Full wwPDB X-ray Structure Validation Report (i)

May 9, 2023 – 10:29 pm BST

PDB ID	:	8B8E
Title	:	Wild-type GH11 from Blastobotrys mokoenaii
Authors	:	Coleman, T.; Ravn, J.L.; Larsbrink, J.
Deposited on	:	2022-10-04
Resolution	:	1.55 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 (1)) were used in the production of this report:

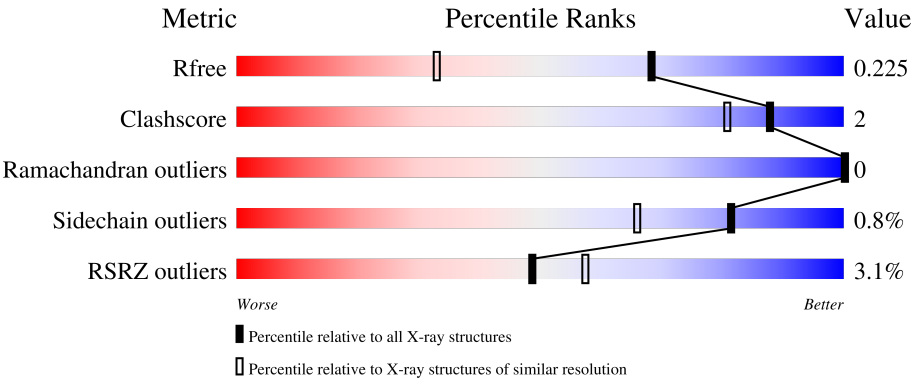
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 1.55 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}	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	225	81% · 15%
1	B	225	81% · 15%
1	C	225	4% 83% · 14%
1	D	225	2% 82% · · 15%
1	E	225	6% 81% · · 15%

2 Entry composition

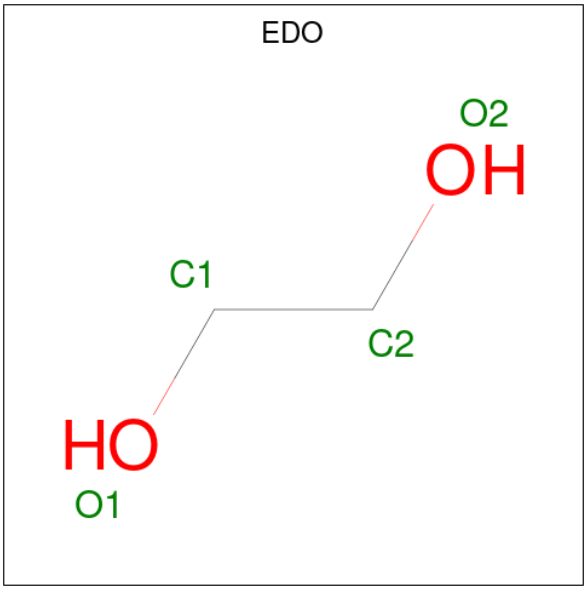
There are 9 unique types of molecules in this entry. The entry contains 15021 atoms, of which 6762 are hydrogens and 0 are deuteriums.

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 BmGH11.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	191	Total	C	H	N	O	S	0	3	0
			2770	914	1304	246	305	1			
1	B	191	Total	C	H	N	O	S	0	3	0
			2770	915	1302	246	306	1			
1	C	193	Total	C	H	N	O	S	0	1	0
			2785	920	1308	251	305	1			
1	D	191	Total	C	H	N	O	S	0	4	0
			2783	918	1312	247	305	1			
1	E	191	Total	C	H	N	O	S	0	8	0
			2806	925	1320	249	311	1			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		

