



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:11 PM UTC

PDB ID : 6E9B / pdb_00006e9b
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

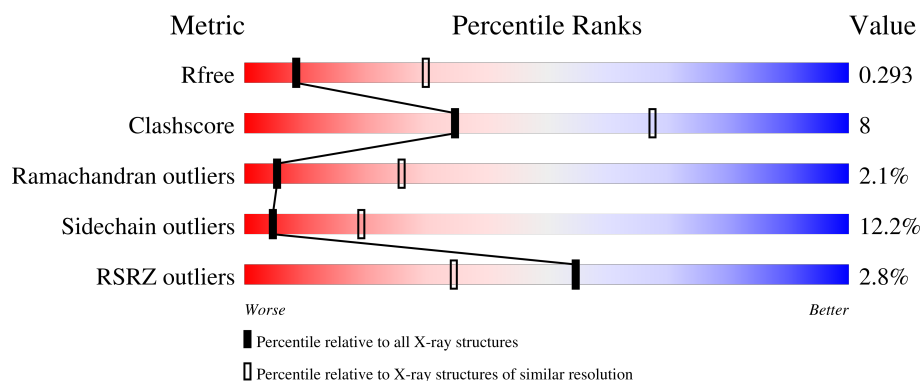
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (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 $\leq 5\%$. 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	420	2% 62% 26% • 9%
1	B	420	3% 65% 23% • 10%
1	C	420	• 63% 26% • 8%
1	D	420	3% 65% 19% • 12%
2	E	7	14% 57% 29%

2 Entry composition

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

Continued on next page...

Continued from previous page...

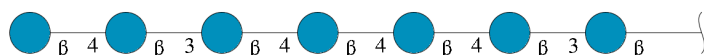
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP A7LY28
B	2	GLY	-	expression tag	UNP A7LY28
B	3	SER	-	expression tag	UNP A7LY28
B	4	SER	-	expression tag	UNP A7LY28
B	5	HIS	-	expression tag	UNP A7LY28
B	6	HIS	-	expression tag	UNP A7LY28
B	7	HIS	-	expression tag	UNP A7LY28
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

Continued on next page...

Continued from previous page...

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	0	0	0
			78	42	36			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

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

Continued on next page...

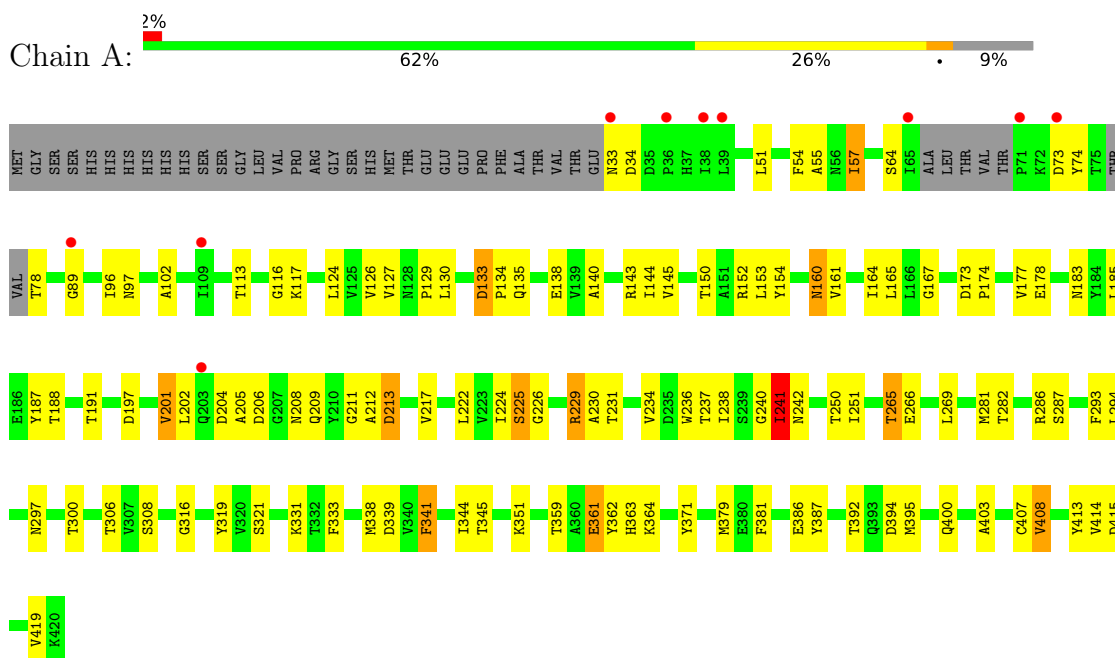
Continued from previous page...

