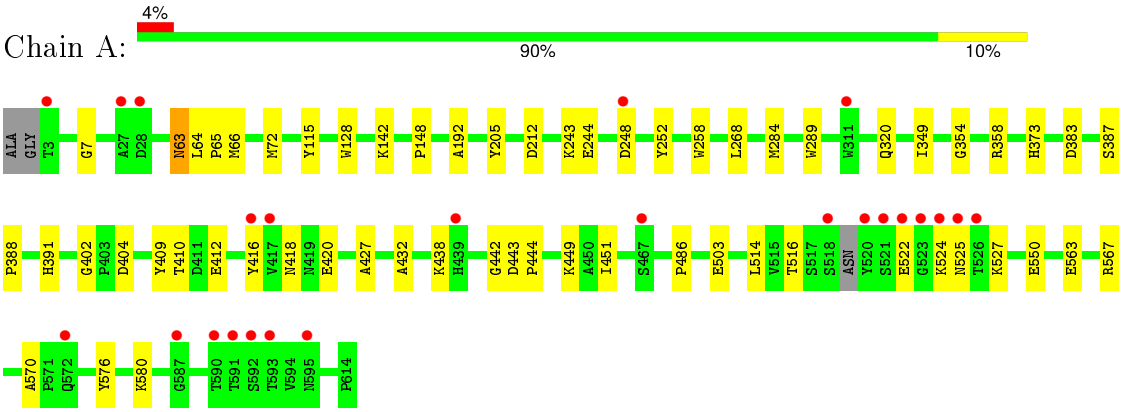
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	322	Total O 322 322	0	0
6	B	347	Total O 347 347	0	0

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.

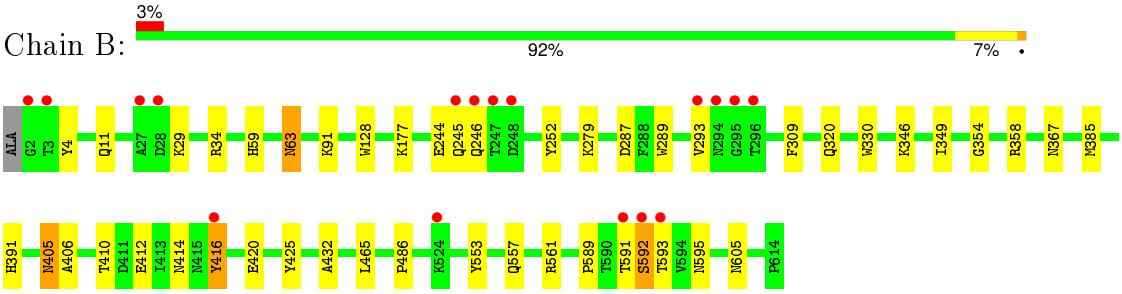
- Molecule 1: ENDOCELLULASE 9G

Chain A:



- Molecule 1: ENDOCELLULASE 9G

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.85Å 57.72Å 86.27Å 94.22° 100.87° 99.61°	Depositor
Resolution (Å)	29.17 – 1.60 29.17 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.17-1.60) 88.7 (29.17-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 1.60Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.174 , 0.200 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	13.1	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 125299 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10380	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CA, MG, EDO

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	0.49	0/4951	0.70	1/6742 (0.0%)
1	B	0.50	0/4949	0.70	0/6743
All	All	0.49	0/9900	0.70	1/13485 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	MET	CG-SD-CE	5.73	109.37	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	4	TYR	Sidechain

