



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:26 AM UTC

PDB ID : 3AXX / pdb_00003axx
Title : Functional analysis of hyperthermophilic endocellulase from the Archaeon Pyrococcus horikoshii
Authors : Kim, H.-W.; Ishikawa, K.
Deposited on : 2011-04-18
Resolution : 1.90 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

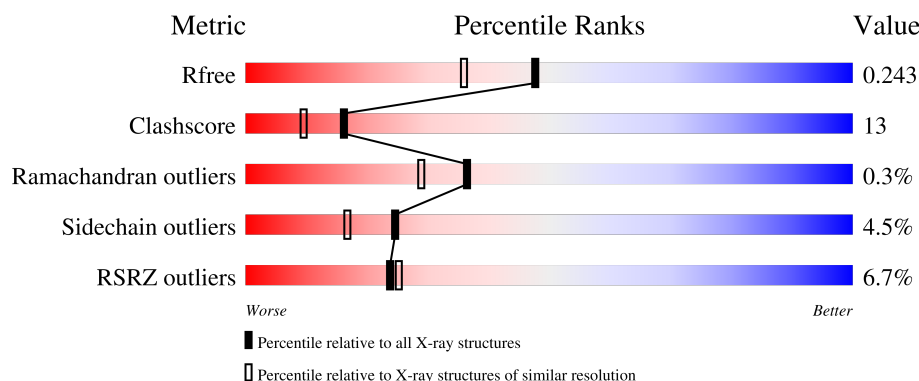
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	458	5% 61% 19% • 18%
1	B	458	4% 60% 20% • 17%
1	C	458	8% 52% 26% • 17%
2	D	2	50% 50%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	 50%50%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9814 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 458aa long hypothetical endo-1,4-beta-glucanase.

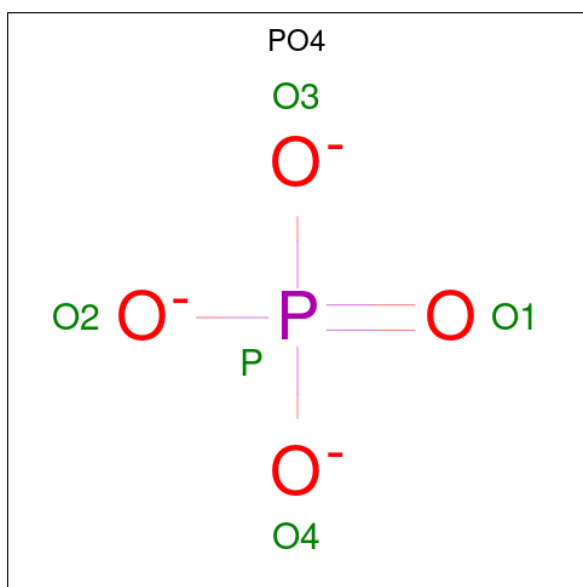
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3071	2002	502	557	10			
1	B	379	Total	C	N	O	S	0	0	0
			3090	2015	504	561	10			
1	C	378	Total	C	N	O	S	0	0	0
			3083	2011	503	559	10			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	2	Total	C	O	0	0	0
			23	12	11			
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

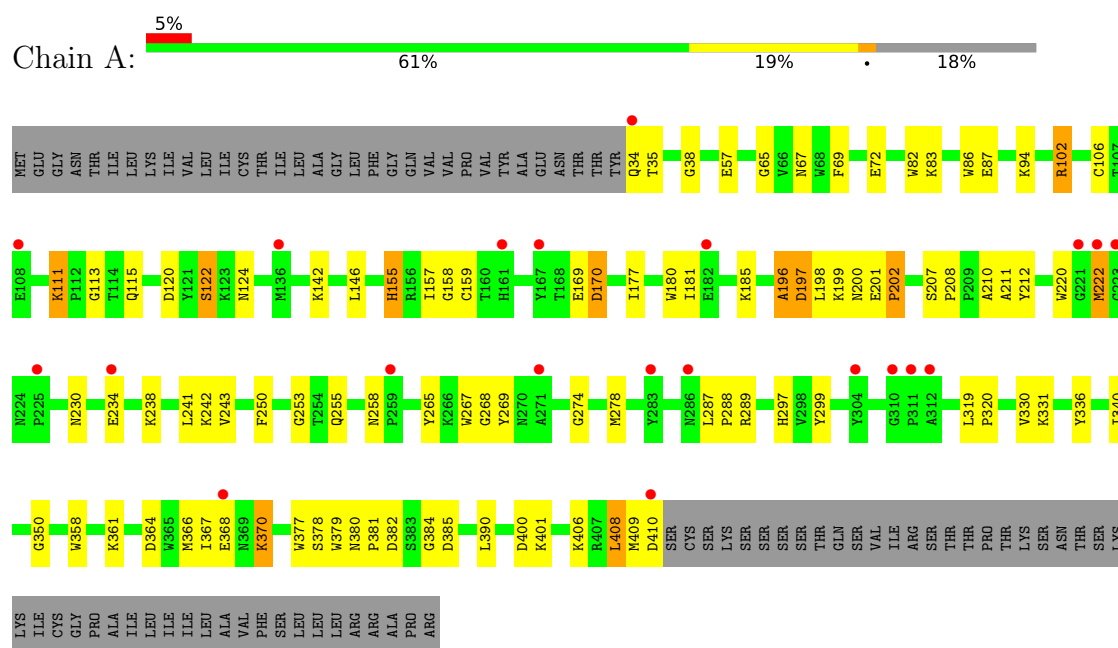
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	192	Total	O	0	0
			192	192		
4	B	189	Total	O	0	0
			189	189		
4	C	105	Total	O	0	0
			105	105		

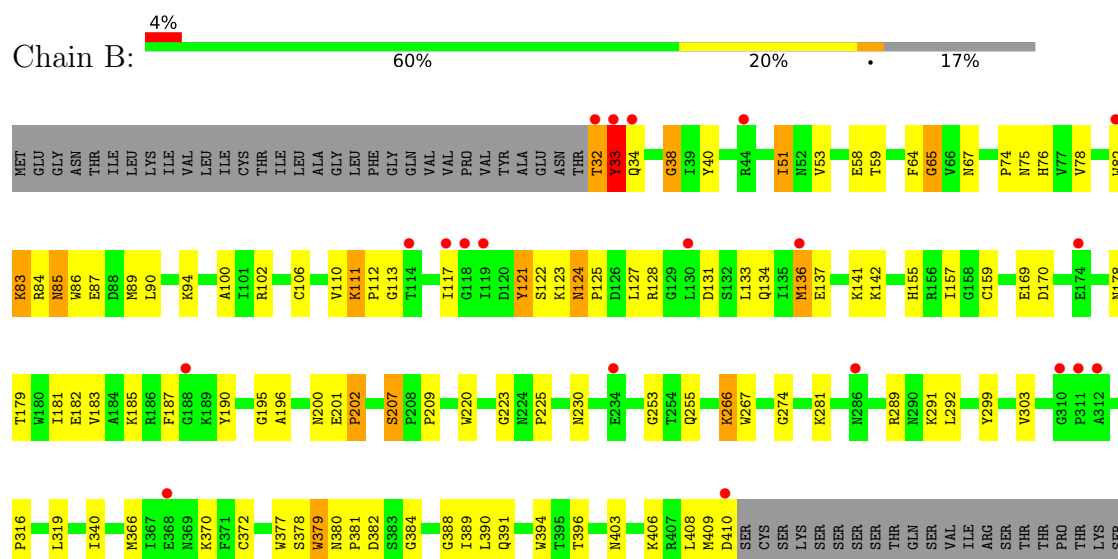
3 Residue-property plots

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: 458aa long hypothetical endo-1,4-beta-glucanase

