



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:35 AM UTC

PDB ID : 2G5B / pdb_00002g5b
Title : Crystal Structure of the anti-Bax monoclonal antibody 6A7 and a Bax peptide.
Authors : Peyerl, F.W.; Dai, S.; Murphy, G.A.; Marrack, P.; Kappler, J.W.
Deposited on : 2006-02-22
Resolution : 2.30 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

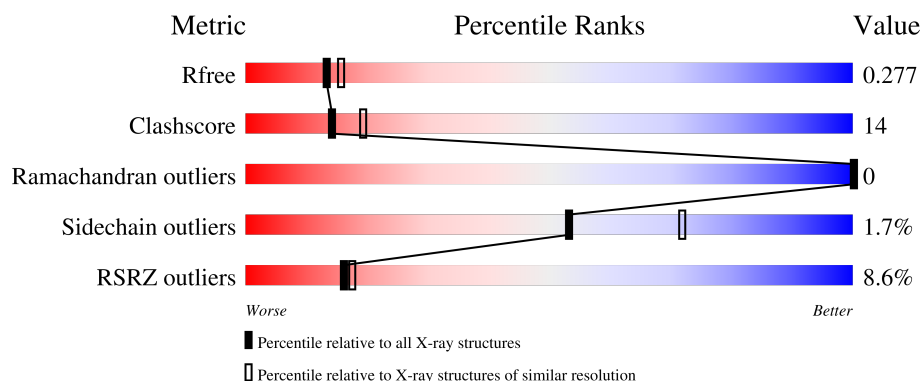
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	217	7% 74% 25% .
1	C	217	16% 77% 22%
1	E	217	6% 76% 24%
1	G	217	6% 78% 21% .
2	B	222	16% 73% 23% ..

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Mol	Chain	Length	Quality of chain
2	D	222	
2	F	222	
2	H	222	
3	I	7	
3	J	7	
3	K	7	
3	L	7	
4	M	3	
4	O	3	
5	N	2	
6	P	3	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14198 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 6A7 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1692	1052	290	343	7			
1	C	217	Total	C	N	O	S	0	0	0
			1692	1052	290	343	7			
1	E	217	Total	C	N	O	S	0	0	0
			1692	1052	290	343	7			
1	G	217	Total	C	N	O	S	0	0	0
			1692	1052	290	343	7			

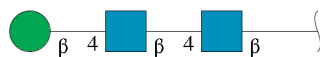
- Molecule 2 is a protein called 6A7 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1654	1050	272	325	7			
2	D	216	Total	C	N	O	S	0	0	0
			1654	1050	272	325	7			
2	F	216	Total	C	N	O	S	0	0	0
			1654	1050	272	325	7			
2	H	216	Total	C	N	O	S	0	0	0
			1654	1050	272	325	7			

- Molecule 3 is a protein called Bax Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	7	Total	C	N	O	0	0	0
			53	31	8	14			
3	J	7	Total	C	N	O	0	0	0
			53	31	8	14			
3	K	7	Total	C	N	O	0	0	0
			53	31	8	14			
3	L	7	Total	C	N	O	0	0	0
			53	31	8	14			

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



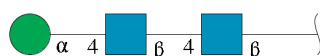
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



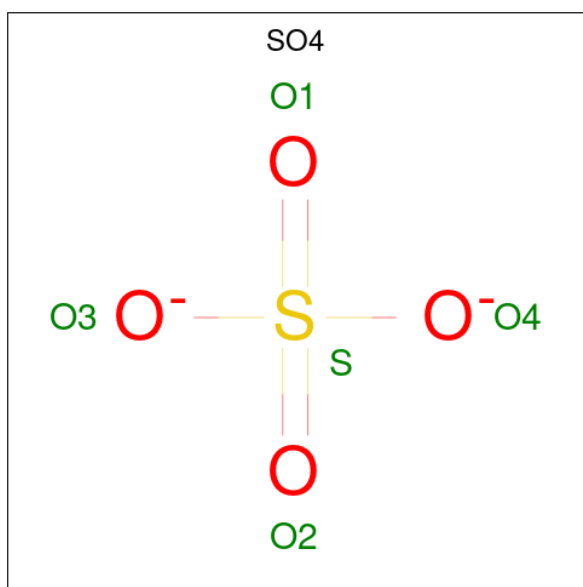
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	P	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	45	Total	O	0	0
			45	45		
8	B	28	Total	O	0	0
			28	28		
8	C	49	Total	O	0	0
			49	49		
8	D	54	Total	O	0	0
			54	54		
8	E	56	Total	O	0	0
			56	56		

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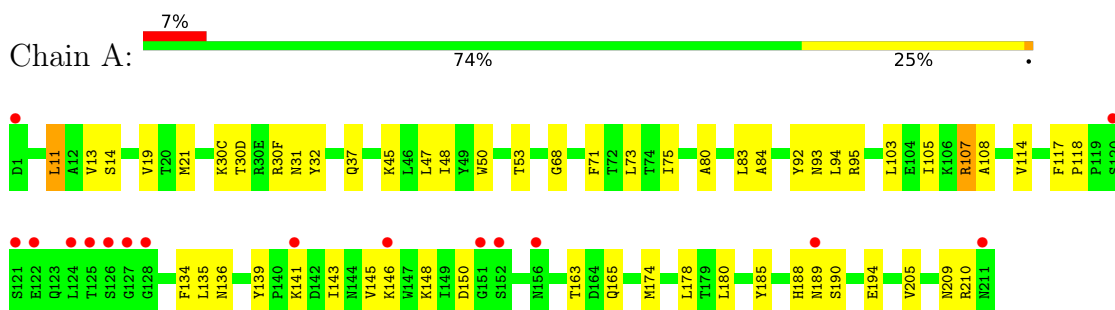
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	57	Total 57	O 57	0	0
8	G	53	Total 53	O 53	0	0
8	H	73	Total 73	O 73	0	0
8	J	3	Total 3	O 3	0	0
8	K	1	Total 1	O 1	0	0
8	L	3	Total 3	O 3	0	0

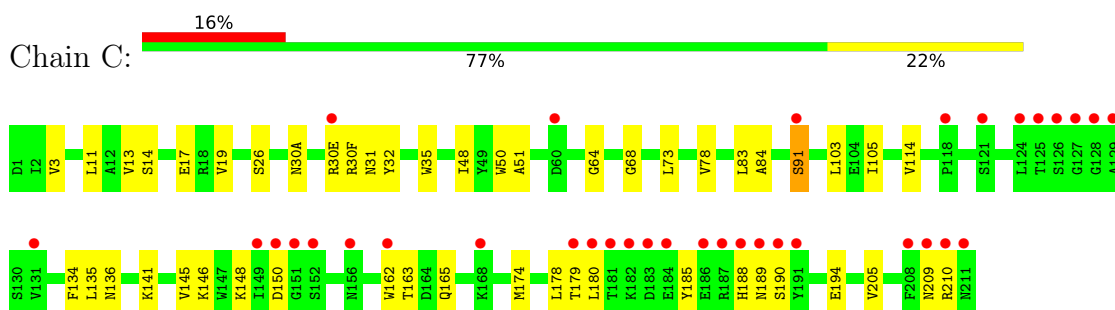
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

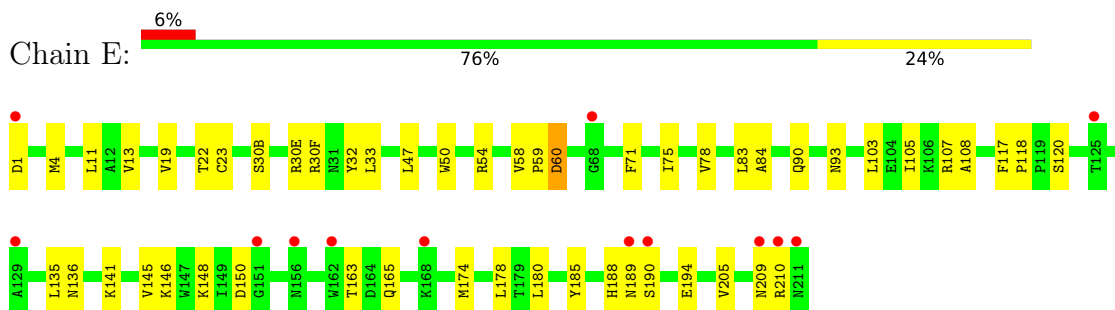
- Molecule 1: 6A7 Fab Light Chain



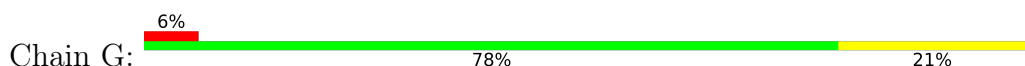
- Molecule 1: 6A7 Fab Light Chain

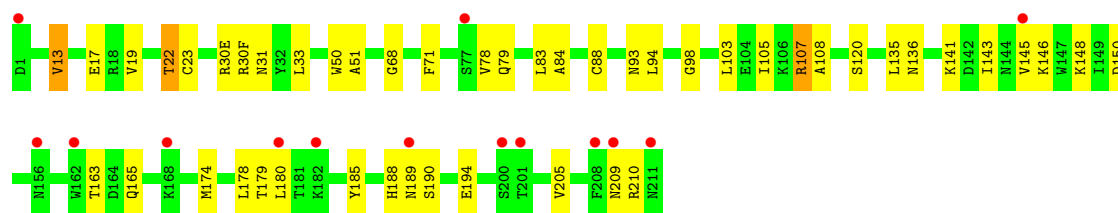


- Molecule 1: 6A7 Fab Light Chain

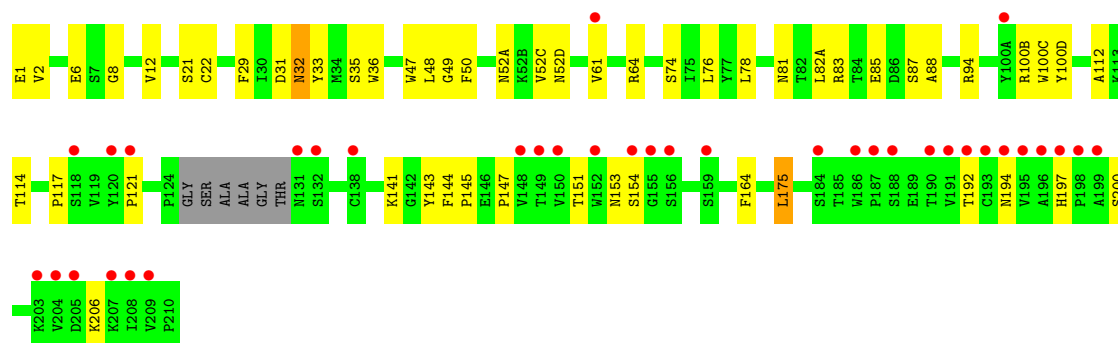
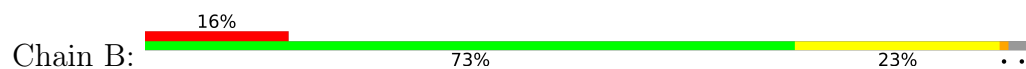