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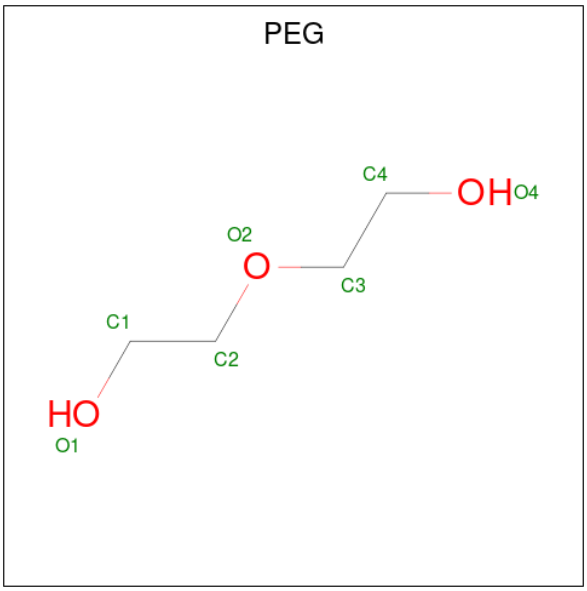
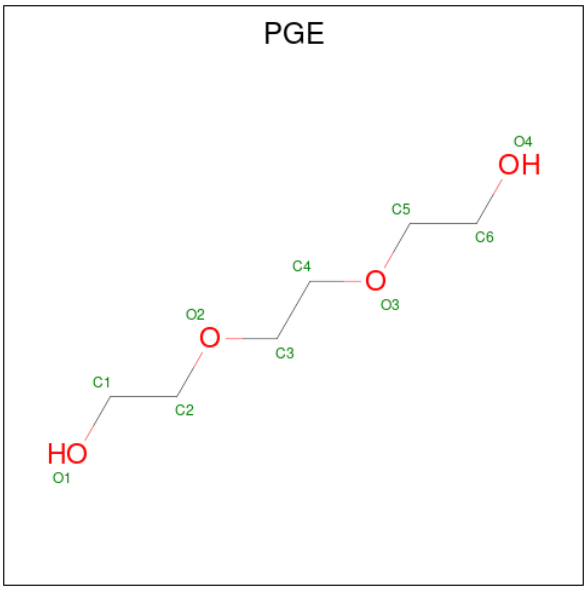
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 10 2 6 2	0	0
2	A	1	Total C H O 10 2 6 2	0	0
2	A	1	Total C H O 10 2 6 2	0	0
2	A	1	Total C H O 10 2 6 2	0	0
2	A	1	Total C H O 10 2 6 2	0	0
2	A	1	Total C H O 10 2 6 2	0	0
2	B	1	Total C H O 10 2 6 2	0	0
2	B	1	Total C H O 10 2 6 2	0	0
2	B	1	Total C H O 10 2 6 2	0	0
2	B	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	E	1	Total C H O 10 2 6 2	0	0
2	E	1	Total C H O 10 2 6 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	E	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

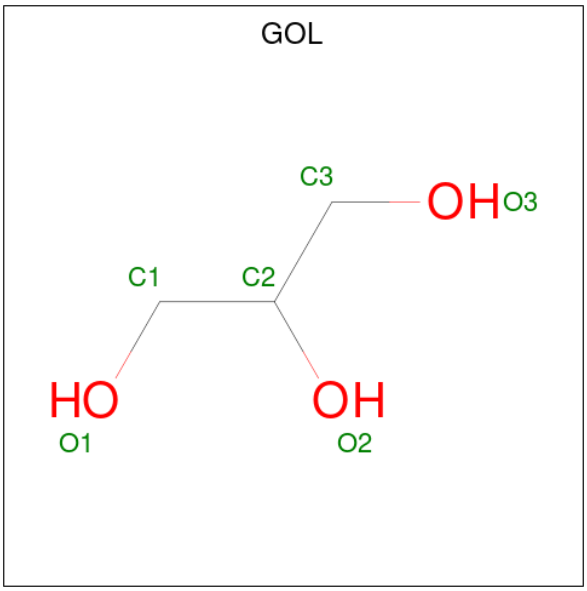


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 24 6 14 4	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	D	2	Total Na 2 2	0	0
5	E	1	Total Na 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C H O 14 3 8 3	0	0
6	B	1	Total C H O 14 3 8 3	0	0
6	B	1	Total C H O 14 3 8 3	0	0
6	B	1	Total C H O 14 3 8 3	0	0
6	E	1	Total C H O 14 3 8 3	0	0