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	4812	0	4528	38	0
1	B	4808	0	4513	36	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
4	A	12	0	18	4	0
4	B	32	0	47	3	0
5	A	24	0	32	0	0
5	B	12	0	16	0	0
6	A	322	0	0	4	0
6	B	347	0	0	5	0
All	All	10380	0	9154	74	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 (74) 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:212:ASP:HB3	4:A:620:EDO:H22	1.28	1.12
1:B:416:TYR:O	1:B:420:GLU:HG2	1.72	0.88
1:B:591:THR:OG1	1:B:593:THR:HG22	1.75	0.87
1:A:416:TYR:O	1:A:420:GLU:HG2	1.75	0.85
1:B:128:TRP:HB2	4:B:625:EDO:H21	1.66	0.76
1:B:91:LYS:HG3	6:B:768:HOH:O	1.90	0.70
1:A:64:LEU:HB3	1:A:65:PRO:HD3	1.74	0.69
1:B:287:ASP:HB3	1:B:293:VAL:HG12	1.76	0.68
1:A:410:THR:HG22	1:A:412:GLU:HG3	1.74	0.68
1:A:449:LYS:HB3	1:A:451:ILE:HD13	1.77	0.67
1:A:524:LYS:NZ	1:A:524:LYS:HB2	2.11	0.66
1:A:212:ASP:CB	4:A:620:EDO:H22	2.16	0.65
1:A:438:LYS:HD2	6:A:817:HOH:O	1.97	0.64
1:B:405:ASN:HD22	1:B:406:ALA:N	1.96	0.64
1:A:65:PRO:HG3	1:A:205:TYR:CD1	2.33	0.64
1:B:244:GLU:HG2	1:B:252:TYR:CE1	2.34	0.63
1:B:465:LEU:O	1:B:591:THR:O	2.18	0.62
1:B:553:TYR:CE2	4:B:628:EDO:H21	2.35	0.62
1:B:346[A]:LYS:HE2	6:B:833:HOH:O	2.01	0.61
1:A:65:PRO:HG3	1:A:205:TYR:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ASN:C	1:B:405:ASN:HD22	2.07	0.59
1:A:524:LYS:HZ2	1:A:524:LYS:HB2	1.69	0.58
1:A:527:LYS:HG2	6:A:937:HOH:O	2.04	0.57
1:B:279:LYS:HD3	1:B:330:TRP:HH2	1.70	0.56
1:B:420:GLU:OE2	1:B:425:TYR:OH	2.24	0.56
1:B:593:THR:O	1:B:593:THR:HG23	2.06	0.55
1:B:279:LYS:HD3	1:B:330:TRP:CH2	2.43	0.52
1:A:244:GLU:HG3	1:A:252:TYR:CE1	2.45	0.52
1:B:287:ASP:CB	1:B:293:VAL:HG12	2.39	0.51
1:B:177:LYS:HE3	6:B:966:HOH:O	2.09	0.51
1:A:516:THR:HA	1:A:567:ARG:O	2.11	0.51
1:A:258:TRP:HE1	4:A:622:EDO:H12	1.74	0.51
1:B:591:THR:OG1	1:B:592:SER:N	2.41	0.50
1:B:59:HIS:HD2	6:B:691:HOH:O	1.94	0.50
1:B:385:MET:HE2	1:B:414:ASN:HB2	1.94	0.50
1:B:289:TRP:CE2	1:B:320:GLN:HG3	2.49	0.48
1:A:349:ILE:HD11	1:A:432:ALA:HB3	1.95	0.47
1:A:522:GLU:HG3	1:A:563:GLU:HB3	1.95	0.47