- Molecule 1: 6A7 Fab Light Chain

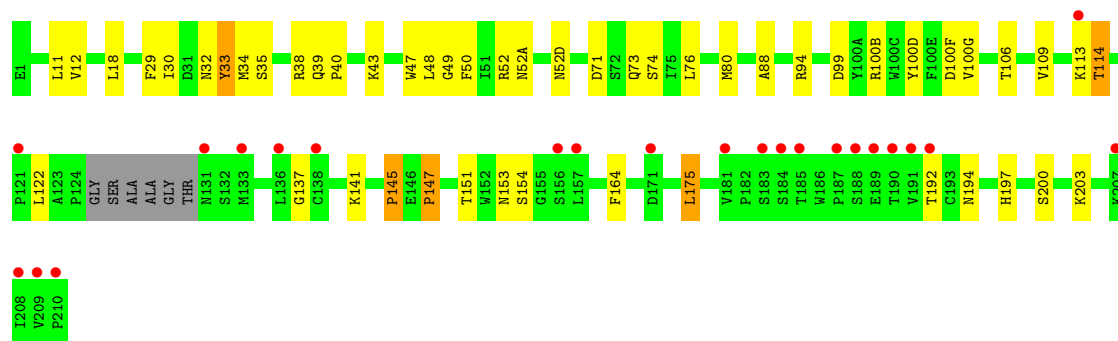
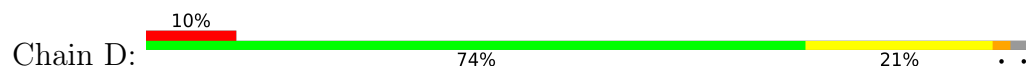




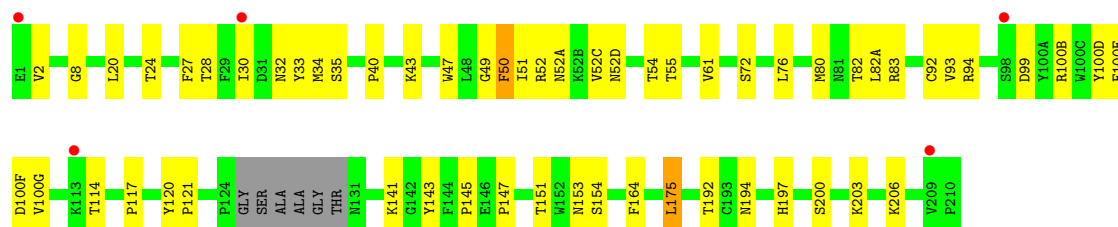
• Molecule 2: 6A7 Fab Heavy Chain



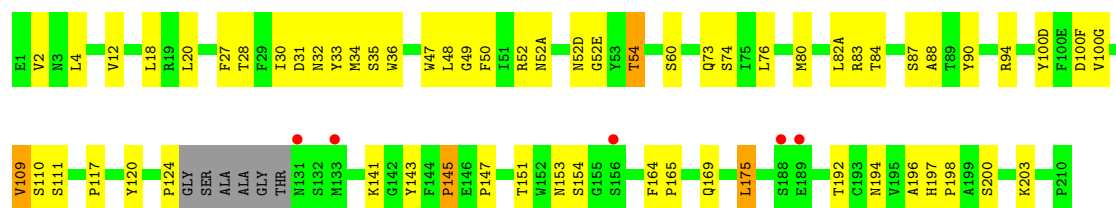
• Molecule 2: 6A7 Fab Heavy Chain



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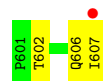
- Molecule 3: Bax Peptide



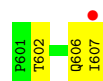
- Molecule 3: Bax Peptide



- Molecule 3: Bax Peptide



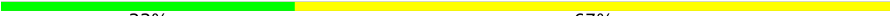
- Molecule 3: Bax Peptide



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  33% 67%

NAG1
NAG2
BGL3

- Molecule 5: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%

NAG1
BGL2

- Molecule 6: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

NAG1
NAG2
MAN3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	166.53Å 183.90Å 67.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.30) 99.5 (20.00-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.275 0.235 , 0.277	Depositor DCC
R_{free} test set	4616 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14198	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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: NDG, MAN, BMA, NAG, 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	0.36	0/1728	0.86	3/2340 (0.1%)
1	C	0.37	0/1728	0.85	3/2340 (0.1%)
1	E	0.37	0/1728	0.86	2/2340 (0.1%)
1	G	0.38	0/1728	0.86	5/2340 (0.2%)
2	B	0.39	0/1699	0.88	3/2324 (0.1%)
2	D	0.41	0/1699	0.91	3/2324 (0.1%)
2	F	0.41	0/1699	0.91	4/2324 (0.2%)
2	H	0.44	0/1699	0.93	6/2324 (0.3%)
3	I	0.49	0/53	0.96	0/69
3	J	0.53	0/53	1.01	0/69
3	K	0.48	0/53	0.99	0/69
3	L	0.51	0/53	1.00	0/69
All	All	0.39	0/13920	0.89	29/18932 (0.2%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	32	ASN	N-CA-C	8.99	124.36	110.42
2	H	32	ASN	N-CA-C	8.05	123.14	110.17
2	H	33	TYR	N-CA-C	-8.05	97.52	110.32
2	D	33	TYR	N-CA-C	-7.95	97.69	110.32
2	B	33	TYR	N-CA-C	-7.87	97.81	110.32
2	D	32	ASN	N-CA-C	7.58	121.88	110.14
2	F	33	TYR	N-CA-C	-7.56	97.26	109.96
2	B	32	ASN	N-CA-C	7.05	121.34	110.42
2	H	60	SER	N-CA-C	7.01	121.49	113.15
1	E	136	ASN	N-CA-C	6.44	120.53	110.17
1	G	136	ASN	N-CA-C	6.41	120.48	110.17
1	C	136	ASN	N-CA-C	6.30	120.32	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASN	N-CA-C	6.24	120.22	110.17
1	G	141	LYS	N-CA-C	6.08	118.70	111.71
1	E	141	LYS	N-CA-C	6.04	118.65	111.71
1	C	141	LYS	N-CA-C	5.97	118.58	111.71
1	A	141	LYS	N-CA-C	5.94	118.54	111.71
1	G	98	GLY	N-CA-C	-5.81	103.72	112.60
2	B	141	LYS	N-CA-C	5.64	118.92	109.95
2	F	61	VAL	N-CA-C	5.61	117.59	112.43
1	G	88	CYS	N-CA-C	-5.59	101.75	110.42
2	F	141	LYS	N-CA-C	5.54	118.75	109.95
1	A	92	TYR	N-CA-C	-5.51	104.91	111.03
2	D	141	LYS	N-CA-C	5.47	118.64	109.95
2	H	141	LYS	N-CA-C	5.45	118.61	109.95
2	H	36	TRP	N-CA-C	-5.41	100.58	109.40
2	H	52(E)	GLY	N-CA-C	5.36	122.75	115.30
1	G	22	THR	N-CA-C	5.14	117.94	109.72
1	C	78	VAL	N-CA-C	5.03	116.71	109.51

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	1692	0	1638	57	0
1	C	1692	0	1638	45	0
1	E	1692	0	1638	45	0
1	G	1692	0	1638	36	0
2	B	1654	0	1602	47	0
2	D	1654	0	1602	51	0
2	F	1654	0	1602	57	0
2	H	1654	0	1602	52	0
3	I	53	0	49	12	0
3	J	53	0	49	10	0
3	K	53	0	49	10	0
3	L	53	0	49	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	39	0	34	4	0
4	O	39	0	34	1	0
5	N	28	0	24	0	0
6	P	39	0	34	4	0
7	A	10	0	0	0	0
7	C	10	0	0	0	0
7	E	10	0	0	0	0
7	G	5	0	0	0	0
8	A	45	0	0	1	0
8	B	28	0	0	1	0
8	C	49	0	0	2	0
8	D	54	0	0	0	0
8	E	56	0	0	1	0
8	F	57	0	0	1	0
8	G	53	0	0	0	0
8	H	73	0	0	3	0
8	J	3	0	0	1	0
8	K	1	0	0	0	0
8	L	3	0	0	0	0
All	All	14198	0	13282	384	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 14.