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

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.

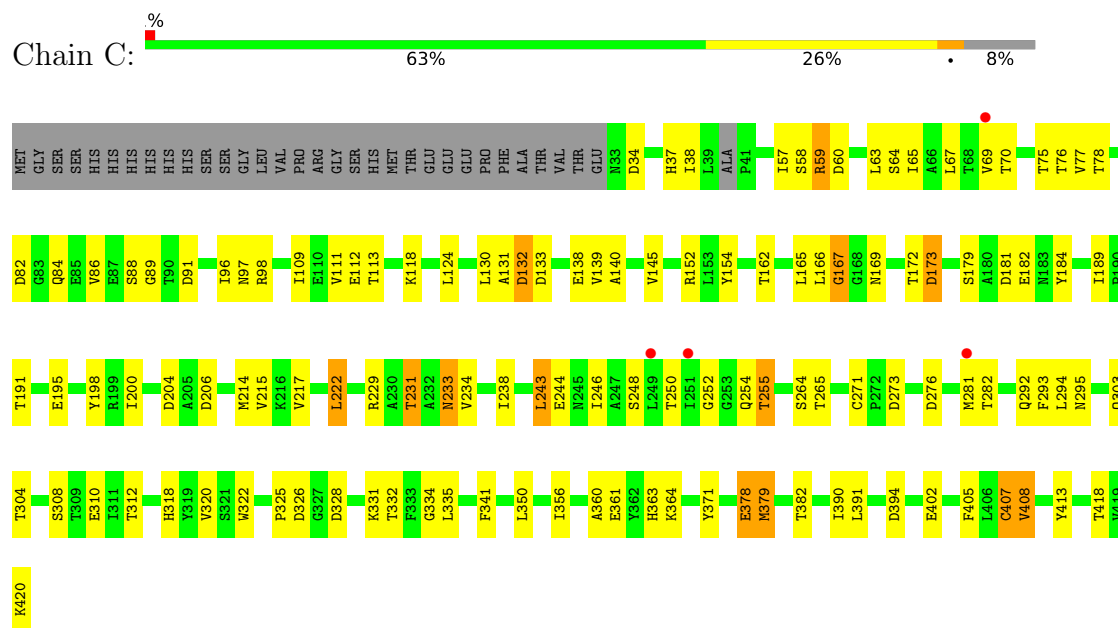
- Molecule 1: Mixed-linkage glucan utilization locus (MLGUL) SGBP-B



