



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:53 AM UTC

PDB ID : 6Z32 / pdb_00006z32
Title : Human cation-independent mannose 6-phosphate/IGF2 receptor domains 7-11
Authors : Bochel, A.J.; Williams, C.; McCoy, A.J.; Hoppe, H.; Winter, A.J.; Nicholls, R.D.; Harlos, K.; Jones, Y.E.; Berger, I.; Hassan, B.; Crump, M.P.
Deposited on : 2020-05-19
Resolution : 3.47 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

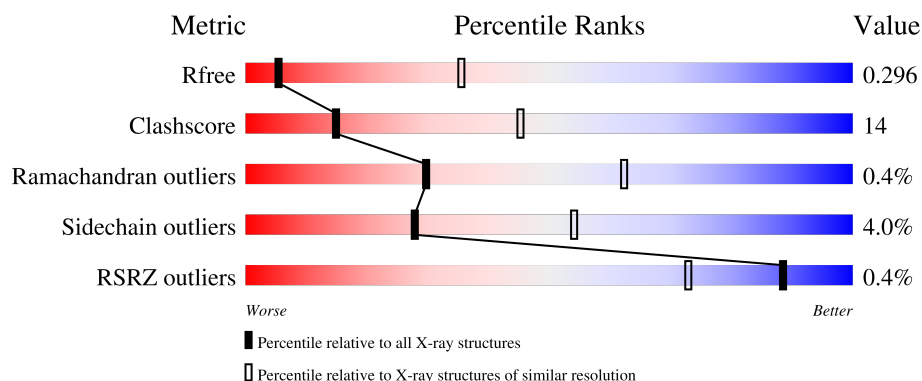
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

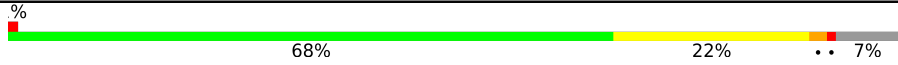
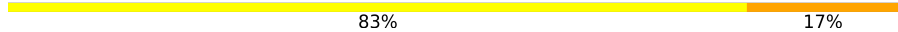
The reported resolution of this entry is 3.47 Å.

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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	737	 68% 22% 7%
1	B	737	 69% 19% 10%
2	C	6	 67% 33%
2	D	6	 83% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	2	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10549 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 Cation-independent mannose-6-phosphate receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5257	3312	887	1011	47			
1	B	665	Total	C	N	O	S	0	0	0
			5101	3212	858	984	47			

There are 30 discrepancies between the modelled and reference sequences:

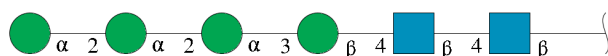
Chain	Residue	Modelled	Actual	Comment	Reference
A	913	GLU	-	expression tag	UNP P11717
A	914	THR	-	expression tag	UNP P11717
A	915	GLY	-	expression tag	UNP P11717
A	916	GLN	-	expression tag	UNP P11717
A	917	LEU	-	expression tag	UNP P11717
A	918	LYS	-	expression tag	UNP P11717
A	919	HIS	-	expression tag	UNP P11717
A	920	HIS	-	expression tag	UNP P11717
A	921	HIS	-	expression tag	UNP P11717
A	922	HIS	-	expression tag	UNP P11717
A	923	HIS	-	expression tag	UNP P11717
A	924	HIS	-	expression tag	UNP P11717
A	925	GLU	-	expression tag	UNP P11717
A	926	PHE	-	expression tag	UNP P11717
A	1619	GLY	ARG	variant	UNP P11717
B	913	GLU	-	expression tag	UNP P11717
B	914	THR	-	expression tag	UNP P11717
B	915	GLY	-	expression tag	UNP P11717
B	916	GLN	-	expression tag	UNP P11717
B	917	LEU	-	expression tag	UNP P11717
B	918	LYS	-	expression tag	UNP P11717
B	919	HIS	-	expression tag	UNP P11717
B	920	HIS	-	expression tag	UNP P11717
B	921	HIS	-	expression tag	UNP P11717
B	922	HIS	-	expression tag	UNP P11717

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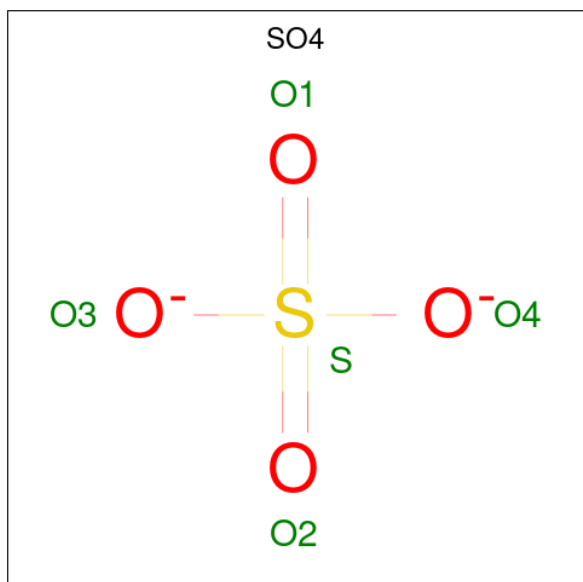
Chain	Residue	Modelled	Actual	Comment	Reference
B	923	HIS	-	expression tag	UNP P11717
B	924	HIS	-	expression tag	UNP P11717
B	925	GLU	-	expression tag	UNP P11717
B	926	PHE	-	expression tag	UNP P11717
B	1619	GLY	ARG	variant	UNP P11717

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



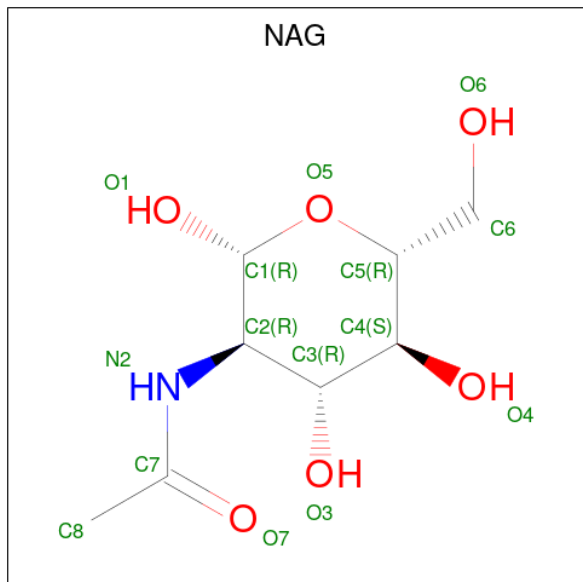
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	D	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