All (384) 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)
2:D:154:SER:H	2:D:194:ASN:HD21	1.07	1.00
2:F:30:ILE:HD11	2:H:196:ALA:HB1	1.44	0.99
2:D:52(A):ASN:HD21	3:J:607:ILE:HG23	1.29	0.98
2:F:154:SER:H	2:F:194:ASN:HD21	1.09	0.97
6:P:2:NAG:H62	6:P:3:MAN:H2	1.48	0.96
2:F:52(A):ASN:HD21	3:K:607:ILE:HG23	1.31	0.95
1:C:105:ILE:H	1:C:165:GLN:HE22	1.14	0.94
2:H:154:SER:H	2:H:194:ASN:HD21	1.09	0.93
2:B:154:SER:H	2:B:194:ASN:HD21	1.08	0.92
2:H:52:ARG:HD2	2:H:54:THR:HG23	1.50	0.92
1:A:93:ASN:HD22	3:I:602:THR:H	1.18	0.91
1:G:105:ILE:H	1:G:165:GLN:HE22	1.14	0.90
2:D:52(A):ASN:HD21	3:J:607:ILE:CG2	1.89	0.86
2:F:93:VAL:HG11	2:F:100(E):PHE:HB3	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ILE:H	1:A:165:GLN:HE22	1.20	0.85
2:H:52(A):ASN:HD21	3:L:607:ILE:HG23	1.40	0.85
2:D:153:ASN:ND2	2:D:192:THR:H	1.79	0.81
2:H:153:ASN:ND2	2:H:192:THR:H	1.78	0.81
2:B:153:ASN:ND2	2:B:192:THR:H	1.79	0.81
2:F:153:ASN:ND2	2:F:192:THR:H	1.80	0.79
2:D:154:SER:H	2:D:194:ASN:ND2	1.80	0.78
2:F:154:SER:H	2:F:194:ASN:ND2	1.81	0.78
1:E:105:ILE:H	1:E:165:GLN:HE22	1.29	0.78
3:I:606:GLN:O	3:I:607:ILE:HG22	1.84	0.77
2:B:154:SER:H	2:B:194:ASN:ND2	1.81	0.77
1:A:30(F):ARG:HH11	1:A:30(F):ARG:HG2	1.49	0.77
1:A:31:ASN:ND2	1:A:68:GLY:H	1.83	0.76
2:H:154:SER:H	2:H:194:ASN:ND2	1.82	0.76
3:J:606:GLN:O	3:J:607:ILE:HG22	1.85	0.76
3:K:606:GLN:O	3:K:607:ILE:HG22	1.85	0.76
1:C:11:LEU:HD11	1:C:19:VAL:HG13	1.68	0.75
1:C:105:ILE:N	1:C:165:GLN:HE22	1.84	0.75
2:F:52:ARG:HD2	2:F:54:THR:HG23	1.67	0.75
3:L:606:GLN:O	3:L:607:ILE:HG22	1.87	0.75
2:F:52(A):ASN:HD21	3:K:607:ILE:CG2	2.00	0.75
2:H:153:ASN:HD21	2:H:192:THR:H	1.35	0.74
2:H:52:ARG:HD2	2:H:54:THR:CG2	2.17	0.74
2:F:52:ARG:HD2	2:F:54:THR:CG2	2.17	0.74
1:G:150:ASP:HA	1:G:190:SER:HB3	1.70	0.73
2:F:153:ASN:HD21	2:F:192:THR:H	1.37	0.73
2:D:153:ASN:HD21	2:D:192:THR:H	1.36	0.73
1:E:150:ASP:HA	1:E:190:SER:HB3	1.70	0.73
1:A:80:ALA:O	1:A:105:ILE:HD11	1.87	0.73
1:E:13:VAL:HG21	1:E:19:VAL:HG22	1.71	0.72
1:C:30(F):ARG:HG2	1:C:30(F):ARG:HH11	1.54	0.72
2:F:52:ARG:HH11	2:F:54:THR:HG23	1.54	0.72
1:A:93:ASN:ND2	3:I:602:THR:H	1.87	0.72
1:A:150:ASP:HA	1:A:190:SER:HB3	1.71	0.72
1:E:93:ASN:HD22	3:K:602:THR:H	1.38	0.71
2:F:30:ILE:HD11	2:H:196:ALA:CB	2.18	0.71
2:B:52(A):ASN:HD21	3:I:607:ILE:HG23	1.54	0.71
2:B:153:ASN:HD21	2:B:192:THR:H	1.36	0.71
1:A:188:HIS:O	1:A:210:ARG:HD3	1.91	0.70
1:G:30(F):ARG:HD3	1:G:50:TRP:CE2	2.26	0.70
1:C:188:HIS:O	1:C:210:ARG:HD3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ASP:HA	1:C:190:SER:HB3	1.71	0.70
2:F:117:PRO:HB3	2:F:143:TYR:HB3	1.72	0.70
2:B:35:SER:OG	2:B:50:PHE:HB3	1.92	0.70
1:G:93:ASN:HD22	3:L:602:THR:H	1.40	0.69
2:B:8:GLY:H	2:D:73:GLN:NE2	1.92	0.68
1:C:105:ILE:H	1:C:165:GLN:NE2	1.90	0.68
1:E:188:HIS:O	1:E:210:ARG:HD3	1.94	0.67
1:G:188:HIS:O	1:G:210:ARG:HD3	1.94	0.67
2:H:52(A):ASN:HD21	3:L:607:ILE:CG2	2.08	0.66
1:G:107:ARG:HD3	1:G:108:ALA:O	1.95	0.66
1:A:19:VAL:HG22	1:A:75:ILE:HB	1.77	0.66
2:B:32:ASN:ND2	4:M:1:NAG:H81	2.11	0.65
2:F:52(D):ASN:HD21	3:K:607:ILE:HG22	1.61	0.64
1:A:30(F):ARG:HD3	1:A:50:TRP:CE2	2.33	0.63
6:P:2:NAG:C6	6:P:3:MAN:H2	2.26	0.63
2:B:175:LEU:C	2:B:175:LEU:HD12	2.23	0.63
2:B:32:ASN:HD21	4:M:1:NAG:H81	1.62	0.63
1:E:194:GLU:HG2	1:E:205:VAL:HG22	1.80	0.63
1:A:194:GLU:HG2	1:A:205:VAL:HG22	1.80	0.63
2:D:52(D):ASN:HD21	3:J:607:ILE:HG22	1.64	0.63
1:A:30(F):ARG:HG2	1:A:30(F):ARG:NH1	2.11	0.62
2:B:12:VAL:HG11	2:B:82(A):LEU:HD13	1.82	0.62
2:F:203:LYS:HE2	2:H:31:ASP:OD1	1.99	0.62
1:A:107:ARG:HD3	1:A:108:ALA:O	1.99	0.62
2:D:154:SER:N	2:D:194:ASN:HD21	1.89	0.61
2:F:47:TRP:CZ2	2:F:49:GLY:HA2	2.35	0.61
2:D:175:LEU:HD12	2:D:175:LEU:C	2.26	0.61
1:E:30(E):ARG:C	1:E:30(F):ARG:HG2	2.25	0.61
1:E:135:LEU:HD21	1:E:145:VAL:HG22	1.83	0.61
2:B:154:SER:N	2:B:194:ASN:HD21	1.91	0.61
1:G:194:GLU:HG2	1:G:205:VAL:HG22	1.82	0.61
1:C:30(E):ARG:HG3	1:C:30(E):ARG:HH11	1.66	0.61
2:D:11:LEU:HD23	2:D:114:THR:HG22	1.82	0.60
2:F:175:LEU:HD12	2:F:175:LEU:C	2.26	0.60
2:B:8:GLY:H	2:D:73:GLN:HE22	1.48	0.60
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.37	0.60
2:H:175:LEU:C	2:H:175:LEU:HD12	2.26	0.60
1:A:135:LEU:HD21	1:A:145:VAL:HG22	1.83	0.60
1:A:30(F):ARG:HD3	1:A:50:TRP:CD2	2.37	0.60
1:C:194:GLU:HG2	1:C:205:VAL:HG22	1.84	0.59
2:H:12:VAL:O	2:H:109:VAL:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52(A):ASN:HD21	3:I:607:ILE:CG2	2.14	0.59
1:A:19:VAL:CG2	1:A:75:ILE:HB	2.33	0.59
1:C:135:LEU:HD21	1:C:145:VAL:HG22	1.85	0.59
1:G:120:SER:OG	2:H:120:TYR:HB3	2.02	0.59
2:D:52(A):ASN:ND2	3:J:607:ILE:HG23	2.10	0.59
1:C:31:ASN:ND2	1:C:68:GLY:H	2.01	0.58
2:D:106:THR:HG21	2:D:147:PRO:HD3	1.84	0.58
2:D:145:PRO:O	2:D:197:HIS:HE1	1.87	0.58
2:B:112:ALA:HB3	2:B:144:PHE:CE2	2.39	0.58
2:H:4:LEU:HD11	2:H:100(G):VAL:HG23	1.85	0.57
2:H:94:ARG:HB3	2:H:100(G):VAL:HG22	1.85	0.57
1:C:30(F):ARG:HD3	1:C:50:TRP:CE2	2.40	0.57
2:F:50:PHE:CD1	2:F:50:PHE:C	2.83	0.57
1:G:135:LEU:HD21	1:G:145:VAL:HG22	1.86	0.57
2:F:154:SER:N	2:F:194:ASN:HD21	1.91	0.57
2:F:100(D):TYR:CE2	2:F:100(F):ASP:HB3	2.40	0.56
1:E:54:ARG:NH1	1:E:54:ARG:HB2	2.20	0.56
1:A:30(D):THR:HG21	1:A:32:TYR:OH	2.05	0.56
1:G:145:VAL:CG2	1:G:174:MET:HE1	2.36	0.56
1:A:45:LYS:HD2	8:A:747:HOH:O	2.04	0.56
1:C:30(F):ARG:HG2	1:C:30(F):ARG:NH1	2.19	0.56
2:B:1:GLU:HG2	2:B:2:VAL:N	2.21	0.56
2:B:145:PRO:O	2:B:197:HIS:HE1	1.88	0.56
1:A:145:VAL:CG2	1:A:174:MET:HE1	2.36	0.56
2:D:52(D):ASN:ND2	3:J:607:ILE:HG22	2.20	0.56
2:H:145:PRO:O	2:H:197:HIS:HE1	1.89	0.56
2:F:145:PRO:O	2:F:197:HIS:HE1	1.89	0.55
2:D:30:ILE:HG22	2:D:71:ASP:HB3	1.88	0.55
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.42	0.55
1:E:11:LEU:HD11	1:E:19:VAL:HG13	1.88	0.55
2:B:31:ASP:OD1	2:D:203:LYS:HE2	2.07	0.55
2:F:8:GLY:H	2:H:73:GLN:NE2	2.04	0.55
1:E:145:VAL:CG2	1:E:174:MET:HE1	2.36	0.55
1:C:30(F):ARG:HD3	1:C:50:TRP:CD2	2.42	0.55
2:H:12:VAL:HG11	2:H:82(A):LEU:HD13	1.89	0.55
2:F:28:THR:HG22	2:F:30:ILE:HG13	1.89	0.55
2:F:151:THR:OG1	2:F:194:ASN:HB2	2.06	0.55
1:A:93:ASN:HD22	3:I:602:THR:N	1.97	0.54
2:D:50:PHE:CD1	2:D:50:PHE:C	2.85	0.54
1:A:31:ASN:HD21	1:A:68:GLY:H	1.52	0.54
2:H:52(D):ASN:HD21	3:L:607:ILE:HG22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ASN:HD21	1:C:68:GLY:H	1.56	0.54
2:B:151:THR:OG1	2:B:194:ASN:HB2	2.08	0.54
2:B:32:ASN:HD21	4:M:1:NAG:C8	2.21	0.53
1:A:80:ALA:HA	1:A:105:ILE:HD13	1.90	0.53
2:B:48:LEU:HD22	2:B:61:VAL:HG11	1.90	0.53
1:C:145:VAL:CG2	1:C:174:MET:HE1	2.38	0.53
6:P:2:NAG:H62	6:P:3:MAN:C2	2.32	0.53
1:C:11:LEU:HD11	1:C:19:VAL:CG1	2.38	0.53
2:B:29:PHE:CD2	2:B:74:SER:HA	2.44	0.53
2:D:151:THR:OG1	2:D:194:ASN:HB2	2.09	0.53
1:C:185:TYR:O	1:C:210:ARG:HD2	2.09	0.53
2:H:151:THR:OG1	2:H:194:ASN:HB2	2.09	0.53
1:C:162:TRP:HE3	8:C:713:HOH:O	1.91	0.52
2:B:117:PRO:HB3	2:B:143:TYR:HB3	1.92	0.52
1:E:185:TYR:O	1:E:210:ARG:HD2	2.09	0.52
1:A:105:ILE:N	1:A:165:GLN:HE22	2.00	0.52
2:D:100(D):TYR:CE2	2:D:100(F):ASP:HB3	2.45	0.52
2:F:93:VAL:HG11	2:F:100(E):PHE:CB	2.32	0.52
1:A:185:TYR:O	1:A:210:ARG:HD2	2.10	0.52
2:B:121:PRO:HD3	2:B:206:LYS:HE2	1.91	0.52
1:G:163:THR:HG23	2:H:164:PHE:CD1	2.44	0.52
2:H:50:PHE:CD1	2:H:50:PHE:C	2.87	0.52
2:H:154:SER:N	2:H:194:ASN:HD21	1.92	0.52
1:C:163:THR:HG23	2:D:164:PHE:CD1	2.45	0.52
2:F:40:PRO:HB2	2:F:43:LYS:HD3	1.92	0.52
2:H:52(D):ASN:ND2	3:L:607:ILE:HG22	2.25	0.52
1:E:75:ILE:CG2	1:E:78:VAL:HG12	2.40	0.51
1:G:146:LYS:HD2	1:G:148:LYS:HE3	1.93	0.51
2:D:12:VAL:O	2:D:109:VAL:HA	2.10	0.51
2:B:50:PHE:CD1	2:B:50:PHE:C	2.89	0.51
2:D:33:TYR:CE2	2:D:52:ARG:HG2	2.45	0.51
1:C:91:SER:HB2	8:C:706:HOH:O	2.09	0.51
1:E:54:ARG:HB2	1:E:54:ARG:HH11	1.75	0.51
2:F:50:PHE:C	2:F:50:PHE:HD1	2.19	0.51
1:G:13:VAL:HG13	1:G:17:GLU:HB2	1.92	0.51
2:D:113:LYS:NZ	2:D:114:THR:HG23	2.26	0.51
2:D:35:SER:OG	2:D:50:PHE:HB3	2.11	0.51
1:E:83:LEU:C	1:E:83:LEU:HD23	2.36	0.51
2:F:99:ASP:OD1	2:F:100(B):ARG:NH1	2.44	0.51
1:A:146:LYS:HD2	1:A:148:LYS:HE3	1.93	0.51
2:B:22:CYS:HB3	2:B:76:LEU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:52(D):ASN:ND2	3:K:607:ILE:HG22	2.25	0.51
2:B:83:ARG:HB2	2:B:85:GLU:HG2	1.93	0.51
2:F:20:LEU:HG	2:F:80:MET:HE2	1.93	0.50
1:E:146:LYS:HD2	1:E:148:LYS:HE3	1.92	0.50
1:A:30(C):LYS:NZ	1:A:30(C):LYS:HB3	2.25	0.50
1:G:185:TYR:O	1:G:210:ARG:HD2	2.11	0.50
2:H:169:GLN:HB3	8:H:663:HOH:O	2.12	0.50
2:F:100(D):TYR:HE2	2:F:100(F):ASP:HB3	1.77	0.50
1:G:78:VAL:HG12	1:G:79:GLN:N	2.27	0.50
1:C:146:LYS:HD2	1:C:148:LYS:HE3	1.92	0.49
2:D:122:LEU:HB2	2:D:137:GLY:C	2.37	0.49
1:E:107:ARG:HG3	1:E:107:ARG:HH11	1.76	0.49
2:F:93:VAL:CG1	2:F:100(E):PHE:HB3	2.36	0.49
2:F:34:MET:HB3	2:F:76:LEU:HD22	1.94	0.49
2:F:94:ARG:CZ	4:O:1:NAG:H83	2.42	0.49
1:G:30(E):ARG:C	1:G:30(F):ARG:HG2	2.37	0.49
2:F:72:SER:HA	2:H:198:PRO:O	2.12	0.49
2:B:36:TRP:CE2	2:B:78:LEU:HB2	2.47	0.49
1:A:163:THR:HG23	2:B:164:PHE:CD1	2.48	0.49
2:H:28:THR:HG22	2:H:30:ILE:HG22	1.95	0.49
2:H:197:HIS:HD2	2:H:200:SER:OG	1.95	0.48
1:A:11:LEU:HD12	1:A:11:LEU:O	2.13	0.48
2:B:32:ASN:ND2	4:M:1:NAG:C8	2.76	0.48
2:D:40:PRO:HB2	2:D:43:LYS:HG3	1.95	0.48
2:H:83:ARG:O	2:H:109:VAL:HG11	2.13	0.48
1:A:93:ASN:ND2	3:I:601:PRO:HA	2.28	0.48