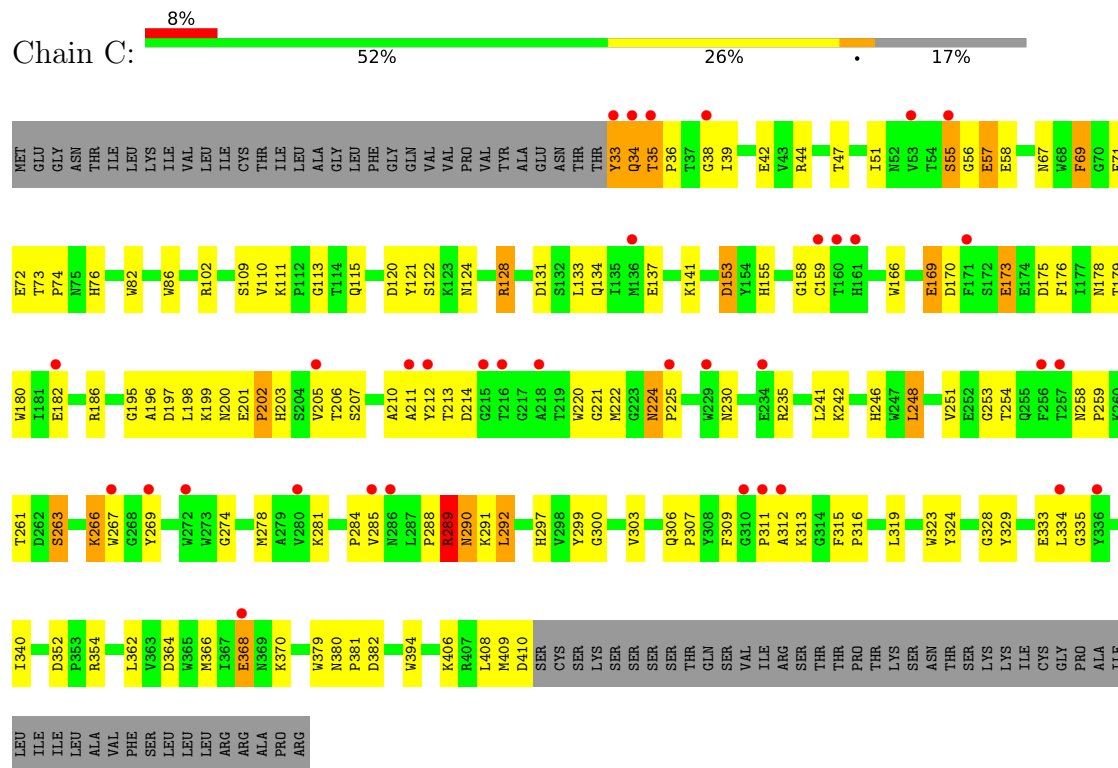


- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase



ASN
THR
SER
LYS
LYS
ILE
CYS
GLY
PRO
ALA
ILE
LEU
ILE
ILE
LEU
ALA
VAL
GLY
PHE
SER
LEU
LEU
ARG
ARG
ALA
PRO
ARG

- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.47Å 58.49Å 138.50Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-1.90) 94.7 (50.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 1.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.241 0.230 , 0.243	Depositor DCC
R_{free} test set	4609 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.8	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	0.95	EDS
Total number of atoms	9814	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: PO4, 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	0.44	0/3182	1.02	24/4344 (0.6%)
1	B	0.47	2/3202 (0.1%)	1.07	33/4372 (0.8%)
1	C	0.42	1/3195 (0.0%)	1.07	25/4362 (0.6%)
All	All	0.45	3/9579 (0.0%)	1.05	82/13078 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	ARG	CA-CB	-6.55	1.42	1.53
1	C	289	ARG	N-CA	-5.84	1.38	1.46
1	B	289	ARG	N-CA	-5.58	1.39	1.46

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	TYR	N-CA-C	12.95	126.82	111.02
1	A	222	MET	N-CA-C	-8.08	102.88	114.12
1	C	379	TRP	N-CA-C	-8.03	102.47	111.14
1	C	56	GLY	N-CA-C	-7.72	105.21	115.40
1	C	38	GLY	N-CA-C	-7.53	105.53	113.58
1	B	289	ARG	CB-CG-CD	-7.39	94.30	111.30
1	C	224	ASN	CA-C-N	7.16	128.79	119.84
1	C	224	ASN	C-N-CA	7.16	128.79	119.84
1	B	384	GLY	N-CA-C	7.15	121.56	112.83
1	B	155	HIS	N-CA-C	6.99	118.97	111.36
1	A	379	TRP	N-CA-C	-6.90	103.84	111.36
1	C	158	GLY	N-CA-C	-6.67	102.41	112.41
1	A	157	ILE	N-CA-C	-6.58	104.44	110.82
1	A	65	GLY	N-CA-C	6.53	123.98	112.10
1	B	202	PRO	N-CA-C	-6.50	101.00	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	TRP	N-CA-C	-6.35	105.54	113.28
1	B	255	GLN	N-CA-C	-6.33	104.27	112.68
1	A	384	GLY	N-CA-C	6.29	120.25	112.64
1	C	195	GLY	N-CA-C	6.29	118.62	110.45
1	C	197	ASP	N-CA-C	-6.20	97.08	107.99
1	A	169	GLU	N-CA-C	-6.18	104.54	111.28
1	B	34	GLN	N-CA-C	6.08	118.52	109.59
1	B	124	ASN	CA-C-N	6.06	125.77	119.05
1	B	124	ASN	C-N-CA	6.06	125.77	119.05
1	B	195	GLY	N-CA-C	6.03	118.29	110.45
1	C	203	HIS	N-CA-C	5.99	115.99	108.45
1	B	85	ASN	N-CA-C	-5.95	99.96	109.96
1	C	202	PRO	N-CA-C	-5.92	101.92	111.03
1	A	155	HIS	N-CA-C	5.91	118.96	111.69
1	A	113	GLY	N-CA-C	5.90	123.20	115.36
1	C	300	GLY	CA-C-N	5.86	126.00	119.32
1	C	300	GLY	C-N-CA	5.86	126.00	119.32
1	A	201	GLU	N-CA-C	5.82	122.68	109.81
1	B	82	TRP	N-CA-C	-5.81	106.23	113.38
1	C	292	LEU	N-CA-C	5.79	118.68	109.24
1	B	157	ILE	N-CA-C	-5.77	104.71	111.00
1	A	202	PRO	N-CA-C	-5.77	102.14	111.14
1	C	248	LEU	N-CA-C	-5.75	100.91	110.17
1	B	292	LEU	N-CA-C	5.74	119.17	109.76
1	B	122	SER	N-CA-C	-5.69	105.16	111.36
1	C	115	GLN	CA-C-N	-5.69	113.35	120.51
1	C	115	GLN	C-N-CA	-5.69	113.35	120.51
1	A	102	ARG	N-CA-C	-5.60	100.05	108.96
1	A	258	ASN	N-CA-C	-5.59	100.89	108.11
1	C	370	LYS	N-CA-C	5.59	119.28	111.74
1	B	379	TRP	N-CA-C	-5.57	105.11	111.07
1	B	121	TYR	N-CA-C	5.54	119.65	113.01
1	B	170	ASP	N-CA-C	5.52	120.13	113.17
1	C	335	GLY	N-CA-C	5.52	121.53	113.48
1	B	319	LEU	N-CA-C	5.51	120.24	112.75
1	C	175	ASP	N-CA-C	-5.50	105.44	111.82
1	C	201	GLU	N-CA-C	5.48	121.92	109.81
1	A	122	SER	N-CA-C	-5.45	105.34	111.28
1	B	207	SER	CA-C-N	5.44	123.58	119.66
1	B	207	SER	C-N-CA	5.44	123.58	119.66
1	A	158	GLY	N-CA-C	-5.43	104.27	112.41
1	A	197	ASP	N-CA-C	-5.41	97.08	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	GLU	N-CA-C	5.38	121.70	109.81
1	A	38	GLY	N-CA-C	-5.37	107.90	115.32
1	C	198	LEU	N-CA-C	5.35	120.14	111.37
1	B	38	GLY	N-CA-C	-5.31	108.37	114.69
1	B	65	GLY	N-CA-C	5.31	121.76	112.10
1	A	198	LEU	N-CA-C	5.30	120.12	111.37
1	B	389	ILE	N-CA-C	-5.26	105.40	110.72
1	C	82	TRP	N-CA-C	-5.26	106.86	113.28
1	B	113	GLY	N-CA-C	5.23	122.01	115.21
1	A	196	ALA	N-CA-C	5.19	117.36	108.90
1	B	370	LYS	N-CA-C	5.19	118.74	111.74
1	A	211	ALA	N-CA-C	5.18	117.59	111.33
1	C	290	ASN	N-CA-C	-5.16	106.84	112.72
1	C	69	PHE	N-CA-C	5.13	118.03	110.59
1	B	196	ALA	N-CA-C	5.12	117.25	108.90
1	B	289	ARG	N-CA-C	5.11	117.58	111.71
1	B	183	VAL	N-CA-C	-5.10	105.42	110.62
1	A	170	ASP	N-CA-C	5.08	117.94	111.69
1	A	319	LEU	N-CA-C	5.08	119.65	112.75
1	A	370	LYS	N-CA-C	5.07	118.58	111.74
1	C	113	GLY	N-CA-C	5.07	122.10	115.36
1	B	111	LYS	CA-C-N	-5.06	114.73	119.89
1	B	111	LYS	C-N-CA	-5.06	114.73	119.89
1	A	208	PRO	N-CA-C	-5.02	104.58	110.70
1	B	59	THR	N-CA-C	5.01	116.88	109.62