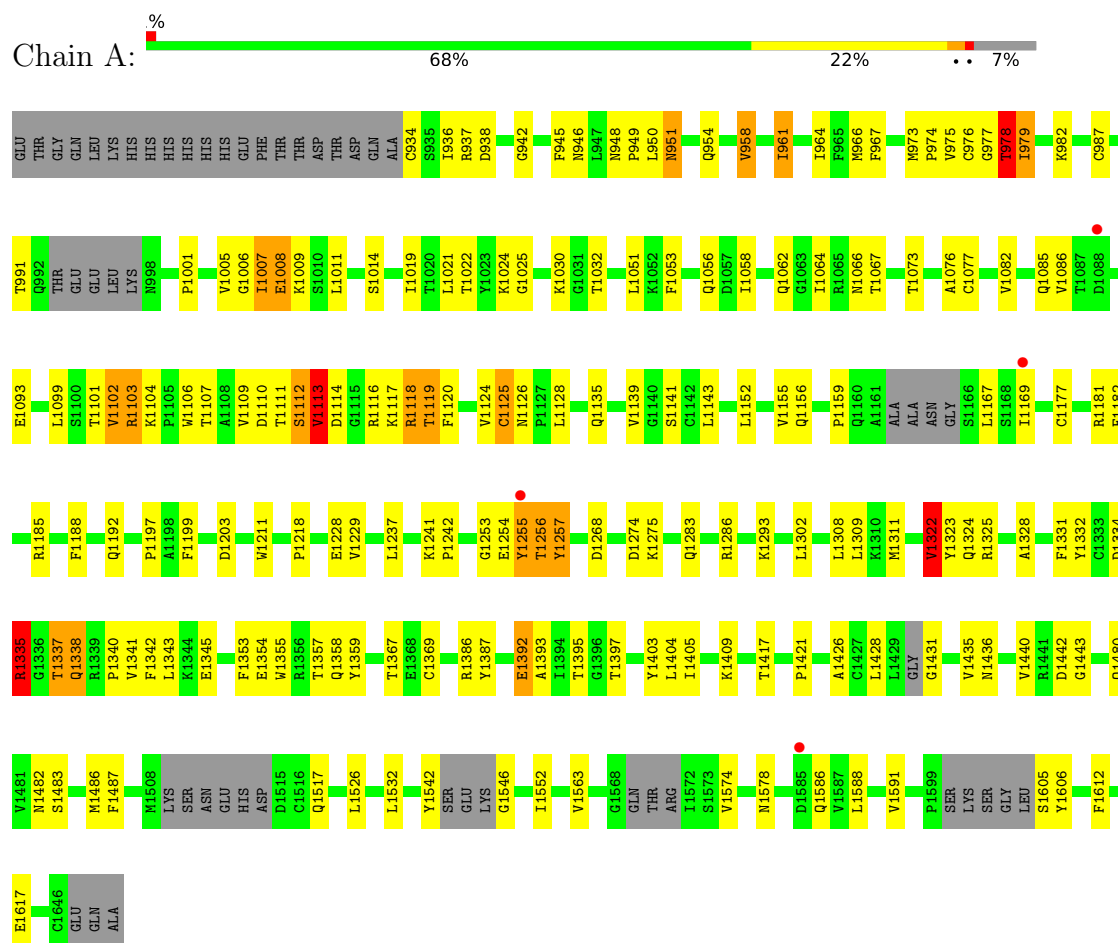


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

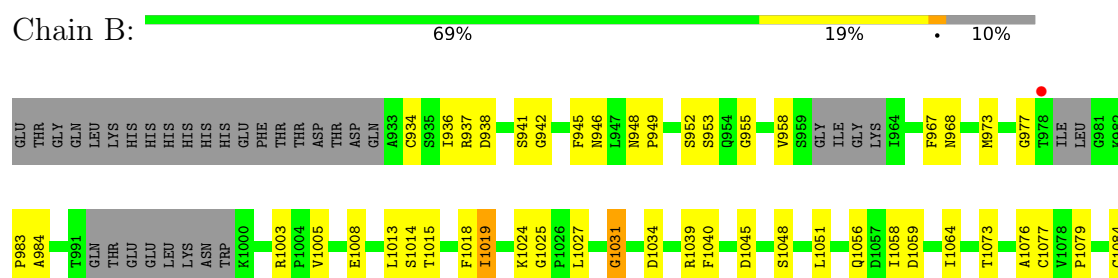
3 Residue-property plots

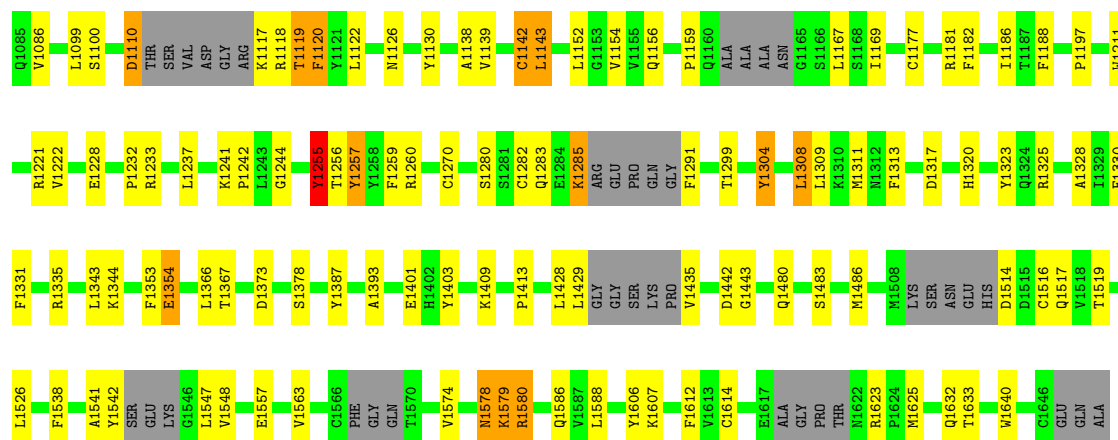
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cation-independent mannose-6-phosphate receptor



• Molecule 1: Cation-independent mannose-6-phosphate receptor





- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 67% 33%



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 83% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.20Å 139.20Å 234.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.72 – 3.47 89.72 – 3.47	Depositor EDS
% Data completeness (in resolution range)	98.5 (89.72-3.47) 98.7 (89.72-3.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.261 , 0.300 0.270 , 0.296	Depositor DCC
R_{free} test set	1493 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	157.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 210.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10549	wwPDB-VP
Average B, all atoms (Å ²)	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: 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	1.04	3/5379 (0.1%)	1.32	21/7300 (0.3%)
1	B	1.03	4/5213 (0.1%)	1.30	21/7067 (0.3%)
All	All	1.04	7/10592 (0.1%)	1.31	42/14367 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1579	LYS	CA-C	8.50	1.63	1.52
1	A	1008	GLU	C-O	-6.29	1.16	1.24
1	A	974	PRO	C-O	-6.15	1.16	1.24
1	B	1256	THR	C-O	-5.36	1.17	1.24
1	B	1270	CYS	N-CA	5.22	1.50	1.46
1	A	973	MET	C-O	-5.16	1.18	1.24
1	B	1138	ALA	C-O	5.01	1.29	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1579	LYS	N-CA-C	8.64	124.88	113.30
1	A	951	ASN	N-CA-C	-7.34	99.29	110.30
1	A	1322	VAL	N-CA-C	7.00	119.76	112.83
1	B	1120	PHE	CB-CA-C	-6.78	98.91	110.16
1	A	1392	GLU	CB-CG-CD	6.75	124.07	112.60
1	B	1580	ARG	N-CA-C	6.70	120.17	108.52
1	B	1579	LYS	CA-C-O	6.53	127.09	119.32
1	A	978	THR	CB-CA-C	6.44	123.23	110.42
1	B	953	SER	CA-C-N	6.34	129.07	120.38
1	B	953	SER	C-N-CA	6.34	129.07	120.38
1	A	951	ASN	CB-CA-C	6.30	118.82	110.06
1	A	1118	ARG	N-CA-C	6.18	119.56	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1110	ASP	CB-CA-C	6.12	121.73	110.10
1	B	1255	TYR	CA-CB-CG	6.05	124.78	113.90
1	A	979	ILE	CB-CA-C	5.89	120.95	111.29
1	B	1119	THR	CB-CA-C	-5.81	99.19	109.70
1	B	1304	TYR	CA-C-O	-5.75	114.37	120.40
1	A	1397	THR	CA-CB-OG1	-5.59	101.22	109.60
1	A	1102	VAL	CA-C-N	5.55	130.00	120.72
1	A	1102	VAL	C-N-CA	5.55	130.00	120.72
1	B	1142	CYS	CA-C-N	5.54	128.57	120.71
1	B	1142	CYS	C-N-CA	5.54	128.57	120.71
1	B	1563	VAL	CA-C-N	5.44	125.99	120.00
1	B	1563	VAL	C-N-CA	5.44	125.99	120.00
1	A	1335	ARG	CA-C-N	-5.41	117.56	122.80
1	A	1335	ARG	C-N-CA	-5.41	117.56	122.80
1	B	1014	SER	CA-C-N	5.37	128.22	120.38
1	B	1014	SER	C-N-CA	5.37	128.22	120.38
1	B	1578	ASN	CA-C-N	5.33	130.75	122.49
1	B	1578	ASN	C-N-CA	5.33	130.75	122.49
1	A	1254	GLU	N-CA-C	-5.30	107.35	113.88
1	A	1268	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	1008	GLU	CA-C-O	-5.27	114.64	120.33
1	A	1431	GLY	CA-C-N	5.27	127.61	120.65
1	A	1431	GLY	C-N-CA	5.27	127.61	120.65
1	A	975	VAL	CA-C-O	-5.16	116.42	121.58
1	A	1563	VAL	CA-C-N	5.11	125.62	120.00
1	A	1563	VAL	C-N-CA	5.11	125.62	120.00
1	B	1118	ARG	N-CA-CB	5.05	120.48	111.69
1	A	977	GLY	O-C-N	5.05	127.68	122.88
1	B	1373	ASP	CA-C-N	5.04	125.57	119.98
1	B	1373	ASP	C-N-CA	5.04	125.57	119.98