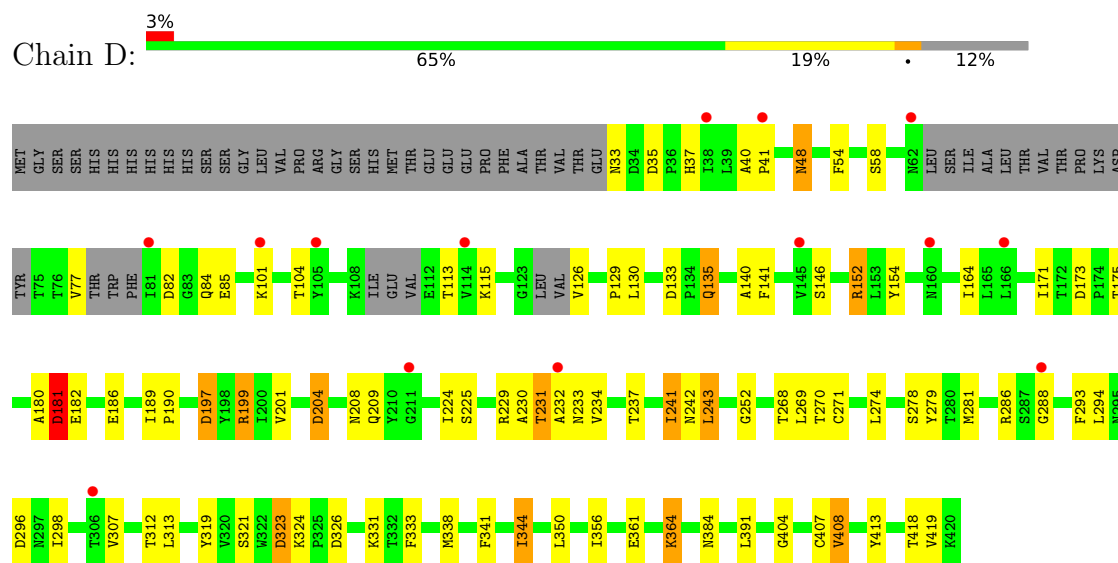
- Molecule 1: Mixed-linkage glucan utilization locus (MLGUL) SGBP-B



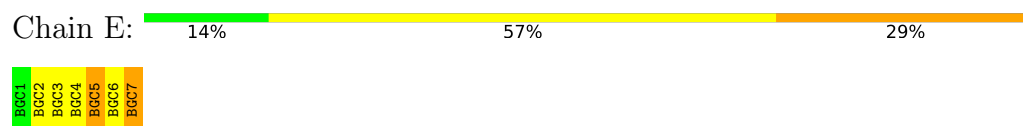
• Molecule 1: Mixed-linkage glucan utilization locus (MLGUL) SGBP-B