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	3071	0	2910	59	0
1	B	3090	0	2926	77	0
1	C	3083	0	2919	100	0
2	D	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	23	0	21	0	0
2	F	23	0	21	1	0
3	A	15	0	0	0	0
4	A	192	0	0	10	1
4	B	189	0	0	9	0
4	C	105	0	0	2	0
All	All	9814	0	8818	236	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 13.

All (236) 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:266:LYS:H	1:C:266:LYS:HD2	1.15	1.10
1:A:212:TYR:HB3	1:A:222:MET:HE2	1.32	1.09
1:C:333:GLU:HG2	1:C:334:LEU:HD23	1.49	0.91
1:C:67:ASN:HD21	1:C:102:ARG:HH11	1.18	0.91
1:A:111:LYS:HB3	1:A:111:LYS:HZ2	1.34	0.91
1:B:372:CYS:HB2	4:B:483:HOH:O	1.75	0.85
1:B:51:ILE:HD13	1:B:58:GLU:HG2	1.60	0.84
1:A:212:TYR:HB3	1:A:222:MET:CE	2.08	0.83
1:A:111:LYS:HB3	1:A:111:LYS:NZ	1.92	0.82
1:C:406:LYS:HA	1:C:409:MET:HE2	1.63	0.81
1:B:83:LYS:O	1:B:83:LYS:HD3	1.80	0.80
1:B:86:TRP:HD1	1:B:124:ASN:HD22	1.27	0.79
1:B:106:CYS:HG	1:B:159:CYS:HG	1.27	0.79
1:C:289:ARG:O	1:C:289:ARG:HG3	1.83	0.78
1:B:406:LYS:HA	1:B:409:MET:HE3	1.66	0.77
1:C:67:ASN:ND2	1:C:102:ARG:HH11	1.81	0.77
1:C:289:ARG:O	1:C:289:ARG:CG	2.32	0.76
1:C:266:LYS:HD2	1:C:266:LYS:N	1.95	0.76
1:C:340:ILE:HD12	1:C:366:MET:HE3	1.67	0.76
1:C:409:MET:O	1:C:410:ASP:HB2	1.86	0.75
1:B:110:VAL:HA	1:B:133:LEU:HD13	1.71	0.73
1:C:35:THR:HB	1:C:246:HIS:HB3	1.68	0.73
1:B:133:LEU:HG	4:B:642:HOH:O	1.87	0.73
1:A:67:ASN:HD21	1:A:102:ARG:HH11	1.35	0.72
1:B:136:MET:HE2	1:B:187:PHE:CZ	2.25	0.72
1:B:33:TYR:HD1	1:B:33:TYR:H	1.35	0.71
1:C:169:GLU:HG3	1:C:170:ASP:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:TYR:CD1	1:C:34:GLN:HG2	2.25	0.71
1:C:128:ARG:HD2	4:C:461:HOH:O	1.89	0.71
1:A:253:GLY:O	1:A:274:GLY:HA2	1.91	0.70
1:A:87:GLU:OE2	1:A:142:LYS:HE3	1.91	0.70
1:C:76:HIS:HE1	1:C:159:CYS:SG	2.13	0.70
1:B:67:ASN:HD21	1:B:102:ARG:HD3	1.57	0.69
1:B:340:ILE:HG13	4:B:486:HOH:O	1.93	0.69
1:A:120:ASP:OD1	1:A:122:SER:HB3	1.92	0.68
1:A:67:ASN:HD21	1:A:102:ARG:HD3	1.57	0.68
1:A:102:ARG:HH22	1:A:200:ASN:HD22	1.40	0.68
1:C:267:TRP:CZ3	1:C:307:PRO:HB2	2.28	0.68
1:B:134:GLN:HG3	4:B:636:HOH:O	1.92	0.67
1:A:106:CYS:HG	1:A:159:CYS:HG	0.67	0.67
1:A:86:TRP:HD1	1:A:124:ASN:HD22	1.43	0.67
1:B:67:ASN:HD21	1:B:102:ARG:HH11	1.42	0.67
1:A:86:TRP:H	1:A:124:ASN:HD21	1.41	0.65
1:A:234:GLU:HB2	4:A:640:HOH:O	1.95	0.65
1:C:33:TYR:HD1	1:C:34:GLN:HG2	1.59	0.65
1:C:333:GLU:HG2	1:C:334:LEU:CD2	2.26	0.65
1:B:123:LYS:C	1:B:125:PRO:HD3	2.22	0.65
1:B:84:ARG:NH1	1:B:394:TRP:O	2.29	0.63
1:C:186:ARG:HG3	1:C:186:ARG:HH11	1.64	0.63
1:C:86:TRP:H	1:C:124:ASN:HD21	1.46	0.62
1:B:391:GLN:HG3	1:B:396:THR:O	2.00	0.62
1:B:121:TYR:CD1	1:B:128:ARG:HG2	2.35	0.62
1:C:199:LYS:HD2	1:C:202:PRO:HG3	1.82	0.61
1:C:311:PRO:C	1:C:313:LYS:H	2.08	0.61
1:B:340:ILE:HD12	1:B:366:MET:HE3	1.82	0.61
1:A:289:ARG:HB3	1:A:289:ARG:CZ	2.31	0.61
1:C:288:PRO:O	1:C:290:ASN:N	2.34	0.61
1:B:86:TRP:H	1:B:124:ASN:ND2	1.99	0.61
1:A:410:ASP:HB3	4:A:631:HOH:O	2.01	0.60
1:A:289:ARG:HH21	1:A:289:ARG:HG3	1.66	0.60
1:C:102:ARG:HH22	1:C:200:ASN:HD22	1.49	0.60
1:A:86:TRP:H	1:A:124:ASN:ND2	2.00	0.60
1:C:212:TYR:O	1:C:222:MET:HE2	2.02	0.60
1:A:242:LYS:HE2	4:A:643:HOH:O	2.02	0.59
1:C:173:GLU:O	1:C:173:GLU:HG3	2.02	0.59
1:C:311:PRO:O	1:C:313:LYS:N	2.35	0.59
1:A:34:GLN:HA	4:A:472:HOH:O	2.02	0.59
1:C:220:TRP:CE2	1:C:230:ASN:HB3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLN:C	1:C:35:THR:HG22	2.27	0.59
1:A:67:ASN:ND2	1:A:102:ARG:HH11	2.01	0.59
1:C:364:ASP:O	1:C:368:GLU:HG3	2.03	0.59
1:B:131:ASP:OD1	1:B:134:GLN:CG	2.51	0.58
1:C:86:TRP:HD1	1:C:124:ASN:HD22	1.49	0.58
1:A:380:ASN:HB3	1:A:382:ASP:OD1	2.02	0.58
1:C:44:ARG:NH1	1:C:58:GLU:OE1	2.35	0.58
1:A:220:TRP:CE2	1:A:230:ASN:HB3	2.39	0.58
1:C:86:TRP:H	1:C:124:ASN:ND2	2.01	0.57
1:B:75:ASN:HA	1:B:117:ILE:HG12	1.86	0.57
1:C:35:THR:HG21	1:C:39:ILE:O	2.05	0.57
1:B:381:PRO:HD2	1:B:394:TRP:CZ2	2.39	0.57
1:B:409:MET:O	1:B:410:ASP:HB2	2.05	0.57
1:A:368:GLU:HG3	4:A:517:HOH:O	2.04	0.57
1:A:102:ARG:HH22	1:A:200:ASN:ND2	2.03	0.57
1:C:67:ASN:HD21	1:C:102:ARG:HD3	1.69	0.56
1:C:120:ASP:OD1	1:C:122:SER:HB3	2.06	0.56
1:B:253:GLY:O	1:B:274:GLY:HA2	2.06	0.56
1:B:266:LYS:HE2	1:B:267:TRP:NE1	2.19	0.56
1:C:35:THR:HB	1:C:246:HIS:CB	2.36	0.55
1:B:64:PHE:CD2	1:B:409:MET:HG2	2.41	0.55
1:C:311:PRO:HA	1:C:315:PHE:HB3	1.88	0.55
1:A:385:ASP:HB3	4:A:647:HOH:O	2.05	0.55
1:B:67:ASN:ND2	1:B:102:ARG:HH11	2.04	0.55
1:A:367:ILE:HG13	1:A:408:LEU:HD13	1.89	0.55
1:B:124:ASN:N	1:B:125:PRO:HD3	2.21	0.55
1:B:209:PRO:HD2	4:B:632:HOH:O	2.07	0.54
1:C:71:PHE:O	1:C:109:SER:OG	2.17	0.54
1:B:86:TRP:H	1:B:124:ASN:HD21	1.55	0.54
1:C:186:ARG:HG3	1:C:186:ARG:NH1	2.21	0.54
1:B:32:THR:HA	1:B:40:TYR:CD2	2.42	0.54
1:B:86:TRP:HD1	1:B:124:ASN:ND2	2.00	0.53
1:C:253:GLY:O	1:C:274:GLY:HA2	2.07	0.53
1:A:180:TRP:CH2	1:A:196:ALA:HB1	2.43	0.53
1:A:207:SER:O	1:A:210:ALA:HB3	2.08	0.53
1:B:83:LYS:HD3	1:B:83:LYS:C	2.29	0.53
1:C:329:TYR:O	1:C:333:GLU:HB3	2.08	0.53
1:B:102:ARG:HH22	1:B:200:ASN:HD22	1.57	0.53
1:C:131:ASP:OD1	1:C:134:GLN:HG3	2.09	0.53
1:B:86:TRP:CD1	1:B:124:ASN:HD22	2.17	0.53
1:C:281:LYS:O	1:C:284:PRO:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:MET:SD	1:C:259:PRO:HD3	2.49	0.52
1:C:267:TRP:HZ3	1:C:307:PRO:HB2	1.73	0.52
1:B:86:TRP:O	1:B:89:MET:HB2	2.10	0.52
1:C:33:TYR:HD1	1:C:34:GLN:N	2.07	0.52
1:C:206:THR:OG1	1:C:214:ASP:OD2	2.25	0.52