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	5257	0	5051	172	0
1	B	5101	0	4894	133	0
2	C	72	0	61	10	0
2	D	72	0	61	4	0
3	A	5	0	0	1	0
4	A	14	0	13	0	0
4	B	28	0	26	1	0
All	All	10549	0	10106	285	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 (285) 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:A:1102:VAL:HG21	1:A:1106:TRP:CZ2	1.74	1.20
1:A:979:ILE:HG21	1:A:1007:ILE:CD1	1.74	1.18
1:A:976:CYS:HB3	1:A:1001:PRO:HB3	1.22	1.16
1:B:1120:PHE:CE1	1:B:1143:LEU:HD12	1.82	1.14
1:A:1338:GLN:HB3	1:B:1130:TYR:CZ	1.81	1.14
1:A:979:ILE:HD13	1:A:1007:ILE:CG1	1.76	1.14
1:A:979:ILE:CD1	1:A:1007:ILE:HG12	1.82	1.09
1:A:1338:GLN:HB3	1:B:1130:TYR:CE1	1.88	1.08
1:A:1335:ARG:HH21	1:A:1335:ARG:HG2	1.17	1.07
1:A:979:ILE:HD13	1:A:1007:ILE:HG12	1.34	1.07
1:B:1120:PHE:CZ	1:B:1143:LEU:CD1	2.54	0.91
1:A:979:ILE:HG21	1:A:1007:ILE:HD13	1.49	0.91
1:A:1102:VAL:HG21	1:A:1106:TRP:HZ2	1.36	0.90
1:B:1120:PHE:CE1	1:B:1143:LEU:CD1	2.55	0.90
1:B:1120:PHE:CZ	1:B:1143:LEU:HD12	2.06	0.90
1:B:1142:CYS:O	1:B:1142:CYS:SG	2.30	0.89
1:A:946:ASN:HD21	1:A:1181:ARG:HD3	1.36	0.89
1:B:1013:LEU:HA	1:B:1018:PHE:O	1.73	0.89
1:A:1337:THR:HG22	1:A:1358:GLN:HG2	1.55	0.89
1:A:1113:VAL:HG23	1:B:1580:ARG:HA	1.53	0.88
1:B:1285:LYS:HD3	1:B:1291:PHE:CE2	2.09	0.86
1:A:1102:VAL:CG2	1:A:1106:TRP:CZ2	2.58	0.85
1:A:976:CYS:CB	1:A:1001:PRO:HB3	2.07	0.84
1:A:1324:GLN:HB2	2:C:2:NAG:C8	2.07	0.84
1:A:1323:TYR:OH	1:B:1320:HIS:CD2	2.31	0.84
1:A:1324:GLN:H	2:C:2:NAG:H81	1.43	0.84
1:A:976:CYS:HB3	1:A:1001:PRO:CB	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:936:ILE:HD11	1:B:1019:ILE:HG12	1.61	0.81
1:A:1102:VAL:CG2	1:A:1106:TRP:HZ2	1.94	0.81
1:A:979:ILE:CD1	1:A:1007:ILE:CG1	2.51	0.81
1:B:1542:TYR:HE2	1:B:1548:VAL:HG23	1.46	0.80
1:B:1027:LEU:HD22	1:B:1031:GLY:HA2	1.64	0.79
1:A:1324:GLN:H	2:C:2:NAG:C8	1.96	0.78
1:A:1111:THR:HG23	1:A:1116:ARG:O	1.85	0.77
1:A:1338:GLN:CB	1:B:1130:TYR:CE1	2.67	0.77
1:A:1335:ARG:HG2	1:A:1335:ARG:NH2	1.92	0.76
1:B:1120:PHE:CD1	1:B:1143:LEU:HD12	2.21	0.76
1:B:1541:ALA:HB3	1:B:1623:ARG:HH22	1.50	0.75
1:A:979:ILE:HG21	1:A:1007:ILE:CG1	2.16	0.75
1:A:979:ILE:HG21	1:A:1007:ILE:HD11	1.68	0.73
1:A:1337:THR:HG21	1:A:1359:TYR:CE2	2.22	0.73
1:A:979:ILE:HD13	1:A:1007:ILE:HG13	1.66	0.73
1:A:934:CYS:HB3	1:A:1011:LEU:CD1	2.18	0.73
1:A:946:ASN:ND2	1:A:1181:ARG:HD3	2.04	0.72
1:A:1113:VAL:CG2	1:B:1580:ARG:HA	2.20	0.72
1:A:1293:LYS:HE2	1:A:1325:ARG:CZ	2.22	0.70
1:A:1337:THR:CG2	1:A:1358:GLN:HG2	2.20	0.70
1:A:1338:GLN:HB3	1:B:1130:TYR:CE2	2.28	0.69
1:B:1019:ILE:HG22	1:B:1040:PHE:HB2	1.73	0.69
1:B:936:ILE:HD12	1:B:1013:LEU:CD2	2.23	0.68
1:B:936:ILE:HD11	1:B:1019:ILE:CG1	2.24	0.68
1:A:979:ILE:HD12	1:A:1007:ILE:HG12	1.72	0.67
1:A:979:ILE:CG2	1:A:1007:ILE:HD13	2.24	0.67
1:A:1324:GLN:HB2	2:C:2:NAG:H81	1.77	0.66
1:A:979:ILE:CG2	1:A:1007:ILE:CD1	2.65	0.66
1:A:1283:GLN:HE21	1:A:1293:LYS:HG3	1.60	0.66
1:B:1255:TYR:OH	2:C:6:MAN:H3	1.96	0.66
1:A:958:VAL:HG11	1:A:1051:LEU:HD22	1.78	0.65
1:A:1143:LEU:HB2	1:A:1152:LEU:HD11	1.79	0.65
1:A:1482:ASN:OD1	1:A:1482:ASN:O	2.15	0.65
1:B:936:ILE:HD12	1:B:1013:LEU:HD21	1.77	0.65
1:B:1159:PRO:HG3	1:B:1169:ILE:HD11	1.79	0.64
1:B:967:PHE:CZ	1:B:1051:LEU:HD11	2.33	0.64
1:B:1143:LEU:H	1:B:1152:LEU:CD1	2.10	0.64
1:B:1323:TYR:CE1	2:D:3:BMA:H61	2.33	0.64
1:B:952:SER:O	1:B:968:ASN:ND2	2.31	0.64
1:B:1542:TYR:CE2	1:B:1548:VAL:HG23	2.32	0.64
1:A:1486:MET:SD	1:B:1614:CYS:HB3	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1013:LEU:CA	1:B:1018:PHE:O	2.46	0.63
1:A:1542:TYR:HD2	1:A:1546:GLY:HA3	1.61	0.63
1:B:968:ASN:HB2	1:B:973:MET:HE2	1.79	0.63
1:B:1100:SER:HB2	1:B:1126:ASN:HD22	1.64	0.63
1:A:934:CYS:HB3	1:A:1011:LEU:HD13	1.80	0.63
1:B:1013:LEU:CD2	1:B:1019:ILE:CG1	2.77	0.62
1:A:979:ILE:HG21	1:A:1007:ILE:HG12	1.81	0.62
1:B:1013:LEU:HD23	1:B:1019:ILE:HG12	1.81	0.62
1:A:1167:LEU:HB2	1:A:1188:PHE:HB2	1.81	0.62
1:B:1574:VAL:HA	1:B:1606:TYR:HB3	1.81	0.62
2:C:3:BMA:O6	2:C:3:BMA:O4	2.07	0.62
1:A:966:MET:HE3	1:A:976:CYS:SG	2.41	0.61
1:B:1366:LEU:HD23	1:B:1367:THR:N	2.15	0.61
1:B:1048:SER:O	1:B:1048:SER:OG	2.18	0.61
1:B:936:ILE:CD1	1:B:1019:ILE:HG12	2.31	0.60
1:B:1019:ILE:CG2	1:B:1040:PHE:HB2	2.30	0.60
1:A:1159:PRO:HG3	1:A:1169:ILE:HD11	1.83	0.60
1:A:1006:GLY:O	1:A:1009:LYS:NZ	2.34	0.60
1:A:1324:GLN:N	2:C:2:NAG:H81	2.15	0.59
1:A:1393:ALA:HB3	1:A:1403:TYR:HB2	1.85	0.59
1:B:936:ILE:HD11	1:B:1019:ILE:CD1	2.33	0.59
1:B:1013:LEU:CD2	1:B:1019:ILE:HG13	2.32	0.59