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



• 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



4 Data and refinement statistics

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 34.33 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.33-3.15) 99.9 (34.33-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.31 , 89.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BGC, 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	0.89	1/2887 (0.0%)	1.40	25/3947 (0.6%)
1	B	0.93	0/2852	1.35	10/3898 (0.3%)
1	C	0.90	1/2929 (0.0%)	1.38	23/4011 (0.6%)
1	D	0.97	1/2694 (0.0%)	1.37	16/3685 (0.4%)
All	All	0.92	3/11362 (0.0%)	1.37	74/15541 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	231	THR	CA-C	7.55	1.56	1.52
1	A	173	ASP	CA-C	5.65	1.59	1.52
1	C	165	LEU	CA-C	-5.05	1.46	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ASP	CA-CB-CG	7.47	120.07	112.60
1	C	378	GLU	N-CA-C	-7.03	99.62	110.10
1	C	133	ASP	CA-CB-CG	7.03	119.63	112.60
1	D	233	ASN	CA-C-N	6.78	129.77	120.35
1	D	233	ASN	C-N-CA	6.78	129.77	120.35
1	C	173	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	241	ILE	CA-C-N	-6.72	113.15	123.17
1	A	241	ILE	C-N-CA	-6.72	113.15	123.17
1	D	197	ASP	CA-C-N	6.69	130.65	120.82
1	D	197	ASP	C-N-CA	6.69	130.65	120.82
1	A	414	VAL	N-CA-C	-6.66	98.84	108.36
1	D	48	ASN	CA-CB-CG	6.64	119.24	112.60
1	D	54	PHE	CA-CB-CG	6.62	120.42	113.80
1	B	133	ASP	CA-CB-CG	6.57	119.17	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	ASN	N-CA-C	-6.43	105.47	113.38
1	C	179	SER	CA-C-N	6.40	129.69	120.79
1	C	179	SER	C-N-CA	6.40	129.69	120.79
1	D	204	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	60	ASP	CA-CB-CG	6.10	118.70	112.60
1	D	189	ILE	N-CA-C	6.04	114.64	109.02
1	D	270	THR	CA-C-N	6.00	129.41	120.83
1	D	270	THR	C-N-CA	6.00	129.41	120.83
1	C	231	THR	CA-C-N	5.95	129.55	121.05
1	C	231	THR	C-N-CA	5.95	129.55	121.05
1	D	408	VAL	N-CA-CB	-5.94	102.48	112.47
1	D	361	GLU	CB-CG-CD	5.93	122.68	112.60
1	A	225	SER	N-CA-C	5.92	117.78	108.96
1	C	360	ALA	CA-C-N	5.88	128.15	120.28
1	C	360	ALA	C-N-CA	5.88	128.15	120.28
1	A	265	THR	N-CA-C	5.87	117.48	111.14
1	C	334	GLY	CA-C-N	5.86	132.74	121.54
1	C	334	GLY	C-N-CA	5.86	132.74	121.54
1	C	204	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	361	GLU	CB-CG-CD	5.71	122.31	112.60
1	C	82	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	106	ASN	CA-CB-CG	5.64	118.24	112.60
1	B	196	GLY	N-CA-C	5.54	118.49	111.85
1	A	33	ASN	CA-CB-CG	5.54	118.14	112.60
1	A	173	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	341	PHE	CA-CB-CG	-5.44	108.36	113.80
1	C	206	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	80	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	160	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	408	VAL	N-CA-CB	-5.42	101.72	112.24
1	B	407	CYS	N-CA-C	-5.40	99.48	108.34
1	B	402	GLU	CA-C-N	5.36	131.77	121.54
1	B	402	GLU	C-N-CA	5.36	131.77	121.54
1	A	403	ALA	N-CA-C	5.35	119.39	112.86
1	A	74	TYR	N-CA-C	-5.34	105.41	112.94
1	A	339	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	323	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	266	GLU	N-CA-C	5.29	117.80	108.75
1	A	237	THR	CA-C-N	5.29	129.93	123.10
1	A	237	THR	C-N-CA	5.29	129.93	123.10
1	A	204	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	286	ARG	N-CA-C	-5.29	105.60	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	MET	N-CA-C	5.28	117.68	110.55
1	A	371	TYR	N-CA-C	-5.23	106.68	113.16
1	A	241	ILE	N-CA-C	5.21	116.38	111.48
1	C	58	SER	CA-C-N	5.21	128.63	120.82
1	C	58	SER	C-N-CA	5.21	128.63	120.82
1	C	182	GLU	CB-CG-CD	5.21	121.45	112.60
1	C	407	CYS	N-CA-C	-5.16	99.88	108.34
1	A	205	ALA	CA-C-N	5.13	127.16	120.28
1	A	205	ALA	C-N-CA	5.13	127.16	120.28
1	C	60	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	173	ASP	CA-CB-CG	5.12	117.72	112.60
1	D	199	ARG	N-CA-C	-5.12	102.18	110.32
1	A	331	LYS	N-CA-C	-5.09	105.82	112.23
1	C	179	SER	N-CA-C	5.07	116.95	108.99
1	D	225	SER	N-CA-C	5.05	116.52	108.79
1	C	255	THR	CA-C-N	5.01	127.87	120.91
1	C	255	THR	C-N-CA	5.01	127.87	120.91
1	A	266	GLU	N-CA-C	5.00	116.59	109.14

