



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:05 AM UTC

PDB ID : 6S21 / pdb_00006s21
Title : Metabolism of multiple glycosaminoglycans by bacteroides thetaiotaomicron is orchestrated by a versatile core genetic locus (BT33494S-sulf)
Authors : Ndeh, D.; Basle, A.; Strahl, H.; Henrissat, B.; Terrapon, N.; Cartmell, A.
Deposited on : 2019-06-19
Resolution : 2.80 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:

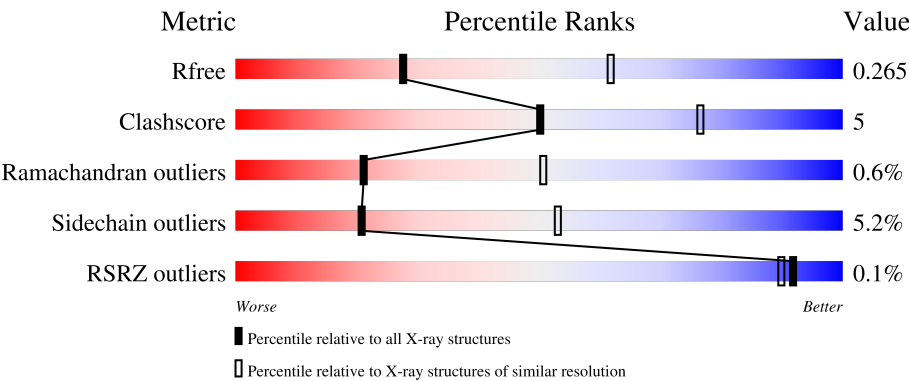
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	513	76%17%• 5%
1	B	513	75%17%• 5%
1	C	513	74%18%• 5%
2	D	3	33%67%
2	E	3	100%

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Mol	Chain	Length	Quality of chain
2	F	3	 A horizontal bar chart showing the quality of chain F. The bar is divided into two segments: a yellow segment on the left representing 33% and an orange segment on the right representing 67%. The percentages are labeled below the bar.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11684 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 Endo-4-O-sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3841	2434	648	740	19			
1	B	485	Total	C	N	O	S	0	0	0
			3824	2424	642	739	19			
1	C	486	Total	C	N	O	S	0	0	0
			3841	2435	650	737	19			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP Q8A2F6
A	-3	GLY	-	expression tag	UNP Q8A2F6
A	-2	SER	-	expression tag	UNP Q8A2F6
A	-1	SER	-	expression tag	UNP Q8A2F6
A	0	HIS	-	expression tag	UNP Q8A2F6
A	1	HIS	-	expression tag	UNP Q8A2F6
A	2	HIS	-	expression tag	UNP Q8A2F6
A	3	HIS	-	expression tag	UNP Q8A2F6
A	4	HIS	-	expression tag	UNP Q8A2F6
A	5	HIS	-	expression tag	UNP Q8A2F6
A	6	SER	-	expression tag	UNP Q8A2F6
A	7	SER	-	expression tag	UNP Q8A2F6
A	8	GLY	-	expression tag	UNP Q8A2F6
A	9	LEU	-	expression tag	UNP Q8A2F6
A	10	VAL	-	expression tag	UNP Q8A2F6
A	11	PRO	-	expression tag	UNP Q8A2F6
A	12	ARG	-	expression tag	UNP Q8A2F6
A	13	GLY	-	expression tag	UNP Q8A2F6
A	14	SER	-	expression tag	UNP Q8A2F6
A	15	HIS	-	expression tag	UNP Q8A2F6
A	16	MET	-	expression tag	UNP Q8A2F6
B	-4	MET	-	initiating methionine	UNP Q8A2F6
B	-3	GLY	-	expression tag	UNP Q8A2F6

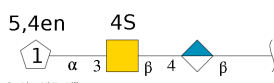
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP Q8A2F6
B	-1	SER	-	expression tag	UNP Q8A2F6
B	0	HIS	-	expression tag	UNP Q8A2F6
B	1	HIS	-	expression tag	UNP Q8A2F6
B	2	HIS	-	expression tag	UNP Q8A2F6
B	3	HIS	-	expression tag	UNP Q8A2F6
B	4	HIS	-	expression tag	UNP Q8A2F6
B	5	HIS	-	expression tag	UNP Q8A2F6
B	6	SER	-	expression tag	UNP Q8A2F6
B	7	SER	-	expression tag	UNP Q8A2F6
B	8	GLY	-	expression tag	UNP Q8A2F6
B	9	LEU	-	expression tag	UNP Q8A2F6
B	10	VAL	-	expression tag	UNP Q8A2F6
B	11	PRO	-	expression tag	UNP Q8A2F6
B	12	ARG	-	expression tag	UNP Q8A2F6
B	13	GLY	-	expression tag	UNP Q8A2F6
B	14	SER	-	expression tag	UNP Q8A2F6
B	15	HIS	-	expression tag	UNP Q8A2F6
B	16	MET	-	expression tag	UNP Q8A2F6
C	-4	MET	-	initiating methionine	UNP Q8A2F6
C	-3	GLY	-	expression tag	UNP Q8A2F6
C	-2	SER	-	expression tag	UNP Q8A2F6
C	-1	SER	-	expression tag	UNP Q8A2F6
C	0	HIS	-	expression tag	UNP Q8A2F6
C	1	HIS	-	expression tag	UNP Q8A2F6
C	2	HIS	-	expression tag	UNP Q8A2F6
C	3	HIS	-	expression tag	UNP Q8A2F6
C	4	HIS	-	expression tag	UNP Q8A2F6
C	5	HIS	-	expression tag	UNP Q8A2F6
C	6	SER	-	expression tag	UNP Q8A2F6
C	7	SER	-	expression tag	UNP Q8A2F6
C	8	GLY	-	expression tag	UNP Q8A2F6
C	9	LEU	-	expression tag	UNP Q8A2F6
C	10	VAL	-	expression tag	UNP Q8A2F6
C	11	PRO	-	expression tag	UNP Q8A2F6
C	12	ARG	-	expression tag	UNP Q8A2F6
C	13	GLY	-	expression tag	UNP Q8A2F6
C	14	SER	-	expression tag	UNP Q8A2F6
C	15	HIS	-	expression tag	UNP Q8A2F6
C	16	MET	-	expression tag	UNP Q8A2F6

- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-4-O-sulfo-beta-D-galactopyranose-(1-4)-beta-D-glucopyranuronic

acid.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	S	0	0	0
			42	20	1	20	1			
2	E	3	Total	C	N	O	S	0	0	0
			42	20	1	20	1			
2	F	3	Total	C	N	O	S	0	0	0
			42	20	1	20	1			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

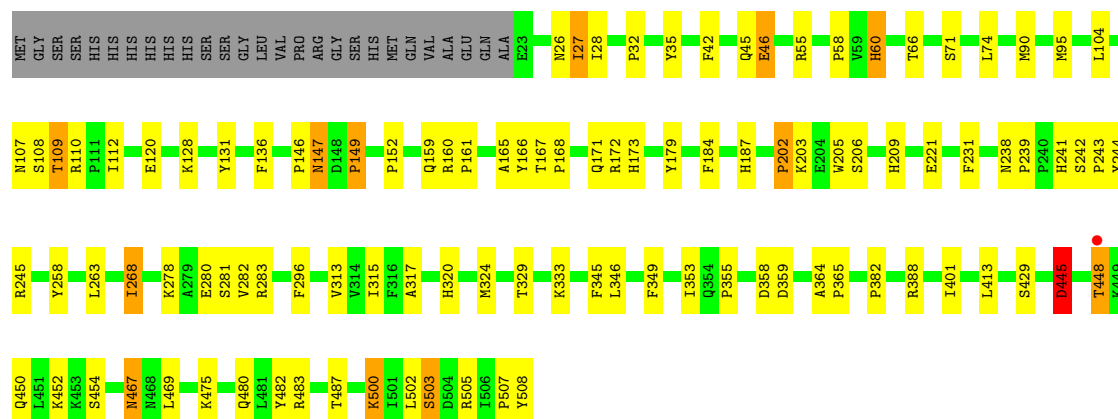
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	16	Total	O	0	0
			16	16		
4	C	17	Total	O	0	0
			17	17		