1:B:557:GLN:O	1:B:561:ARG:HG2	2.13	0.47
1:A:580:LYS:HE3	6:A:752:HOH:O	2.14	0.47
1:A:148:PRO:HB3	1:A:192:ALA:HB1	1.96	0.47
1:A:373:HIS:CE1	1:A:416:TYR:CE2	3.03	0.46
1:A:64:LEU:HB3	1:A:65:PRO:CD	2.43	0.46
1:A:63:ASN:HD22	1:A:63:ASN:N	2.13	0.46
1:A:525:ASN:HB2	1:A:550:GLU:OE2	2.15	0.46
1:A:409:TYR:CD1	1:A:418:ASN:HB3	2.51	0.45
1:B:591:THR:HG1	1:B:593:THR:HG22	1.78	0.45
1:B:405:ASN:ND2	1:B:405:ASN:C	2.69	0.45
1:A:258:TRP:HE1	4:A:622:EDO:C1	2.29	0.45
1:B:349:ILE:HD11	1:B:432:ALA:HB3	1.99	0.45
1:B:367:ASN:ND2	6:B:752:HOH:O	2.49	0.44
1:B:245:GLN:HB3	1:B:246:GLN:NE2	2.32	0.44
1:B:246:GLN:N	1:B:246:GLN:NE2	2.66	0.44
1:B:410:THR:HG22	1:B:412:GLU:HG3	1.98	0.44
1:B:287:ASP:CB	1:B:293:VAL:CG1	2.95	0.44
1:A:289:TRP:CE2	1:A:320:GLN:HG3	2.53	0.44
1:B:63:ASN:N	1:B:63:ASN:HD22	2.15	0.43
1:A:514:LEU:HD22	1:A:570:ALA:HA	2.01	0.43
1:A:503:GLU:HG3	1:A:576:TYR:O	2.18	0.43
1:B:553:TYR:CE2	4:B:628:EDO:C2	3.01	0.42
1:B:29:LYS:HE2	1:B:34:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:PRO:HB3	1:B:595:ASN:HD22	1.85	0.42
1:A:7:GLY:HA3	1:A:442:GLY:O	2.19	0.42
1:A:72:MET:HB2	1:A:427:ALA:HB1	2.02	0.42
1:B:246:GLN:CD	1:B:246:GLN:N	2.73	0.42
1:A:387:SER:HA	1:A:388:PRO:C	2.40	0.42
1:A:115:TYR:CD1	1:A:142:LYS:HB3	2.54	0.42
1:A:252:TYR:CD2	1:A:284:MET:HG2	2.54	0.41
1:A:404:ASP:HB2	6:A:923:HOH:O	2.21	0.41
1:A:243:LYS:HD3	1:A:248:ASP:HA	2.02	0.41
1:B:252:TYR:CE2	1:B:293:VAL:HG21	2.57	0.40
1:A:402:GLY:O	1:A:418:ASN:HA	2.22	0.40
1:A:443:ASP:HA	1:A:444:PRO:HD3	1.97	0.40
1:A:128:TRP:O	1:A:383:ASP:HA	2.21	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	611/614 (100%)	594 (97%)	16 (3%)	1 (0%)	52	28
1	B	613/614 (100%)	597 (97%)	14 (2%)	2 (0%)	46	23
All	All	1224/1228 (100%)	1191 (97%)	30 (2%)	3 (0%)	52	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	592	SER
1	A	354	GLY
1	B	354	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	508/507 (100%)	502 (99%)	6 (1%)	78 60
1	B	507/507 (100%)	498 (98%)	9 (2%)	66 41
All	All	1015/1014 (100%)	1000 (98%)	15 (2%)	74 50