1:A:967:PHE:CZ	1:A:1051:LEU:HD11	2.38	0.59
1:B:1233:ARG:HH22	1:B:1413:PRO:HB2	1.68	0.58
1:A:978:THR:HA	1:A:982:LYS:O	2.02	0.58
1:A:1099:LEU:O	1:A:1106:TRP:NE1	2.36	0.58
1:B:1317:ASP:OD1	1:B:1325:ARG:NH1	2.35	0.58
1:A:1338:GLN:O	1:A:1355:TRP:NE1	2.36	0.58
2:C:2:NAG:O7	2:C:2:NAG:O3	2.22	0.58
1:B:955:GLY:HA3	1:B:973:MET:HE1	1.86	0.57
1:A:1337:THR:O	1:A:1337:THR:OG1	2.21	0.57
1:B:1167:LEU:HB2	1:B:1188:PHE:HB2	1.85	0.57
1:A:1110:ASP:OD2	1:A:1199:PHE:CD2	2.57	0.57
1:B:1013:LEU:CD2	1:B:1019:ILE:HG12	2.35	0.57
1:B:1003:ARG:HB3	1:B:1034:ASP:OD2	2.05	0.57
1:A:1283:GLN:CG	1:A:1293:LYS:HB2	2.35	0.57
1:B:1309:LEU:HB2	1:B:1331:PHE:HB2	1.87	0.57
1:A:1323:TYR:HH	1:B:1320:HIS:CD2	2.20	0.56
1:A:1542:TYR:CG	1:A:1542:TYR:O	2.56	0.56
1:A:1086:VAL:HG21	1:A:1159:PRO:HB2	1.87	0.56
1:B:1079:PRO:HB3	1:B:1154:VAL:CG1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1578:ASN:OD1	1:B:1579:LYS:N	2.38	0.56
1:B:1323:TYR:CZ	2:D:3:BMA:H61	2.41	0.56
1:A:938:ASP:HB2	1:A:945:PHE:HE2	1.71	0.56
1:A:1337:THR:HA	1:A:1357:THR:HA	1.88	0.56
1:A:1345:GLU:OE2	2:D:6:MAN:O4	2.24	0.55
1:B:1177:CYS:O	1:B:1177:CYS:SG	2.63	0.55
1:B:1393:ALA:HB3	1:B:1403:TYR:HB2	1.87	0.55
1:A:1203:ASP:CG	1:B:1607:LYS:HZ1	2.13	0.55
1:B:1257:TYR:CD2	1:B:1353:PHE:HZ	2.25	0.55
1:A:1102:VAL:HG12	1:A:1104:LYS:H	1.72	0.55
1:A:1255:TYR:N	1:A:1255:TYR:CD2	2.76	0.54
1:A:1337:THR:HG21	1:A:1359:TYR:CD2	2.42	0.54
1:A:1229:VAL:HG12	1:A:1302:LEU:HD23	1.90	0.54
1:A:1338:GLN:HB3	1:B:1130:TYR:CD1	2.41	0.54
1:B:1122:LEU:HD23	1:B:1186:ILE:HD11	1.89	0.54
1:B:1056:GLN:HE21	1:B:1058:ILE:HG12	1.71	0.54
1:A:1574:VAL:HA	1:A:1606:TYR:HB3	1.89	0.54
1:A:961:ILE:HG22	1:A:961:ILE:O	2.08	0.54
1:A:1335:ARG:O	1:A:1358:GLN:OE1	2.26	0.54
1:B:1541:ALA:CB	1:B:1623:ARG:HH22	2.18	0.53
1:A:976:CYS:CB	1:A:1001:PRO:CB	2.77	0.53
1:B:1541:ALA:HB3	1:B:1623:ARG:NH2	2.23	0.53
1:B:1073:THR:HG23	1:B:1076:ALA:H	1.73	0.53
1:B:1299:THR:HG22	1:B:1313:PHE:HD1	1.73	0.53
1:A:1542:TYR:O	1:A:1542:TYR:CD2	2.61	0.53
4:B:1701:NAG:O6	4:B:1701:NAG:O4	2.22	0.53
1:B:1086:VAL:HG21	1:B:1159:PRO:HB2	1.89	0.53
1:A:1032:THR:CG2	1:A:1062:GLN:O	2.57	0.53
1:A:1128:LEU:HD12	1:A:1139:VAL:HG12	1.90	0.53
1:A:1255:TYR:N	1:A:1255:TYR:HD2	2.07	0.53
1:A:1324:GLN:HB2	2:C:2:NAG:H82	1.86	0.53
1:A:1103:ARG:O	1:A:1103:ARG:HG2	2.06	0.52
1:A:964:ILE:HD12	1:A:991:THR:HG22	1.90	0.52
1:A:1056:GLN:HB2	1:A:1067:THR:HG22	1.91	0.52
1:B:1285:LYS:CD	1:B:1291:PHE:CE2	2.89	0.52
1:A:1617:GLU:OE1	1:A:1617:GLU:N	2.42	0.52
1:A:1395:THR:HG22	1:A:1487:PHE:HB3	1.92	0.52
1:B:1139:VAL:HG11	1:B:1142:CYS:HB3	1.92	0.52
1:B:936:ILE:CD1	1:B:1013:LEU:HD21	2.40	0.51
1:B:938:ASP:HB2	1:B:945:PHE:HE2	1.76	0.51
1:A:1255:TYR:HD2	1:A:1255:TYR:H	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:958:VAL:HG11	1:B:1051:LEU:HD22	1.92	0.51
1:A:1228:GLU:HB3	1:A:1237:LEU:HD11	1.93	0.51
1:A:1480:GLN:HB3	1:A:1483:SER:HB3	1.92	0.51
1:B:1442:ASP:OD1	1:B:1443:GLY:N	2.44	0.51
1:A:1203:ASP:HB2	1:B:1607:LYS:HE2	1.93	0.51
1:B:1255:TYR:HB2	1:B:1257:TYR:HE1	1.76	0.50
1:A:1337:THR:HB	1:A:1357:THR:OG1	2.11	0.50
1:B:1285:LYS:HD3	1:B:1291:PHE:HE2	1.73	0.50
1:B:1013:LEU:HD23	1:B:1019:ILE:CG1	2.42	0.50
1:A:961:ILE:HD11	1:A:1053:PHE:HZ	1.76	0.50
1:A:1064:ILE:HD11	1:A:1066:ASN:HD22	1.76	0.50
1:B:1005:VAL:HG23	1:B:1025:GLY:N	2.26	0.50
1:A:1082:VAL:HG23	1:A:1155:VAL:HG12	1.94	0.50
1:B:1308:LEU:HD11	1:B:1330:PHE:HB3	1.94	0.49
1:B:1221:ARG:HA	1:B:1304:TYR:O	2.12	0.49
1:B:938:ASP:HB3	1:B:941:SER:HB3	1.93	0.49
1:A:1442:ASP:OD1	1:A:1443:GLY:N	2.46	0.49
1:A:1073:THR:HG23	1:A:1076:ALA:H	1.78	0.49
1:B:977:GLY:O	1:B:983:PRO:HA	2.13	0.49
1:B:1323:TYR:OH	2:D:3:BMA:H61	2.12	0.49
1:A:950:LEU:O	1:A:951:ASN:C	2.55	0.48
1:A:1311:MET:O	1:A:1328:ALA:HA	2.13	0.48
1:A:1113:VAL:HG21	1:B:1579:LYS:O	2.13	0.48
1:B:1311:MET:O	1:B:1328:ALA:HA	2.13	0.48
1:A:1343:LEU:HD11	1:A:1354:GLU:HB3	1.96	0.48
1:A:1532:LEU:HB2	1:A:1552:ILE:HD11	1.95	0.48
1:A:936:ILE:HD11	1:A:1019:ILE:HG12	1.94	0.48
1:B:1241:LYS:N	1:B:1242:PRO:CD	2.77	0.48
1:A:979:ILE:HD13	1:A:1007:ILE:CD1	2.41	0.48
1:B:1517:GLN:HB2	1:B:1526:LEU:HD21	1.96	0.48
1:A:1293:LYS:HE2	1:A:1325:ARG:NH2	2.29	0.47
1:B:1588:LEU:HB2	1:B:1612:PHE:HB2	1.95	0.47
1:A:1338:GLN:CB	1:B:1130:TYR:CD1	2.96	0.47
1:A:1058:ILE:O	1:A:1058:ILE:HG22	2.15	0.47
1:A:1008:GLU:HB3	1:A:1024:LYS:HB2	1.97	0.47
1:A:1114:ASP:HB2	1:B:1514:ASP:OD2	2.14	0.47
1:B:1018:PHE:CG	1:B:1039:ARG:NH1	2.82	0.47
1:A:1056:GLN:CB	1:A:1067:THR:HG22	2.45	0.47