- Molecule 1: Endo-4-O-sulfatase





- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-4-O-sulfo-beta-D-galactopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain D: 33% 67%

BDP1
ASG2
GCD3

- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-4-O-sulfo-beta-D-galactopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain E: 100%

BDP1
ASG2
GCD3

- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-4-O-sulfo-beta-D-galactopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain F: 33% 67%

BDP1
ASG2
GCD3

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.91Å 93.91Å 304.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.98 – 2.80 68.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.98-2.80) 99.9 (68.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.189 , 0.261 0.198 , 0.265	Depositor DCC
R_{free} test set	1856 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11684	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: ASG, GCD, CA, BDP

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	1.21	5/3950 (0.1%)	1.56	23/5384 (0.4%)
1	B	1.20	8/3933 (0.2%)	1.57	28/5364 (0.5%)
1	C	1.21	8/3950 (0.2%)	1.58	30/5383 (0.6%)
All	All	1.21	21/11833 (0.2%)	1.57	81/16131 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
All	All	0	9

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	PRO	C-O	-8.30	1.13	1.24
1	C	355	PRO	C-O	-7.75	1.13	1.24
1	A	187	HIS	CE1-NE2	7.50	1.40	1.32
1	A	111	PRO	C-O	-6.05	1.16	1.24
1	C	149	PRO	C-O	-5.94	1.16	1.24
1	C	507	PRO	C-O	-5.83	1.17	1.23
1	B	312	THR	C-O	5.79	1.30	1.23
1	B	173	HIS	CE1-NE2	5.79	1.38	1.32
1	B	149	PRO	C-O	-5.78	1.17	1.24
1	B	219	LYS	C-O	-5.76	1.16	1.24
1	A	149	PRO	C-O	-5.75	1.16	1.24
1	B	187	HIS	CE1-NE2	5.75	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	187	HIS	CE1-NE2	5.69	1.38	1.32
1	C	165	ALA	C-O	5.50	1.30	1.23
1	B	300	LEU	C-O	5.49	1.30	1.24
1	C	353	ILE	C-O	-5.41	1.18	1.24
1	B	353	ILE	C-O	-5.41	1.18	1.24
1	B	111	PRO	C-O	-5.34	1.17	1.24
1	C	60	HIS	CA-CB	5.27	1.59	1.53
1	A	411	GLN	C-O	5.11	1.29	1.24
1	C	445	ASP	C-O	5.03	1.30	1.23

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	PRO	N-CA-C	-7.63	100.54	111.22
1	C	60	HIS	CB-CA-C	7.42	123.78	111.31
1	A	508	TYR	CA-C-O	7.29	133.20	120.80
1	A	202	PRO	N-CA-C	-7.07	101.32	111.22
1	B	152	PRO	N-CA-C	6.63	124.53	113.78
1	B	202	PRO	N-CA-C	-6.62	101.95	111.22
1	C	66	THR	CA-CB-OG1	-6.51	99.83	109.60
1	B	167	THR	CB-CA-C	6.49	116.95	110.33
1	A	60	HIS	CB-CA-C	6.47	122.17	111.31
1	A	245	ARG	N-CA-C	-6.38	106.13	114.04
1	B	475	LYS	CB-CA-C	6.23	121.13	110.79
1	B	329	THR	CA-C-O	-6.20	112.84	119.97
1	A	296	PHE	CA-C-N	6.17	126.96	119.99
1	A	296	PHE	C-N-CA	6.17	126.96	119.99
1	C	152	PRO	N-CA-C	6.14	125.12	112.47
1	A	168	PRO	CA-C-O	-6.04	114.35	122.08
1	B	108	SER	CA-C-N	6.01	129.44	120.31
1	B	108	SER	C-N-CA	6.01	129.44	120.31
1	B	205	TRP	CB-CA-C	5.93	118.70	110.16
1	C	329	THR	CA-C-O	-5.93	113.16	119.97
1	C	205	TRP	CB-CA-C	5.91	118.67	110.16
1	A	108	SER	CA-C-N	5.90	129.28	120.31
1	A	108	SER	C-N-CA	5.90	129.28	120.31
1	C	487	THR	CA-CB-OG1	-5.90	100.75	109.60
1	A	404	PRO	CA-C-N	5.88	128.15	120.28
1	A	404	PRO	C-N-CA	5.88	128.15	120.28
1	B	203	LYS	N-CA-C	-5.78	101.62	109.54
1	B	296	PHE	CA-C-N	5.73	126.47	119.99
1	B	296	PHE	C-N-CA	5.73	126.47	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	PRO	CA-C-O	-5.71	114.78	122.08
1	C	167	THR	CB-CA-C	5.69	116.14	110.33
1	C	245	ARG	N-CA-C	-5.67	107.01	114.04
1	A	167	THR	CB-CA-C	5.64	116.08	110.33
1	C	35	TYR	CA-C-N	5.62	128.82	120.90
1	C	35	TYR	C-N-CA	5.62	128.82	120.90
1	C	359	ASP	N-CA-C	-5.60	106.34	112.72
1	A	203	LYS	N-CA-C	-5.58	101.89	109.54
1	B	36	ARG	CB-CA-C	-5.58	100.72	109.70
1	A	36	ARG	CB-CA-C	-5.55	100.84	109.61
1	A	66	THR	CA-CB-OG1	-5.54	101.29	109.60
1	B	55	ARG	CB-CA-C	5.50	119.31	110.29
1	B	168	PRO	CA-C-O	-5.49	115.06	122.08
1	A	258	TYR	CA-C-N	5.47	129.89	121.19
1	A	258	TYR	C-N-CA	5.47	129.89	121.19
1	B	258	TYR	CA-C-N	5.47	129.03	120.82
1	B	258	TYR	C-N-CA	5.47	129.03	120.82
1	C	108	SER	CA-C-N	5.47	128.63	120.31
1	C	108	SER	C-N-CA	5.47	128.63	120.31
1	C	171	GLN	N-CA-CB	-5.47	102.86	111.39
1	C	296	PHE	CA-C-N	5.41	126.10	119.99
1	C	296	PHE	C-N-CA	5.41	126.10	119.99
1	B	500	LYS	CA-C-N	5.41	128.33	120.98
1	B	500	LYS	C-N-CA	5.41	128.33	120.98
1	C	258	TYR	CA-C-N	5.40	129.77	121.19
1	C	258	TYR	C-N-CA	5.40	129.77	121.19
1	A	35	TYR	CA-C-N	5.38	129.33	121.31
1	A	35	TYR	C-N-CA	5.38	129.33	121.31
1	B	462	ASP	CB-CA-C	5.38	118.26	111.21
1	B	475	LYS	N-CA-C	-5.38	105.41	111.28
1	B	35	TYR	CA-C-N	5.33	128.42	120.90
1	B	35	TYR	C-N-CA	5.33	128.42	120.90
1	C	203	LYS	N-CA-C	-5.31	99.73	108.49
1	A	329	THR	CA-C-O	-5.26	113.92	119.97
1	A	359	ASP	N-CA-C	-5.17	106.83	112.72
1	C	502	LEU	CA-C-N	5.14	131.36	121.54
1	C	502	LEU	C-N-CA	5.14	131.36	121.54
1	C	46	GLU	CB-CA-C	5.14	118.44	109.65
1	B	202	PRO	CA-C-N	-5.14	115.47	122.87
1	B	202	PRO	C-N-CA	-5.14	115.47	122.87
1	B	31	PHE	CA-CB-CG	5.12	118.92	113.80
1	B	60	HIS	CB-CA-C	5.11	119.90	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	PRO	CB-CA-C	-5.09	103.16	111.56
1	B	448	THR	CB-CA-C	5.06	120.71	110.38
1	C	475	LYS	CB-CA-C	5.05	119.18	110.79
1	A	359	ASP	CB-CA-C	5.05	119.27	110.94
1	A	109	THR	CA-CB-CG2	5.05	119.08	110.50
1	C	448	THR	CA-CB-CG2	5.04	119.08	110.50
1	B	185	ASP	CA-CB-CG	5.03	117.62	112.60
1	C	508	TYR	CA-C-O	-5.02	112.27	120.80
1	C	500	LYS	CA-C-N	5.01	127.80	120.98
1	C	500	LYS	C-N-CA	5.01	127.80	120.98