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	268[A]	LEU
1	A	268[B]	LEU
1	A	358	ARG
1	A	391	HIS
1	A	486	PRO
1	B	11	GLN
1	B	63	ASN
1	B	309	PHE
1	B	358	ARG
1	B	391	HIS
1	B	405	ASN
1	B	416	TYR
1	B	486	PRO
1	B	605	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	89	GLN
1	A	117	GLN
1	A	135	GLN
1	A	240	ASN
1	A	276	GLN
1	A	418	ASN

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Mol	Chain	Res	Type
1	A	466	ASN
1	A	525	ASN
1	A	551	ASN
1	A	557	GLN
1	A	565	GLN
1	B	59	HIS
1	B	63	ASN
1	B	89	GLN
1	B	117	GLN
1	B	245	GLN
1	B	246	GLN
1	B	276	GLN
1	B	294	ASN
1	B	367	ASN
1	B	405	ASN
1	B	466	ASN
1	B	557	GLN
1	B	572	GLN
1	B	595	ASN
1	B	605	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 28 ligands modelled in this entry, 11 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	EDO	A	620	-	3,3,3	1.75	2 (66%)	2,2,2	0.58	0
4	EDO	A	621	-	3,3,3	2.11	2 (66%)	2,2,2	0.52	0
4	EDO	A	622	-	3,3,3	1.92	1 (33%)	2,2,2	0.54	0
5	GOL	A	623	-	5,5,5	0.97	0	5,5,5	0.73	0
5	GOL	A	624	-	5,5,5	0.94	0	5,5,5	0.87	0
5	GOL	A	625	-	5,5,5	1.10	0	5,5,5	0.77	0
5	GOL	A	626	-	5,5,5	0.98	0	5,5,5	0.95	0
4	EDO	B	621	-	3,3,3	2.07	2 (66%)	2,2,2	0.56	0
4	EDO	B	622	-	3,3,3	1.99	1 (33%)	2,2,2	0.61	0
4	EDO	B	623	-	3,3,3	2.01	1 (33%)	2,2,2	0.39	0
4	EDO	B	624	3	3,3,3	2.05	1 (33%)	2,2,2	0.47	0
4	EDO	B	625	-	3,3,3	2.06	2 (66%)	2,2,2	0.45	0
4	EDO	B	626	-	3,3,3	2.14	2 (66%)	2,2,2	0.49	0
4	EDO	B	627	-	3,3,3	2.27	2 (66%)	2,2,2	0.56	0
4	EDO	B	628	-	3,3,3	1.94	2 (66%)	2,2,2	0.37	0
5	GOL	B	629	-	5,5,5	1.15	0	5,5,5	0.68	0
5	GOL	B	630	-	5,5,5	0.97	0	5,5,5	0.84	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
4	EDO	A	620	-	-	0/1/1/1	0/0/0/0
4	EDO	A	621	-	-	0/1/1/1	0/0/0/0
4	EDO	A	622	-	-	0/1/1/1	0/0/0/0
5	GOL	A	623	-	-	0/4/4/4	0/0/0/0
5	GOL	A	624	-	-	0/4/4/4	0/0/0/0
5	GOL	A	625	-	-	0/4/4/4	0/0/0/0
5	GOL	A	626	-	-	0/4/4/4	0/0/0/0
4	EDO	B	621	-	-	0/1/1/1	0/0/0/0
4	EDO	B	622	-	-	0/1/1/1	0/0/0/0
4	EDO	B	623	-	-	0/1/1/1	0/0/0/0
4	EDO	B	624	3	-	0/1/1/1	0/0/0/0
4	EDO	B	625	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	626	-	-	0/1/1/1	0/0/0/0
4	EDO	B	627	-	-	0/1/1/1	0/0/0/0
4	EDO	B	628	-	-	0/1/1/1	0/0/0/0
5	GOL	B	629	-	-	0/4/4/4	0/0/0/0
5	GOL	B	630	-	-	0/4/4/4	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	620	EDO	O2-C2	2.05	1.53	1.42
4	B	626	EDO	O1-C1	2.14	1.53	1.42
4	A	620	EDO	O1-C1	2.18	1.53	1.42
4	B	621	EDO	O1-C1	2.19	1.53	1.42
4	A	621	EDO	O1-C1	2.22	1.54	1.42
4	B	628	EDO	O2-C2	2.25	1.54	1.42
4	B	627	EDO	O1-C1	2.29	1.54	1.42
4	B	625	EDO	O1-C1	2.30	1.54	1.42
4	B	628	EDO	O1-C1	2.37	1.54	1.42
4	B	625	EDO	O2-C2	2.52	1.55	1.42
4	B	621	EDO	O2-C2	2.62	1.56	1.42
4	B	622	EDO	O2-C2	2.73	1.56	1.42
4	A	621	EDO	O2-C2	2.77	1.57	1.42
4	B	624	EDO	O2-C2	2.82	1.57	1.42
