Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 09:31 AM EDT

PDB ID	:	6E9B
Title	:	Bacteroides ovatus mixed-linkage glucan utilization locus (MLGUL) SGBP-B in complex with mixed-linkage heptasaccharide
Authors	:	Tamura, K.; Gardill, B.R.; Brumer, H.; Van Petegem, F.
Deposited on	:	2018-07-31
Resolution	:	3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

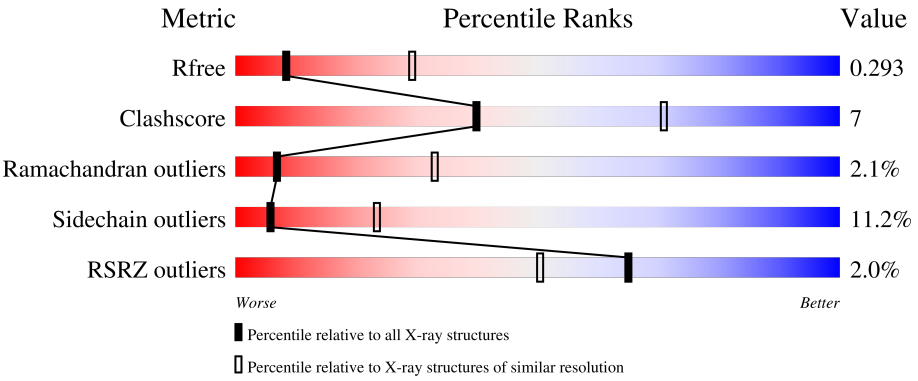
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	420	66% 24% • 9%
1	B	420	67% 22% • 10%
1	C	420	68% 22% • 8%
1	D	420	3% 68% 19% • 12%
2	E	7	14% 57% 29%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11363 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 Mixed-linkage glucan utilization locus (MLGUL) SGBP-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2836	1769	464	595	8			
1	B	378	Total	C	N	O	S	0	0	0
			2804	1742	462	593	7			
1	C	387	Total	C	N	O	S	0	0	0
			2877	1792	466	611	8			
1	D	368	Total	C	N	O	S	0	0	0
			2651	1641	440	562	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A7LY28
A	2	GLY	-	expression tag	UNP A7LY28
A	3	SER	-	expression tag	UNP A7LY28
A	4	SER	-	expression tag	UNP A7LY28
A	5	HIS	-	expression tag	UNP A7LY28
A	6	HIS	-	expression tag	UNP A7LY28
A	7	HIS	-	expression tag	UNP A7LY28
A	8	HIS	-	expression tag	UNP A7LY28
A	9	HIS	-	expression tag	UNP A7LY28
A	10	HIS	-	expression tag	UNP A7LY28
A	11	SER	-	expression tag	UNP A7LY28
A	12	SER	-	expression tag	UNP A7LY28
A	13	GLY	-	expression tag	UNP A7LY28
A	14	LEU	-	expression tag	UNP A7LY28
A	15	VAL	-	expression tag	UNP A7LY28
A	16	PRO	-	expression tag	UNP A7LY28
A	17	ARG	-	expression tag	UNP A7LY28
A	18	GLY	-	expression tag	UNP A7LY28
A	19	SER	-	expression tag	UNP A7LY28
A	20	HIS	-	expression tag	UNP A7LY28
A	21	MET	-	expression tag	UNP A7LY28

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP A7LY28
B	2	GLY	-	expression tag	UNP A7LY28
B	3	SER	-	expression tag	UNP A7LY28
B	4	SER	-	expression tag	UNP A7LY28
B	5	HIS	-	expression tag	UNP A7LY28
B	6	HIS	-	expression tag	UNP A7LY28
B	7	HIS	-	expression tag	UNP A7LY28
B	8	HIS	-	expression tag	UNP A7LY28
B	9	HIS	-	expression tag	UNP A7LY28
B	10	HIS	-	expression tag	UNP A7LY28
B	11	SER	-	expression tag	UNP A7LY28
B	12	SER	-	expression tag	UNP A7LY28
B	13	GLY	-	expression tag	UNP A7LY28
B	14	LEU	-	expression tag	UNP A7LY28
B	15	VAL	-	expression tag	UNP A7LY28
B	16	PRO	-	expression tag	UNP A7LY28
B	17	ARG	-	expression tag	UNP A7LY28
B	18	GLY	-	expression tag	UNP A7LY28
B	19	SER	-	expression tag	UNP A7LY28
B	20	HIS	-	expression tag	UNP A7LY28
B	21	MET	-	expression tag	UNP A7LY28
C	1	MET	-	initiating methionine	UNP A7LY28
C	2	GLY	-	expression tag	UNP A7LY28
C	3	SER	-	expression tag	UNP A7LY28
C	4	SER	-	expression tag	UNP A7LY28
C	5	HIS	-	expression tag	UNP A7LY28
C	6	HIS	-	expression tag	UNP A7LY28
C	7	HIS	-	expression tag	UNP A7LY28
C	8	HIS	-	expression tag	UNP A7LY28
C	9	HIS	-	expression tag	UNP A7LY28
C	10	HIS	-	expression tag	UNP A7LY28
C	11	SER	-	expression tag	UNP A7LY28
C	12	SER	-	expression tag	UNP A7LY28
C	13	GLY	-	expression tag	UNP A7LY28
C	14	LEU	-	expression tag	UNP A7LY28
C	15	VAL	-	expression tag	UNP A7LY28
C	16	PRO	-	expression tag	UNP A7LY28
C	17	ARG	-	expression tag	UNP A7LY28
C	18	GLY	-	expression tag	UNP A7LY28
C	19	SER	-	expression tag	UNP A7LY28
C	20	HIS	-	expression tag	UNP A7LY28
C	21	MET	-	expression tag	UNP A7LY28