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	43	0
1	B	2804	0	2592	48	0
1	C	2877	0	2678	37	0
1	D	2651	0	2405	39	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
4	A	13	0	0	0	0
4	B	13	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	23	0	0	1	0
4	D	18	0	0	0	0
All	All	11363	0	10392	163	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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:D:338:MET:HE3	1:D:404:GLY:H	1.68	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
1:D:344:ILE:HG12	1:D:419:VAL:HG21	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:232:ALA:C	1:D:234:VAL:H	2.17	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:D:281:MET:HE3	1:D:293:PHE:CE1	2.45	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ILE:HA	1:B:285:THR:HA	1.93	0.49
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:D:296:ASP:C	1:D:298:ILE:H	2.21	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: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:A:281:MET:HE3	1:A:293:PHE:CE1	2.50	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:166:LEU:O	1:C:167:GLY:C	2.61	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:D:286:ARG:C	1:D:288:GLY:H	2.28	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	4	23
1	B	368/420 (88%)	314 (85%)	47 (13%)	7 (2%)	6	28
1	C	383/420 (91%)	339 (88%)	36 (9%)	8 (2%)	5	26
1	D	358/420 (85%)	299 (84%)	52 (14%)	7 (2%)	6	27
All	All	1484/1680 (88%)	1287 (87%)	166 (11%)	31 (2%)	5	26

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	335	LEU
1	D	181	ASP
1	A	167	GLY
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 ⓘ

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%)	273 (90%)	31 (10%)	7	26
1	B	298/358 (83%)	264 (89%)	34 (11%)	5	21
1	C	310/358 (87%)	260 (84%)	50 (16%)	2	11
1	D	271/358 (76%)	242 (89%)	29 (11%)	6	24
All	All	1183/1432 (83%)	1039 (88%)	144 (12%)	5	19

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	51	LEU
1	A	57	ILE
1	A	73	ASP
1	A	78	THR
1	A	126	VAL
1	A	150	THR
1	A	160	ASN
1	A	164	ILE
1	A	188	THR
1	A	191	THR
1	A	197	ASP
1	A	201	VAL
1	A	206	ASP
1	A	213	ASP
1	A	225	SER
1	A	229	ARG
1	A	238	ILE
1	A	241	ILE
1	A	265	THR
1	A	269	LEU
1	A	282	THR
1	A	287	SER
1	A	297	ASN
1	A	300	THR
1	A	306	THR
1	A	308	SER
1	A	345	THR
1	A	359	THR
1	A	386	GLU
1	A	408	VAL
1	B	57	ILE
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	100	LEU
1	B	112	GLU
1	B	141	PHE
1	B	142	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	179	SER
1	B	204	ASP
1	B	223	VAL
1	B	224	ILE
1	B	229	ARG
1	B	251	ILE
1	B	263	SER
1	B	265	THR
1	B	286	ARG
1	B	292	GLN
1	B	295	ASN
1	B	300	THR
1	B	322	TRP
1	B	338	MET
1	B	339	ASP
1	B	340	VAL
1	B	356	ILE
1	B	361	GLU
1	B	379	MET
1	B	388	THR
1	B	390	ILE
1	B	407	CYS
1	B	418	THR
1	C	34	ASP
1	C	37	HIS
1	C	57	ILE
1	C	59	ARG
1	C	64	SER
1	C	65	ILE
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	109	ILE
1	C	113	THR
1	C	124	LEU
1	C	138	GLU
1	C	139	VAL
1	C	152	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	162	THR
1	C	169	ASN
1	C	172	THR
1	C	191	THR
1	C	195	GLU
1	C	200	ILE
1	C	215	VAL
1	C	217	VAL
1	C	222	LEU
1	C	229	ARG
1	C	233	ASN
1	C	238	ILE
1	C	244	GLU
1	C	248	SER
1	C	255	THR
1	C	264	SER
1	C	265	THR
1	C	273	ASP
1	C	282	THR
1	C	292	GLN
1	C	295	ASN
1	C	308	SER
1	C	320	VAL
1	C	322	TRP
1	C	356	ILE
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	77	VAL
1	D	82	ASP
1	D	84	GLN
1	D	101	LYS
1	D	135	GLN
1	D	152	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	164	ILE
1	D	181	ASP
1	D	197	ASP
1	D	201	VAL
1	D	209	GLN
1	D	224	ILE
1	D	229	ARG
1	D	237	THR
1	D	243	LEU
1	D	268	THR
1	D	269	LEU
1	D	278	SER
1	D	294	LEU
1	D	326	ASP
1	D	344	ILE
1	D	356	ILE
1	D	364	LYS
1	D	408	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	62	ASN
1	A	97	ASN
1	A	157	ASN
1	A	169	ASN
1	A	183	ASN
1	A	228	ASN
1	A	393	GLN
1	A	397	ASN
1	A	400	GLN
1	B	157	ASN
1	B	203	GLN
1	B	209	GLN
1	B	292	GLN
1	C	50	GLN
1	C	84	GLN
1	C	128	ASN
1	C	303	GLN
1	D	48	ASN
1	D	56	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	169	ASN
1	D	228	ASN
1	D	297	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 ⓘ