1:B:380:ASN:O	1:B:388:GLY:HA3	2.09	0.52
1:B:141:LYS:HD2	4:B:476:HOH:O	2.10	0.51
1:C:340:ILE:HD12	1:C:366:MET:CE	2.40	0.51
1:B:136:MET:CE	1:B:187:PHE:CZ	2.94	0.51
1:B:181:ILE:O	1:B:185:LYS:HG3	2.12	0.50
1:B:379:TRP:CE2	1:B:390:LEU:HD11	2.46	0.50
1:C:352:ASP:OD1	1:C:354:ARG:HB2	2.11	0.50
1:C:55:SER:C	1:C:57:GLU:H	2.18	0.50
1:A:94:LYS:NZ	1:A:146:LEU:O	2.33	0.50
1:B:86:TRP:N	1:B:124:ASN:HD21	2.09	0.50
1:A:289:ARG:HH21	1:A:289:ARG:CG	2.25	0.50
1:B:223:GLY:O	1:B:225:PRO:HD3	2.12	0.50
1:B:131:ASP:OD1	1:B:134:GLN:HG3	2.12	0.49
1:C:42:GLU:OE1	1:C:51:ILE:HD11	2.13	0.49
1:B:202:PRO:HD2	1:B:253:GLY:O	2.12	0.49
1:C:263:SER:HB3	1:C:269:TYR:OH	2.12	0.49
1:C:51:ILE:HG12	1:C:58:GLU:HB2	1.95	0.49
1:C:133:LEU:O	1:C:137:GLU:HG3	2.13	0.49
1:B:179:THR:O	1:B:182:GLU:HG3	2.13	0.49
1:C:258:ASN:ND2	1:C:261:THR:OG1	2.46	0.49
1:B:131:ASP:OD1	1:B:134:GLN:HG2	2.13	0.48
1:C:334:LEU:HD23	1:C:334:LEU:N	2.27	0.48
1:C:206:THR:O	1:C:211:ALA:HB2	2.13	0.48
1:C:311:PRO:C	1:C:313:LYS:N	2.72	0.48
1:B:409:MET:O	1:B:410:ASP:CB	2.60	0.48
1:B:33:TYR:CD1	1:B:33:TYR:N	2.76	0.48
1:B:190:TYR:N	1:B:190:TYR:CD2	2.82	0.47
1:B:220:TRP:CE2	1:B:230:ASN:HB3	2.49	0.47
1:B:291:LYS:HE2	1:B:291:LYS:HA	1.95	0.47
1:A:86:TRP:N	1:A:124:ASN:HD21	2.11	0.47
1:C:288:PRO:O	1:C:289:ARG:C	2.57	0.47
1:A:381:PRO:HB3	1:A:390:LEU:O	2.14	0.47
1:B:178:ASN:O	1:B:182:GLU:HG2	2.14	0.47
1:B:299:TYR:CD1	1:B:303:VAL:HG21	2.49	0.47
1:C:299:TYR:CD1	1:C:303:VAL:HG21	2.49	0.47
1:B:85:ASN:HA	1:B:124:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:TYR:OH	1:A:269:TYR:HE1	1.98	0.47
1:C:324:TYR:HA	1:C:328:GLY:HA3	1.97	0.47
1:A:255:GLN:HB3	4:A:477:HOH:O	2.15	0.46
1:C:55:SER:HB2	1:C:57:GLU:HB2	1.97	0.46
1:A:177:ILE:HG22	1:A:181:ILE:HD12	1.97	0.46
1:B:124:ASN:HB3	1:B:127:LEU:HD12	1.97	0.46
1:A:409:MET:O	1:A:410:ASP:HB2	2.15	0.45
1:B:87:GLU:CB	4:B:647:HOH:O	2.64	0.45
1:B:381:PRO:HD2	1:B:394:TRP:CH2	2.51	0.45
1:C:380:ASN:HB3	1:C:382:ASP:OD1	2.16	0.45
1:C:153:ASP:OD1	1:C:153:ASP:C	2.58	0.45
1:C:221:GLY:HA2	4:C:557:HOH:O	2.15	0.45
1:B:74:PRO:O	1:B:76:HIS:CD2	2.69	0.45
1:B:38:GLY:O	1:B:53:VAL:HG22	2.17	0.45
1:C:291:LYS:HE2	1:C:291:LYS:HA	1.98	0.45
1:B:74:PRO:HD3	1:B:159:CYS:O	2.17	0.45
1:C:200:ASN:ND2	1:C:297:HIS:HE1	2.15	0.45
1:C:306:GLN:HB2	1:C:309:PHE:CD2	2.52	0.45
1:A:265:TYR:CE2	1:A:267:TRP:HB2	2.52	0.44
1:A:330:VAL:HG12	1:A:336:TYR:HB2	1.98	0.44
1:B:137:GLU:CD	4:B:642:HOH:O	2.59	0.44
1:A:370:LYS:HE2	4:A:544:HOH:O	2.18	0.44
1:B:380:ASN:HB3	1:B:382:ASP:OD1	2.18	0.44
1:C:137:GLU:OE2	1:C:186:ARG:NH1	2.51	0.44
1:C:235:ARG:HH11	1:C:235:ARG:HG3	1.82	0.44
1:A:331:LYS:HE3	1:A:370:LYS:O	2.18	0.43
1:C:306:GLN:NE2	2:F:1:BGC:O2	2.47	0.43
1:C:212:TYR:HB3	1:C:222:MET:HE2	2.00	0.43
1:A:367:ILE:HG13	1:A:408:LEU:CD1	2.48	0.43
1:B:111:LYS:O	1:B:112:PRO:C	2.58	0.43
1:C:281:LYS:NZ	1:C:281:LYS:HB3	2.33	0.43
1:C:121:TYR:HB3	1:C:128:ARG:HD3	1.99	0.43
1:C:278:MET:HA	1:C:329:TYR:OH	2.18	0.43
1:C:86:TRP:N	1:C:124:ASN:HD21	2.12	0.43
1:C:169:GLU:HG3	1:C:170:ASP:H	1.79	0.43
1:A:340:ILE:HD12	1:A:366:MET:HE3	2.01	0.43
1:C:36:PRO:HD2	1:C:246:HIS:CE1	2.53	0.43
1:C:316:PRO:O	1:C:319:LEU:HG	2.19	0.43
1:C:381:PRO:HD2	1:C:394:TRP:CH2	2.54	0.43
1:C:102:ARG:HH22	1:C:200:ASN:ND2	2.15	0.43
1:C:224:ASN:HA	1:C:225:PRO:HD2	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:HD12	1:B:142:LYS:CG	2.48	0.43
1:C:110:VAL:HA	1:C:133:LEU:HD13	1.99	0.43
1:C:176:PHE:O	1:C:179:THR:HB	2.19	0.43
1:A:287:LEU:O	1:A:288:PRO:C	2.60	0.43
1:B:87:GLU:HB2	4:B:647:HOH:O	2.18	0.43
1:C:408:LEU:HD12	1:C:408:LEU:O	2.19	0.43
1:B:133:LEU:O	1:B:136:MET:HB2	2.20	0.42
1:C:35:THR:HG21	1:C:39:ILE:C	2.43	0.42
1:C:166:TRP:CD1	1:C:173:GLU:HB2	2.54	0.42
1:A:200:ASN:ND2	1:A:297:HIS:HE1	2.17	0.42
1:B:121:TYR:CE1	1:B:128:ARG:HA	2.54	0.42
1:B:377:TRP:HA	1:B:378:SER:HA	1.79	0.42
1:B:67:ASN:ND2	1:B:102:ARG:HB3	2.34	0.42
1:B:87:GLU:CD	1:B:142:LYS:HE3	2.45	0.42
1:C:261:THR:HG22	1:C:278:MET:HG3	2.01	0.42
1:C:155:HIS:CE1	1:C:200:ASN:CG	2.98	0.42
1:A:361:LYS:HD2	4:A:615:HOH:O	2.20	0.42
1:B:64:PHE:CG	1:B:409:MET:HG2	2.55	0.41
1:B:89:MET:HE1	1:B:394:TRP:CE3	2.55	0.41
1:B:65:GLY:HA2	1:B:100:ALA:O	2.21	0.41
1:A:377:TRP:HA	1:A:378:SER:HA	1.75	0.41
1:A:400:ASP:OD1	1:A:401:LYS:N	2.53	0.41
1:C:241:LEU:HD23	1:C:241:LEU:HA	1.84	0.41
1:B:281:LYS:HB3	1:B:281:LYS:HE2	1.95	0.41
1:C:178:ASN:O	1:C:182:GLU:HG3	2.20	0.41
1:B:85:ASN:HA	1:B:124:ASN:HD21	1.84	0.41
1:A:299:TYR:C	1:A:358:TRP:CZ2	2.99	0.41
1:A:197:ASP:HA	1:A:250:PHE:HB2	2.02	0.41
1:A:234:GLU:O	1:A:238:LYS:HG3	2.21	0.41
1:A:350:GLY:HA2	4:A:484:HOH:O	2.20	0.41
1:A:364:ASP:O	1:A:368:GLU:HG3	2.21	0.41
1:A:406:LYS:HB2	1:A:406:LYS:HE3	1.82	0.41
1:C:202:PRO:HB2	1:C:254:THR:HG22	2.02	0.41
1:A:241:LEU:HD23	1:A:241:LEU:HA	1.93	0.41
1:A:199:LYS:CD	1:A:202:PRO:HG3	2.51	0.40
1:C:324:TYR:CE2	1:C:329:TYR:HB3	2.55	0.40
1:C:69:PHE:HB2	1:C:72:GLU:OE2	2.21	0.40
1:C:155:HIS:HA	1:C:200:ASN:HB3	2.02	0.40
1:C:180:TRP:CH2	1:C:196:ALA:HB1	2.57	0.40
1:C:251:VAL:HG11	1:C:285:VAL:HG21	2.03	0.40
1:A:69:PHE:HB2	1:A:72:GLU:OE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:THR:HB	1:C:74:PRO:CD	2.52	0.40
1:A:155:HIS:HA	1:A:200:ASN:HB3	2.03	0.40
1:A:268:GLY:HA2	1:A:278:MET:HE1	2.03	0.40
1:C:323:TRP:CH2	1:C:362:LEU:HA	2.56	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)
4:A:558:HOH:O	4:A:558:HOH:O[2_555]	1.97	0.23