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	TYR	Peptide
1	A	146	PRO	Peptide
1	A	147	ASN	Peptide
1	B	131	TYR	Peptide
1	B	146	PRO	Peptide
1	B	147	ASN	Peptide
1	C	131	TYR	Peptide
1	C	146	PRO	Peptide
1	C	147	ASN	Peptide

5.2 Too-close contacts [i](#)

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	3841	0	3585	36	1
1	B	3824	0	3558	40	0
1	C	3841	0	3594	41	1
2	D	42	0	20	2	0
2	E	42	0	20	0	0
2	F	42	0	20	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	16	0	0	0	0
4	B	16	0	0	4	0
4	C	17	0	0	2	0
All	All	11684	0	10797	118	1

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 5.

All (118) 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:483:ARG:CB	4:C:716:HOH:O	2.16	0.93
1:A:185:ASP:OD2	2:D:2:ASG:O6	2.00	0.79
1:A:107:ASN:OD1	1:A:109:THR:HB	1.86	0.76
1:A:242:SER:HB2	2:D:1:BDP:H1	1.69	0.75
1:B:107:ASN:OD1	1:B:109:THR:HB	1.87	0.75
1:B:147:ASN:ND2	1:B:166:TYR:O	2.21	0.73
1:C:107:ASN:OD1	1:C:109:THR:HB	1.88	0.73
1:C:147:ASN:ND2	1:C:166:TYR:O	2.22	0.72
1:A:451:LEU:O	1:B:247:LEU:HD12	1.90	0.70
1:C:238:ASN:HB3	1:C:239:PRO:HD3	1.74	0.70
1:A:238:ASN:HB3	1:A:239:PRO:HD3	1.74	0.70
1:B:238:ASN:HB3	1:B:239:PRO:HD3	1.74	0.70
1:B:179:TYR:HH	1:B:209:HIS:HE2	1.41	0.69
1:B:297:GLY:O	1:B:301:GLU:HG2	1.95	0.67
1:C:120:GLU:HG2	1:C:382:PRO:HG3	1.78	0.65
1:A:109:THR:HG22	1:A:110:ARG:HG3	1.82	0.62
1:C:448:THR:O	1:C:450:GLN:N	2.32	0.62
1:A:202:PRO:HG3	1:A:209:HIS:CE1	2.35	0.61
1:B:346:LEU:HD12	1:B:346:LEU:N	2.17	0.60
1:B:202:PRO:HG3	1:B:209:HIS:CE1	2.37	0.59
1:A:448:THR:O	1:A:450:GLN:N	2.33	0.59
1:B:179:TYR:OH	1:B:209:HIS:NE2	2.30	0.58
1:B:109:THR:HG22	1:B:110:ARG:HG3	1.86	0.58
1:B:304:LYS:HE3	1:B:309:ASP:OD2	2.03	0.58
1:C:346:LEU:HD12	1:C:346:LEU:N	2.19	0.57
1:B:345:PHE:C	1:B:346:LEU:HD12	2.29	0.57
1:C:345:PHE:C	1:C:346:LEU:HD12	2.29	0.57
1:C:467:ASN:O	1:C:469:LEU:HD13	2.04	0.57
1:A:345:PHE:C	1:A:346:LEU:HD12	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ASN:ND2	4:B:701:HOH:O	2.38	0.56
1:A:55:ARG:HB3	1:A:268:ILE:HD12	1.88	0.56
1:C:109:THR:HG22	1:C:110:ARG:HG3	1.87	0.55
1:C:243:PRO:O	4:C:701:HOH:O	2.18	0.55
1:C:202:PRO:HG3	1:C:209:HIS:CE1	2.42	0.55
1:C:280:GLU:OE2	1:C:283:ARG:NH1	2.39	0.54
1:A:346:LEU:HD12	1:A:346:LEU:N	2.22	0.54
1:C:58:PRO:HD3	1:C:268:ILE:HD13	1.90	0.54
1:C:364:ALA:HB3	1:C:365:PRO:HD3	1.90	0.54
1:C:179:TYR:OH	1:C:209:HIS:NE2	2.37	0.53
1:C:448:THR:O	1:C:448:THR:HG23	2.10	0.52
1:B:160:ARG:HA	1:B:161:PRO:C	2.34	0.51
1:C:179:TYR:HH	1:C:209:HIS:HE2	1.57	0.51
1:A:160:ARG:HA	1:A:161:PRO:C	2.35	0.51
1:B:364:ALA:HB3	1:B:365:PRO:HD3	1.92	0.51
1:C:445:ASP:OD1	1:C:448:THR:HG22	2.11	0.51
1:B:282:VAL:N	1:B:324:MET:HE2	2.26	0.51
1:C:282:VAL:N	1:C:324:MET:HE2	2.26	0.51
1:A:445:ASP:OD1	1:A:448:THR:HG22	2.11	0.50
1:A:364:ALA:HB3	1:A:365:PRO:HD3	1.94	0.50
1:B:90:MET:HG2	1:B:95:MET:O	2.12	0.49
1:A:448:THR:O	1:A:448:THR:HG23	2.13	0.49
1:B:105:ASN:HB3	4:B:701:HOH:O	2.14	0.48
1:A:90:MET:HG2	1:A:95:MET:O	2.14	0.48
1:C:278:LYS:O	1:C:281:SER:HB2	2.13	0.48
1:A:27:ILE:HA	1:A:313:VAL:O	2.14	0.48
1:B:152:PRO:CG	4:B:713:HOH:O	2.62	0.48
1:A:254:ASP:OD1	1:A:294:ARG:NH1	2.31	0.48
1:B:315:ILE:HA	1:B:346:LEU:O	2.14	0.48
1:B:445:ASP:OD2	1:B:448:THR:HG22	2.13	0.48
1:C:90:MET:HG2	1:C:95:MET:O	2.14	0.48
1:A:282:VAL:N	1:A:324:MET:HE2	2.28	0.47
1:A:315:ILE:HA	1:A:346:LEU:O	2.15	0.47
1:A:413:LEU:HD12	1:A:429:SER:HB3	1.97	0.47
1:A:313:VAL:HG22	1:A:349:PHE:CD2	2.50	0.47
1:B:110:ARG:NH1	4:B:701:HOH:O	2.47	0.47
1:A:179:TYR:OH	1:A:209:HIS:NE2	2.30	0.47
1:C:160:ARG:HA	1:C:161:PRO:C	2.39	0.47
1:B:482:TYR:CE2	1:B:505:ARG:HB3	2.48	0.47
2:F:2:ASG:H6B	2:F:2:ASG:OSC	2.15	0.47
1:B:313:VAL:HG22	1:B:349:PHE:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:TYR:CE2	1:A:505:ARG:HB3	2.51	0.46
1:B:413:LEU:HD12	1:B:429:SER:HB3	1.96	0.46
1:A:149:PRO:HG3	1:A:166:TYR:CE2	2.51	0.46
1:B:27:ILE:HA	1:B:313:VAL:O	2.16	0.46
1:B:313:VAL:HG22	1:B:349:PHE:CG	2.50	0.46
1:C:315:ILE:HA	1:C:346:LEU:O	2.15	0.46
1:C:482:TYR:CE2	1:C:505:ARG:HB3	2.51	0.45
1:B:149:PRO:HG3	1:B:166:TYR:CE2	2.51	0.45
1:B:241:HIS:ND1	1:B:242:SER:O	2.43	0.45
1:C:27:ILE:HA	1:C:313:VAL:O	2.16	0.45
1:B:261:GLN:HG3	1:B:262:PRO:HD2	1.98	0.45
1:C:313:VAL:HG22	1:C:349:PHE:CG	2.52	0.45
1:A:313:VAL:HG22	1:A:349:PHE:CG	2.53	0.44
1:A:261:GLN:HG3	1:A:262:PRO:HD2	2.00	0.44
1:C:32:PRO:HD2	1:C:317:ALA:O	2.18	0.44
1:B:258:TYR:OH	1:B:290:THR:OG1	2.33	0.43
1:C:42:PHE:HA	1:C:45:GLN:CD	2.44	0.43
1:C:320:HIS:CE1	1:C:333:LYS:HE3	2.53	0.43
1:B:263:LEU:HD12	1:B:263:LEU:HA	1.83	0.43
1:A:32:PRO:HD2	1:A:317:ALA:O	2.19	0.43
1:A:263:LEU:HD12	1:A:263:LEU:HA	1.83	0.43
1:C:282:VAL:CA	1:C:324:MET:HE2	2.49	0.43
1:B:282:VAL:CA	1:B:324:MET:HE2	2.50	0.42
1:B:85:SER:N	1:B:86:PRO:CD	2.82	0.42
1:B:467:ASN:O	1:B:469:LEU:HD13	2.18	0.42
1:C:241:HIS:ND1	1:C:242:SER:O	2.42	0.42
1:A:278:LYS:O	1:A:281:SER:HB2	2.19	0.42
1:A:172:ARG:O	1:A:173:HIS:C	2.63	0.42
1:C:448:THR:O	1:C:448:THR:CG2	2.68	0.42
2:F:1:BDP:O6B	2:F:1:BDP:O4	2.38	0.41
1:B:42:PHE:HA	1:B:45:GLN:CD	2.45	0.41
1:C:26:ASN:HB3	1:C:231:PHE:CE1	2.55	0.41
1:C:445:ASP:OD1	1:C:448:THR:N	2.47	0.41
1:C:313:VAL:HG22	1:C:349:PHE:CD2	2.55	0.41
1:A:273:ASP:HB3	1:A:276:MET:HG3	2.03	0.41
1:A:393:LEU:HB2	1:A:401:ILE:HG21	2.03	0.41
1:B:172:ARG:O	1:B:173:HIS:C	2.64	0.41
1:A:74:LEU:HA	1:A:358:ASP:O	2.20	0.41
1:C:413:LEU:HD12	1:C:429:SER:HB3	2.02	0.41
1:A:205:TRP:CH2	1:A:291:GLY:HA3	2.55	0.41
1:A:276:MET:O	1:A:277:LYS:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:PHE:HA	1:C:179:TYR:O	2.21	0.41
1:B:108:SER:HB3	1:B:162:VAL:HB	2.02	0.41
1:B:281:SER:HB2	1:B:324:MET:HE1	2.03	0.41
1:B:32:PRO:HD2	1:B:317:ALA:O	2.21	0.40
1:C:74:LEU:HA	1:C:358:ASP:O	2.20	0.40
1:C:149:PRO:HG3	1:C:166:TYR:CE2	2.55	0.40
1:C:172:ARG:O	1:C:173:HIS:C	2.64	0.40