1:A:1185:ARG:NH2	1:B:1633:THR:HG22	2.29	0.47
1:A:1241:LYS:N	1:A:1242:PRO:CD	2.78	0.47
1:A:1334:ASP:O	1:A:1358:GLN:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1486:MET:CE	1:B:1586:GLN:HE21	2.28	0.47
1:A:1340:PRO:HD3	1:A:1355:TRP:CE2	2.49	0.47
1:A:948:ASN:N	1:A:949:PRO:CD	2.78	0.47
1:A:1283:GLN:HG2	1:A:1293:LYS:HB2	1.97	0.47
1:A:1308:LEU:HD13	1:A:1332:TYR:CE1	2.50	0.46
1:B:1079:PRO:HB3	1:B:1154:VAL:HG11	1.96	0.46
1:A:1335:ARG:HH21	1:A:1335:ARG:CG	2.05	0.46
1:B:948:ASN:N	1:B:949:PRO:CD	2.78	0.46
1:A:1367:THR:OG1	1:A:1440:VAL:CG1	2.64	0.46
1:B:1366:LEU:HD23	1:B:1367:THR:H	1.79	0.46
1:A:1387:TYR:CD1	1:A:1409:LYS:HE3	2.50	0.46
1:A:1428:LEU:HB3	1:A:1435:VAL:HB	1.97	0.46
1:A:1586:GLN:HB3	1:B:1486:MET:HE1	1.98	0.46
1:A:1101:THR:HG22	1:A:1101:THR:O	2.14	0.46
1:A:1322:VAL:O	1:A:1322:VAL:CG2	2.63	0.46
1:B:1257:TYR:CZ	1:B:1283:GLN:OE1	2.69	0.46
1:A:1085:GLN:NE2	1:A:1093:GLU:OE2	2.49	0.46
1:A:1107:THR:HA	1:A:1120:PHE:O	2.15	0.46
1:B:936:ILE:CD1	1:B:1013:LEU:CD2	2.91	0.46
1:A:1578:ASN:ND2	1:A:1591:VAL:O	2.44	0.45
1:A:1586:GLN:NE2	1:B:1486:MET:HE2	2.30	0.45
1:B:1008:GLU:HB3	1:B:1024:LYS:HB2	1.98	0.45
1:A:1218:PRO:HB2	1:A:1417:THR:HG23	1.99	0.45
1:A:1077:CYS:O	1:A:1156:GLN:NE2	2.49	0.45
1:B:1142:CYS:HA	1:B:1152:LEU:HD12	1.98	0.45
1:A:937:ARG:NH1	1:A:942:GLY:HA2	2.32	0.45
1:A:1064:ILE:HD11	1:A:1066:ASN:ND2	2.32	0.45
1:A:1203:ASP:CG	1:B:1607:LYS:CE	2.90	0.45
1:B:936:ILE:HD11	1:B:1019:ILE:HD11	1.98	0.45
1:B:1480:GLN:HB3	1:B:1483:SER:HB3	1.99	0.45
1:B:937:ARG:NH1	1:B:942:GLY:HA2	2.32	0.44
1:A:1338:GLN:H	1:A:1338:GLN:HG3	1.50	0.44
1:A:1064:ILE:HG12	1:A:1066:ASN:HB2	1.99	0.44
1:B:1110:ASP:O	1:B:1117:LYS:HA	2.18	0.44
1:A:1309:LEU:HB2	1:A:1331:PHE:HB2	1.99	0.44
1:A:1517:GLN:HB3	1:A:1526:LEU:HD11	2.00	0.44
1:B:1143:LEU:H	1:B:1152:LEU:HD13	1.82	0.44
1:B:1197:PRO:HD3	1:B:1211:TRP:CZ2	2.53	0.44
1:B:1428:LEU:O	1:B:1429:LEU:C	2.60	0.44
1:A:1120:PHE:CE2	1:A:1143:LEU:HD13	2.53	0.44
1:A:1283:GLN:HE21	1:A:1293:LYS:CG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1482:ASN:O	1:A:1482:ASN:CG	2.60	0.44
1:A:1586:GLN:HE21	1:B:1486:MET:CE	2.31	0.43
1:B:1257:TYR:HD2	1:B:1353:PHE:HZ	1.64	0.43
1:B:1343:LEU:HD11	1:B:1354:GLU:HB3	1.99	0.43
1:B:1387:TYR:CD1	1:B:1409:LYS:HE3	2.52	0.43
1:A:1005:VAL:HG23	1:A:1025:GLY:N	2.33	0.43
1:A:1257:TYR:CD2	1:A:1353:PHE:HZ	2.36	0.43
1:A:1112:SER:OG	1:A:1116:ARG:HB3	2.18	0.43
1:A:1335:ARG:O	1:A:1358:GLN:HB3	2.19	0.43
1:A:1403:TYR:CE1	1:A:1428:LEU:HD13	2.53	0.43
1:B:946:ASN:ND2	1:B:1181:ARG:HD3	2.34	0.43
1:B:977:GLY:HA2	1:B:984:ALA:HB3	1.99	0.43
1:B:1335:ARG:HB2	1:B:1387:TYR:CE2	2.54	0.43
1:A:1120:PHE:CD2	1:A:1143:LEU:HD13	2.53	0.43
1:A:1111:THR:CG2	1:A:1116:ARG:O	2.63	0.42
1:A:1197:PRO:HD3	1:A:1211:TRP:CZ2	2.53	0.42
1:A:1311:MET:HE3	1:A:1311:MET:HB2	1.97	0.42
1:A:1124:VAL:HG12	1:A:1125:CYS:SG	2.59	0.42
1:B:1244:GLY:O	1:B:1260:ARG:HD2	2.19	0.42
1:B:1282:CYS:SG	1:B:1283:GLN:N	2.93	0.42
1:A:946:ASN:HD21	1:A:1181:ARG:CD	2.20	0.42
1:A:1124:VAL:C	1:A:1126:ASN:H	2.26	0.42
1:A:1141:SER:OG	1:A:1152:LEU:HB2	2.20	0.42
1:A:1177:CYS:HB2	1:A:1182:PHE:CZ	2.55	0.42
1:A:1203:ASP:CG	1:B:1607:LYS:NZ	2.77	0.42
1:A:1392:GLU:H	1:A:1392:GLU:CD	2.23	0.42
1:B:1335:ARG:HB2	1:B:1387:TYR:CZ	2.55	0.42
1:B:1428:LEU:HB3	1:B:1435:VAL:HB	2.02	0.42
1:A:1421:PRO:HG2	1:A:1436:ASN:HB2	2.02	0.42
1:B:1222:VAL:HG21	1:B:1232:PRO:HD3	2.01	0.42
1:A:1324:GLN:CB	2:C:2:NAG:H81	2.47	0.41
1:A:1323:TYR:OH	1:B:1320:HIS:NE2	2.38	0.41
1:A:1082:VAL:HG23	1:A:1155:VAL:CG1	2.51	0.41
1:A:1404:LEU:O	1:A:1426:ALA:HA	2.20	0.41
1:B:1625:MET:HA	1:B:1625:MET:HE2	2.03	0.41
1:A:1102:VAL:HG21	1:A:1106:TRP:CE2	2.45	0.41
1:B:1632:GLN:HG3	1:B:1633:THR:HG23	2.03	0.41
1:A:1021:LEU:HD23	1:A:1022:THR:N	2.35	0.41
1:A:1342:PHE:HA	1:A:1353:PHE:CD1	2.56	0.41
1:A:1588:LEU:HB2	1:A:1612:PHE:HB2	2.01	0.41
1:A:1109:VAL:HG22	1:A:1119:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1256:THR:OG1	1:A:1286:ARG:NH1	2.52	0.41
1:A:1386:ARG:HA	3:A:1701:SO4:O3	2.20	0.40
1:A:1542:TYR:CD2	1:A:1546:GLY:HA3	2.49	0.40
1:B:1059:ASP:HB3	1:B:1064:ILE:HG23	2.04	0.40
1:B:1228:GLU:HB3	1:B:1237:LEU:HD11	2.03	0.40
1:B:1259:PHE:HA	1:B:1280:SER:O	2.21	0.40
1:B:1401:GLU:HB2	1:B:1428:LEU:HD11	2.03	0.40
1:B:1177:CYS:HB3	1:B:1182:PHE:CZ	2.56	0.40
1:A:1110:ASP:OD2	1:A:1199:PHE:HD2	2.02	0.40
1:B:1045:ASP:N	1:B:1045:ASP:OD1	2.52	0.40
1:B:1538:PHE:CE2	1:B:1640:TRP:HH2	2.39	0.40
1:B:1077:CYS:O	1:B:1156:GLN:NE2	2.51	0.40