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	375/458 (82%)	364 (97%)	11 (3%)	0	100	100
1	B	377/458 (82%)	364 (97%)	13 (3%)	0	100	100
1	C	376/458 (82%)	337 (90%)	36 (10%)	3 (1%)	16	8
All	All	1128/1374 (82%)	1065 (94%)	60 (5%)	3 (0%)	36	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	312	ALA
1	C	289	ARG
1	C	210	ALA

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	324/396 (82%)	314 (97%)	10 (3%)	35	29
1	B	326/396 (82%)	313 (96%)	13 (4%)	28	20
1	C	325/396 (82%)	304 (94%)	21 (6%)	15	8
All	All	975/1188 (82%)	931 (96%)	44 (4%)	24	17

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	57	GLU
1	A	83	LYS
1	A	111	LYS
1	A	115	GLN
1	A	170	ASP
1	A	185	LYS
1	A	243	VAL
1	A	320	PRO
1	A	408	LEU
1	B	32	THR
1	B	33	TYR
1	B	51	ILE
1	B	78	VAL
1	B	83	LYS
1	B	94	LYS
1	B	136	MET
1	B	169	GLU
1	B	207	SER
1	B	266	LYS
1	B	316	PRO
1	B	403	ASN
1	B	408	LEU
1	C	33	TYR
1	C	34	GLN
1	C	35	THR

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Mol	Chain	Res	Type
1	C	47	THR
1	C	55	SER
1	C	57	GLU
1	C	111	LYS
1	C	128	ARG
1	C	141	LYS
1	C	153	ASP
1	C	169	GLU
1	C	173	GLU
1	C	205	VAL
1	C	207	SER
1	C	213	THR
1	C	242	LYS
1	C	248	LEU
1	C	263	SER
1	C	266	LYS
1	C	292	LEU
1	C	368	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	76	HIS
1	A	115	GLN
1	A	124	ASN
1	A	200	ASN
1	A	359	GLN
1	B	62	HIS
1	B	67	ASN
1	B	76	HIS
1	B	124	ASN
1	B	134	GLN
1	B	200	ASN
1	B	359	GLN
1	C	67	ASN
1	C	76	HIS
1	C	115	GLN
1	C	124	ASN
1	C	161	HIS
1	C	200	ASN
1	C	270	ASN

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Mol	Chain	Res	Type
1	C	359	GLN

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 ⓘ

6 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	D	1	2	12,12,12	0.49	0	17,17,17	1.30	4 (23%)
2	BGC	D	2	2	11,11,12	0.34	0	15,15,17	0.69	0
2	BGC	E	1	2	12,12,12	0.49	0	17,17,17	1.29	2 (11%)
2	BGC	E	2	2	11,11,12	0.32	0	15,15,17	0.70	0
2	BGC	F	1	2	12,12,12	0.59	0	17,17,17	1.92	6 (35%)
2	BGC	F	2	2	11,11,12	0.37	0	15,15,17	1.93	4 (26%)