All (1) 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:A:60:HIS:NE2	1:C:60:HIS:NE2[1_455]	2.10	0.10

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	484/513 (94%)	451 (93%)	29 (6%)	4 (1%)	16	44
1	B	483/513 (94%)	449 (93%)	33 (7%)	1 (0%)	43	72
1	C	484/513 (94%)	448 (93%)	32 (7%)	4 (1%)	16	44
All	All	1451/1539 (94%)	1348 (93%)	94 (6%)	9 (1%)	21	51

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	B	159	GLN
1	C	184	PHE
1	C	159	GLN
1	C	500	LYS

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Mol	Chain	Res	Type
1	C	503	SER
1	A	84	SER
1	A	184	PHE
1	A	503	SER

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	415/458 (91%)	396 (95%)	19 (5%)	24	58
1	B	413/458 (90%)	389 (94%)	24 (6%)	18	49
1	C	415/458 (91%)	393 (95%)	22 (5%)	20	52
All	All	1243/1374 (90%)	1178 (95%)	65 (5%)	21	53

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	71	SER
1	A	104	LEU
1	A	109	THR
1	A	112	ILE
1	A	206	SER
1	A	244	TYR
1	A	261	GLN
1	A	263	LEU
1	A	280	GLU
1	A	384	GLU
1	A	388	ARG
1	A	401	ILE
1	A	454	SER
1	A	472	ASP
1	A	476	GLU
1	A	480	GLN
1	A	491	GLU

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Mol	Chain	Res	Type
1	A	503	SER
1	B	27	ILE
1	B	28	ILE
1	B	71	SER
1	B	104	LEU
1	B	109	THR
1	B	112	ILE
1	B	160	ARG
1	B	206	SER
1	B	223	ASN
1	B	240	PRO
1	B	242	SER
1	B	244	TYR
1	B	263	LEU
1	B	301	GLU
1	B	379	ASP
1	B	383	SER
1	B	388	ARG
1	B	401	ILE
1	B	448	THR
1	B	452	LYS
1	B	454	SER
1	B	472	ASP
1	B	480	GLN
1	B	491	GLU
1	C	27	ILE
1	C	28	ILE
1	C	46	GLU
1	C	55	ARG
1	C	71	SER
1	C	104	LEU
1	C	109	THR
1	C	112	ILE
1	C	128	LYS
1	C	206	SER
1	C	221	GLU
1	C	244	TYR
1	C	263	LEU
1	C	268	ILE
1	C	388	ARG
1	C	401	ILE
1	C	445	ASP

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Mol	Chain	Res	Type
1	C	452	LYS
1	C	454	SER
1	C	467	ASN
1	C	480	GLN
1	C	503	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	411	GLN
1	A	474	ASN
1	B	78	GLN
1	B	159	GLN
1	B	238	ASN
1	B	411	GLN
1	B	474	ASN
1	C	159	GLN
1	C	474	ASN