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
2	BGC	E	2	2	11,11,12	0.30	0	15,15,17	1.14	2 (13%)
2	BGC	E	3	2	11,11,12	0.45	0	15,15,17	1.16	1 (6%)
2	BGC	E	4	2	11,11,12	0.42	0	15,15,17	1.22	2 (13%)
2	BGC	E	5	2	11,11,12	0.56	0	15,15,17	1.37	1 (6%)
2	BGC	E	6	2	11,11,12	0.50	0	15,15,17	1.11	2 (13%)
2	BGC	E	7	2	11,11,12	0.56	0	15,15,17	0.79	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 (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	BGC	C1-O5-C5	4.39	118.08	112.19
2	E	4	BGC	C1-O5-C5	2.98	116.17	112.19
2	E	6	BGC	C2-C3-C4	2.48	115.22	110.86
2	E	3	BGC	O2-C2-C3	-2.42	105.14	110.15
2	E	2	BGC	O3-C3-C2	-2.24	105.48	110.05
2	E	6	BGC	C1-C2-C3	2.15	112.78	109.64
2	E	4	BGC	O3-C3-C2	-2.11	105.75	110.05
2	E	2	BGC	O4-C4-C3	-2.08	105.47	110.38
2	E	7	BGC	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

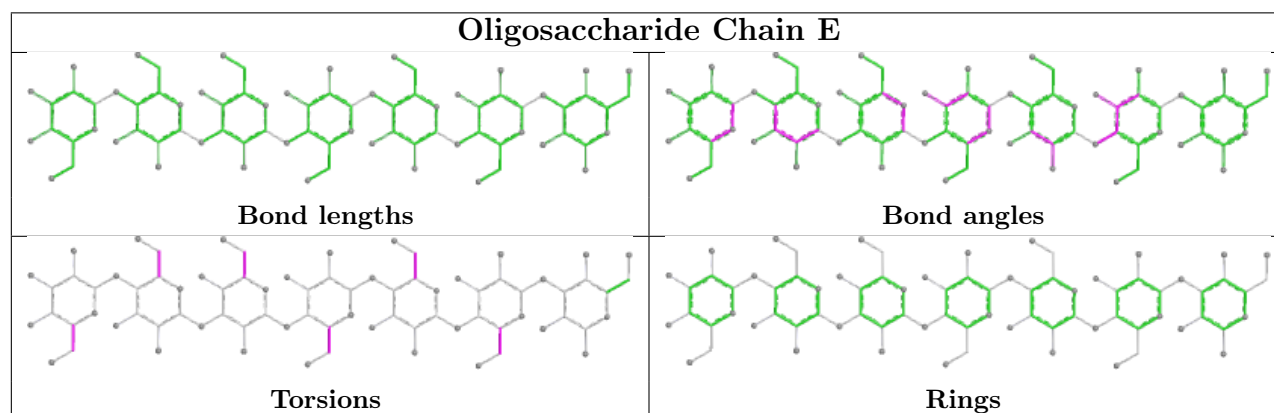
Mol	Chain	Res	Type	Atoms
2	E	4	BGC	O5-C5-C6-O6
2	E	7	BGC	O5-C5-C6-O6
2	E	5	BGC	O5-C5-C6-O6
2	E	3	BGC	O5-C5-C6-O6
2	E	2	BGC	O5-C5-C6-O6
2	E	4	BGC	C4-C5-C6-O6
2	E	7	BGC	C4-C5-C6-O6
2	E	6	BGC	O5-C5-C6-O6