2:D:39:GLN:C	2:D:88:ALA:HB1	2.39	0.48
1:E:105:ILE:N	1:E:165:GLN:HE22	2.05	0.48
2:H:100(D):TYR:HE1	2:H:100(F):ASP:HB3	1.78	0.48
2:D:99:ASP:OD1	2:D:100(B):ARG:NH1	2.47	0.48
2:F:117:PRO:CB	2:F:143:TYR:HB3	2.43	0.48
1:G:145:VAL:HG21	1:G:174:MET:HE1	1.96	0.47
1:C:83:LEU:O	1:C:84:ALA:HB2	2.15	0.47
1:A:93:ASN:O	1:A:94:LEU:HB2	2.15	0.47
1:E:22:THR:HG22	1:E:23:CYS:N	2.31	0.47
1:E:33:LEU:HG	1:E:71:PHE:CG	2.50	0.47
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.50	0.47
2:B:32:ASN:ND2	2:B:94:ARG:HD2	2.30	0.46
1:C:103:LEU:HD23	1:C:103:LEU:C	2.40	0.46
2:B:154:SER:N	2:B:194:ASN:ND2	2.58	0.46
2:D:154:SER:N	2:D:194:ASN:ND2	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:THR:HG23	2:F:164:PHE:CD1	2.50	0.46
2:D:197:HIS:HD2	2:D:200:SER:OG	1.98	0.46
2:F:24:THR:HB	2:F:27:PHE:HE1	1.80	0.46
1:E:145:VAL:HG21	1:E:174:MET:CE	2.46	0.46
1:A:189:ASN:O	1:A:209:ASN:HA	2.16	0.46
1:E:145:VAL:HG21	1:E:174:MET:HE1	1.98	0.46
1:G:31:ASN:ND2	1:G:68:GLY:H	2.13	0.46
1:G:150:ASP:OD2	1:G:188:HIS:HB3	2.16	0.46
1:E:107:ARG:HG3	1:E:108:ALA:O	2.15	0.46
2:F:154:SER:N	2:F:194:ASN:ND2	2.58	0.46
1:A:145:VAL:HG21	1:A:174:MET:HE1	1.98	0.46
1:C:178:LEU:HG	1:C:180:LEU:HD13	1.98	0.46
1:E:189:ASN:O	1:E:209:ASN:HA	2.16	0.46
2:F:52:ARG:CD	2:F:54:THR:HG23	2.42	0.46
1:A:145:VAL:HG21	1:A:174:MET:CE	2.46	0.45
1:C:189:ASN:O	1:C:209:ASN:HA	2.16	0.45
1:E:30(F):ARG:HD3	1:E:50:TRP:CE2	2.51	0.45
1:E:150:ASP:OD2	1:E:188:HIS:HB3	2.17	0.45
2:F:30:ILE:HD12	2:H:203:LYS:HB2	1.97	0.45
2:H:35:SER:OG	2:H:50:PHE:HB3	2.16	0.45
2:H:18:LEU:HB3	2:H:80:MET:HE3	1.98	0.45
2:H:84:THR:HG22	8:H:634:HOH:O	2.16	0.45
2:F:35:SER:OG	2:F:50:PHE:HB3	2.16	0.45
1:G:83:LEU:O	1:G:84:ALA:HB2	2.17	0.45
1:G:145:VAL:HG21	1:G:174:MET:CE	2.46	0.45
1:G:178:LEU:HG	1:G:180:LEU:HD13	1.98	0.45
1:A:178:LEU:HG	1:A:180:LEU:HD13	1.99	0.45
1:E:117:PHE:HA	1:E:118:PRO:HD3	1.84	0.45
2:F:80:MET:HB3	2:F:82(A):LEU:HD21	1.98	0.45
2:D:11:LEU:HD23	2:D:114:THR:CG2	2.47	0.45
1:E:120:SER:OG	2:F:120:TYR:HB3	2.17	0.45
2:F:197:HIS:HD2	2:F:200:SER:OG	1.99	0.45
1:G:31:ASN:HD21	1:G:68:GLY:H	1.64	0.45
1:A:150:ASP:OD2	1:A:188:HIS:HB3	2.17	0.45
1:C:13:VAL:HG22	1:C:14:SER:N	2.31	0.45
1:C:150:ASP:OD2	1:C:188:HIS:HB3	2.16	0.45
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.52	0.45
2:F:52(D):ASN:ND2	3:K:607:ILE:CG2	2.80	0.45
2:F:153:ASN:HD21	2:F:192:THR:N	2.11	0.45
2:H:73:GLN:O	2:H:74:SER:HB2	2.16	0.45
1:A:83:LEU:O	1:A:84:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:ARG:CD	2:D:48:LEU:HD21	2.47	0.44
2:F:121:PRO:HD3	2:F:206:LYS:HE2	1.99	0.44
1:G:33:LEU:C	1:G:33:LEU:HD13	2.42	0.44
2:H:20:LEU:HG	2:H:80:MET:HE2	2.00	0.44
2:H:48:LEU:HD11	2:H:90:TYR:CE2	2.52	0.44
2:H:52:ARG:CD	2:H:54:THR:HG23	2.33	0.44
1:A:30(C):LYS:HE3	3:I:604:SER:HB3	1.98	0.44
2:B:64:ARG:HG2	2:B:81:ASN:O	2.18	0.44
2:B:175:LEU:C	2:B:175:LEU:CD1	2.91	0.44
2:H:100(D):TYR:CE1	2:H:100(F):ASP:HB3	2.52	0.44
1:G:189:ASN:O	1:G:209:ASN:HA	2.17	0.44
1:E:54:ARG:HD2	1:E:59:PRO:O	2.18	0.44
2:F:2:VAL:HG13	2:F:27:PHE:CD1	2.52	0.44
2:B:12:VAL:CG1	2:B:82(A):LEU:HD13	2.48	0.44
1:C:145:VAL:HG21	1:C:174:MET:CE	2.48	0.44
2:H:153:ASN:HD21	2:H:192:THR:N	2.09	0.44
2:F:93:VAL:HG13	2:F:100(G):VAL:O	2.18	0.44
1:G:135:LEU:N	1:G:135:LEU:HD12	2.33	0.44
3:K:606:GLN:O	3:K:607:ILE:CG2	2.63	0.44
1:A:11:LEU:HD12	1:A:103:LEU:HA	2.00	0.43
2:B:12:VAL:HG11	2:B:82(A):LEU:CD1	2.49	0.43
2:B:197:HIS:HD2	2:B:200:SER:OG	2.00	0.43
2:D:50:PHE:C	2:D:50:PHE:HD1	2.25	0.43
2:D:153:ASN:HD21	2:D:192:THR:N	2.10	0.43
2:F:51:ILE:HG13	2:F:55:THR:HG22	1.99	0.43
1:A:37:GLN:HB2	1:A:47:LEU:HD11	2.01	0.43
2:D:113:LYS:HZ2	2:D:114:THR:HG23	1.83	0.43
1:E:178:LEU:HG	1:E:180:LEU:HD13	2.00	0.43
2:B:100(C):TRP:HA	2:B:100(C):TRP:CE3	2.54	0.43
3:I:606:GLN:O	3:I:607:ILE:CG2	2.63	0.43
2:B:52(D):ASN:HD21	3:I:607:ILE:HG22	1.84	0.43
1:C:13:VAL:CG2	1:C:17:GLU:HB2	2.49	0.43
2:F:82:THR:HG22	2:F:82:THR:O	2.17	0.43
3:J:606:GLN:HA	8:J:435:HOH:O	2.17	0.43
1:C:3:VAL:HB	1:C:26:SER:HB3	2.01	0.43
1:C:145:VAL:HG21	1:C:174:MET:HE1	2.00	0.43
1:G:13:VAL:HG21	1:G:19:VAL:HG22	2.01	0.43
2:B:6:GLU:HA	2:B:21:SER:O	2.18	0.43
2:D:38:ARG:NE	2:D:48:LEU:HD21	2.33	0.43
2:F:52(C):VAL:HG23	8:F:611:HOH:O	2.17	0.43
1:G:33:LEU:HG	1:G:71:PHE:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:HD2	1:A:139:TYR:CG	2.53	0.43
1:C:30(A):ASN:O	1:C:30(E):ARG:N	2.51	0.43
1:C:50:TRP:O	1:C:51:ALA:HB3	2.19	0.43
1:E:32:TYR:O	1:E:90:GLN:HA	2.19	0.43
2:D:52(A):ASN:HD21	3:J:607:ILE:HG21	1.80	0.42
1:C:189:ASN:HD22	1:C:210:ARG:H	1.67	0.42
1:E:93:ASN:ND2	3:K:602:THR:H	2.12	0.42
3:J:606:GLN:O	3:J:607:ILE:CG2	2.63	0.42
2:D:18:LEU:HB3	2:D:80:MET:HE3	2.01	0.42
1:A:135:LEU:HD23	1:A:143:ILE:CD1	2.50	0.42
1:C:48:ILE:HD13	1:C:64:GLY:N	2.35	0.42
1:G:93:ASN:O	1:G:94:LEU:HB2	2.19	0.42
6:P:1:NAG:H83	6:P:1:NAG:O3	2.19	0.42
1:E:135:LEU:N	1:E:135:LEU:HD12	2.35	0.42
1:G:189:ASN:HD22	1:G:210:ARG:H	1.66	0.42
1:A:13:VAL:HG22	1:A:14:SER:N	2.34	0.42
1:C:30(E):ARG:HG3	1:C:30(E):ARG:NH1	2.33	0.42
1:E:30(B):SER:O	1:E:30(E):ARG:HD2	2.19	0.42
1:G:50:TRP:O	1:G:51:ALA:HB3	2.20	0.42
1:A:50:TRP:CZ2	2:B:100(B):ARG:HA	2.54	0.42
2:D:94:ARG:HB3	2:D:100(G):VAL:CG1	2.50	0.42
1:E:47:LEU:HD22	1:E:58:VAL:HG13	2.00	0.42
1:G:189:ASN:ND2	1:G:210:ARG:H	2.17	0.42
2:H:50:PHE:C	2:H:50:PHE:HD1	2.27	0.42
1:A:93:ASN:ND2	3:I:602:THR:HG23	2.35	0.41
2:B:29:PHE:HB3	8:B:610:HOH:O	2.18	0.41
1:E:1:ASP:N	8:E:749:HOH:O	2.53	0.41
1:E:54:ARG:NE	1:E:60:ASP:HA	2.35	0.41
1:E:145:VAL:HG23	1:E:174:MET:HE1	2.02	0.41
1:G:179:THR:O	1:G:180:LEU:HD12	2.20	0.41
1:A:189:ASN:HD22	1:A:210:ARG:H	1.66	0.41
2:B:8:GLY:N	2:D:73:GLN:HE22	2.15	0.41
2:D:11:LEU:CD2	2:D:114:THR:HG22	2.47	0.41
2:F:203:LYS:CE	2:H:31:ASP:OD1	2.65	0.41
2:H:154:SER:N	2:H:194:ASN:ND2	2.59	0.41
1:A:48:ILE:HG23	1:A:53:THR:O	2.20	0.41
1:A:21:MET:HG3	1:A:73:LEU:HB3	2.02	0.41
1:C:135:LEU:N	1:C:135:LEU:HD12	2.34	0.41
2:D:29:PHE:CD2	2:D:74:SER:HA	2.56	0.41
2:H:175:LEU:C	2:H:175:LEU:CD1	2.93	0.41
1:C:189:ASN:ND2	1:C:210:ARG:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:LEU:C	2:D:175:LEU:CD1	2.93	0.41
2:F:52(A):ASN:ND2	3:K:607:ILE:HG23	2.15	0.41
1:E:83:LEU:O	1:E:84:ALA:HB2	2.20	0.41
1:A:30(C):LYS:NZ	1:A:30(C):LYS:CB	2.83	0.41
1:A:135:LEU:HD12	1:A:135:LEU:N	2.36	0.41
1:A:189:ASN:ND2	1:A:210:ARG:H	2.18	0.41
2:B:87:SER:O	2:B:88:ALA:HB2	2.21	0.41
2:D:52(D):ASN:ND2	3:J:607:ILE:CG2	2.83	0.41
2:D:100(B):ARG:HB3	2:D:100(D):TYR:CE1	2.56	0.41
1:E:189:ASN:HD22	1:E:210:ARG:H	1.68	0.41
1:E:189:ASN:ND2	1:E:210:ARG:H	2.19	0.41
1:A:21:MET:CG	1:A:73:LEU:HB3	2.50	0.41
2:D:30:ILE:HG22	2:D:71:ASP:CB	2.51	0.41
1:E:75:ILE:HG21	1:E:78:VAL:HG12	2.02	0.41
2:H:117:PRO:HB3	2:H:143:TYR:HB3	2.02	0.41
1:A:117:PHE:HA	1:A:118:PRO:HD3	1.85	0.41
2:B:52(C):VAL:HG21	3:I:607:ILE:CD1	2.51	0.41
2:B:100(B):ARG:HB3	2:B:100(D):TYR:CE1	2.55	0.41
1:C:31:ASN:O	1:C:50:TRP:HA	2.21	0.41
1:C:179:THR:O	1:C:180:LEU:HD12	2.21	0.41
2:D:34:MET:HB3	2:D:76:LEU:HD22	2.02	0.41
1:E:4:MET:HE3	1:E:23:CYS:SG	2.60	0.41
2:F:83:ARG:HD3	2:F:83:ARG:HA	1.81	0.41
2:H:87:SER:O	2:H:88:ALA:HB2	2.19	0.41
1:A:145:VAL:HG23	1:A:174:MET:HE1	2.02	0.41
1:C:35:TRP:CE2	1:C:73:LEU:HB2	2.56	0.41
1:G:22:THR:HG22	1:G:23:CYS:N	2.36	0.41
1:G:145:VAL:HG23	1:G:174:MET:HE1	2.02	0.41
1:A:71:PHE:CD1	1:A:71:PHE:N	2.88	0.40
2:H:164:PHE:HA	2:H:165:PRO:HD3	1.97	0.40
1:A:114:VAL:HA	1:A:134:PHE:O	2.22	0.40
1:C:32:TYR:HB3	1:C:91:SER:HB3	2.04	0.40
1:E:22:THR:CG2	1:E:23:CYS:N	2.85	0.40
2:F:76:LEU:HD23	2:F:92:CYS:SG	2.61	0.40
1:A:94:LEU:O	1:A:95:ARG:HG3	2.22	0.40
1:A:103:LEU:C	1:A:103:LEU:HD23	2.46	0.40
1:C:114:VAL:HA	1:C:134:PHE:O	2.21	0.40
2:D:100(D):TYR:HE2	2:D:100(F):ASP:HB3	1.86	0.40
2:H:34:MET:HB3	2:H:76:LEU:HD22	2.03	0.40
2:H:124:PRO:C	8:H:649:HOH:O	2.63	0.40
1:C:14:SER:O	1:C:17:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:LEU:HD23	1:G:143:ILE:CD1	2.51	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	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
1	C	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
1	E	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
1	G	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
2	B	212/222 (96%)	200 (94%)	12 (6%)	0	100	100
2	D	212/222 (96%)	205 (97%)	7 (3%)	0	100	100
2	F	212/222 (96%)	208 (98%)	4 (2%)	0	100	100
2	H	212/222 (96%)	206 (97%)	6 (3%)	0	100	100
3	I	5/7 (71%)	5 (100%)	0	0	100	100
3	J	5/7 (71%)	5 (100%)	0	0	100	100
3	K	5/7 (71%)	5 (100%)	0	0	100	100
3	L	5/7 (71%)	5 (100%)	0	0	100	100
All	All	1728/1784 (97%)	1671 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/193 (100%)	191 (99%)	2 (1%)	68	82
1	C	193/193 (100%)	192 (100%)	1 (0%)	81	90
1	E	193/193 (100%)	191 (99%)	2 (1%)	68	82
1	G	193/193 (100%)	190 (98%)	3 (2%)	55	73
2	B	189/191 (99%)	186 (98%)	3 (2%)	55	73
2	D	189/191 (99%)	185 (98%)	4 (2%)	47	66
2	F	189/191 (99%)	185 (98%)	4 (2%)	47	66
2	H	189/191 (99%)	182 (96%)	7 (4%)	30	45
3	I	7/7 (100%)	7 (100%)	0	100	100
3	J	7/7 (100%)	7 (100%)	0	100	100
3	K	7/7 (100%)	7 (100%)	0	100	100
3	L	7/7 (100%)	7 (100%)	0	100	100
All	All	1556/1564 (100%)	1530 (98%)	26 (2%)	53	72