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	D	1	2	-	0/2/22/22	0/1/1/1
2	BGC	D	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	1/2/22/22	0/1/1/1
2	BGC	F	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	BGC	C3-C4-C5	4.46	118.33	110.23
2	F	1	BGC	O5-C1-C2	-4.15	103.00	110.30
2	F	2	BGC	O5-C5-C6	-3.87	100.13	107.66
2	E	1	BGC	C1-O5-C5	-3.43	107.01	113.65
2	F	2	BGC	C2-C3-C4	-3.32	105.02	110.86
2	E	1	BGC	O5-C5-C6	2.55	112.76	106.44
2	D	1	BGC	O5-C5-C4	2.36	113.96	109.70
2	F	1	BGC	O6-C6-C5	-2.34	103.37	111.33
2	F	1	BGC	O5-C5-C6	-2.33	100.67	106.44
2	D	1	BGC	O5-C5-C6	2.32	112.18	106.44
2	D	1	BGC	C6-C5-C4	-2.30	107.38	113.02
2	D	1	BGC	C1-O5-C5	-2.27	109.26	113.65
2	F	2	BGC	O5-C1-C2	-2.21	105.52	110.79
2	F	1	BGC	C1-C2-C3	2.18	114.80	110.36
2	F	2	BGC	C1-O5-C5	2.14	115.06	112.19
2	F	1	BGC	O1-C1-O5	-2.07	104.25	110.41

There are no chirality outliers.

All (1) torsion outliers are listed below:

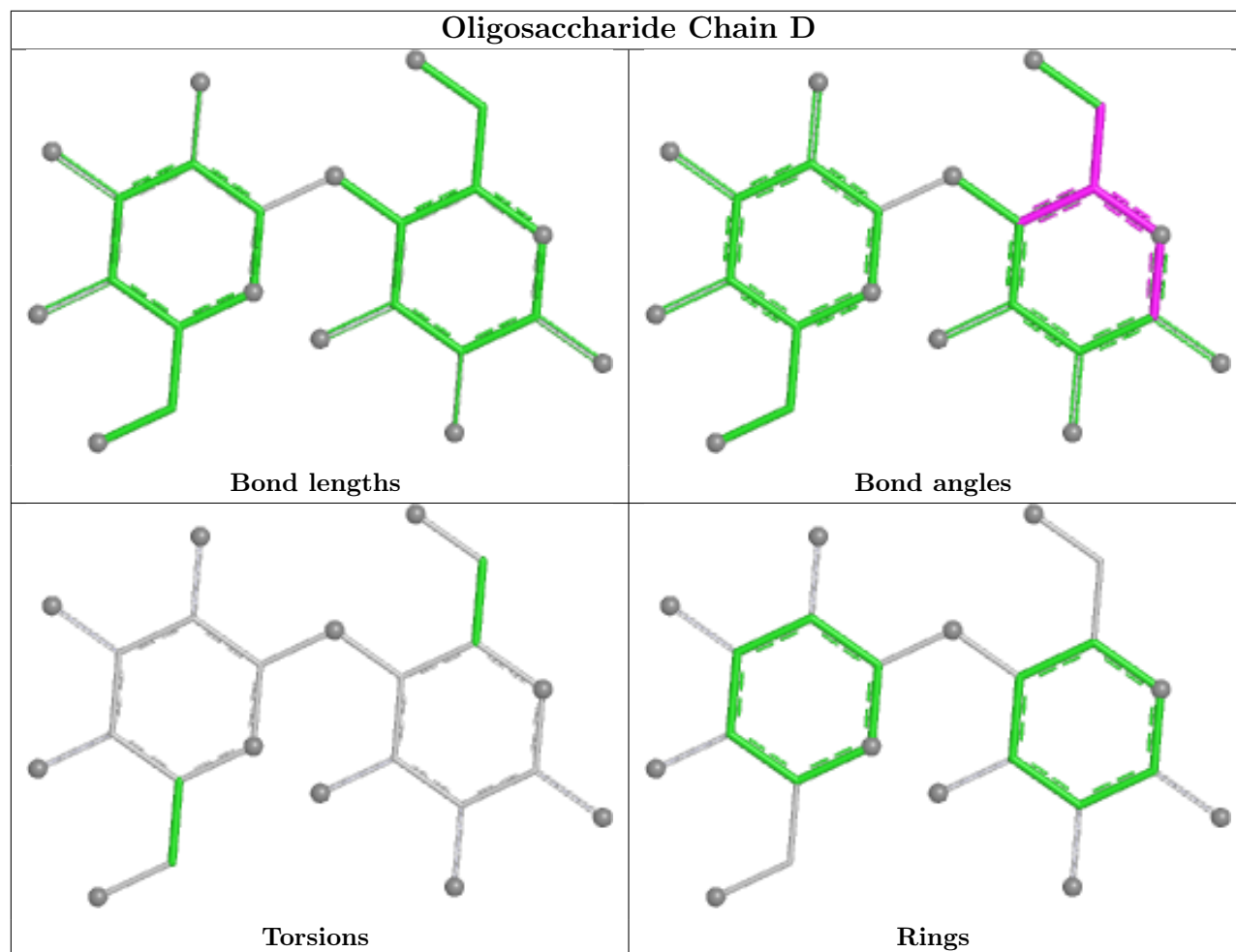
Mol	Chain	Res	Type	Atoms
2	F	1	BGC	O5-C5-C6-O6

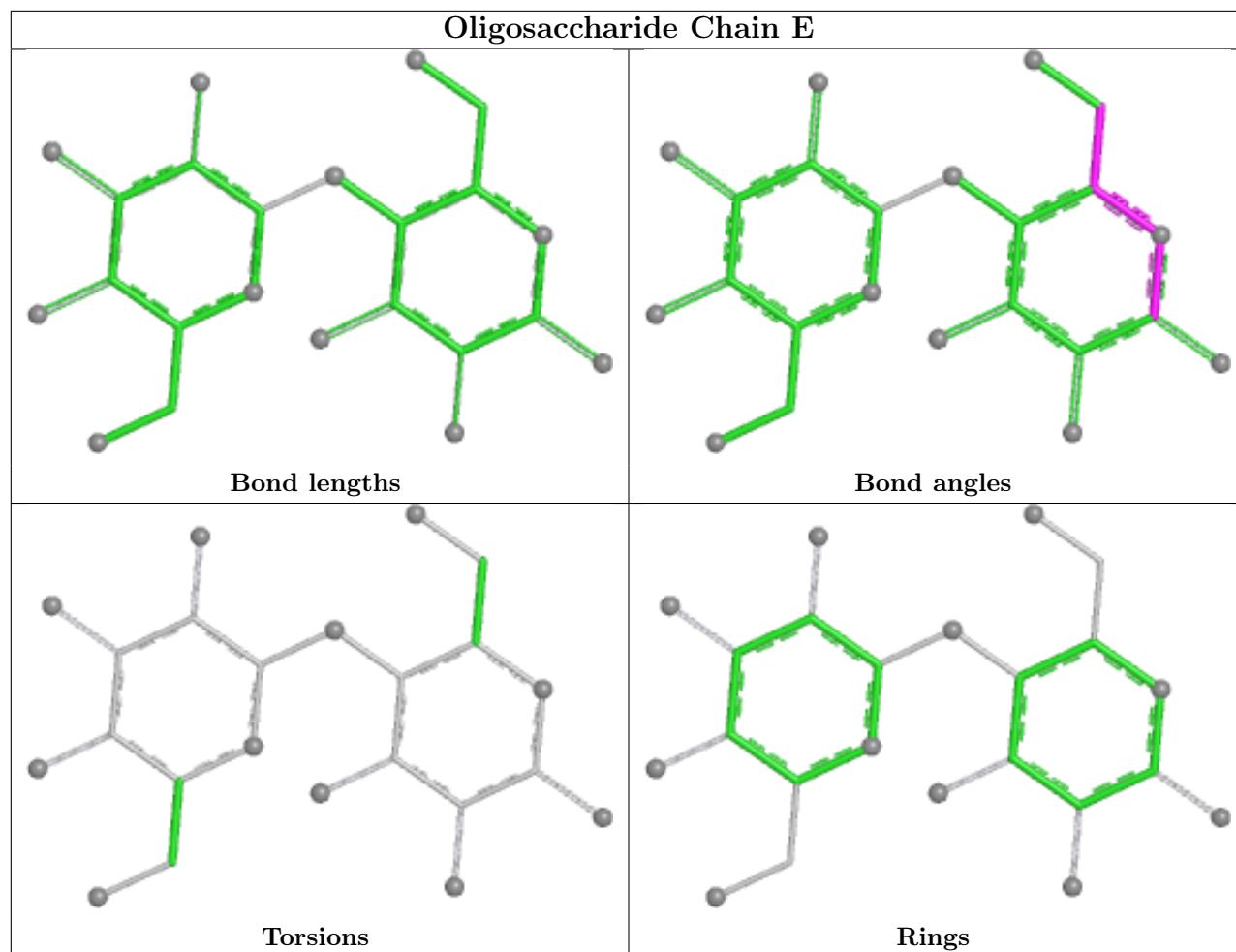
There are no ring outliers.