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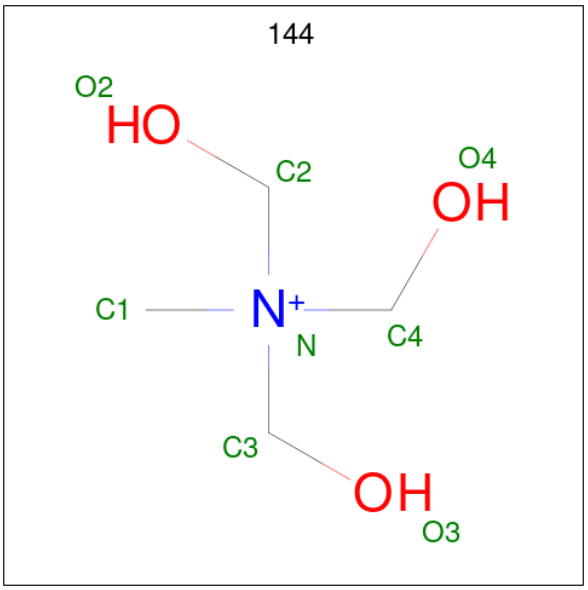
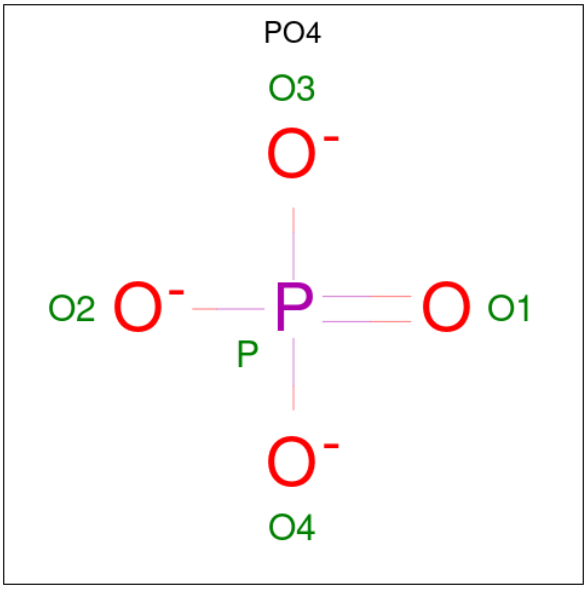
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	E	1	14	3	8	3	0	0

- Molecule 7 is TRIS-HYDROXYMETHYL-METHYL-AMMONIUM (three-letter code: 144) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
7	B	1	20	4	12	1	3	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 9 is water.

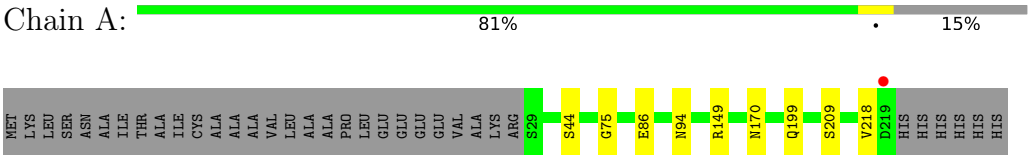
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	160	Total O 160 160	0	0
9	B	174	Total O 174 174	0	0
9	C	142	Total O 142 142	0	0
9	D	143	Total O 143 143	0	0
9	E	112	Total O 112 112	0	0

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.