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	107	ARG
2	B	114	THR
2	B	147	PRO
2	B	175	LEU
1	C	91	SER
2	D	114	THR
2	D	145	PRO
2	D	147	PRO
2	D	175	LEU
1	E	60	ASP
1	E	103	LEU
2	F	50	PHE
2	F	114	THR
2	F	147	PRO
2	F	175	LEU
1	G	13	VAL
1	G	103	LEU

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Mol	Chain	Res	Type
1	G	107	ARG
2	H	54	THR
2	H	109	VAL
2	H	110	SER
2	H	111	SER
2	H	145	PRO
2	H	147	PRO
2	H	175	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	79	GLN
1	A	93	ASN
1	A	165	GLN
1	A	189	ASN
1	A	209	ASN
1	A	211	ASN
2	B	13	GLN
2	B	32	ASN
2	B	52(A)	ASN
2	B	52(D)	ASN
2	B	81	ASN
2	B	153	ASN
2	B	194	ASN
2	B	197	HIS
1	C	31	ASN
1	C	42	GLN
1	C	79	GLN
1	C	165	GLN
1	C	189	ASN
1	C	209	ASN
1	C	211	ASN
2	D	52(A)	ASN
2	D	52(D)	ASN
2	D	73	GLN
2	D	153	ASN
2	D	194	ASN
2	D	197	HIS
1	E	79	GLN
1	E	93	ASN

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Mol	Chain	Res	Type
1	E	136	ASN
1	E	165	GLN
1	E	189	ASN
1	E	209	ASN
1	E	211	ASN
2	F	3	ASN
2	F	52(A)	ASN
2	F	52(D)	ASN
2	F	153	ASN
2	F	194	ASN
2	F	197	HIS
1	G	31	ASN
1	G	42	GLN
1	G	79	GLN
1	G	93	ASN
1	G	136	ASN
1	G	165	GLN
1	G	189	ASN
1	G	209	ASN
1	G	211	ASN
2	H	3	ASN
2	H	52(A)	ASN
2	H	52(D)	ASN
2	H	73	GLN
2	H	79	GLN
2	H	153	ASN
2	H	194	ASN
2	H	197	HIS
3	J	606	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 ⓘ

11 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	$\# Z > 2$
4	NAG	M	1	2,4	14,14,15	0.55	0	17,19,21	0.75	0
4	NAG	M	2	4	14,14,15	0.55	0	17,19,21	0.78	1 (5%)
4	BMA	M	3	4	11,11,12	0.94	1 (9%)	15,15,17	1.02	1 (6%)
5	NAG	N	1	5,2	14,14,15	0.63	0	17,19,21	0.82	1 (5%)
5	NDG	N	2	5	14,14,15	0.72	0	17,19,21	0.70	0
4	NAG	O	1	2,4	14,14,15	0.68	0	17,19,21	0.75	0
4	NAG	O	2	4	14,14,15	0.48	0	17,19,21	0.81	1 (5%)
4	BMA	O	3	4	11,11,12	0.82	0	15,15,17	0.76	0
6	NAG	P	1	6,2	14,14,15	0.61	0	17,19,21	0.76	1 (5%)
6	NAG	P	2	6	14,14,15	0.74	0	17,19,21	1.22	2 (11%)
6	MAN	P	3	6	11,11,12	0.99	1 (9%)	15,15,17	0.92	2 (13%)