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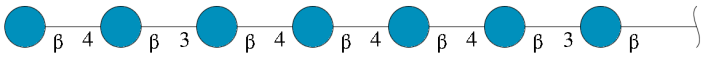
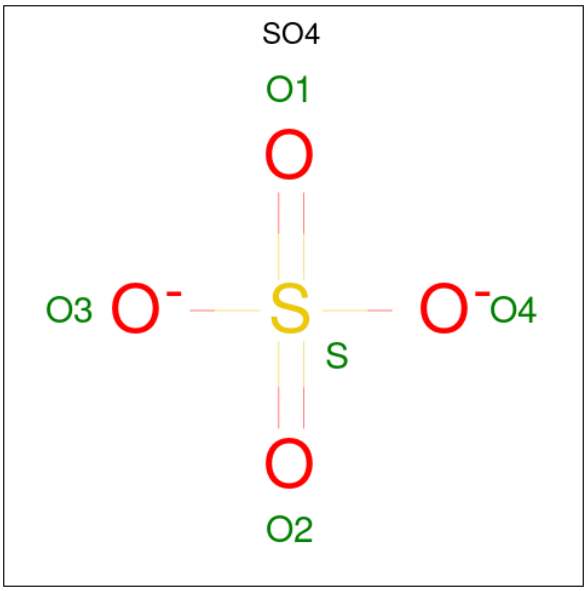
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP A7LY28
D	2	GLY	-	expression tag	UNP A7LY28
D	3	SER	-	expression tag	UNP A7LY28
D	4	SER	-	expression tag	UNP A7LY28
D	5	HIS	-	expression tag	UNP A7LY28
D	6	HIS	-	expression tag	UNP A7LY28
D	7	HIS	-	expression tag	UNP A7LY28
D	8	HIS	-	expression tag	UNP A7LY28
D	9	HIS	-	expression tag	UNP A7LY28
D	10	HIS	-	expression tag	UNP A7LY28
D	11	SER	-	expression tag	UNP A7LY28
D	12	SER	-	expression tag	UNP A7LY28
D	13	GLY	-	expression tag	UNP A7LY28
D	14	LEU	-	expression tag	UNP A7LY28
D	15	VAL	-	expression tag	UNP A7LY28
D	16	PRO	-	expression tag	UNP A7LY28
D	17	ARG	-	expression tag	UNP A7LY28
D	18	GLY	-	expression tag	UNP A7LY28
D	19	SER	-	expression tag	UNP A7LY28
D	20	HIS	-	expression tag	UNP A7LY28
D	21	MET	-	expression tag	UNP A7LY28

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	7	Total C O 78 42 36	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0
4	B	13	Total O 13 13	0	0

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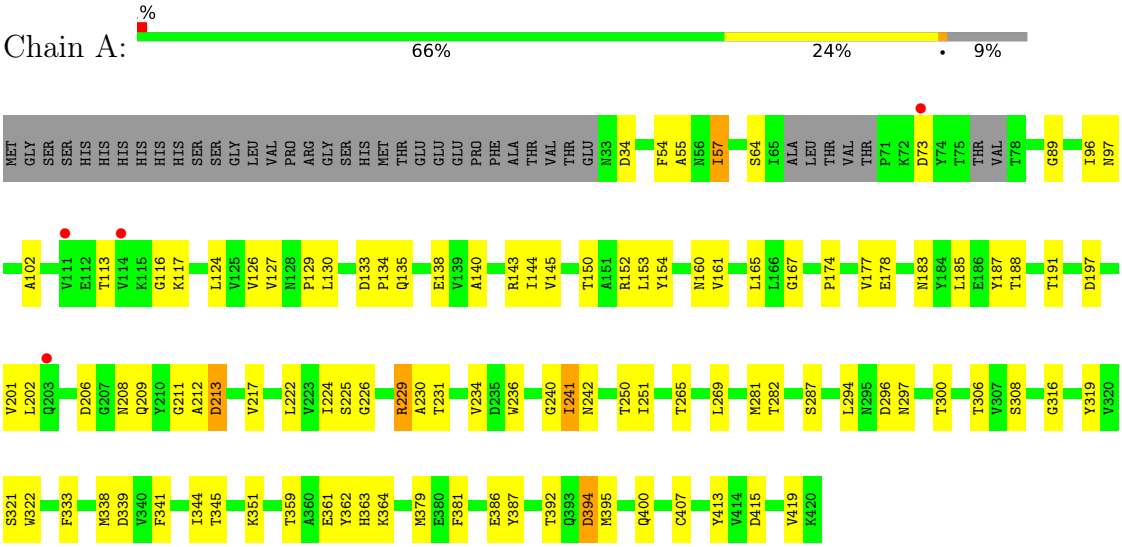
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	23	Total O 23 23	0	0
4	D	18	Total O 18 18	0	0

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.

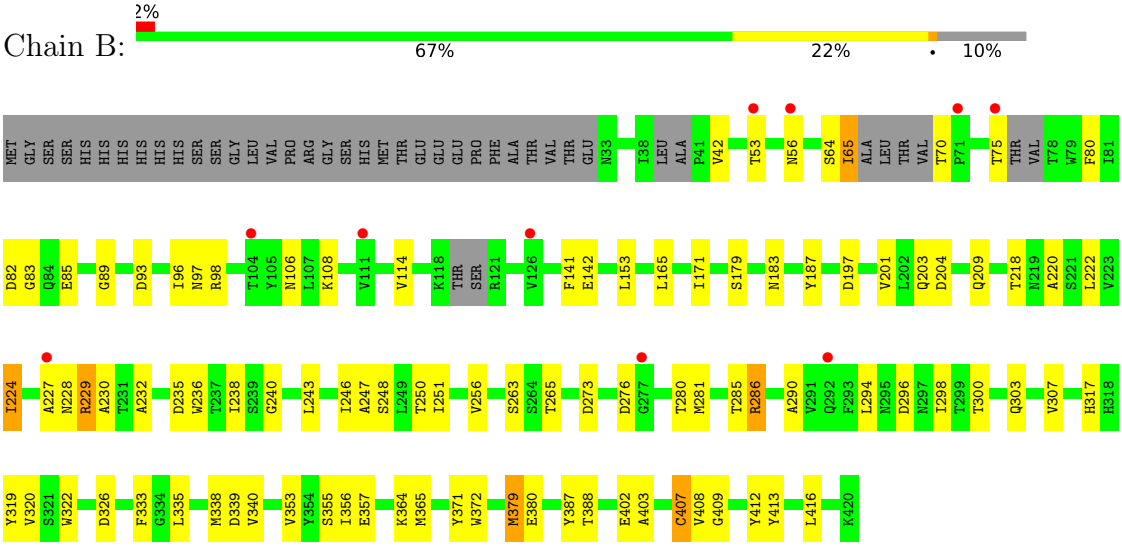
• Molecule 1: Mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain A:



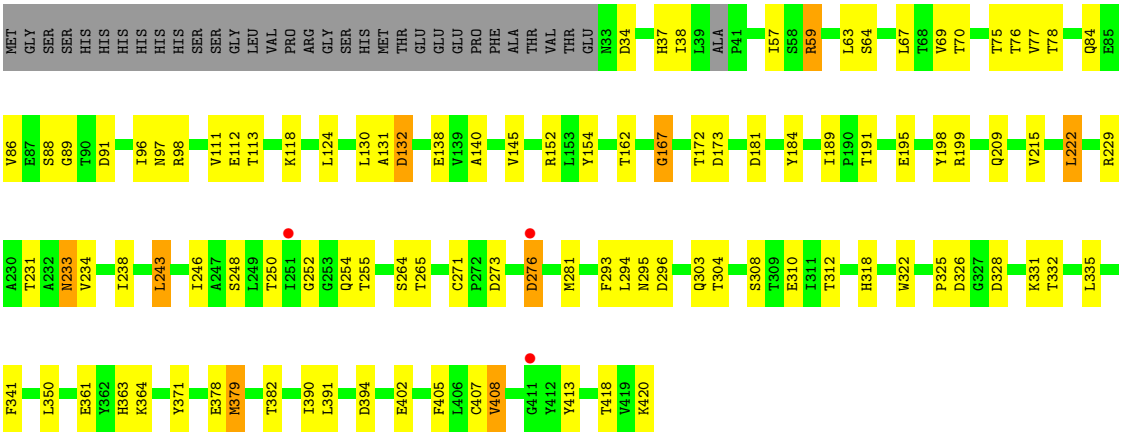
• Molecule 1: Mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain B:



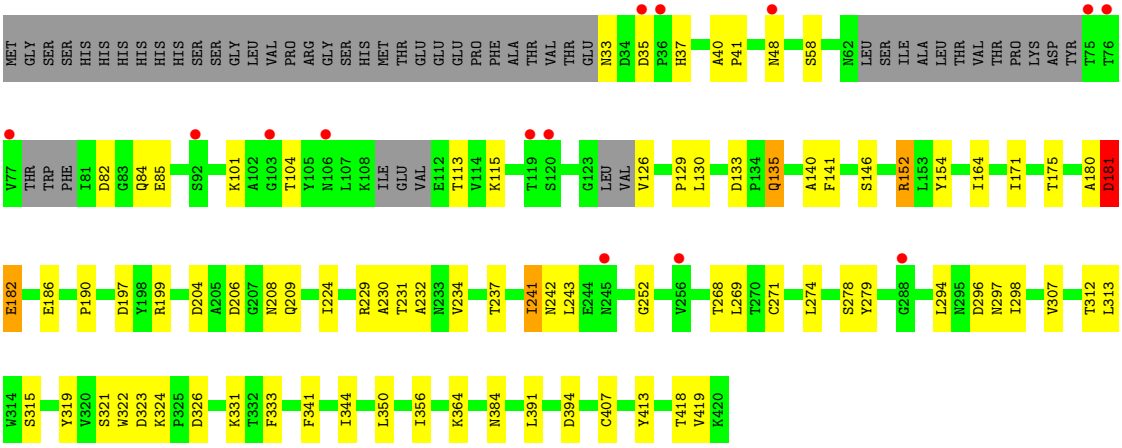
• Molecule 1: Mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain C:



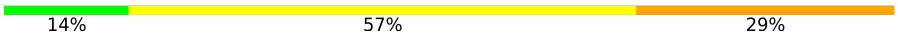
• Molecule 1: Mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain D:



• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	156.29Å 242.21Å 75.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.33 – 3.15 34.32 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.33-3.15) 99.9 (34.32-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.18Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.221 , 0.272 0.240 , 0.293	Depositor DCC
R_{free} test set	2505 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	90.3	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 87.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11363	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: SO4, BGC

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	0.52	0/2887	0.78	0/3947
1	B	0.51	0/2852	0.75	0/3898
1	C	0.52	0/2929	0.78	0/4011
1	D	0.54	0/2694	0.76	0/3685
All	All	0.52	0/11362	0.77	0/15541

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	2836	0	2651	42	0
1	B	2804	0	2592	48	0
1	C	2877	0	2678	36	0
1	D	2651	0	2405	36	0
2	E	78	0	66	2	0
3	A	20	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	13	0	0	0	0
4	B	13	0	0	0	0
4	C	23	0	0	1	0
4	D	18	0	0	0	0
All	All	11363	0	10392	158	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 7.