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	0.34	0	6,6,6	0.07	0
3	SO4	A	502	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	A	501	-	4,4,4	0.33	0	6,6,6	0.09	0
3	SO4	A	504	-	4,4,4	0.38	0	6,6,6	0.39	0
3	SO4	D	508	-	4,4,4	0.31	0	6,6,6	0.31	0
3	SO4	B	502	-	4,4,4	0.29	0	6,6,6	0.06	0
3	SO4	C	501	-	4,4,4	0.33	0	6,6,6	0.21	0
3	SO4	A	503	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	D	509	-	4,4,4	0.26	0	6,6,6	0.24	0
3	SO4	C	502	-	4,4,4	0.26	0	6,6,6	0.24	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, 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	381/420 (90%)	0.12	10 (2%) 57 36	41, 84, 154, 174	0
1	B	378/420 (90%)	0.36	14 (3%) 45 26	63, 111, 156, 188	0
1	C	387/420 (92%)	0.05	4 (1%) 79 62	48, 93, 125, 140	0
1	D	368/420 (87%)	0.40	14 (3%) 44 26	41, 114, 171, 189	0
All	All	1514/1680 (90%)	0.23	42 (2%) 55 34	41, 100, 158, 189	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	38	ILE	4.1
1	A	65	ILE	4.0
1	A	109	ILE	4.0
1	D	81	ILE	3.9
1	B	51	LEU	3.8
1	D	288	GLY	3.8
1	B	111	VAL	3.3
1	A	39	LEU	3.3
1	A	203	GLN	3.2
1	B	65	ILE	3.0
1	A	89	GLY	3.0
1	A	71	PRO	3.0
1	A	36	PRO	2.8
1	C	69	VAL	2.8
1	B	41	PRO	2.6
1	A	38	ILE	2.5
1	C	251	ILE	2.5
1	D	101	LYS	2.4
1	D	211	GLY	2.4
1	D	62	ASN	2.4
1	B	86	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	109	ILE	2.4
1	B	251	ILE	2.4
1	B	110	GLU	2.3
1	B	252	GLY	2.3
1	A	33	ASN	2.3
1	D	145	VAL	2.2
1	C	281	MET	2.2
1	D	105	TYR	2.2
1	D	160	ASN	2.2
1	D	232	ALA	2.2
1	A	73	ASP	2.2
1	B	336	ILE	2.1
1	C	249	LEU	2.1
1	B	278	SER	2.1
1	D	306	THR	2.1
1	B	290	ALA	2.1
1	D	41	PRO	2.1
1	B	114	VAL	2.1
1	D	114	VAL	2.1
1	D	38	ILE	2.1
1	D	166	LEU	2.0