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
4	NAG	M	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	M	2	4	-	4/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1
5	NAG	N	1	5,2	-	4/6/23/26	0/1/1/1
5	NDG	N	2	5	-	3/6/23/26	0/1/1/1
4	NAG	O	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	4/6/23/26	0/1/1/1
4	BMA	O	3	4	-	0/2/19/22	0/1/1/1
6	NAG	P	1	6,2	-	4/6/23/26	0/1/1/1
6	NAG	P	2	6	-	4/6/23/26	0/1/1/1
6	MAN	P	3	6	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	3	MAN	O5-C5	2.04	1.47	1.43
4	M	3	BMA	O5-C1	2.03	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	2	NAG	C4-C3-C2	-2.97	106.66	111.02
4	O	2	NAG	C2-N2-C7	-2.53	119.50	122.90
6	P	2	NAG	C2-N2-C7	-2.45	119.61	122.90
4	M	3	BMA	C2-C3-C4	-2.44	106.57	110.86
6	P	1	NAG	C2-N2-C7	-2.31	119.81	122.90
6	P	3	MAN	C3-C4-C5	-2.26	106.14	110.23
4	M	2	NAG	C2-N2-C7	-2.13	120.04	122.90
6	P	3	MAN	C2-C3-C4	-2.11	107.14	110.86
5	N	1	NAG	C2-N2-C7	-2.06	120.14	122.90

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	O	2	NAG	C8-C7-N2-C2
4	O	2	NAG	O7-C7-N2-C2
5	N	1	NAG	C8-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
5	N	2	NDG	C8-C7-N2-C2
5	N	2	NDG	O7-C7-N2-C2
6	P	1	NAG	C8-C7-N2-C2
6	P	1	NAG	O7-C7-N2-C2
6	P	2	NAG	O7-C7-N2-C2
6	P	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O5-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2

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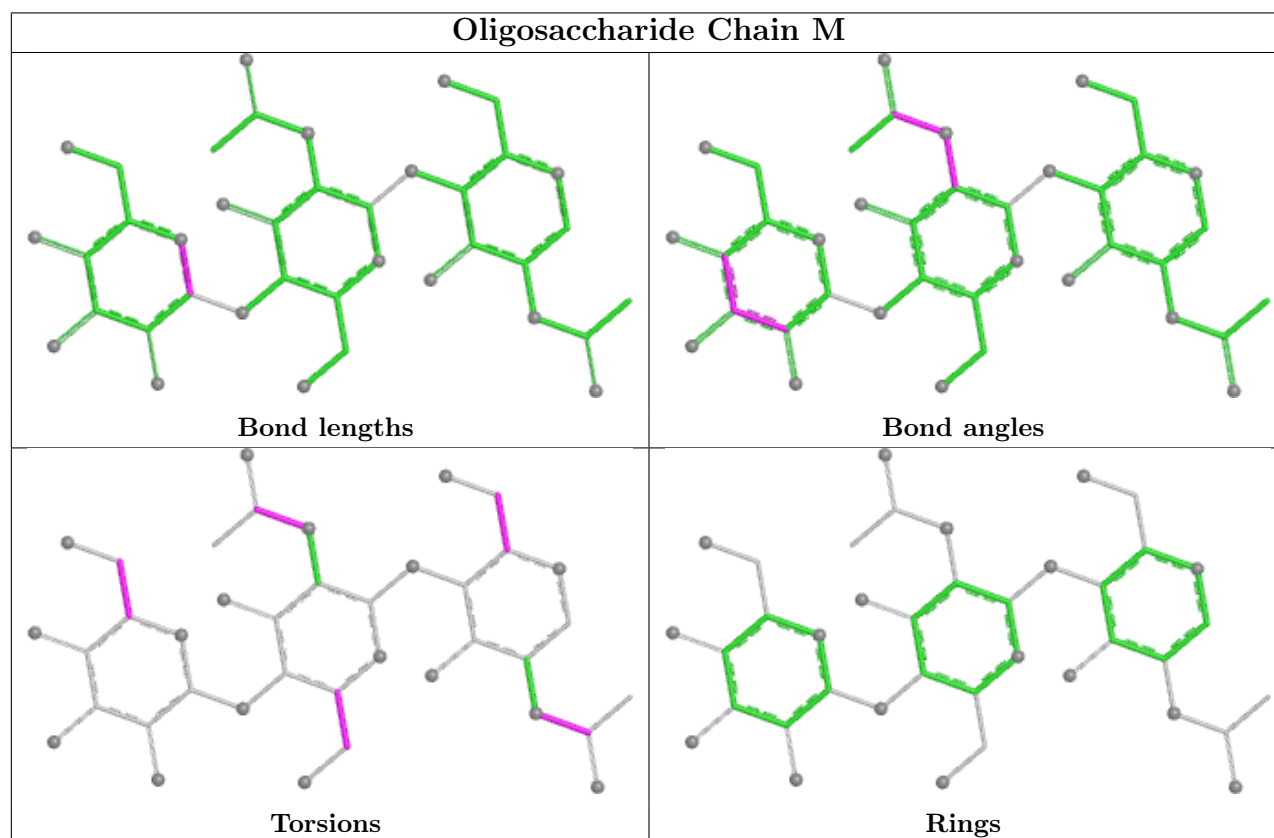
Mol	Chain	Res	Type	Atoms
5	N	1	NAG	C4-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
6	P	2	NAG	C4-C5-C6-O6
6	P	1	NAG	C4-C5-C6-O6
6	P	1	NAG	O5-C5-C6-O6
5	N	2	NDG	O5-C5-C6-O6
4	M	1	NAG	O7-C7-N2-C2

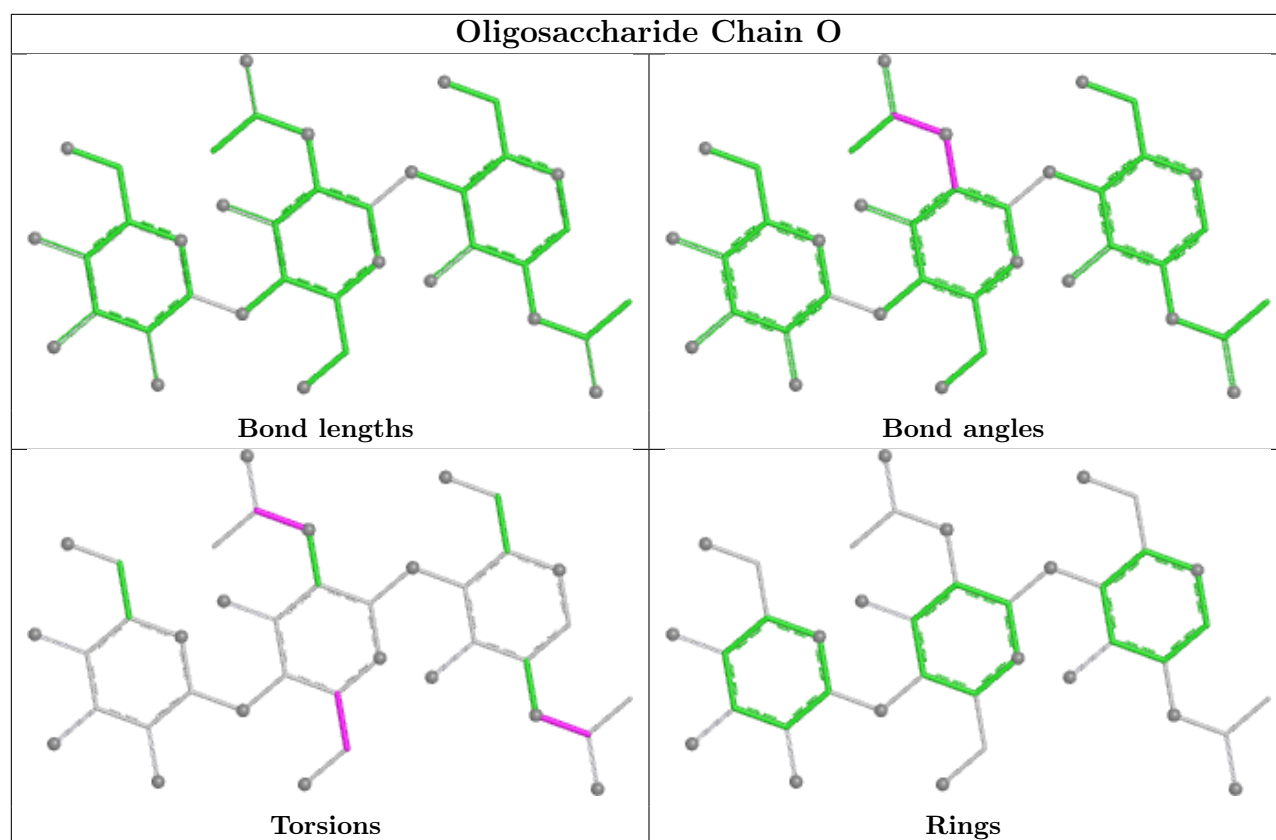
There are no ring outliers.

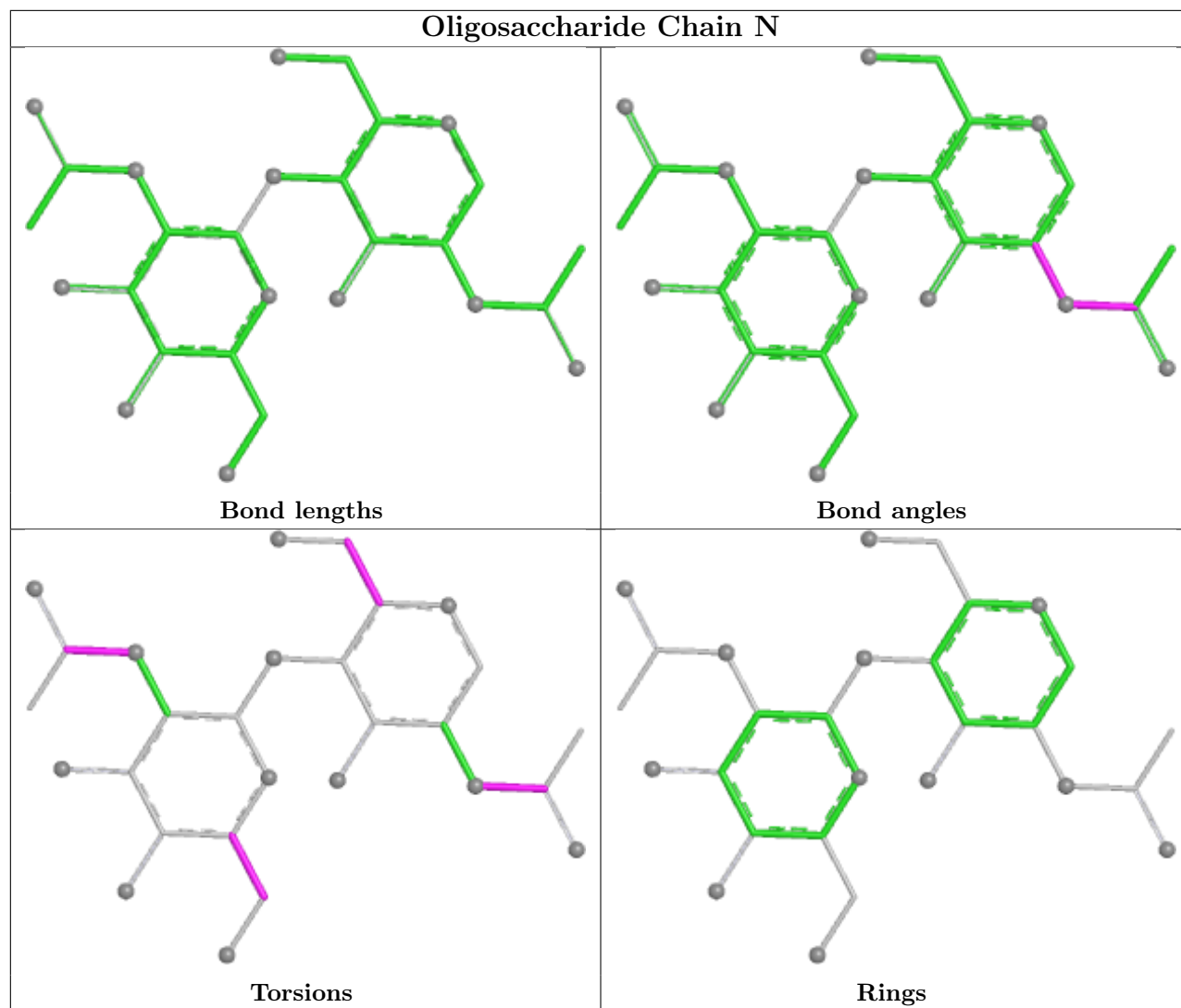
5 monomers are involved in 9 short contacts:

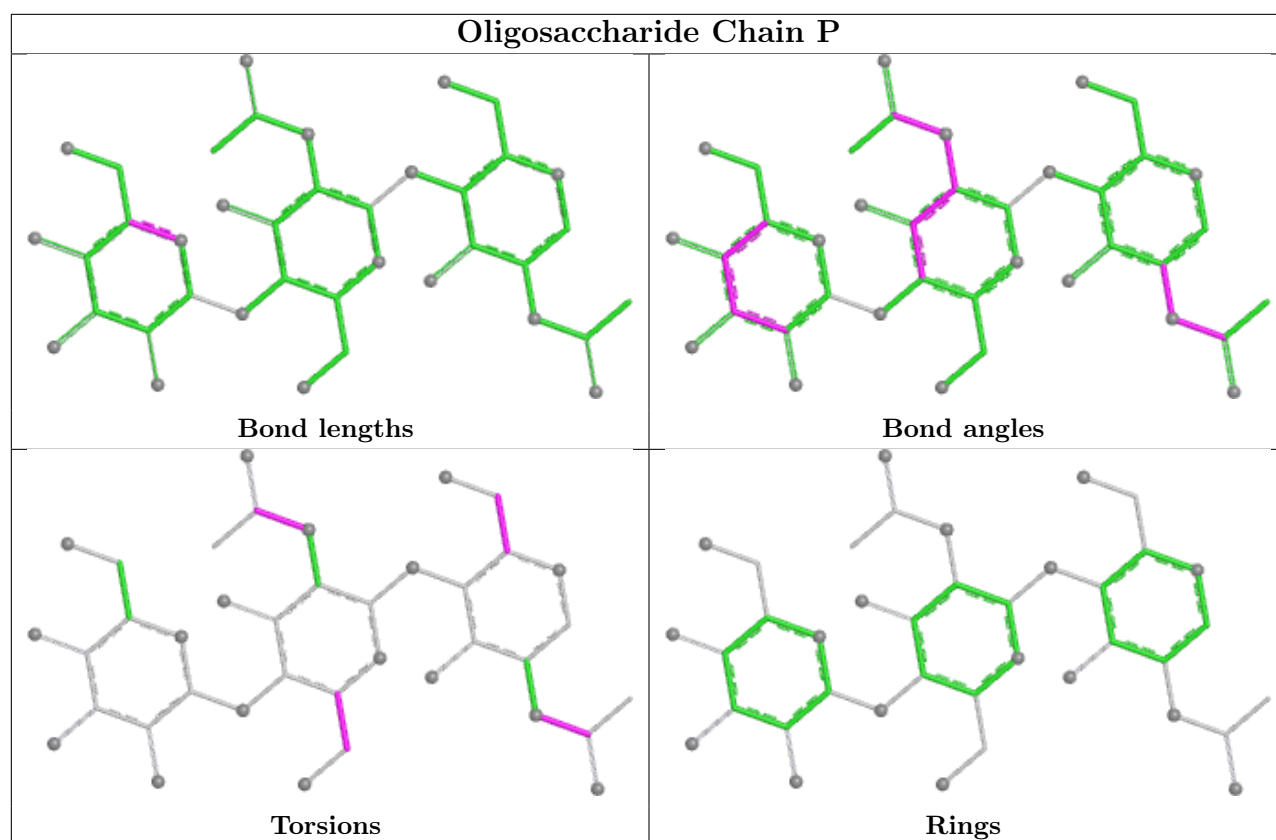
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	1	NAG	1	0
6	P	3	MAN	3	0
4	O	1	NAG	1	0
4	M	1	NAG	4	0
6	P	2	NAG	3	0

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](#)

7 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	$\# Z > 2$
7	SO4	C	705	-	4,4,4	0.36	0	6,6,6	0.13	0
7	SO4	E	701	-	4,4,4	0.39	0	6,6,6	0.11	0
7	SO4	A	704	-	4,4,4	0.34	0	6,6,6	0.18	0
7	SO4	C	703	-	4,4,4	0.38	0	6,6,6	0.12	0
7	SO4	A	702	-	4,4,4	0.40	0	6,6,6	0.10	0
7	SO4	E	706	-	4,4,4	0.38	0	6,6,6	0.10	0
7	SO4	G	707	-	4,4,4	0.39	0	6,6,6	0.07	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.

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	217/217 (100%)	0.43	16 (7%) 20 22	21, 41, 74, 117	0
1	C	217/217 (100%)	0.57	35 (16%) 4 5	19, 40, 102, 134	0
1	E	217/217 (100%)	0.30	13 (5%) 27 29	20, 37, 81, 152	0
1	G	217/217 (100%)	0.25	14 (6%) 25 27	19, 36, 80, 119	0
2	B	216/222 (97%)	0.75	36 (16%) 4 5	23, 43, 90, 129	0
2	D	216/222 (97%)	0.27	23 (10%) 11 12	17, 34, 86, 125	0
2	F	216/222 (97%)	-0.01	5 (2%) 61 63	17, 32, 63, 104	0
2	H	216/222 (97%)	-0.06	5 (2%) 61 63	16, 31, 59, 126	0
3	I	7/7 (100%)	1.00	1 (14%) 6 7	42, 55, 61, 67	0
3	J	7/7 (100%)	0.78	1 (14%) 6 7	29, 36, 66, 74	0
3	K	7/7 (100%)	0.72	1 (14%) 6 7	35, 36, 50, 66	0
3	L	7/7 (100%)	0.38	1 (14%) 6 7	32, 33, 59, 72	0
All	All	1760/1784 (98%)	0.32	151 (8%) 16 17	16, 37, 82, 152	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	184	SER	5.5
2	D	187	PRO	5.1
2	B	156	SER	4.9
1	E	211	ASN	4.7
2	D	188	SER	4.7
2	B	191	VAL	4.6
3	J	607	ILE	4.5
2	F	113	LYS	4.4
1	E	1	ASP	4.2
1	A	122	GLU	4.1
1	A	125	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	151	GLY	4.0
2	B	190	THR	4.0
1	E	190	SER	3.9
1	C	180	LEU	3.8
2	B	155	GLY	3.8
2	D	190	THR	3.8
1	G	1	ASP	3.7
1	C	124	LEU	3.6
1	A	121	SER	3.6
2	D	185	THR	3.6
2	B	204	VAL	3.6
2	B	199	ALA	3.6
1	G	162	TRP	3.5
3	K	607	ILE	3.5
1	C	152	SER	3.5
1	E	68	GLY	3.5
2	B	187	PRO	3.4
2	B	203	LYS	3.4
1	E	156	ASN	3.4
2	D	208	ILE	3.3
1	C	190	SER	3.3
3	L	607	ILE	3.3
2	B	192	THR	3.3
2	B	61	VAL	3.3
1	C	118	PRO	3.2
2	D	189	GLU	3.2
2	D	192	THR	3.2
1	A	156	ASN	3.2
1	C	125	THR	3.1
1	C	150	ASP	3.1
2	D	207	LYS	3.1
1	C	208	PHE	3.0
1	C	181	THR	3.0
1	C	151	GLY	3.0
2	B	150	VAL	3.0
1	E	125	THR	3.0
2	B	120	TYR	3.0
1	C	128	GLY	3.0
1	C	186	GLU	3.0
2	H	189	GLU	3.0
2	H	131	ASN	2.9
2	B	197	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	209	VAL	2.9
1	C	179	THR	2.9
1	A	1	ASP	2.9
1	A	211	ASN	2.9
1	G	211	ASN	2.9
2	D	113	LYS	2.8
2	B	196	ALA	2.8
2	D	191	VAL	2.8
1	A	189	ASN	2.8
1	C	126	SER	2.8
2	B	209	VAL	2.8
1	E	209	ASN	2.7
2	B	205	ASP	2.7
2	B	193	CYS	2.7
1	G	201	THR	2.7
1	A	126	SER	2.7
2	B	132	SER	2.7
1	C	210	ARG	2.7
1	E	162	TRP	2.7
2	D	133	MET	2.7
1	E	129	ALA	2.7
1	C	189	ASN	2.7
1	C	156	ASN	2.6
1	C	209	ASN	2.6
1	G	180	LEU	2.6
2	F	209	VAL	2.6
1	G	145	VAL	2.6
1	C	121	SER	2.6
1	C	187	ARG	2.6
1	G	200	SER	2.6
2	B	154	SER	2.6
2	D	183	SER	2.6
1	C	149	ILE	2.5
2	D	171	ASP	2.5
2	B	149	THR	2.5
2	B	159	SER	2.5
2	D	181	VAL	2.5
2	D	156	SER	2.5
1	C	188	HIS	2.4
1	G	156	ASN	2.4
1	E	168	LYS	2.4
1	G	208	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	207	LYS	2.4
1	C	211	ASN	2.4
1	G	209	ASN	2.4
1	A	128	GLY	2.4
1	C	127	GLY	2.4
2	B	148	VAL	2.4
2	D	157	LEU	2.4
1	C	91	SER	2.3
3	I	607	ILE	2.3
2	B	131	ASN	2.3
1	A	146	LYS	2.3
1	C	162	TRP	2.3
2	B	118	SER	2.3
1	G	182	LYS	2.3
2	B	198	PRO	2.3
1	A	127	GLY	2.3
2	B	186	TRP	2.3
1	A	152	SER	2.3
2	F	98	SER	2.3
2	D	131	ASN	2.2
2	B	121	PRO	2.2
1	E	210	ARG	2.2
1	G	189	ASN	2.2
1	C	131	VAL	2.2
1	E	189	ASN	2.2
1	C	184	GLU	2.2
1	C	168	LYS	2.2
1	C	129	ALA	2.2
2	B	208	ILE	2.2
2	B	194	ASN	2.2
1	E	151	GLY	2.2
2	D	138	CYS	2.2
2	F	30	ILE	2.1
2	B	188	SER	2.1
2	H	133	MET	2.1
2	B	152	TRP	2.1
1	C	30(E)	ARG	2.1
2	B	138	CYS	2.1
1	A	120	SER	2.1
1	G	77	SER	2.1
2	B	184	SER	2.1
2	D	136	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	191	TYR	2.1
2	H	188	SER	2.1
1	A	141	LYS	2.1
1	C	182	LYS	2.1
1	A	124	LEU	2.1
2	B	100(A)	TYR	2.1
2	D	210	PRO	2.1
2	B	195	VAL	2.1
2	H	156	SER	2.0
2	F	1	GLU	2.0
1	C	60	ASP	2.0
1	C	183	ASP	2.0
2	D	121	PRO	2.0
1	G	168	LYS	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](#)