All (158) 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:C:131:ALA:O	1:C:132:ASP:HB2	1.68	0.91
1:D:152:ARG:HG3	1:D:152:ARG:HH11	1.40	0.83
1:C:181:ASP:HA	1:D:181:ASP:HA	1.67	0.76
1:A:153:LEU:HG	1:A:187:TYR:HE1	1.57	0.70
1:A:202:LEU:HG	1:A:212:ALA:HB2	1.74	0.70
1:D:152:ARG:HH11	1:D:152:ARG:CG	2.05	0.68
1:B:247:ALA:HB2	1:B:286:ARG:HG3	1.76	0.67
1:C:86:VAL:HG21	1:C:98:ARG:NH2	2.09	0.67
1:A:153:LEU:HG	1:A:187:TYR:CE1	2.29	0.67
1:A:392:THR:HG22	1:A:394:ASP:H	1.62	0.65
1:B:364:LYS:HG3	1:B:380:GLU:HG3	1.79	0.64
1:D:333:PHE:HB3	1:D:407:CYS:HB2	1.79	0.64
1:A:361:GLU:HG2	1:A:362:TYR:HD1	1.62	0.63
1:B:372:TRP:CZ3	1:B:408:VAL:HG21	2.34	0.62
1:B:89:GLY:HA3	1:B:97:ASN:H	1.64	0.61
1:A:364:LYS:HA	1:A:379:MET:O	2.01	0.61
1:B:372:TRP:HZ3	1:B:408:VAL:HG21	1.66	0.60
1:B:408:VAL:HG22	1:B:409:GLY:H	1.66	0.60
1:A:113:THR:HG22	1:A:117:LYS:H	1.67	0.60
1:A:333:PHE:HB3	1:A:407:CYS:HB2	1.83	0.60
1:D:241:ILE:H	1:D:243:LEU:HD13	1.67	0.60
1:B:80:PHE:HB2	1:B:108:LYS:HB2	1.84	0.59
1:B:364:LYS:HA	1:B:379:MET:O	2.03	0.59
1:A:344:ILE:HG12	1:A:419:VAL:HG21	1.84	0.59
1:D:312:THR:HA	1:D:418:THR:HG22	1.83	0.59
1:B:227:ALA:HB2	1:B:238:ILE:HD11	1.84	0.58
1:C:88:SER:HA	1:C:96:ILE:HG13	1.84	0.58
1:C:89:GLY:HA3	1:C:97:ASN:O	2.04	0.58
1:B:250:THR:O	1:B:281:MET:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:ILE:HG12	1:D:419:VAL:HG21	1.85	0.57
1:C:131:ALA:O	1:C:132:ASP:CB	2.44	0.57
1:C:59:ARG:HD2	1:C:130:LEU:HG	1.86	0.56
1:B:153:LEU:HG	1:B:187:TYR:CE1	2.40	0.56
1:B:153:LEU:HG	1:B:187:TYR:HE1	1.70	0.56
1:C:312:THR:HA	1:C:418:THR:HG22	1.89	0.55
1:D:130:LEU:HB2	1:D:133:ASP:HB2	1.88	0.55
1:B:224:ILE:HG12	1:B:240:GLY:HA2	1.89	0.55
1:D:313:LEU:HD11	1:D:344:ILE:HD11	1.89	0.55
1:A:222:LEU:HD21	1:A:294:LEU:HD12	1.88	0.55
1:C:145:VAL:HB	1:C:189:ILE:HG13	1.89	0.54
1:B:353:VAL:HB	1:B:416:LEU:HB3	1.90	0.54
1:A:392:THR:HB	1:A:395:MET:HG3	1.90	0.53
1:B:320:VAL:HG11	1:B:408:VAL:HA	1.91	0.53
1:D:252:GLY:HA2	1:D:279:TYR:HB3	1.90	0.53
1:A:251:ILE:HG13	1:A:281:MET:HG3	1.90	0.53
1:C:250:THR:O	1:C:281:MET:HA	2.09	0.53
1:D:331:LYS:HE3	2:E:5:BGC:O6	2.09	0.53
1:A:226:GLY:HA2	1:A:229:ARG:HH12	1.74	0.52
1:C:293:PHE:HB3	1:C:303:GLN:HE21	1.74	0.52
1:C:332:THR:HG22	1:C:408:VAL:HG23	1.90	0.52
1:D:323:ASP:HB2	3:D:509:SO4:O2	2.09	0.52
1:A:174:PRO:HB2	1:A:185:LEU:HD11	1.91	0.52
1:A:250:THR:O	1:A:281:MET:HA	2.09	0.52
1:D:146:SER:HB2	1:D:242:ASN:HD21	1.73	0.51
1:A:351:LYS:HA	1:A:387:TYR:O	2.10	0.51
1:A:319:TYR:CE2	1:A:321:SER:HB2	2.45	0.51
1:D:230:ALA:HB3	1:D:307:VAL:HG22	1.93	0.51
1:C:371:TYR:CG	1:C:402:GLU:HB3	2.46	0.51
1:A:338:MET:CE	1:A:400:GLN:HA	2.41	0.51
1:C:154:TYR:CE1	1:C:184:TYR:HB3	2.46	0.50
1:B:320:VAL:HB	1:B:412:TYR:CE1	2.47	0.50
1:C:63:LEU:O	1:C:97:ASN:HA	2.11	0.50
1:A:129:PRO:HG2	1:A:135:GLN:HG2	1.92	0.50
1:D:232:ALA:O	1:D:271:CYS:HB3	2.10	0.50
1:B:319:TYR:HB2	1:B:413:TYR:CE1	2.47	0.50
1:B:165:LEU:HB2	1:B:201:VAL:CG1	2.42	0.50
1:A:102:ALA:HB3	1:A:211:GLY:HA3	1.93	0.49
1:A:130:LEU:O	1:A:133:ASP:HB2	2.13	0.49
1:C:363:HIS:HD2	1:C:382:THR:HA	1.77	0.49
1:B:246:ILE:HA	1:B:285:THR:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:THR:HA	1:C:254:GLN:O	2.13	0.49
1:B:333:PHE:HD2	1:B:407:CYS:HB2	1.76	0.49
1:C:341:PHE:CE2	1:C:405:PHE:HB3	2.48	0.49
1:B:317:HIS:HB3	1:D:384:ASN:HD21	1.78	0.49
1:C:112:GLU:HG3	1:C:118:LYS:HE2	1.94	0.48
1:B:218:THR:OG1	1:B:220:ALA:HB3	2.14	0.48
1:C:326:ASP:HA	1:C:331:LYS:HD2	1.95	0.48
1:D:232:ALA:C	1:D:234:VAL:H	2.17	0.48
1:C:318:HIS:O	1:C:413:TYR:HA	2.12	0.48
1:D:341:PHE:HA	1:D:344:ILE:HD12	1.95	0.48
1:B:280:THR:HA	1:B:303:GLN:O	2.14	0.48
1:A:316:GLY:O	1:A:415:ASP:HA	2.13	0.48