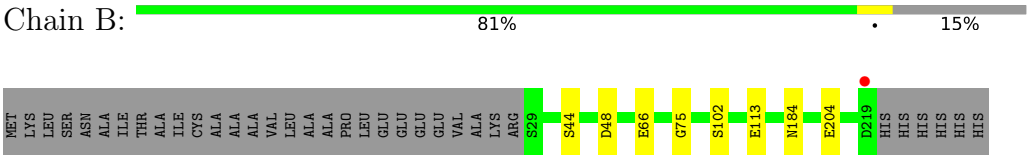
• Molecule 1: BmGH11

Chain A:



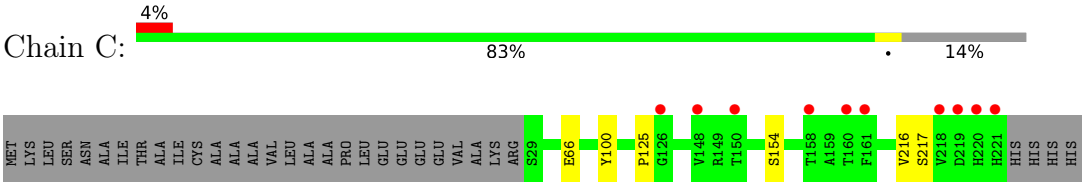
• Molecule 1: BmGH11

Chain B:



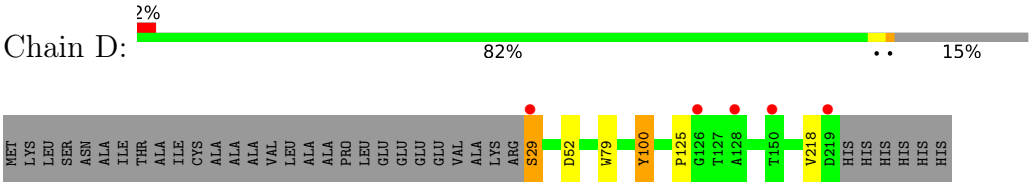
• Molecule 1: BmGH11

Chain C:



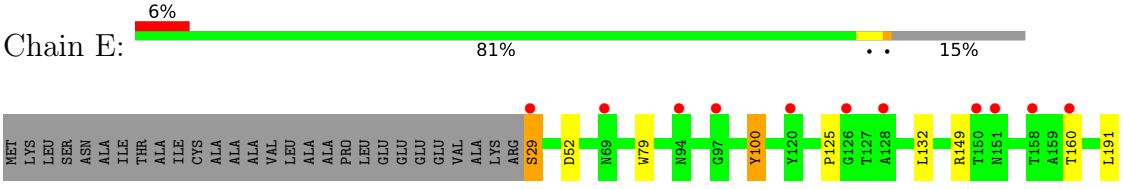
• Molecule 1: BmGH11

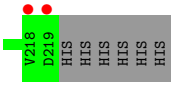
Chain D:



• Molecule 1: BmGH11

Chain E:




V218
D219
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.04Å 37.86Å 142.61Å 90.00° 104.27° 90.00°	Depositor
Resolution (Å)	63.11 – 1.55 63.11 – 1.55	Depositor EDS
% Data completeness (in resolution range)	98.9 (63.11-1.55) 98.9 (63.11-1.55)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.193 , 0.225 0.192 , 0.225	Depositor DCC
R_{free} test set	1998 reflections (1.60%)	wwPDB-VP
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15021	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% 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, 0.333 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: PGE, EDO, NA, PO4, 144, PEG, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.75	0/1519	0.74	0/2077
1	B	0.79	0/1521	0.79	1/2081 (0.0%)
1	C	0.69	0/1526	0.73	0/2087
1	D	0.69	0/1527	0.71	0/2087
1	E	0.65	0/1552	0.71	0/2122
All	All	0.72	0/7645	0.74	1/10454 (0.0%)

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	B	48	ASP	CB-CG-OD1	5.40	123.16	118.30