There are no symmetry-related clashes.

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	670/737 (91%)	632 (94%)	34 (5%)	4 (1%)	21	53
1	B	641/737 (87%)	607 (95%)	33 (5%)	1 (0%)	43	74
All	All	1311/1474 (89%)	1239 (94%)	67 (5%)	5 (0%)	30	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1253	GLY
1	A	1113	VAL
1	A	1125	CYS
1	B	1031	GLY
1	A	961	ILE

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	589/632 (93%)	561 (95%)	28 (5%)	23	49
1	B	574/632 (91%)	556 (97%)	18 (3%)	35	60
All	All	1163/1264 (92%)	1117 (96%)	46 (4%)	28	54

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	954	GLN
1	A	958	VAL
1	A	978	THR
1	A	987	CYS
1	A	1007	ILE
1	A	1014	SER
1	A	1030	LYS
1	A	1103	ARG
1	A	1112	SER
1	A	1113	VAL
1	A	1117	LYS
1	A	1118	ARG
1	A	1119	THR
1	A	1135	GLN
1	A	1192	GLN
1	A	1255	TYR
1	A	1256	THR
1	A	1257	TYR
1	A	1274	ASP
1	A	1275	LYS
1	A	1322	VAL
1	A	1335	ARG
1	A	1337	THR
1	A	1338	GLN
1	A	1341	VAL
1	A	1369	CYS
1	A	1405	ILE

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Mol	Chain	Res	Type
1	A	1605	SER
1	B	934	CYS
1	B	1015	THR
1	B	1019	ILE
1	B	1084	CYS
1	B	1099	LEU
1	B	1119	THR
1	B	1143	LEU
1	B	1255	TYR
1	B	1257	TYR
1	B	1285	LYS
1	B	1308	LEU
1	B	1344	LYS
1	B	1354	GLU
1	B	1378	SER
1	B	1516	CYS
1	B	1519	THR
1	B	1547	LEU
1	B	1557	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	946	ASN
1	A	1043	ASN
1	A	1055	HIS
1	A	1056	GLN
1	A	1151	ASN
1	A	1202	GLN
1	A	1283	GLN
1	A	1358	GLN
1	A	1558	ASN
1	B	1043	ASN
1	B	1056	GLN
1	B	1062	GLN
1	B	1202	GLN
1	B	1292	HIS
1	B	1320	HIS
1	B	1480	GLN
1	B	1586	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 ⓘ

12 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	NAG	C	1	1,2	14,14,15	1.03	1 (7%)	17,19,21	3.17	8 (47%)
2	NAG	C	2	2	14,14,15	0.31	0	17,19,21	0.70	0
2	BMA	C	3	2	11,11,12	2.06	6 (54%)	15,15,17	2.68	9 (60%)
2	MAN	C	4	2	11,11,12	0.33	0	15,15,17	0.91	1 (6%)
2	MAN	C	5	2	11,11,12	1.85	3 (27%)	15,15,17	2.25	5 (33%)
2	MAN	C	6	2	11,11,12	1.71	3 (27%)	15,15,17	2.32	7 (46%)
2	NAG	D	1	1,2	14,14,15	1.26	1 (7%)	17,19,21	3.40	6 (35%)
2	NAG	D	2	2	14,14,15	0.88	0	17,19,21	2.51	9 (52%)
2	BMA	D	3	2	11,11,12	0.24	0	15,15,17	0.72	0
2	MAN	D	4	2	11,11,12	1.94	4 (36%)	15,15,17	1.98	5 (33%)
2	MAN	D	5	2	11,11,12	1.18	2 (18%)	15,15,17	2.84	9 (60%)
2	MAN	D	6	2	11,11,12	1.98	5 (45%)	15,15,17	2.90	9 (60%)

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	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1
2	MAN	D	4	2	-	1/2/19/22	0/1/1/1
2	MAN	D	5	2	-	2/2/19/22	0/1/1/1
2	MAN	D	6	2	-	0/2/19/22	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	MAN	C2-C3	-4.16	1.46	1.52
2	D	1	NAG	O5-C1	-3.50	1.37	1.43
2	D	4	MAN	C2-C3	-3.31	1.47	1.52
2	C	3	BMA	O5-C1	-3.22	1.38	1.43
2	C	5	MAN	O5-C5	-3.17	1.37	1.43
2	D	6	MAN	C2-C3	-3.17	1.47	1.52
2	D	4	MAN	O2-C2	-3.07	1.36	1.43
2	D	4	MAN	O5-C1	-3.06	1.38	1.43
2	D	6	MAN	O5-C1	-2.97	1.38	1.43
2	D	4	MAN	O5-C5	-2.94	1.37	1.43
2	C	3	BMA	C4-C5	-2.93	1.46	1.53
2	D	6	MAN	C4-C5	-2.92	1.46	1.53
2	D	6	MAN	O5-C5	-2.89	1.37	1.43
2	C	3	BMA	O5-C5	-2.70	1.38	1.43
2	C	5	MAN	C4-C5	-2.68	1.47	1.53
2	C	3	BMA	C4-C3	-2.48	1.45	1.52
2	C	6	MAN	O5-C1	-2.42	1.39	1.43
2	C	3	BMA	O2-C2	-2.30	1.38	1.43
2	C	5	MAN	O3-C3	-2.28	1.37	1.43
2	C	1	NAG	O7-C7	-2.22	1.18	1.23
2	C	3	BMA	C2-C3	-2.10	1.49	1.52
2	D	5	MAN	C4-C3	-2.10	1.46	1.52
2	D	5	MAN	C1-C2	2.04	1.57	1.52
2	D	6	MAN	C4-C3	-2.02	1.47	1.52
2	C	6	MAN	O5-C5	-2.00	1.39	1.43