1:C:231:THR:O	1:C:234:VAL:HG22	2.13	0.47
1:D:274:LEU:HB3	1:D:279:TYR:CE2	2.49	0.47
1:D:364:LYS:NZ	2:E:7:BGC:H6C1	2.28	0.47
1:B:371:TYR:HB2	1:B:402:GLU:HB3	1.97	0.47
1:C:350:LEU:HB2	1:C:391:LEU:HD11	1.96	0.47
1:A:102:ALA:HA	1:A:127:VAL:HB	1.96	0.47
1:A:144:ILE:HG22	1:A:241:ILE:HD13	1.96	0.47
1:B:230:ALA:HB3	1:B:307:VAL:HG22	1.96	0.47
1:C:233:ASN:HA	1:C:271:CYS:O	2.14	0.47
1:D:231:THR:HB	1:D:234:VAL:HG11	1.97	0.47
1:B:65:ILE:HB	1:B:96:ILE:HG22	1.96	0.47
1:C:77:VAL:HB	1:C:111:VAL:HG22	1.97	0.46
1:A:145:VAL:CG2	1:A:217:VAL:HG22	2.45	0.46
1:B:165:LEU:HD12	1:B:201:VAL:HG13	1.98	0.46
1:C:89:GLY:H	1:C:97:ASN:H	1.63	0.46
1:C:310:GLU:HG3	1:C:420:LYS:HD3	1.98	0.46
1:B:80:PHE:HD2	1:B:83:GLY:HA2	1.80	0.46
1:A:89:GLY:HA3	1:A:97:ASN:HB3	1.98	0.46
1:B:80:PHE:CB	1:B:108:LYS:HB2	2.46	0.46
1:B:203:GLN:HG3	1:B:209:GLN:HG3	1.98	0.46
1:C:304:THR:HG22	4:C:602:HOH:O	2.15	0.45
1:A:363:HIS:HB2	1:A:381:PHE:O	2.17	0.45
1:D:129:PRO:HG2	1:D:135:GLN:HG2	1.99	0.45
1:D:104:THR:H	1:D:199:ARG:HH22	1.64	0.45
1:D:324:LYS:O	1:D:331:LYS:HD3	2.17	0.45
1:C:222:LEU:HD11	1:C:294:LEU:HB2	1.97	0.45
1:C:364:LYS:HA	1:C:379:MET:O	2.17	0.45
1:A:231:THR:HB	1:A:234:VAL:HG22	1.98	0.45
1:D:204:ASP:HB3	1:D:208:ASN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:HB2	1:A:201:VAL:HB	1.99	0.44
1:B:365:MET:HG3	1:B:412:TYR:CE2	2.51	0.44
1:D:154:TYR:HE2	1:D:182:GLU:HB3	1.83	0.44
1:D:154:TYR:CE2	1:D:182:GLU:HB3	2.53	0.44
1:D:296:ASP:C	1:D:298:ILE:H	2.21	0.44
1:C:243:LEU:HA	1:C:246:ILE:HG13	1.99	0.44
1:A:138:GLU:HB2	1:A:143:ARG:HG3	1.99	0.44
1:D:113:THR:HG23	1:D:115:LYS:H	1.82	0.44
1:D:350:LEU:HB2	1:D:391:LEU:HD11	2.00	0.44
1:A:54:PHE:HB2	1:A:124:LEU:O	2.19	0.43
1:A:341:PHE:HA	1:A:344:ILE:HD12	2.00	0.43
1:A:177:VAL:HG13	1:B:380:GLU:HB3	2.00	0.43
1:B:82:ASP:HA	1:B:106:ASN:HB3	2.01	0.43
1:A:178:GLU:HA	1:A:183:ASN:OD1	2.19	0.43
1:A:224:ILE:HG13	1:A:240:GLY:HA2	2.01	0.42
1:C:378:GLU:O	1:D:175:THR:HA	2.19	0.42
1:B:371:TYR:HD2	1:B:402:GLU:HA	1.85	0.42
1:B:227:ALA:HB1	1:B:303:GLN:HG2	2.02	0.42
1:A:230:ALA:HB2	1:A:236:TRP:CE2	2.54	0.42
1:D:319:TYR:HB2	1:D:413:TYR:CE2	2.54	0.42
1:B:53:THR:HG21	1:B:56:ASN:HD22	1.84	0.42
1:B:165:LEU:HB2	1:B:201:VAL:HG13	2.01	0.42
1:B:296:ASP:O	1:B:298:ILE:HG12	2.20	0.42
1:D:40:ALA:HB3	1:D:41:PRO:HD3	2.02	0.42
1:A:319:TYR:HB2	1:A:413:TYR:CE2	2.54	0.42
1:A:143:ARG:O	1:A:145:VAL:HG13	2.20	0.41
1:B:171:ILE:HG21	1:B:187:TYR:HB2	2.01	0.41
1:B:248:SER:HA	1:B:256:VAL:O	2.20	0.41
1:C:167:GLY:HA3	1:C:198:TYR:CD2	2.55	0.41
1:C:310:GLU:HG2	1:C:418:THR:HB	2.01	0.41
1:A:152:ARG:CD	1:A:154:TYR:CE2	3.03	0.41
1:B:355:SER:OG	1:B:413:TYR:HB2	2.20	0.41
1:C:38:ILE:HD12	1:C:67:LEU:HB3	2.02	0.41
1:D:171:ILE:HD11	1:D:190:PRO:HD3	2.02	0.41
1:C:325:PRO:HG2	1:C:328:ASP:HB2	2.03	0.41
1:B:230:ALA:HB2	1:B:236:TRP:CZ2	2.56	0.41
1:A:54:PHE:HB3	1:A:55:ALA:H	1.61	0.41
1:A:241:ILE:HG23	1:A:242:ASN:HD22	1.85	0.41
1:D:319:TYR:CE2	1:D:321:SER:HB2	2.56	0.41
1:B:240:GLY:HA3	1:B:243:LEU:HD21	2.03	0.40
1:A:64:SER:HA	1:A:96:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:GLU:HB2	1:B:413:TYR:CE2	2.56	0.40
1:D:104:THR:HG23	1:D:126:VAL:HG22	2.03	0.40
1:B:222:LEU:HD11	1:B:294:LEU:N	2.36	0.40
1:B:364:LYS:O	1:B:409:GLY:HA3	2.22	0.40
1:B:228:ASN:HB3	1:B:229:ARG:HD3	2.04	0.40
1:B:408:VAL:HG22	1:B:409:GLY:N	2.36	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	375/420 (89%)	335 (89%)	31 (8%)	9 (2%)	6 30
1	B	368/420 (88%)	314 (85%)	47 (13%)	7 (2%)	8 36
1	C	383/420 (91%)	339 (88%)	36 (9%)	8 (2%)	7 33
1	D	358/420 (85%)	299 (84%)	52 (14%)	7 (2%)	7 34
All	All	1484/1680 (88%)	1287 (87%)	166 (11%)	31 (2%)	7 33