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	1466	1304	1309	8	0
1	B	1468	1302	1308	3	1
1	C	1477	1308	1310	4	0
1	D	1471	1312	1320	4	0
1	E	1486	1320	1319	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	28	42	42	0	0
2	B	16	24	24	0	0
2	C	16	24	24	0	0
2	E	8	12	12	1	0
3	A	7	10	10	2	0
3	B	7	10	10	0	0
3	C	7	10	9	0	0
3	E	7	10	10	0	0
4	A	10	14	14	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	1
6	B	24	32	32	0	0
6	E	12	16	16	0	0
7	B	8	12	12	3	0
8	D	5	0	0	0	0
9	A	160	0	0	4	5
9	B	174	0	0	1	1
9	C	142	0	0	2	4
9	D	143	0	0	0	4
9	E	112	0	0	0	1
All	All	8259	6762	6781	29	11

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 2.

All (29) 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:199:GLN:NE2	9:A:401:HOH:O	2.11	0.83
1:A:149:ARG:NH2	9:A:403:HOH:O	2.20	0.71
1:B:113:GLU:OE2	7:B:307:144:H13	1.94	0.67
1:A:170:ASN:OD1	9:A:402:HOH:O	2.13	0.66
1:A:94:ASN:ND2	9:A:404:HOH:O	2.24	0.65
1:C:66:GLU:OE1	9:C:401:HOH:O	2.16	0.63
1:E:29[A]:SER:N	1:E:52:ASP:OD1	2.33	0.62
1:B:204:GLU:OE2	7:B:307:144:H12	2.02	0.59
1:D:29:SER:N	1:D:52:ASP:OD1	2.36	0.58
1:D:79:TRP:CZ2	1:D:218:VAL:HG22	2.41	0.55
1:D:79:TRP:CZ2	1:D:218:VAL:CG2	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:SER:O	9:C:402:HOH:O	2.20	0.50
1:E:100:TYR:CZ	1:E:125:PRO:HB3	2.47	0.50
1:C:100:TYR:CZ	1:C:125:PRO:HB3	2.47	0.49
1:D:100:TYR:CZ	1:D:125:PRO:HB3	2.49	0.47
1:E:149:ARG:O	1:E:160:THR:HA	2.14	0.47
1:A:209:SER:OG	3:A:303:PEG:C1	2.62	0.47
7:B:307:144:H11	9:B:467:HOH:O	2.15	0.46
1:A:209:SER:OG	3:A:303:PEG:H12	2.16	0.46
1:C:216:VAL:HG12	1:C:217:SER:N	2.33	0.44
1:E:132:LEU:HD12	1:E:191:LEU:HD11	1.99	0.44
1:A:44:SER:O	1:A:75:GLY:HA2	2.20	0.42
1:A:86:GLU:O	1:A:218:VAL:HG23	2.21	0.40
1:B:44:SER:O	1:B:75:GLY:HA2	2.22	0.40

All (11) 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:B:184:ASN:HD21	5:E:306:NA:NA[1_545]	1.31	0.29
9:C:434:HOH:O	9:D:524:HOH:O[1_655]	1.97	0.23
9:C:534:HOH:O	9:D:459:HOH:O[1_655]	1.97	0.23
9:C:523:HOH:O	9:D:527:HOH:O[2_656]	2.04	0.16
9:A:537:HOH:O	9:A:548:HOH:O[2_555]	2.07	0.13
9:A:549:HOH:O	9:E:430:HOH:O[2_645]	2.12	0.08
9:B:443:HOH:O	9:B:558:HOH:O[1_545]	2.12	0.08
9:A:418:HOH:O	9:A:499:HOH:O[1_565]	2.15	0.05
9:C:534:HOH:O	9:D:537:HOH:O[1_655]	2.15	0.05
9:A:524:HOH:O	9:A:559:HOH:O[2_545]	2.17	0.03
9:A:530:HOH:O	9:A:537:HOH:O[2_545]	2.18	0.02