4	A	622	EDO	O2-C2	2.82	1.57	1.42
4	B	626	EDO	O2-C2	2.90	1.57	1.42
4	B	623	EDO	O2-C2	2.96	1.58	1.42
4	B	627	EDO	O2-C2	3.09	1.58	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	620	EDO	2	0
4	A	622	EDO	2	0
4	B	625	EDO	1	0
4	B	628	EDO	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	611/614 (99%)	-0.15	24 (3%) 43 40	8, 15, 29, 47	0
1	B	613/614 (99%)	-0.33	17 (2%) 56 54	8, 14, 24, 41	0
All	All	1224/1228 (99%)	-0.24	41 (3%) 50 47	8, 14, 26, 47	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	591	THR	5.6
1	A	3	THR	5.3
1	B	591	THR	5.1
1	B	592	SER	4.7
1	A	248	ASP	4.7
1	A	592	SER	4.4
1	B	593	THR	4.3
1	A	27	ALA	4.1
1	A	520	TYR	4.0
1	A	521	SER	3.8
1	A	518	SER	3.8
1	A	590	THR	3.5
1	B	416	TYR	3.5
1	B	294	ASN	3.4
1	A	416	TYR	3.4
1	A	524	LYS	3.3
1	B	28	ASP	3.3
1	B	248	ASP	3.2
1	B	245	GLN	3.2
1	B	524	LYS	3.1
1	A	572	GLN	3.0
1	A	439	HIS	2.9
1	A	525	ASN	2.9
1	A	523	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	417	VAL	2.8
1	A	593	THR	2.8
1	A	28	ASP	2.7
1	A	311	TRP	2.7
1	A	526	THR	2.6
1	A	522	GLU	2.6
1	B	296	THR	2.6
1	B	246	GLN	2.4
1	B	27	ALA	2.3
1	B	2	GLY	2.3
1	B	247	THR	2.3
1	B	295	GLY	2.3
1	B	3	THR	2.2
1	A	467	SER	2.2
1	A	587	GLY	2.2
1	A	595	ASN	2.1
1	B	293	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no 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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	EDO	A	620	4/4	0.83	0.16	12.30	25,25,25,28	0
5	GOL	A	625	6/6	0.88	0.14	11.82	17,24,25,26	0
5	GOL	A	626	6/6	0.80	0.18	10.54	28,29,30,32	0
4	EDO	B	625	4/4	0.89	0.17	5.06	24,24,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	EDO	B	628	4/4	0.85	0.21	4.35	25,26,27,27	0
4	EDO	B	622	4/4	0.78	0.14	3.90	21,23,24,26	0
4	EDO	B	627	4/4	0.90	0.11	3.47	29,29,30,30	0
4	EDO	B	623	4/4	0.89	0.16	2.10	23,25,26,27	0
5	GOL	B	630	6/6	0.79	0.17	2.04	36,37,37,38	0
5	GOL	B	629	6/6	0.92	0.12	1.59	17,18,20,20	0
5	GOL	A	623	6/6	0.86	0.15	1.50	24,27,27,27	0
4	EDO	B	621	4/4	0.92	0.11	1.49	15,16,19,20	0
4	EDO	B	626	4/4	0.93	0.14	1.02	23,25,25,27	0
4	EDO	B	624	4/4	0.92	0.10	0.90	20,21,21,22	0
4	EDO	A	622	4/4	0.89	0.14	0.69	24,24,24,25	0
2	CA	B	615	1/1	0.99	0.06	-0.12	12,12,12,12	0
2	CA	B	616	1/1	1.00	0.04	-1.31	11,11,11,11	0
2	CA	A	616	1/1	1.00	0.04	-1.46	10,10,10,10	0
2	CA	A	615	1/1	1.00	0.02	-4.87	10,10,10,10	0
3	MG	B	618	1/1	0.97	0.13	-	24,24,24,24	0
3	MG	A	619	1/1	0.85	0.22	-	38,38,38,38	0
3	MG	B	617	1/1	0.99	0.03	-	18,18,18,18	0
4	EDO	A	621	4/4	0.87	0.20	-	27,27,28,29	0
3	MG	A	617	1/1	0.92	0.49	-	67,67,67,67	0
3	MG	A	618	1/1	0.97	0.10	-	32,32,32,32	0
5	GOL	A	624	6/6	0.76	0.12	-	31,33,34,34	0
3	MG	B	620	1/1	0.98	0.21	-	27,27,27,27	0
3	MG	B	619	1/1	0.95	0.21	-	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.