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	A	213	ASP
1	B	232	ALA
1	B	335	LEU
1	B	403	ALA
1	C	167	GLY
1	C	335	LEU
1	D	181	ASP
1	A	167	GLY

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Mol	Chain	Res	Type
1	B	290	ALA
1	C	132	ASP
1	C	173	ASP
1	C	252	GLY
1	D	85	GLU
1	A	140	ALA
1	A	208	ASN
1	B	273	ASP
1	C	140	ALA
1	C	276	ASP
1	D	141	PHE
1	D	241	ILE
1	A	57	ILE
1	B	42	VAL
1	B	114	VAL
1	D	140	ALA
1	A	161	VAL
1	D	180	ALA
1	D	186	GLU
1	C	243	LEU
1	A	134	PRO
1	A	116	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	304/358 (85%)	275 (90%)	29 (10%)	8 30
1	B	298/358 (83%)	266 (89%)	32 (11%)	6 25
1	C	310/358 (87%)	267 (86%)	43 (14%)	3 15
1	D	271/358 (76%)	242 (89%)	29 (11%)	6 25
All	All	1183/1432 (83%)	1050 (89%)	133 (11%)	6 23

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	57	ILE
1	A	73	ASP
1	A	126	VAL
1	A	150	THR
1	A	160	ASN
1	A	188	THR
1	A	191	THR
1	A	197	ASP
1	A	206	ASP
1	A	213	ASP
1	A	225	SER
1	A	229	ARG
1	A	241	ILE
1	A	265	THR
1	A	269	LEU
1	A	282	THR
1	A	287	SER
1	A	296	ASP
1	A	297	ASN
1	A	300	THR
1	A	306	THR
1	A	308	SER
1	A	322	TRP
1	A	339	ASP
1	A	345	THR
1	A	359	THR
1	A	386	GLU
1	A	394	ASP
1	B	64	SER
1	B	65	ILE
1	B	70	THR
1	B	75	THR
1	B	85	GLU
1	B	93	ASP
1	B	98	ARG
1	B	141	PHE
1	B	142	GLU
1	B	179	SER
1	B	183	ASN
1	B	197	ASP
1	B	204	ASP
1	B	224	ILE

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Mol	Chain	Res	Type
1	B	229	ARG
1	B	235	ASP
1	B	251	ILE
1	B	263	SER
1	B	265	THR
1	B	276	ASP
1	B	286	ARG
1	B	300	THR
1	B	322	TRP
1	B	326	ASP
1	B	338	MET
1	B	339	ASP
1	B	340	VAL
1	B	356	ILE
1	B	379	MET
1	B	387	TYR
1	B	388	THR
1	B	407	CYS
1	C	34	ASP
1	C	37	HIS
1	C	57	ILE
1	C	59	ARG
1	C	64	SER
1	C	69	VAL
1	C	70	THR
1	C	75	THR
1	C	76	THR
1	C	78	THR
1	C	84	GLN
1	C	91	ASP
1	C	113	THR
1	C	124	LEU
1	C	138	GLU
1	C	152	ARG
1	C	162	THR
1	C	172	THR
1	C	191	THR
1	C	195	GLU
1	C	199	ARG
1	C	209	GLN
1	C	215	VAL
1	C	222	LEU

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Mol	Chain	Res	Type
1	C	229	ARG
1	C	233	ASN
1	C	238	ILE
1	C	248	SER
1	C	255	THR
1	C	264	SER
1	C	265	THR
1	C	273	ASP
1	C	276	ASP
1	C	295	ASN
1	C	296	ASP
1	C	308	SER
1	C	322	TRP
1	C	361	GLU
1	C	379	MET
1	C	390	ILE
1	C	394	ASP
1	C	407	CYS
1	C	408	VAL
1	D	33	ASN
1	D	35	ASP
1	D	37	HIS
1	D	48	ASN
1	D	58	SER
1	D	82	ASP
1	D	84	GLN
1	D	101	LYS
1	D	135	GLN
1	D	152	ARG
1	D	164	ILE
1	D	181	ASP
1	D	182	GLU
1	D	197	ASP
1	D	206	ASP
1	D	209	GLN
1	D	224	ILE
1	D	229	ARG
1	D	237	THR
1	D	268	THR
1	D	269	LEU
1	D	278	SER
1	D	294	LEU