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	192/225 (85%)	188 (98%)	4 (2%)	0	100	100
1	B	192/225 (85%)	188 (98%)	4 (2%)	0	100	100
1	C	192/225 (85%)	188 (98%)	4 (2%)	0	100	100
1	D	193/225 (86%)	187 (97%)	6 (3%)	0	100	100
1	E	196/225 (87%)	189 (96%)	7 (4%)	0	100	100
All	All	965/1125 (86%)	940 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	156/179 (87%)	156 (100%)	0	100	100
1	B	156/179 (87%)	153 (98%)	3 (2%)	57	28
1	C	156/179 (87%)	156 (100%)	0	100	100
1	D	157/179 (88%)	155 (99%)	2 (1%)	69	44
1	E	161/179 (90%)	158 (98%)	3 (2%)	57	28
All	All	786/895 (88%)	778 (99%)	8 (1%)	81	57

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	66[A]	GLU
1	B	66[B]	GLU
1	B	102	SER
1	D	29	SER
1	D	100	TYR
1	E	29[A]	SER
1	E	29[B]	SER
1	E	100	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	151	ASN
1	C	207	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 5 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
7	144	B	307	-	1,7,7	1.79	0	3,9,9	0.31	0
2	EDO	C	302	-	3,3,3	0.49	0	2,2,2	0.30	0
2	EDO	A	304	-	3,3,3	0.48	0	2,2,2	0.23	0
6	GOL	E	302	-	5,5,5	0.73	0	5,5,5	1.04	0
2	EDO	E	301	-	3,3,3	0.55	0	2,2,2	0.23	0
8	PO4	D	301	-	4,4,4	0.58	0	6,6,6	0.40	0
3	PEG	B	305	-	6,6,6	0.19	0	5,5,5	0.10	0
3	PEG	E	304	-	6,6,6	0.11	0	5,5,5	0.10	0
2	EDO	C	301	-	3,3,3	0.58	0	2,2,2	0.27	0
6	GOL	E	303	-	5,5,5	0.79	0	5,5,5	1.11	0
2	EDO	A	309	-	3,3,3	0.50	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	B	302	-	3,3,3	0.46	0	2,2,2	0.36	0
3	PEG	A	303	-	6,6,6	0.11	0	5,5,5	0.38	0
6	GOL	B	301	-	5,5,5	1.18	1 (20%)	5,5,5	0.99	0
2	EDO	B	304	-	3,3,3	0.50	0	2,2,2	0.36	0
6	GOL	B	306	-	5,5,5	0.84	0	5,5,5	1.16	0
2	EDO	A	302	-	3,3,3	0.59	0	2,2,2	0.26	0
2	EDO	A	306	-	3,3,3	0.59	0	2,2,2	0.25	0
2	EDO	B	309	-	3,3,3	0.61	0	2,2,2	0.35	0
2	EDO	E	305	-	3,3,3	0.44	0	2,2,2	0.38	0
2	EDO	C	304	-	3,3,3	0.58	0	2,2,2	0.40	0
6	GOL	B	303	-	5,5,5	0.88	0	5,5,5	1.20	1 (20%)
2	EDO	A	307	-	3,3,3	0.66	0	2,2,2	0.45	0
2	EDO	A	308	-	3,3,3	0.78	0	2,2,2	0.38	0
6	GOL	B	308	-	5,5,5	1.09	1 (20%)	5,5,5	1.17	0
2	EDO	B	310	-	3,3,3	0.34	0	2,2,2	0.28	0
4	PGE	A	305	-	9,9,9	0.32	0	8,8,8	0.59	0
3	PEG	C	303	-	6,6,6	0.58	0	5,5,5	0.17	0
2	EDO	A	301	-	3,3,3	0.49	0	2,2,2	0.45	0
2	EDO	C	305	-	3,3,3	0.50	0	2,2,2	0.32	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
7	144	B	307	-	-	0/0/9/9	-
2	EDO	C	302	-	-	0/1/1/1	-
2	EDO	A	304	-	-	1/1/1/1	-
6	GOL	E	302	-	-	3/4/4/4	-
2	EDO	E	301	-	-	0/1/1/1	-
3	PEG	B	305	-	-	2/4/4/4	-
3	PEG	E	304	-	-	3/4/4/4	-
2	EDO	C	301	-	-	0/1/1/1	-
6	GOL	E	303	-	-	2/4/4/4	-
2	EDO	A	309	-	-	0/1/1/1	-
2	EDO	B	302	-	-	0/1/1/1	-
3	PEG	A	303	-	-	4/4/4/4	-
6	GOL	B	301	-	-	0/4/4/4	-
2	EDO	B	304	-	-	1/1/1/1	-
6	GOL	B	306	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	302	-	-	1/1/1/1	-
2	EDO	A	306	-	-	1/1/1/1	-
2	EDO	B	309	-	-	0/1/1/1	-
2	EDO	E	305	-	-	0/1/1/1	-
2	EDO	C	304	-	-	1/1/1/1	-
6	GOL	B	303	-	-	2/4/4/4	-
2	EDO	A	307	-	-	0/1/1/1	-
2	EDO	A	308	-	-	1/1/1/1	-
6	GOL	B	308	-	-	2/4/4/4	-
2	EDO	B	310	-	-	0/1/1/1	-
4	PGE	A	305	-	-	6/7/7/7	-
3	PEG	C	303	-	-	3/4/4/4	-
2	EDO	A	301	-	-	0/1/1/1	-
2	EDO	C	305	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	301	GOL	O2-C2	-2.18	1.36	1.43
6	B	308	GOL	O2-C2	-2.01	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	303	GOL	C3-C2-C1	-2.14	103.39	111.70