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](#)

9 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	BDP	D	1	2	13,13,13	1.33	2 (15%)	18,19,19	2.50	8 (44%)
2	ASG	D	2	3,2	18,18,19	1.24	0	21,26,28	3.68	9 (42%)
2	GCD	D	3	2	10,11,12	2.67	5 (50%)	12,15,17	1.47	3 (25%)
2	BDP	E	1	2	13,13,13	1.97	4 (30%)	18,19,19	2.48	10 (55%)
2	ASG	E	2	3,2	18,18,19	1.04	2 (11%)	21,26,28	2.77	9 (42%)
2	GCD	E	3	2	10,11,12	2.05	2 (20%)	12,15,17	2.90	5 (41%)
2	BDP	F	1	2	13,13,13	1.08	0	18,19,19	2.13	8 (44%)
2	ASG	F	2	3,2	18,18,19	1.08	1 (5%)	21,26,28	2.86	10 (47%)
2	GCD	F	3	2	10,11,12	2.46	4 (40%)	12,15,17	1.50	3 (25%)

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	BDP	D	1	2	-	0/4/24/24	0/1/1/1
2	ASG	D	2	3,2	-	4/11/28/31	0/1/1/1
2	GCD	D	3	2	-	0/4/17/20	0/1/1/1
2	BDP	E	1	2	-	0/4/24/24	0/1/1/1
2	ASG	E	2	3,2	-	4/11/28/31	0/1/1/1
2	GCD	E	3	2	-	0/4/17/20	0/1/1/1
2	BDP	F	1	2	-	0/4/24/24	0/1/1/1
2	ASG	F	2	3,2	-	4/11/28/31	0/1/1/1
2	GCD	F	3	2	-	0/4/17/20	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	GCD	O5-C5	5.95	1.45	1.37
2	D	3	GCD	O5-C5	5.73	1.45	1.37
2	F	3	GCD	O5-C5	5.57	1.44	1.37
2	D	3	GCD	O5-C1	-3.94	1.38	1.45
2	E	1	BDP	C1-C2	3.72	1.60	1.52
2	F	3	GCD	O5-C1	-3.41	1.39	1.45
2	E	1	BDP	O1-C1	3.05	1.49	1.39
2	D	1	BDP	O1-C1	2.74	1.48	1.39
2	D	3	GCD	C3-C4	2.64	1.53	1.50
2	F	3	GCD	O2-C2	2.49	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	BDP	C4-C5	2.34	1.57	1.53
2	F	3	GCD	O6B-C6	-2.28	1.24	1.30
2	F	2	ASG	OSA-S	2.23	1.64	1.50
2	E	2	ASG	OSA-S	2.16	1.63	1.50
2	D	3	GCD	O6A-C6	2.12	1.27	1.22
2	D	3	GCD	O6B-C6	-2.10	1.24	1.30
2	E	1	BDP	C4-C5	2.08	1.56	1.53
2	E	3	GCD	O6B-C6	-2.05	1.25	1.30
2	E	1	BDP	O5-C5	2.03	1.47	1.43
2	E	2	ASG	O5-C1	2.01	1.47	1.43

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	ASG	OSA-S-OSC	-9.17	76.46	108.56
2	D	2	ASG	OSA-S-O4	7.83	124.37	106.37
2	F	2	ASG	O5-C1-C2	-6.67	100.97	111.29
2	F	2	ASG	C1-C2-N2	6.36	120.46	110.43
2	E	2	ASG	OSA-S-O4	6.14	120.48	106.37
2	D	2	ASG	C8-C7-N2	6.09	126.22	116.12
2	E	3	GCD	O5-C5-C4	-5.99	119.44	124.94
2	D	1	BDP	C3-C4-C5	5.86	119.38	109.30
2	E	2	ASG	C4-O4-S	5.63	132.54	119.04
2	D	2	ASG	C1-O5-C5	5.30	119.29	112.19
2	D	2	ASG	OSC-S-OSB	-4.74	93.95	112.24
2	E	2	ASG	O5-C1-C2	-4.73	103.98	111.29
2	E	2	ASG	C1-C2-N2	4.38	117.34	110.43
2	D	1	BDP	O5-C5-C4	4.19	117.76	109.48
2	E	3	GCD	O5-C5-C6	4.11	119.41	111.85
2	D	2	ASG	O7-C7-C8	-4.09	114.77	122.05
2	E	1	BDP	O1-C1-C2	4.08	120.81	108.98
2	F	2	ASG	C8-C7-N2	4.05	122.83	116.12
2	F	1	BDP	O5-C1-C2	-4.03	103.21	110.30
2	E	1	BDP	O2-C2-C3	-3.99	100.98	110.38
2	E	1	BDP	C4-C3-C2	3.97	117.80	110.83
2	F	2	ASG	C4-O4-S	3.93	128.46	119.04
2	E	3	GCD	O6B-C6-C5	3.90	122.90	114.06
2	F	2	ASG	O7-C7-C8	-3.89	115.12	122.05
2	E	3	GCD	O3-C3-C4	-3.86	100.55	109.27
2	F	1	BDP	O4-C4-C5	-3.65	101.43	109.76
2	D	1	BDP	O1-C1-C2	3.53	119.22	108.98
2	E	2	ASG	OSA-S-OSB	-3.51	96.28	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	BDP	O5-C5-C6	3.49	117.07	106.14
2	D	1	BDP	C1-O5-C5	3.43	117.27	112.22
2	E	3	GCD	O6B-C6-O6A	-3.31	116.02	123.90
2	F	2	ASG	C1-O5-C5	3.24	116.53	112.19
2	E	2	ASG	O7-C7-N2	-3.20	116.33	121.98
2	E	1	BDP	O5-C5-C4	3.16	115.72	109.48
2	F	2	ASG	OSA-S-O4	3.16	113.63	106.37
2	E	1	BDP	O2-C2-C1	3.10	116.41	109.25
2	D	2	ASG	OSA-S-OSB	3.00	119.07	108.56
2	D	3	GCD	O5-C5-C4	-2.92	122.26	124.94
2	E	1	BDP	C1-C2-C3	2.83	116.12	110.36
2	D	1	BDP	O2-C2-C3	-2.81	103.75	110.38
2	F	1	BDP	C1-C2-C3	-2.77	104.71	110.36
2	F	1	BDP	C3-C4-C5	-2.73	104.60	109.30
2	E	1	BDP	O3-C3-C2	-2.73	103.94	110.38
2	D	2	ASG	C1-C2-N2	2.73	114.73	110.43
2	F	1	BDP	O3-C3-C4	-2.73	103.95	110.38
2	D	3	GCD	O5-C5-C6	2.71	116.83	111.85
2	E	2	ASG	C1-O5-C5	2.70	115.81	112.19
2	E	1	BDP	C1-O5-C5	2.70	116.19	112.22
2	D	1	BDP	O3-C3-C2	2.60	116.51	110.38
2	E	2	ASG	C8-C7-N2	2.60	120.43	116.12
2	E	2	ASG	O5-C5-C4	2.52	114.58	110.06
2	F	3	GCD	C1-O5-C5	2.45	120.61	115.42
2	D	2	ASG	O5-C5-C6	2.37	112.28	107.66
2	D	3	GCD	O2-C2-C1	2.36	114.63	109.22
2	F	2	ASG	OSA-S-OSB	-2.32	100.44	108.56
2	D	1	BDP	O4-C4-C5	-2.31	104.48	109.76
2	F	1	BDP	O6B-C6-O6A	-2.28	118.91	124.08
2	F	1	BDP	O6B-C6-C5	2.26	121.78	113.64
2	E	1	BDP	O6A-C6-C5	-2.22	112.81	120.81
2	F	2	ASG	OSA-S-OSC	2.20	116.25	108.56
2	D	1	BDP	O6B-C6-C5	2.16	121.42	113.64
2	F	3	GCD	C3-C4-C5	-2.10	117.90	121.45
2	F	3	GCD	O2-C2-C1	2.08	114.00	109.22
2	E	1	BDP	O4-C4-C5	2.02	114.37	109.76
2	F	2	ASG	OSC-S-OSB	-2.01	104.47	112.24

There are no chirality outliers.