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Mol	Chain	Res	Type
1	D	297	ASN
1	D	315	SER
1	D	322	TRP
1	D	326	ASP
1	D	356	ILE
1	D	394	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	ASN
1	B	62	ASN
1	B	292	GLN
1	C	50	GLN
1	C	233	ASN
1	C	303	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)

7 monosaccharides 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	BGC	E	1	2	12,12,12	0.35	0	17,17,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	E	2	2	11,11,12	0.31	0	15,15,17	1.20	2 (13%)
2	BGC	E	3	2	11,11,12	0.46	0	15,15,17	1.25	2 (13%)
2	BGC	E	4	2	11,11,12	0.42	0	15,15,17	1.29	2 (13%)
2	BGC	E	5	2	11,11,12	0.58	0	15,15,17	1.42	1 (6%)
2	BGC	E	6	2	11,11,12	0.52	0	15,15,17	1.20	2 (13%)
2	BGC	E	7	2	11,11,12	0.57	0	15,15,17	0.83	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
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	1/2/19/22	0/1/1/1
2	BGC	E	3	2	-	1/2/19/22	0/1/1/1
2	BGC	E	4	2	-	2/2/19/22	0/1/1/1
2	BGC	E	5	2	-	1/2/19/22	0/1/1/1
2	BGC	E	6	2	-	1/2/19/22	0/1/1/1
2	BGC	E	7	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	5	BGC	C1-O5-C5	4.34	118.08	112.19
2	E	4	BGC	C1-O5-C5	2.94	116.17	112.19
2	E	6	BGC	C1-C2-C3	2.53	112.78	109.67
2	E	6	BGC	C2-C3-C4	2.50	115.22	110.89
2	E	3	BGC	O2-C2-C3	-2.50	105.14	110.14
2	E	2	BGC	O3-C3-C2	-2.36	105.48	109.99
2	E	4	BGC	O3-C3-C2	-2.22	105.75	109.99
2	E	3	BGC	C1-C2-C3	-2.21	106.94	109.67
2	E	2	BGC	O4-C4-C3	-2.11	105.47	110.35
2	E	7	BGC	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

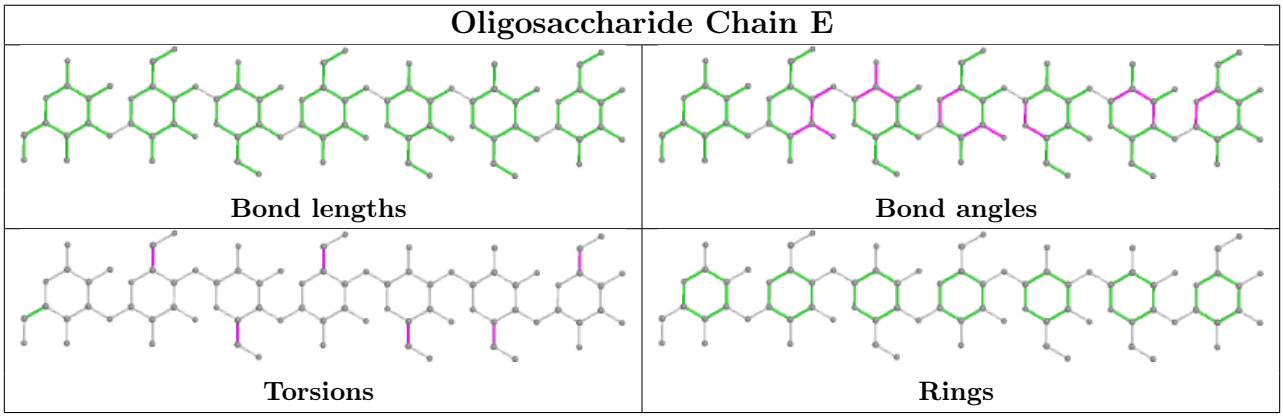
Mol	Chain	Res	Type	Atoms
2	E	4	BGC	O5-C5-C6-O6
2	E	7	BGC	O5-C5-C6-O6
2	E	5	BGC	O5-C5-C6-O6
2	E	3	BGC	O5-C5-C6-O6
2	E	2	BGC	O5-C5-C6-O6
2	E	4	BGC	C4-C5-C6-O6
2	E	7	BGC	C4-C5-C6-O6
2	E	6	BGC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	7	BGC	1	0
2	E	5	BGC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

10 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	$\#\|Z\|>2$
3	SO4	B	501	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.20	0
3	SO4	D	509	-	4,4,4	0.19	0	6,6,6	0.23	0
3	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	A	502	-	4,4,4	0.12	0	6,6,6	0.12	0
3	SO4	A	501	-	4,4,4	0.21	0	6,6,6	0.09	0
3	SO4	C	502	-	4,4,4	0.16	0	6,6,6	0.23	0
3	SO4	A	504	-	4,4,4	0.27	0	6,6,6	0.36	0
3	SO4	D	508	-	4,4,4	0.21	0	6,6,6	0.33	0
3	SO4	B	502	-	4,4,4	0.18	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	509	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	381/420 (90%)	-0.07	4 (1%) 82 73	41, 84, 154, 174	0
1	B	378/420 (90%)	0.09	10 (2%) 56 40	63, 111, 156, 188	0
1	C	387/420 (92%)	-0.14	3 (0%) 86 78	48, 93, 125, 140	0
1	D	368/420 (87%)	0.11	14 (3%) 40 25	41, 114, 171, 189	0
All	All	1514/1680 (90%)	-0.01	31 (2%) 65 50	41, 100, 158, 189	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	ASP	4.2
1	D	288	GLY	3.6
1	D	119	THR	3.3
1	A	203	GLN	3.3
1	D	36	PRO	3.2
1	D	76	THR	3.2
1	B	104	THR	3.0
1	D	48	ASN	2.9
1	D	103	GLY	2.8
1	D	75	THR	2.6
1	D	120	SER	2.5
1	A	111	VAL	2.4
1	C	251	ILE	2.4
1	D	245	ASN	2.3
1	C	276	ASP	2.3
1	C	411	GLY	2.3
1	A	114	VAL	2.3
1	B	126	VAL	2.2
1	D	35	ASP	2.1
1	D	106	ASN	2.1
1	B	75	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	227	ALA	2.1
1	D	77	VAL	2.1
1	B	71	PRO	2.1
1	B	277	GLY	2.1
1	B	53	THR	2.1
1	B	111	VAL	2.1
1	B	292	GLN	2.0
1	B	56	ASN	2.0
1	D	92	SER	2.0
1	D	256	VAL	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)