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	303	GOL	C1-C2-C3-O3
6	B	306	GOL	C1-C2-C3-O3
6	E	302	GOL	C1-C2-C3-O3
6	E	303	GOL	C1-C2-C3-O3
6	E	303	GOL	O2-C2-C3-O3
4	A	305	PGE	C6-C5-O3-C4
6	B	306	GOL	O2-C2-C3-O3
3	C	303	PEG	O1-C1-C2-O2
3	E	304	PEG	O1-C1-C2-O2
3	A	303	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	305	PEG	O1-C1-C2-O2
6	B	308	GOL	C1-C2-C3-O3
6	B	303	GOL	O2-C2-C3-O3
6	E	302	GOL	O2-C2-C3-O3
2	A	306	EDO	O1-C1-C2-O2
2	A	308	EDO	O1-C1-C2-O2
3	C	303	PEG	O2-C3-C4-O4
3	E	304	PEG	O2-C3-C4-O4
4	A	305	PGE	O2-C3-C4-O3
4	A	305	PGE	C4-C3-O2-C2
2	C	304	EDO	O1-C1-C2-O2
2	A	304	EDO	O1-C1-C2-O2
3	B	305	PEG	O2-C3-C4-O4
6	B	308	GOL	O2-C2-C3-O3
3	C	303	PEG	C1-C2-O2-C3
2	A	302	EDO	O1-C1-C2-O2
2	C	305	EDO	O1-C1-C2-O2
4	A	305	PGE	O1-C1-C2-O2
3	A	303	PEG	C1-C2-O2-C3
2	B	304	EDO	O1-C1-C2-O2
6	E	302	GOL	O1-C1-C2-C3
4	A	305	PGE	C3-C4-O3-C5
3	E	304	PEG	C1-C2-O2-C3
3	A	303	PEG	C4-C3-O2-C2
3	A	303	PEG	O2-C3-C4-O4
4	A	305	PGE	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	307	144	3	0
3	A	303	PEG	2	0
2	E	305	EDO	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	191/225 (84%)	-0.12	1 (0%)	91	93	11, 18, 27, 54	0
1	B	191/225 (84%)	-0.20	1 (0%)	91	93	11, 16, 24, 58	0
1	C	193/225 (85%)	0.04	10 (5%)	27	31	13, 19, 37, 52	0
1	D	191/225 (84%)	-0.04	5 (2%)	56	63	13, 19, 36, 57	0
1	E	191/225 (84%)	0.34	13 (6%)	17	20	15, 23, 42, 58	0
All	All	957/1125 (85%)	0.00	30 (3%)	49	57	11, 19, 37, 58	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	218[A]	VAL	4.5
1	C	221	HIS	4.2
1	D	219	ASP	4.1
1	C	160	THR	3.7
1	E	126	GLY	3.6
1	C	218	VAL	3.6
1	C	219	ASP	3.5
1	B	219	ASP	2.9
1	C	126	GLY	2.9
1	A	219	ASP	2.8
1	E	158	THR	2.7
1	E	219	ASP	2.7
1	E	128	ALA	2.7
1	E	97	GLY	2.6
1	C	148	VAL	2.6
1	E	69[A]	ASN	2.5
1	D	29	SER	2.5
1	D	128	ALA	2.5
1	E	150	THR	2.4