All (12) torsion outliers are listed below:

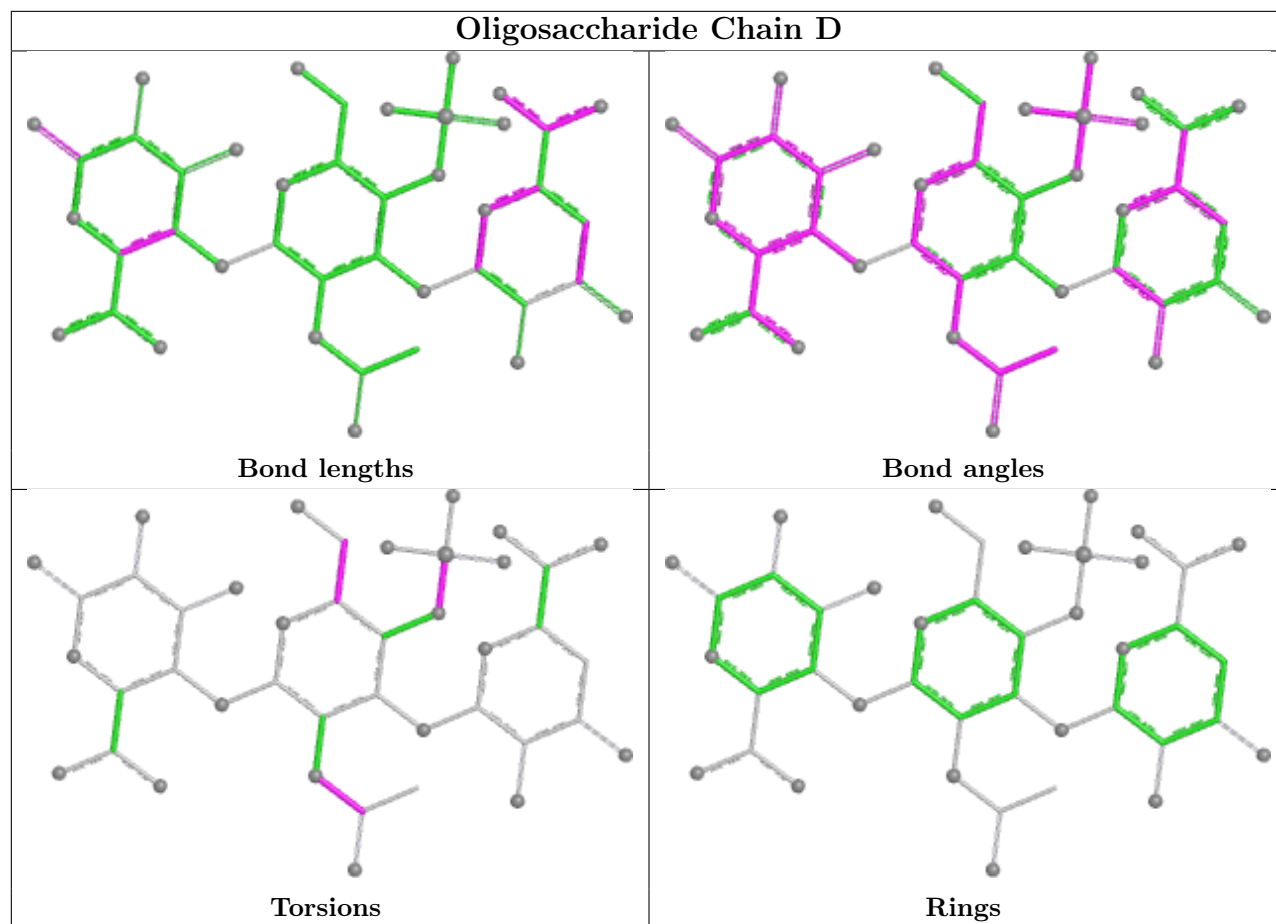
Mol	Chain	Res	Type	Atoms
2	D	2	ASG	C4-O4-S-OSA
2	E	2	ASG	C8-C7-N2-C2
2	E	2	ASG	O7-C7-N2-C2
2	F	2	ASG	C8-C7-N2-C2
2	F	2	ASG	O7-C7-N2-C2
2	E	2	ASG	C4-C5-C6-O6
2	D	2	ASG	C8-C7-N2-C2
2	D	2	ASG	O7-C7-N2-C2
2	F	2	ASG	C4-C5-C6-O6
2	F	2	ASG	O5-C5-C6-O6
2	E	2	ASG	O5-C5-C6-O6
2	D	2	ASG	O5-C5-C6-O6

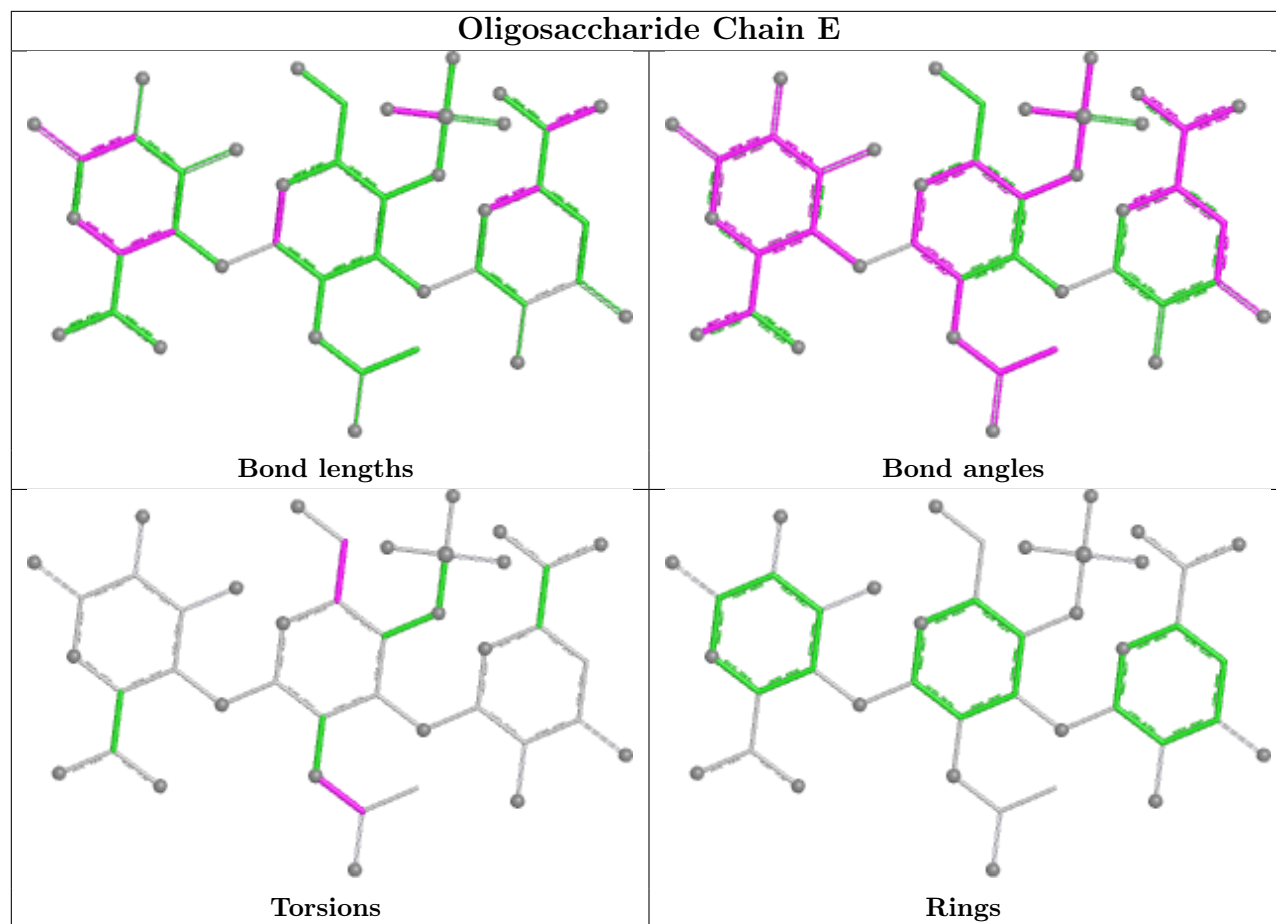
There are no ring outliers.