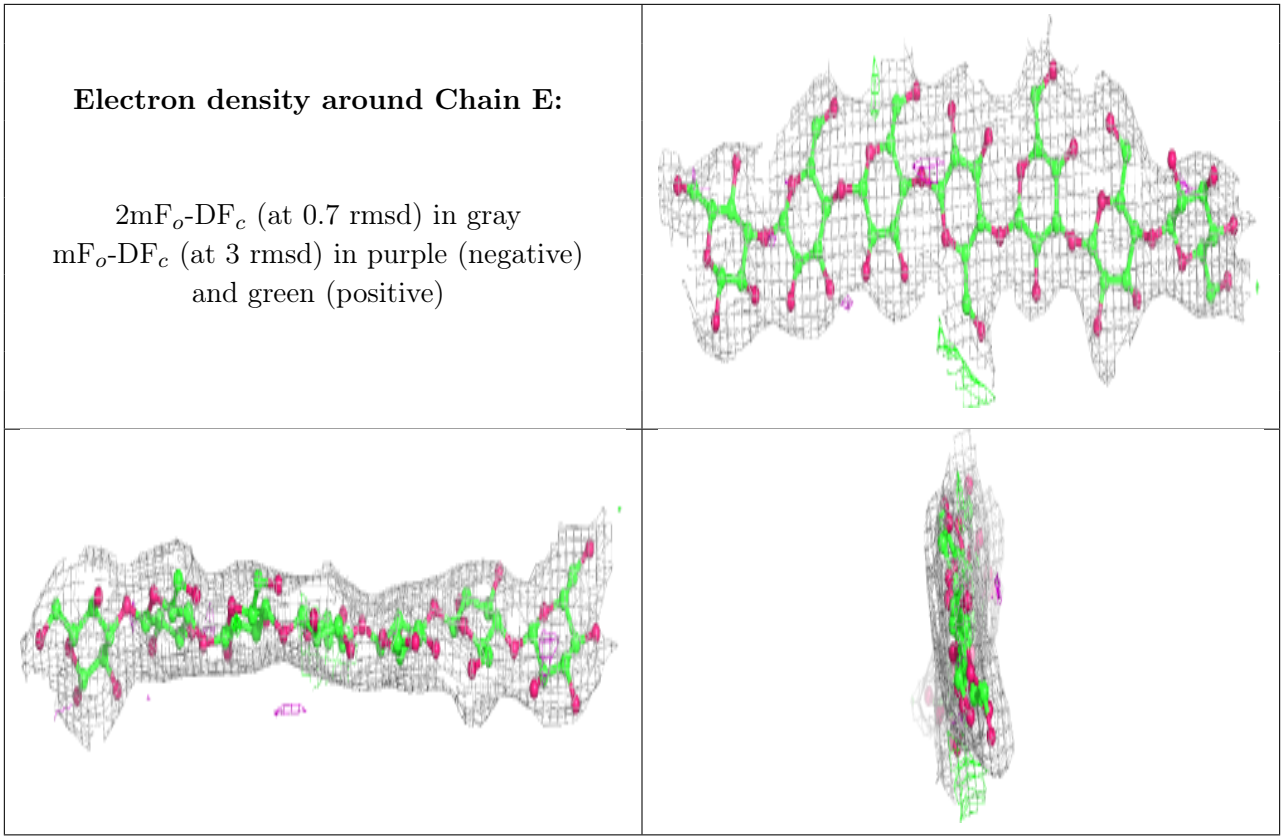
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	BGC	E	1	12/12	0.87	0.17	92,104,111,112	0
2	BGC	E	7	11/12	0.88	0.29	85,91,100,100	0
2	BGC	E	6	11/12	0.91	0.18	60,71,79,82	0
2	BGC	E	4	11/12	0.94	0.28	55,58,74,79	0
2	BGC	E	2	11/12	0.95	0.19	57,60,73,77	0
2	BGC	E	3	11/12	0.97	0.23	44,57,65,66	0
2	BGC	E	5	11/12	0.97	0.18	50,61,68,70	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



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. 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
3	SO4	C	502	5/5	0.75	0.33	152,152,153,154	0
3	SO4	A	503	5/5	0.76	0.38	189,189,189,190	0
3	SO4	A	502	5/5	0.78	0.28	179,179,179,180	0
3	SO4	D	509	5/5	0.82	0.24	137,138,139,139	0
3	SO4	B	502	5/5	0.83	0.13	172,172,173,173	0
3	SO4	B	501	5/5	0.85	0.21	153,154,154,155	0
3	SO4	C	501	5/5	0.90	0.21	127,129,129,131	0
3	SO4	A	501	5/5	0.91	0.21	139,139,139,141	0
3	SO4	A	504	5/5	0.93	0.14	122,122,124,124	0
3	SO4	D	508	5/5	0.95	0.20	115,116,117,120	0

6.5 Other polymers

There are no such residues in this entry.