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

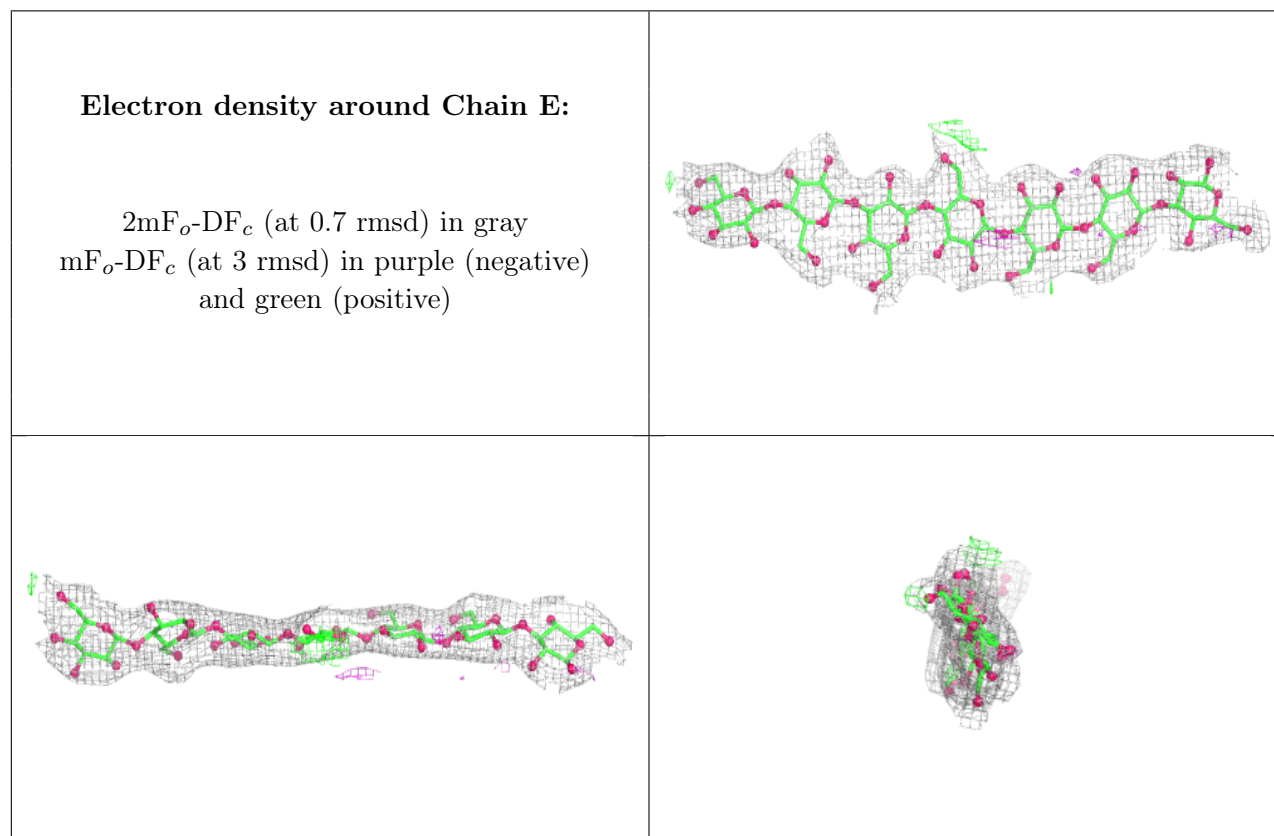
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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, 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	B-factors(Å ²)	Q<0.9
2	BGC	E	1	12/12	0.78	0.11	92,104,111,112	0
2	BGC	E	7	11/12	0.85	0.12	85,91,100,100	0
2	BGC	E	4	11/12	0.93	0.10	55,58,74,79	0
2	BGC	E	6	11/12	0.94	0.09	60,71,79,82	0
2	BGC	E	2	11/12	0.94	0.09	57,60,73,77	0
2	BGC	E	3	11/12	0.95	0.10	44,57,65,66	0
2	BGC	E	5	11/12	0.96	0.09	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.



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, 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	B-factors(Å ²)	Q<0.9
3	SO4	A	502	5/5	0.61	0.14	179,179,179,180	0
3	SO4	B	502	5/5	0.62	0.09	172,172,173,173	0
3	SO4	C	502	5/5	0.75	0.13	152,152,153,154	0
3	SO4	A	503	5/5	0.81	0.16	189,189,189,190	0
3	SO4	A	501	5/5	0.85	0.12	139,139,139,141	0
3	SO4	A	504	5/5	0.85	0.11	122,122,124,124	0
3	SO4	D	509	5/5	0.85	0.15	137,138,139,139	0
3	SO4	B	501	5/5	0.86	0.12	153,154,154,155	0
3	SO4	D	508	5/5	0.89	0.09	115,116,117,120	0
3	SO4	C	501	5/5	0.94	0.07	127,129,129,131	0

6.5 Other polymers ⓘ

There are no such residues in this entry.