1	E	151	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	150	THR	2.3
1	E	160	THR	2.3
1	C	220	HIS	2.2
1	D	126	GLY	2.2
1	C	161	PHE	2.2
1	E	29[A]	SER	2.2
1	C	150	THR	2.2
1	C	158	THR	2.2
1	E	94	ASN	2.1
1	E	120	TYR	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 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
5	NA	E	306	1/1	0.03	0.23	39,39,39,39	0
5	NA	D	302	1/1	0.51	0.21	45,45,45,45	0
2	EDO	A	308	4/4	0.56	0.24	36,45,59,59	0
6	GOL	E	302	6/6	0.68	0.19	38,47,51,57	0
2	EDO	A	301	4/4	0.69	0.13	34,40,42,50	0
2	EDO	B	309	4/4	0.69	0.18	27,32,37,42	0
3	PEG	A	303	7/7	0.69	0.35	31,38,49,59	0
2	EDO	C	304	4/4	0.71	0.18	44,53,63,63	0
4	PGE	A	305	10/10	0.73	0.31	32,52,63,63	0
3	PEG	C	303	7/7	0.74	0.20	28,35,44,44	0
2	EDO	E	301	4/4	0.75	0.17	33,45,50,55	0
2	EDO	C	301	4/4	0.76	0.16	26,40,47,48	0
2	EDO	A	307	4/4	0.77	0.28	26,36,49,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	C	302	4/4	0.78	0.32	47,57,60,68	0
2	EDO	A	309	4/4	0.79	0.23	45,54,58,69	0
2	EDO	A	306	4/4	0.80	0.19	31,37,42,43	0
2	EDO	B	304	4/4	0.81	0.22	39,46,54,54	0
2	EDO	A	302	4/4	0.81	0.13	26,31,42,50	0
2	EDO	A	304	4/4	0.82	0.17	27,41,46,55	0
5	NA	D	303	1/1	0.82	0.20	29,29,29,29	0
3	PEG	B	305	7/7	0.83	0.24	27,33,48,58	0
3	PEG	E	304	7/7	0.85	0.25	42,58,65,65	0
7	144	B	307	8/8	0.85	0.11	15,21,30,30	0
2	EDO	C	305	4/4	0.87	0.17	28,34,40,44	0
8	PO4	D	301	5/5	0.87	0.16	36,39,48,57	0
2	EDO	B	302	4/4	0.89	0.24	27,34,43,52	0
6	GOL	B	308	6/6	0.90	0.09	19,28,47,47	0
2	EDO	B	310	4/4	0.91	0.19	28,35,43,48	0
6	GOL	B	303	6/6	0.92	0.11	22,30,36,36	0
6	GOL	E	303	6/6	0.92	0.14	25,34,44,53	0
5	NA	A	310	1/1	0.93	0.09	32,32,32,32	0
2	EDO	E	305	4/4	0.93	0.21	36,43,45,49	0
6	GOL	B	306	6/6	0.94	0.08	23,27,32,32	0
6	GOL	B	301	6/6	0.95	0.08	16,20,23,24	0
5	NA	B	311	1/1	0.96	0.05	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.