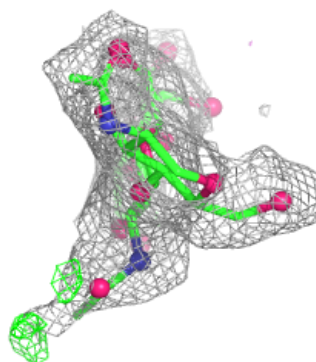
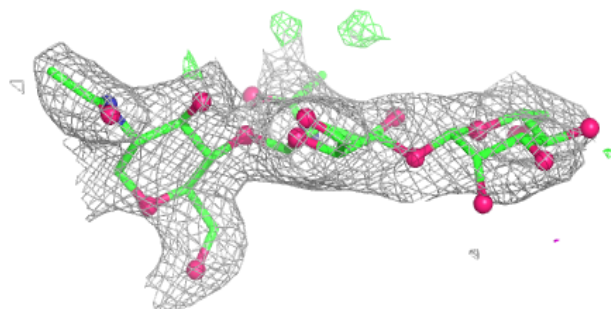
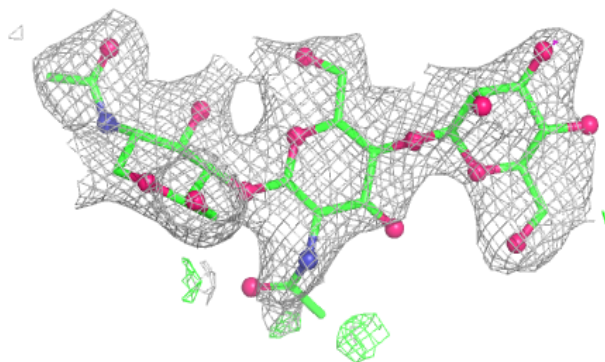
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	O	3	11/12	0.27	0.19	90,90,90,90	0
4	BMA	M	3	11/12	0.43	0.16	93,93,93,93	0
5	NDG	N	2	14/15	0.55	0.18	89,94,96,96	0
4	NAG	M	2	14/15	0.61	0.17	85,90,92,92	0
6	MAN	P	3	11/12	0.61	0.13	80,80,80,80	0
6	NAG	P	2	14/15	0.68	0.15	76,81,82,83	0
4	NAG	O	2	14/15	0.71	0.14	79,84,85,86	0
5	NAG	N	1	14/15	0.73	0.22	76,81,82,83	0
4	NAG	M	1	14/15	0.82	0.11	51,56,58,58	0
6	NAG	P	1	14/15	0.84	0.14	52,57,59,59	0
4	NAG	O	1	14/15	0.87	0.10	38,43,45,45	0

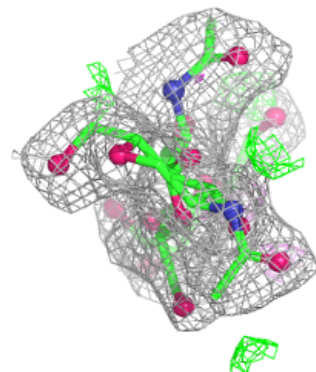
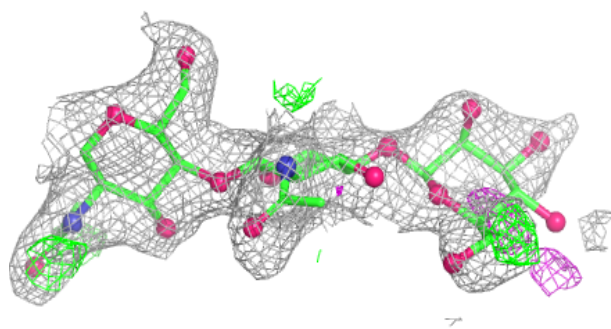
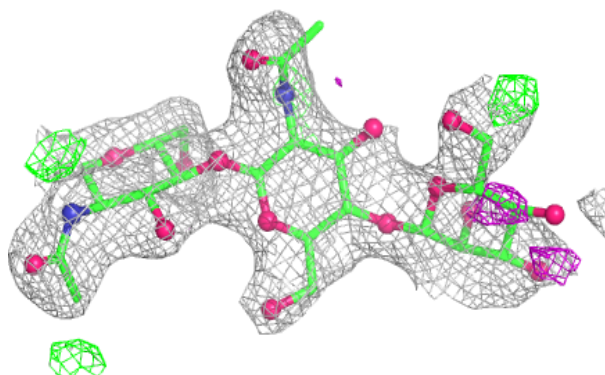
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

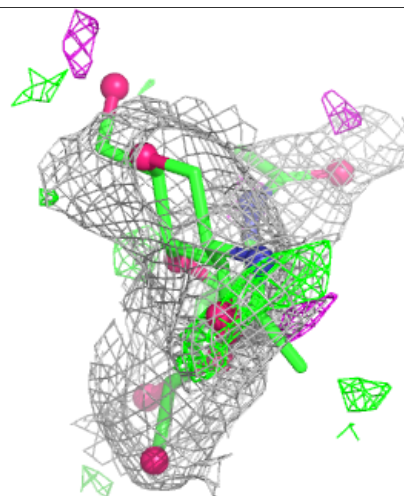
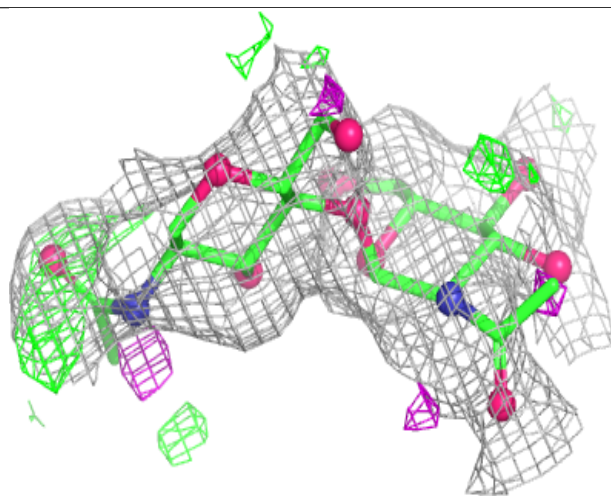
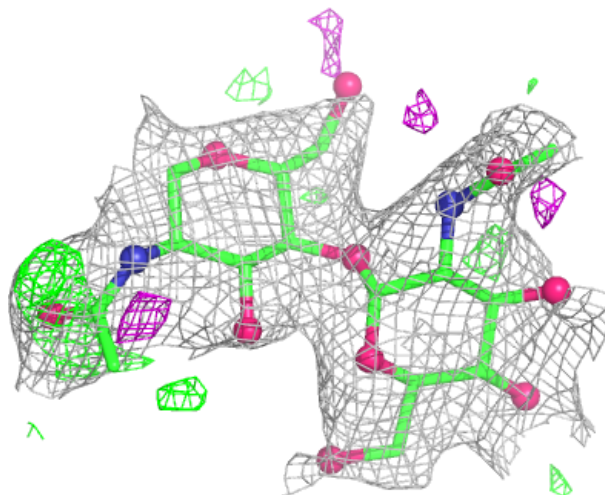
**Electron density around Chain O:**

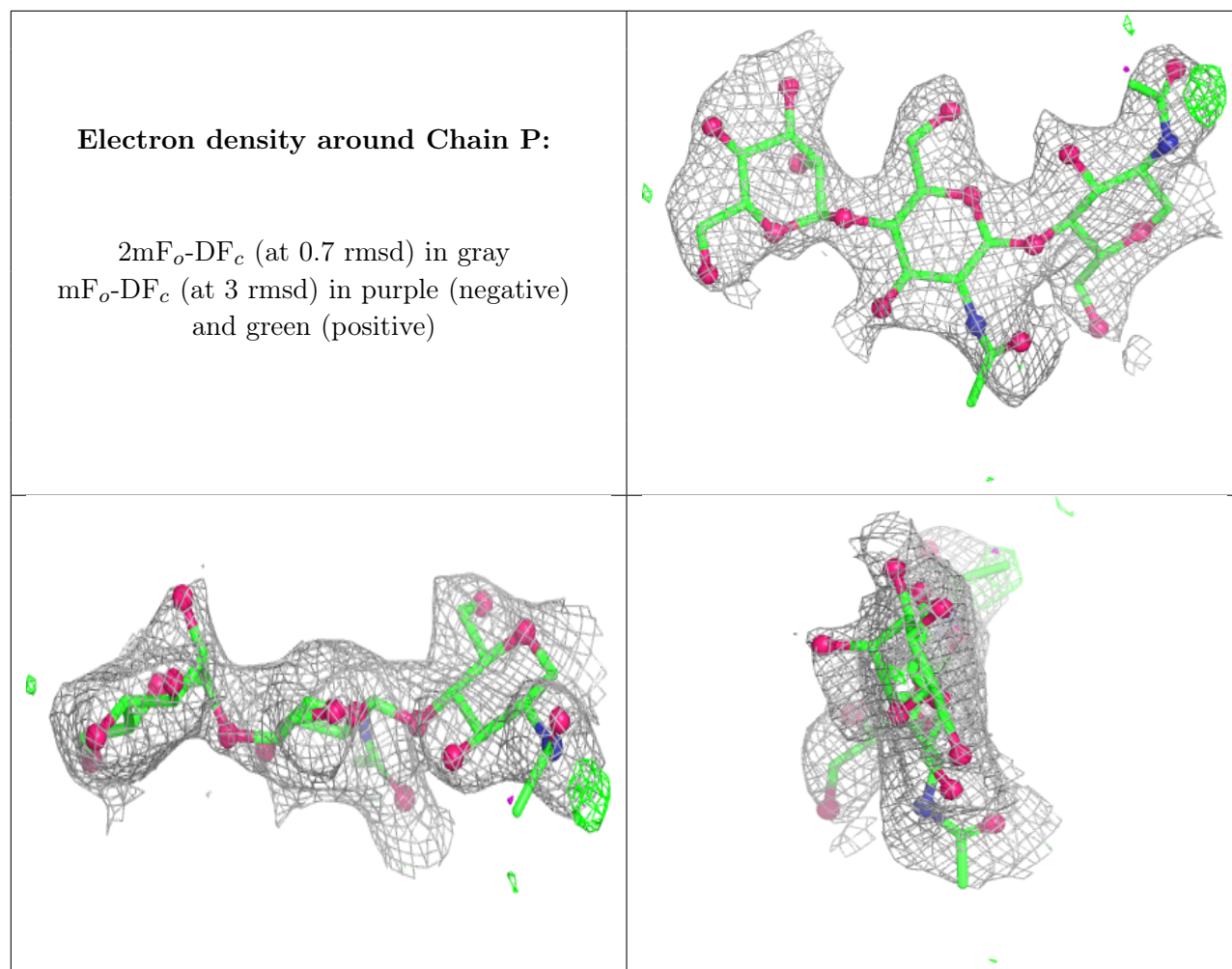
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain N:

$2mF_o-DF_c$ (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
7	SO4	A	702	5/5	0.74	0.13	46,47,47,48	5
7	SO4	E	701	5/5	0.90	0.09	46,47,47,48	5
7	SO4	C	703	5/5	0.92	0.09	46,47,47,47	5
7	SO4	A	704	5/5	0.94	0.08	46,47,47,47	5
7	SO4	G	707	5/5	0.94	0.07	46,47,47,47	5
7	SO4	E	706	5/5	0.95	0.07	46,47,47,47	5
7	SO4	C	705	5/5	0.95	0.06	46,47,47,47	5

6.5 Other polymers [i](#)

There are no such residues in this entry.