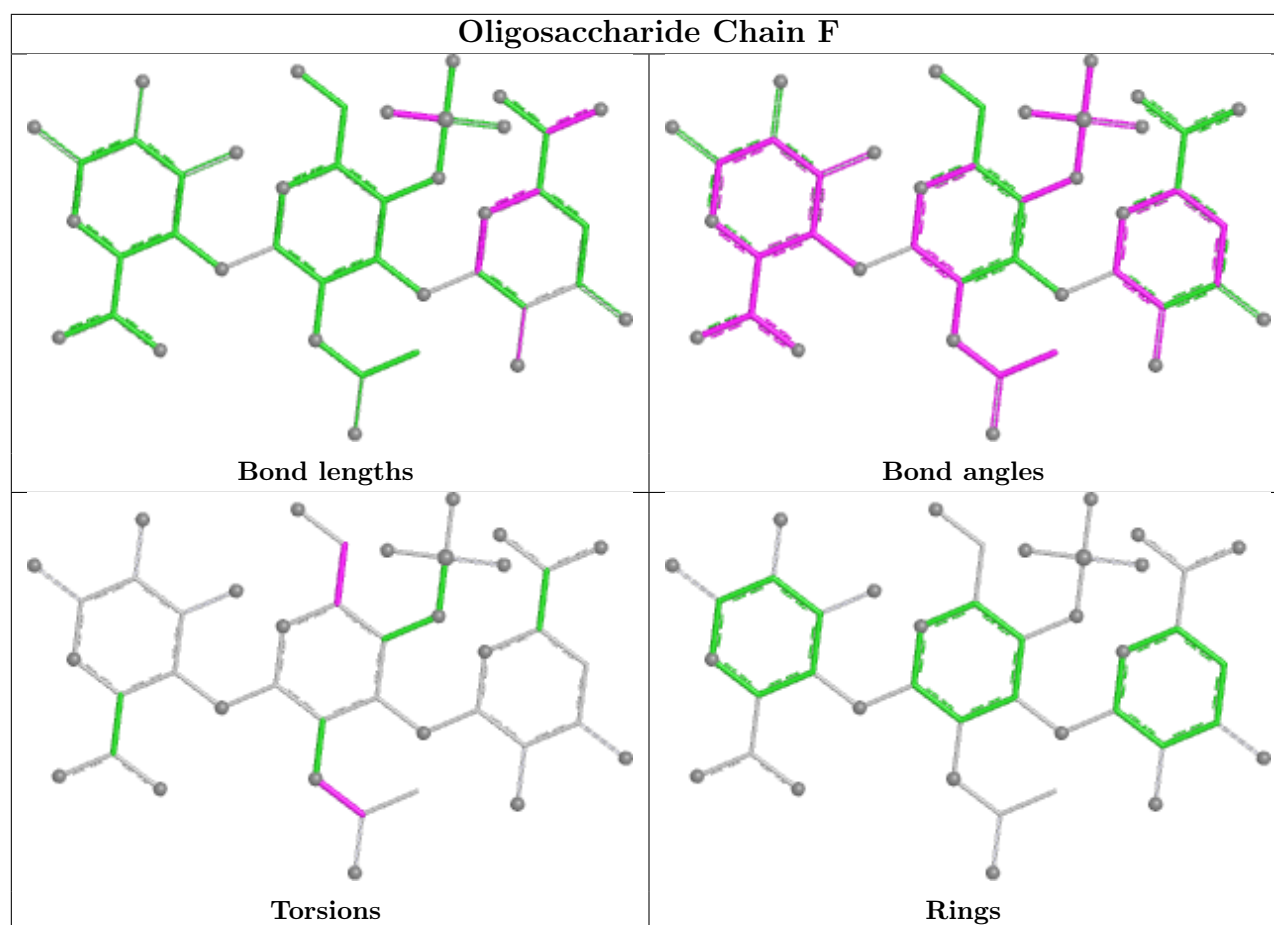
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	ASG	1	0
2	F	1	BDP	1	0
2	F	2	ASG	1	0
2	D	1	BDP	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	486/513 (94%)	-0.37	1 (0%) 91 88	20, 32, 50, 68	0
1	B	485/513 (94%)	-0.21	0 100 100	23, 38, 59, 72	0
1	C	486/513 (94%)	-0.35	1 (0%) 91 88	22, 34, 49, 68	0
All	All	1457/1539 (94%)	-0.31	2 (0%) 92 90	20, 35, 54, 72	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	448	THR	2.3
1	A	23	GLU	2.1

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, 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.