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	-10.15	98.59	112.19
2	C	3	BMA	C1-O5-C5	-6.91	102.93	112.19
2	D	1	NAG	C1-C2-N2	6.89	121.30	110.43
2	D	6	MAN	C6-C5-C4	-6.30	97.55	113.02
2	C	1	NAG	C1-O5-C5	6.03	120.27	112.19
2	C	1	NAG	C2-N2-C7	-5.72	115.23	122.90
2	C	5	MAN	C1-C2-C3	-5.47	101.68	109.64
2	D	5	MAN	O2-C2-C3	-5.25	99.28	110.15
2	D	5	MAN	O4-C4-C3	-5.13	98.29	110.38
2	C	1	NAG	C1-C2-N2	4.78	117.96	110.43
2	D	4	MAN	O2-C2-C3	-4.62	100.58	110.15
2	C	6	MAN	O5-C1-C2	-4.48	100.10	110.79
2	C	6	MAN	C1-C2-C3	-4.36	103.30	109.64
2	D	2	NAG	C1-O5-C5	4.33	117.99	112.19
2	C	5	MAN	O5-C5-C4	-4.25	100.48	110.83
2	C	1	NAG	O3-C3-C2	-4.23	100.62	109.40
2	D	2	NAG	C2-N2-C7	4.20	128.53	122.90
2	C	1	NAG	O4-C4-C3	-4.15	100.60	110.38
2	D	6	MAN	C1-O5-C5	4.11	117.70	112.19
2	C	1	NAG	O5-C5-C6	-4.08	99.73	107.66
2	D	6	MAN	O2-C2-C3	-3.86	102.17	110.15
2	C	6	MAN	O2-C2-C1	3.75	117.82	109.22
2	D	1	NAG	C6-C5-C4	3.63	121.94	113.02
2	C	3	BMA	O3-C3-C4	-3.61	101.86	110.38
2	D	4	MAN	O2-C2-C1	3.54	117.33	109.22
2	C	1	NAG	O5-C1-C2	-3.40	106.04	111.29
2	D	2	NAG	O4-C4-C5	3.39	117.68	109.32
2	D	5	MAN	C1-C2-C3	3.29	114.44	109.64
2	D	5	MAN	O5-C1-C2	-3.29	102.94	110.79
2	D	6	MAN	C1-C2-C3	3.26	114.39	109.64
2	D	2	NAG	C4-C3-C2	-3.24	106.27	111.02
2	D	5	MAN	O2-C2-C1	3.22	116.59	109.22
2	D	6	MAN	O4-C4-C5	-3.16	101.54	109.32
2	C	5	MAN	O3-C3-C4	-3.16	102.93	110.38
2	D	4	MAN	O3-C3-C4	3.15	117.81	110.38
2	D	2	NAG	O4-C4-C3	3.15	117.80	110.38
2	D	2	NAG	C1-C2-N2	3.03	115.20	110.43
2	D	6	MAN	O5-C5-C6	-2.97	101.88	107.66
2	D	6	MAN	O5-C1-C2	-2.89	103.89	110.79
2	D	2	NAG	O5-C1-C2	-2.81	106.94	111.29
2	D	5	MAN	O3-C3-C4	-2.78	103.82	110.38
2	C	3	BMA	C2-C3-C4	-2.75	106.03	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	6	MAN	O4-C4-C3	-2.74	103.92	110.38
2	D	1	NAG	O3-C3-C2	-2.73	103.72	109.40
2	D	2	NAG	O7-C7-C8	-2.72	117.22	122.05
2	D	5	MAN	C2-C3-C4	-2.66	106.19	110.86
2	D	1	NAG	O4-C4-C3	2.46	116.17	110.38
2	C	6	MAN	C2-C3-C4	-2.44	106.57	110.86
2	C	4	MAN	O2-C2-C3	-2.43	105.11	110.15
2	D	5	MAN	O3-C3-C2	2.41	114.96	110.05
2	D	4	MAN	C1-C2-C3	-2.40	106.14	109.64
2	C	1	NAG	C6-C5-C4	-2.37	107.19	113.02
2	C	5	MAN	O4-C4-C3	-2.37	104.79	110.38
2	D	2	NAG	O3-C3-C4	-2.35	104.83	110.38
2	C	3	BMA	O5-C5-C4	-2.30	105.22	110.83
2	C	3	BMA	O6-C6-C5	-2.30	103.52	111.33
2	C	6	MAN	O4-C4-C5	-2.27	103.73	109.32
2	C	3	BMA	O3-C3-C2	2.26	114.67	110.05
2	D	5	MAN	O4-C4-C5	-2.25	103.78	109.32
2	C	3	BMA	C6-C5-C4	-2.24	107.52	113.02
2	D	1	NAG	O5-C5-C4	-2.21	105.45	110.83
2	D	6	MAN	O3-C3-C4	-2.18	105.23	110.38
2	C	3	BMA	O4-C4-C5	-2.18	103.96	109.32
2	C	5	MAN	C1-O5-C5	-2.12	109.34	112.19
2	C	3	BMA	O5-C5-C6	2.10	111.76	107.66
2	C	6	MAN	O2-C2-C3	-2.09	105.83	110.15
2	D	4	MAN	C2-C3-C4	-2.07	107.22	110.86
2	C	6	MAN	C6-C5-C4	-2.06	107.95	113.02

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C1-C2-N2-C7
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2
2	D	5	MAN	C4-C5-C6-O6
2	D	5	MAN	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

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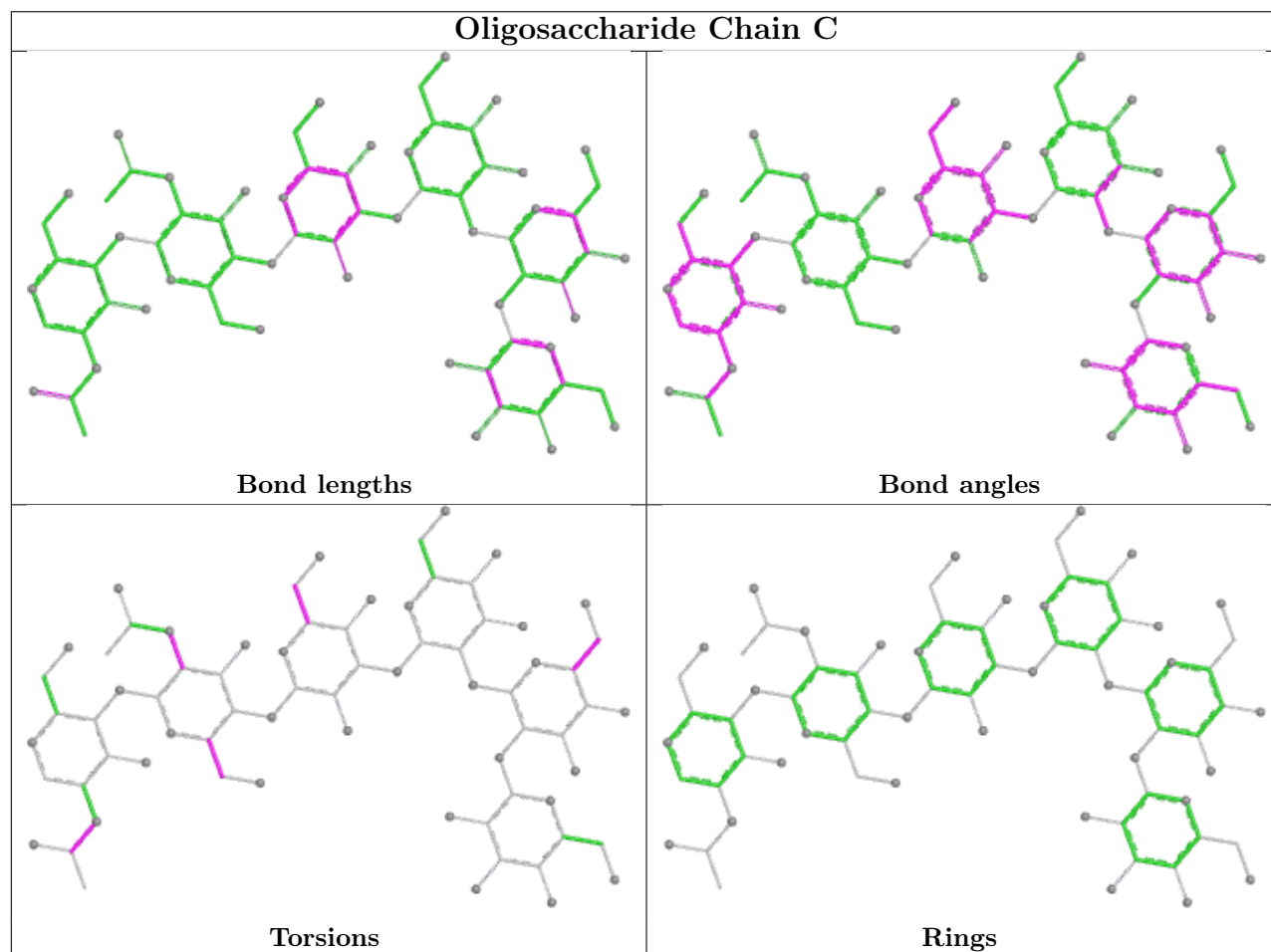
Mol	Chain	Res	Type	Atoms
2	C	5	MAN	C4-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7
2	D	4	MAN	O5-C5-C6-O6
2	D	2	NAG	O7-C7-N2-C2
2	C	5	MAN	O5-C5-C6-O6