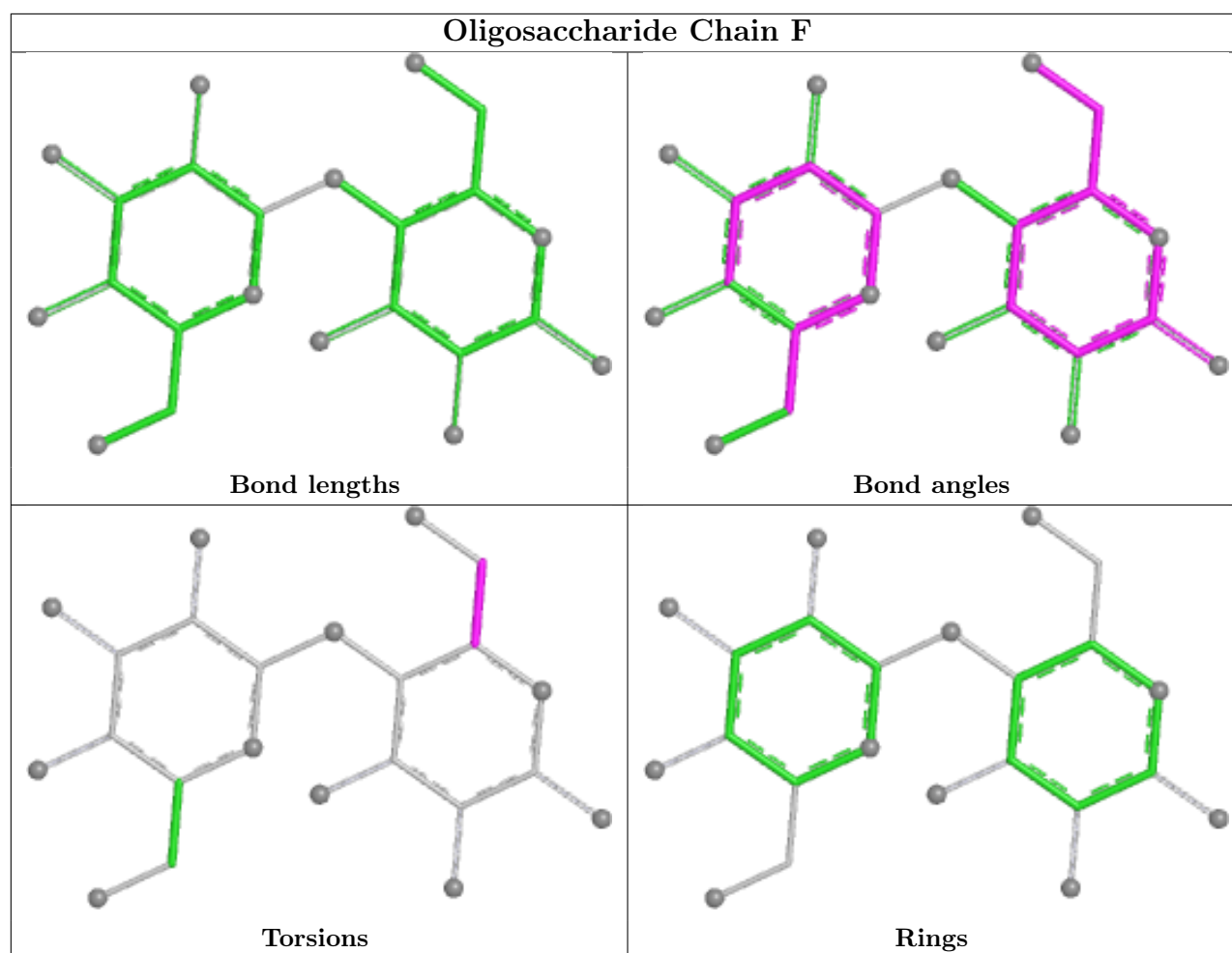
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	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](#)

3 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	PO4	A	461	-	4,4,4	1.69	0	6,6,6	0.46	0
3	PO4	A	460	-	4,4,4	1.74	1 (25%)	6,6,6	0.46	0
3	PO4	A	462	-	4,4,4	1.73	1 (25%)	6,6,6	0.45	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	462	PO4	P-O2	-2.03	1.48	1.54
3	A	460	PO4	P-O3	-2.02	1.48	1.54

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 [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	377/458 (82%)	0.39	21 (5%)	30 32	8, 29, 49, 58	11 (2%)
1	B	379/458 (82%)	0.54	20 (5%)	32 34	8, 32, 56, 66	10 (2%)
1	C	378/458 (82%)	0.93	35 (9%)	14 15	14, 43, 62, 79	9 (2%)
All	All	1134/1374 (82%)	0.62	76 (6%)	24 25	8, 34, 58, 79	30 (2%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	311	PRO	9.7
1	B	312	ALA	9.4
1	C	312	ALA	9.0
1	C	311	PRO	8.4
1	A	311	PRO	8.0
1	B	310	GLY	7.8
1	A	312	ALA	7.6
1	C	161	HIS	7.5
1	A	310	GLY	7.5
1	B	44	ARG	6.6
1	C	136	MET	6.6
1	C	310	GLY	6.3
1	C	368	GLU	5.8
1	C	286	ASN	5.8
1	A	161	HIS	5.6
1	A	286	ASN	5.5
1	C	33	TYR	5.3
1	B	32	THR	5.1
1	B	174	GLU	5.1
1	B	136	MET	5.0
1	B	34	GLN	4.8
1	A	234	GLU	4.8
1	A	136	MET	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	33	TYR	4.5
1	A	108	GLU	4.4
1	A	368	GLU	4.4
1	B	234	GLU	4.4
1	C	182	GLU	4.4
1	B	286	ASN	4.3
1	A	34	GLN	4.2
1	A	182	GLU	3.9
1	C	234	GLU	3.9
1	B	368	GLU	3.7
1	B	117	ILE	3.5
1	C	53	VAL	3.3
1	C	216	THR	3.3
1	A	167	TYR	3.3
1	B	82	TRP	3.3
1	B	119	ILE	3.2
1	C	267	TRP	3.2
1	A	221	GLY	3.1
1	B	410	ASP	2.9
1	A	259	PRO	2.9
1	C	160	THR	2.8
1	C	55	SER	2.7
1	C	256	PHE	2.7
1	A	223	GLY	2.6
1	C	336	TYR	2.5
1	C	171	PHE	2.5
1	C	229	TRP	2.5
1	C	269	TYR	2.5
1	A	222	MET	2.5
1	C	218	ALA	2.4
1	C	34	GLN	2.4
1	A	410	ASP	2.4
1	C	35	THR	2.4
1	C	211	ALA	2.3
1	C	280	VAL	2.3
1	C	285	VAL	2.3
1	C	159	CYS	2.2
1	C	257	THR	2.2
1	C	334	LEU	2.2
1	A	283	TYR	2.2
1	B	188	GLY	2.2
1	B	114	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	130	LEU	2.2
1	C	215	GLY	2.2
1	A	225	PRO	2.2
1	C	212	TYR	2.1
1	C	272	TRP	2.1
1	C	205	VAL	2.1
1	B	118	GLY	2.0
1	C	38	GLY	2.0
1	C	225	PRO	2.0
1	A	271	ALA	2.0
1	A	304	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