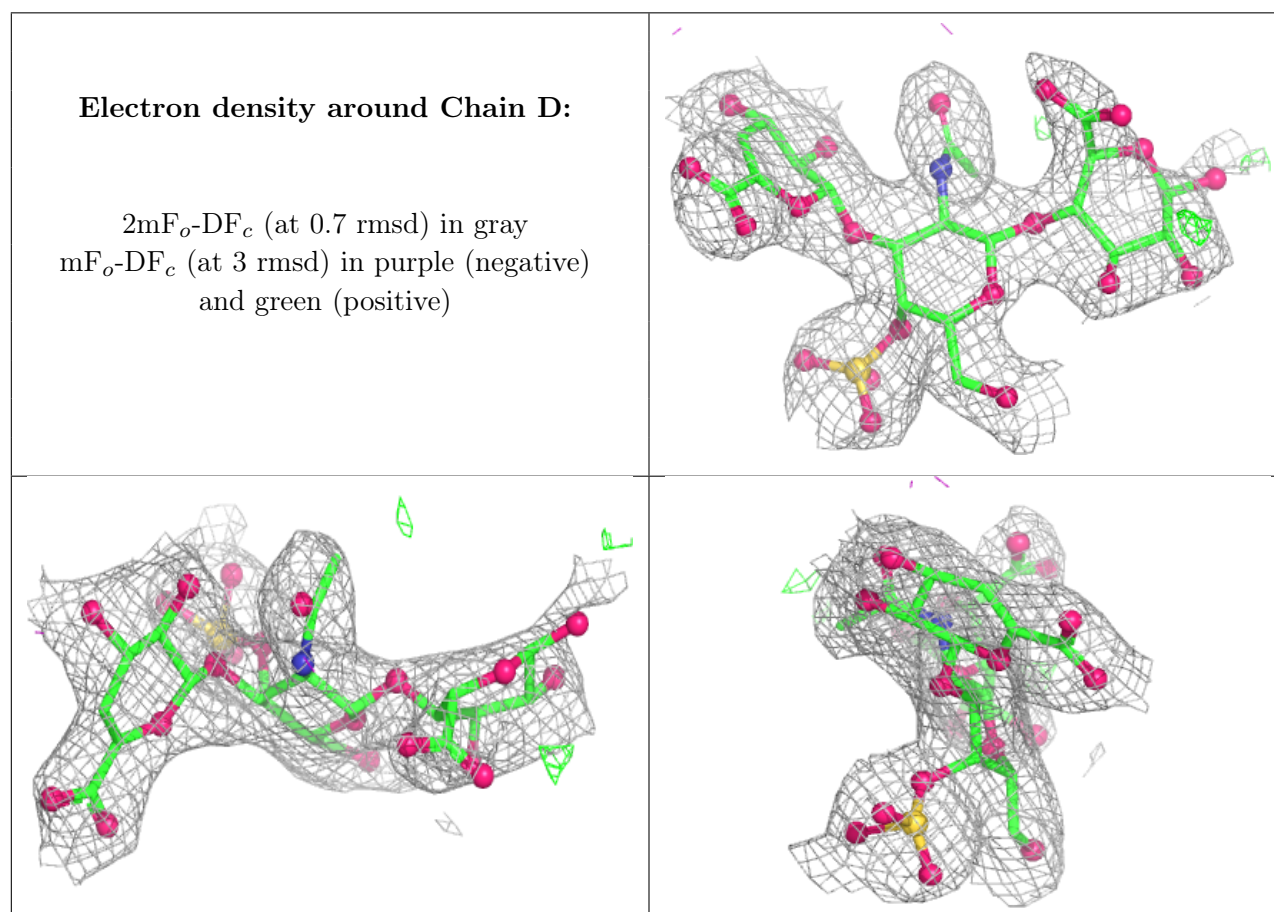
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BDP	F	1	13/13	0.73	0.12	63,70,77,80	0
2	BDP	D	1	13/13	0.82	0.12	48,67,80,87	0
2	BDP	E	1	13/13	0.86	0.09	39,49,63,65	0
2	ASG	E	2	18/19	0.91	0.09	33,49,66,71	0
2	ASG	F	2	18/19	0.91	0.10	29,56,72,72	0
2	GCD	F	3	11/12	0.94	0.08	24,27,31,35	0

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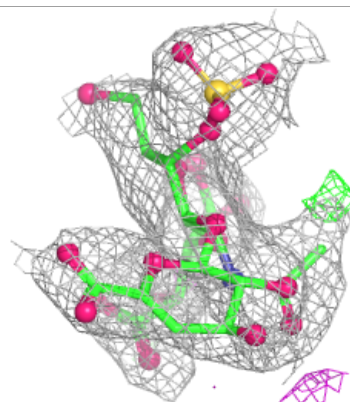
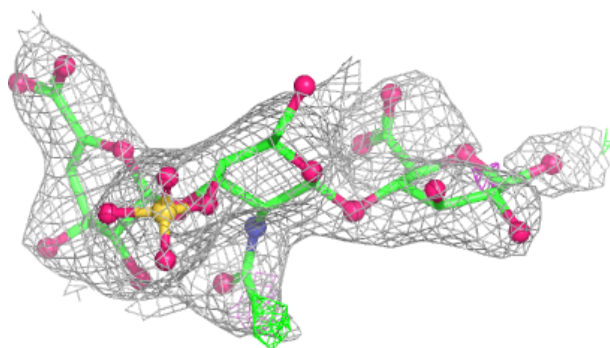
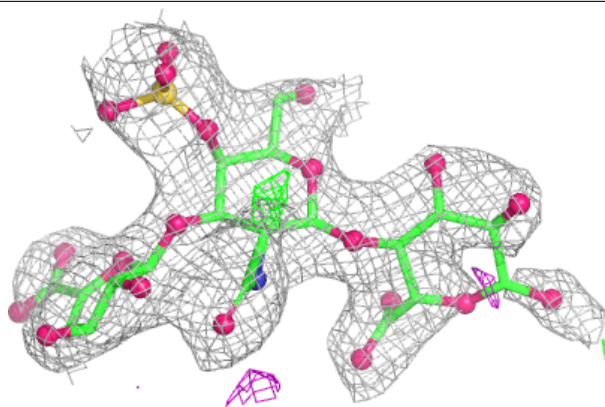
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ASG	D	2	18/19	0.95	0.08	29,49,57,57	0
2	GCD	E	3	11/12	0.96	0.07	33,37,46,49	0
2	GCD	D	3	11/12	0.96	0.05	23,28,32,34	0

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.

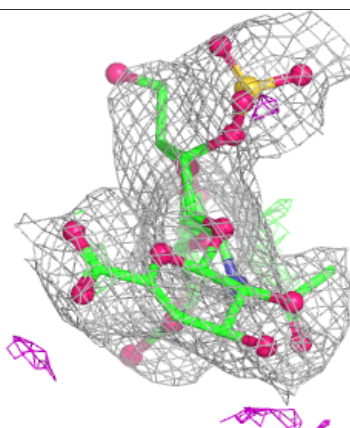
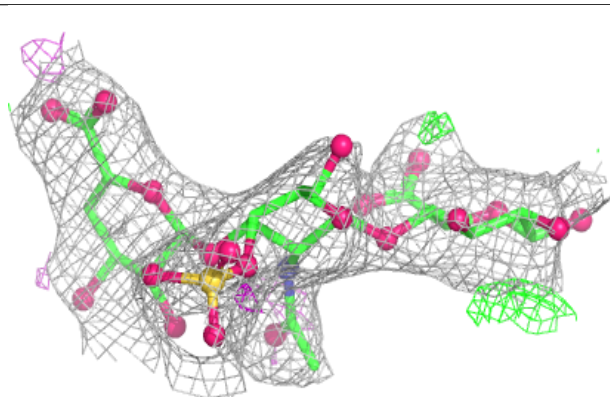
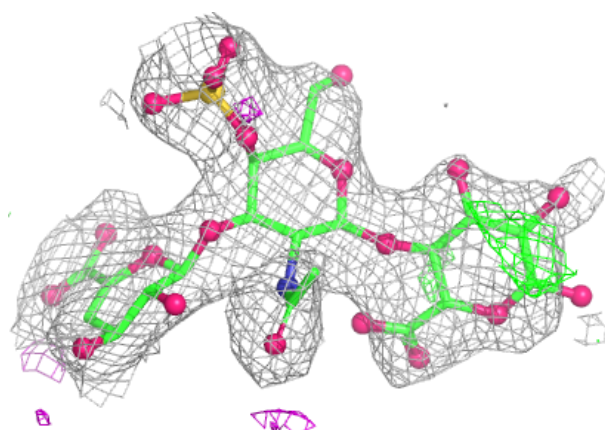


Electron density around Chain E:

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

**Electron density around Chain F:**

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



6.4 Ligands [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, 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	CA	A	601	1/1	0.91	0.07	47,47,47,47	0
3	CA	B	601	1/1	0.96	0.08	63,63,63,63	0
3	CA	C	601	1/1	0.97	0.07	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.