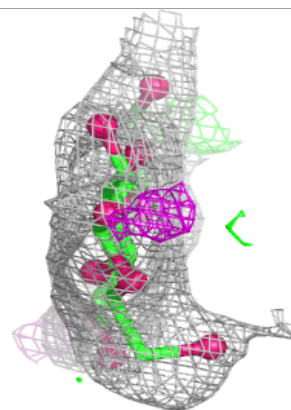
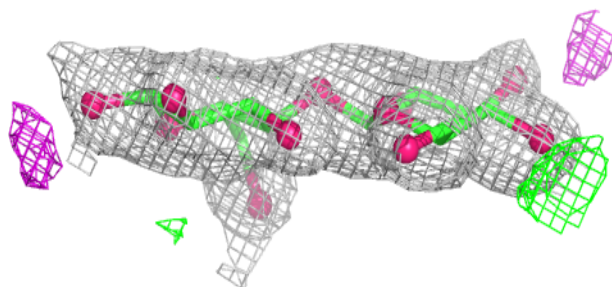
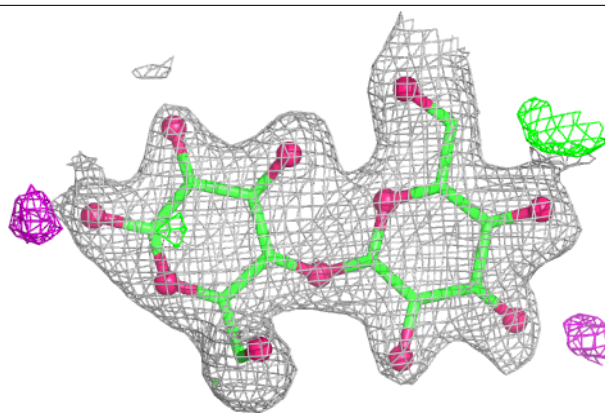
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	D	1	12/12	0.79	0.12	44,50,51,53	0
2	BGC	D	2	11/12	0.82	0.12	46,48,49,49	0
2	BGC	F	1	12/12	0.82	0.12	53,54,54,57	0
2	BGC	E	2	11/12	0.86	0.12	39,40,42,45	0
2	BGC	F	2	11/12	0.86	0.11	51,52,53,53	0
2	BGC	E	1	12/12	0.89	0.12	30,38,42,47	0

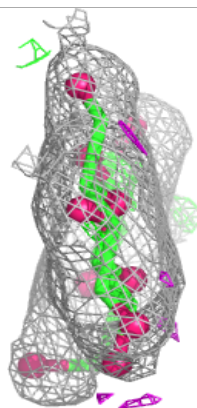
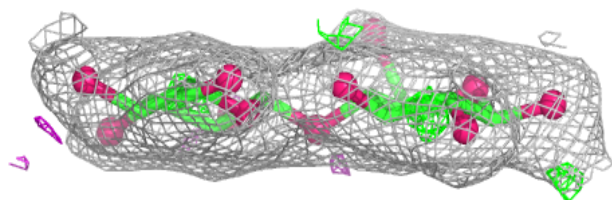
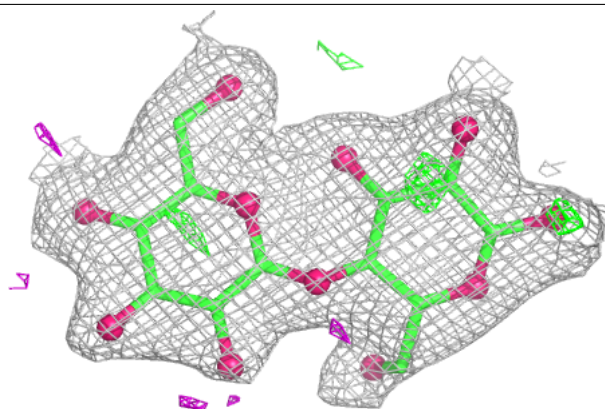
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

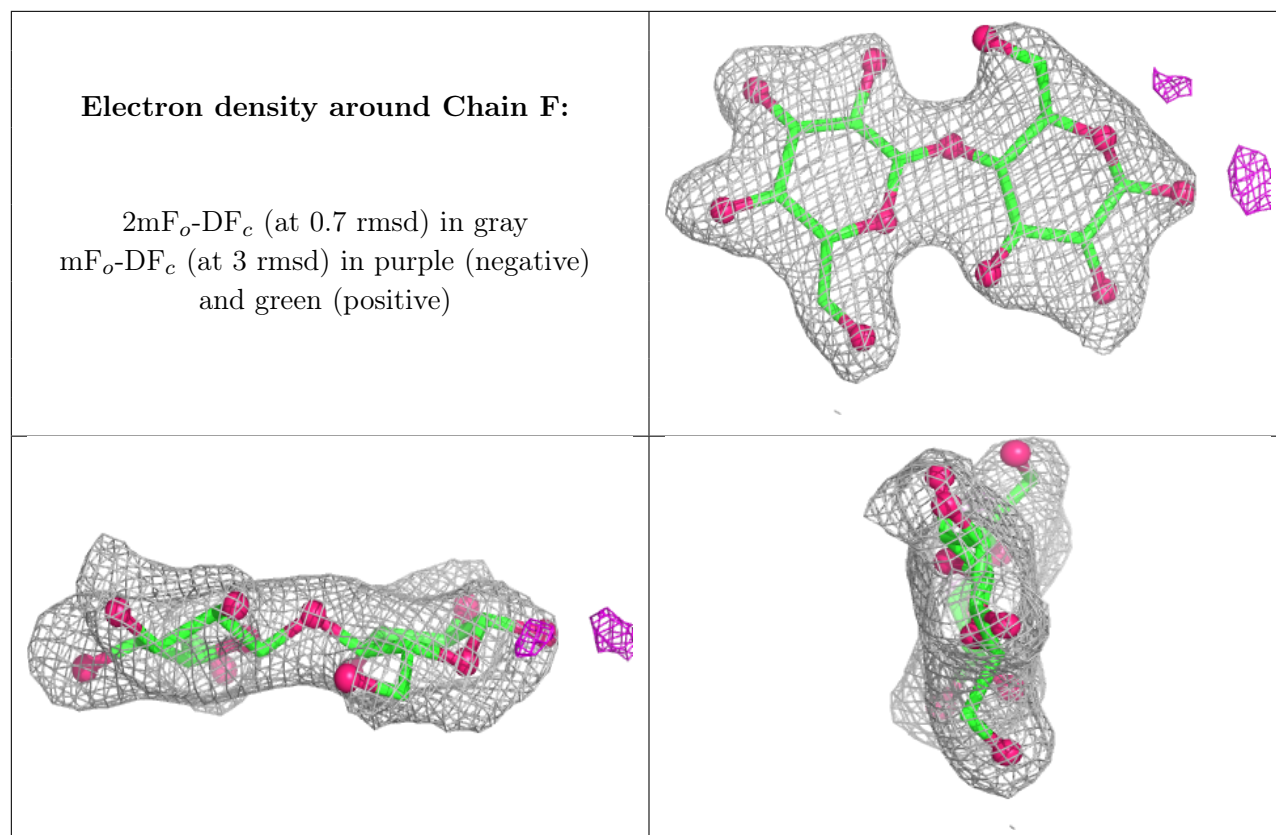
Electron density around Chain D:

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

**Electron density around Chain 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 [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($\text{\AA}^2$)	Q<0.9
3	PO4	A	462	5/5	0.89	0.10	58,59,60,61	0
3	PO4	A	461	5/5	0.94	0.12	45,46,47,48	0
3	PO4	A	460	5/5	0.94	0.08	39,39,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.