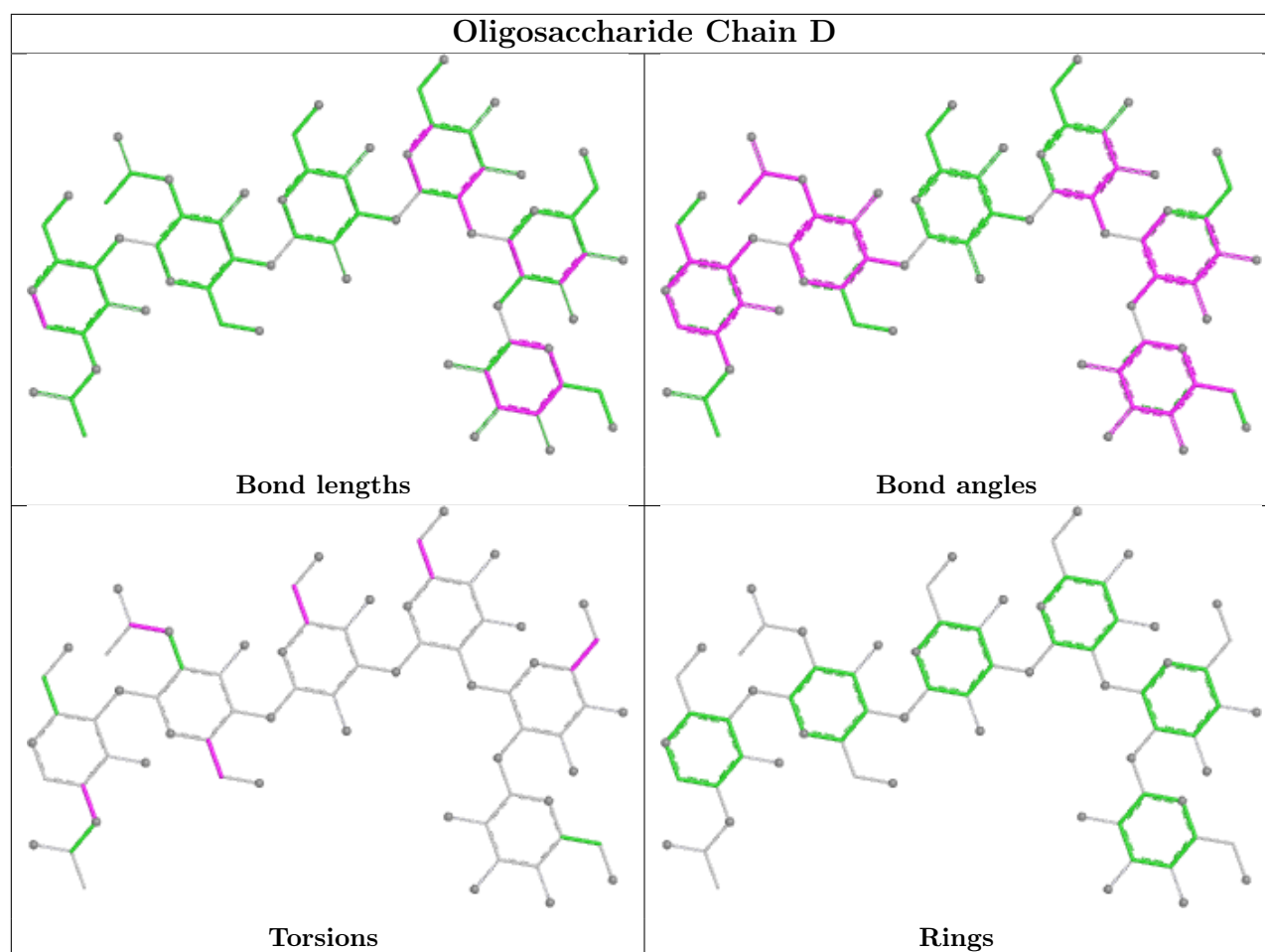
There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	MAN	1	0
2	D	6	MAN	1	0
2	D	3	BMA	3	0
2	C	3	BMA	1	0
2	C	2	NAG	8	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](#)

4 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	$\# Z > 2$
4	NAG	B	1702	1	14,14,15	1.30	2 (14%)	17,19,21	3.47	9 (52%)
4	NAG	A	1702	1	14,14,15	1.55	3 (21%)	17,19,21	1.70	5 (29%)
3	SO4	A	1701	-	4,4,4	0.34	0	6,6,6	0.07	0
4	NAG	B	1701	1	14,14,15	0.88	0	17,19,21	2.45	6 (35%)

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	B	1702	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1702	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1701	1	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1702	NAG	O5-C1	-3.51	1.37	1.43
4	B	1702	NAG	O5-C5	-3.29	1.37	1.43
4	A	1702	NAG	O5-C5	-2.74	1.38	1.43
4	B	1702	NAG	C4-C5	-2.50	1.47	1.53
4	A	1702	NAG	C1-C2	-2.41	1.49	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1702	NAG	O5-C1-C2	-9.20	97.05	111.29
4	B	1701	NAG	C4-C3-C2	-6.39	101.65	111.02
4	B	1702	NAG	C1-C2-N2	4.68	117.80	110.43
4	B	1702	NAG	C4-C3-C2	-4.34	104.66	111.02
4	B	1702	NAG	C1-O5-C5	4.11	117.69	112.19
4	B	1702	NAG	O4-C4-C3	3.76	119.23	110.38
4	A	1702	NAG	C2-N2-C7	3.59	127.71	122.90
4	B	1701	NAG	C1-C2-N2	3.42	115.83	110.43
4	B	1701	NAG	C6-C5-C4	-3.35	104.79	113.02
4	B	1702	NAG	O7-C7-N2	3.32	127.85	121.98
4	B	1701	NAG	O7-C7-N2	-3.26	116.21	121.98
4	A	1702	NAG	C4-C3-C2	3.26	115.80	111.02
4	B	1701	NAG	O5-C5-C6	3.22	113.93	107.66
4	B	1702	NAG	C6-C5-C4	-3.10	105.41	113.02
4	B	1702	NAG	C8-C7-N2	-2.82	111.44	116.12
4	B	1702	NAG	O5-C5-C4	-2.80	104.02	110.83
4	B	1701	NAG	C3-C4-C5	-2.57	105.57	110.23
4	A	1702	NAG	O5-C1-C2	-2.54	107.35	111.29
4	A	1702	NAG	O5-C5-C4	-2.29	105.25	110.83
4	A	1702	NAG	C1-C2-N2	-2.06	107.19	110.43

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1702	NAG	C8-C7-N2-C2
4	B	1702	NAG	O7-C7-N2-C2
4	A	1702	NAG	O5-C5-C6-O6
4	B	1701	NAG	C8-C7-N2-C2
4	B	1701	NAG	O7-C7-N2-C2
4	A	1702	NAG	C4-C5-C6-O6
4	B	1701	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1701	SO4	1	0
4	B	1701	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	686/737 (93%)	-0.52	4 (0%)	85 66	113, 187, 275, 334	0
1	B	665/737 (90%)	-0.53	1 (0%)	91 82	118, 200, 248, 294	0
All	All	1351/1474 (91%)	-0.53	5 (0%)	88 73	113, 195, 266, 334	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1088	ASP	2.3
1	A	1585	ASP	2.3
1	A	1169	ILE	2.3
1	A	1255	TYR	2.1
1	B	978	THR	2.0

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

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

6.3 Carbohydrates

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

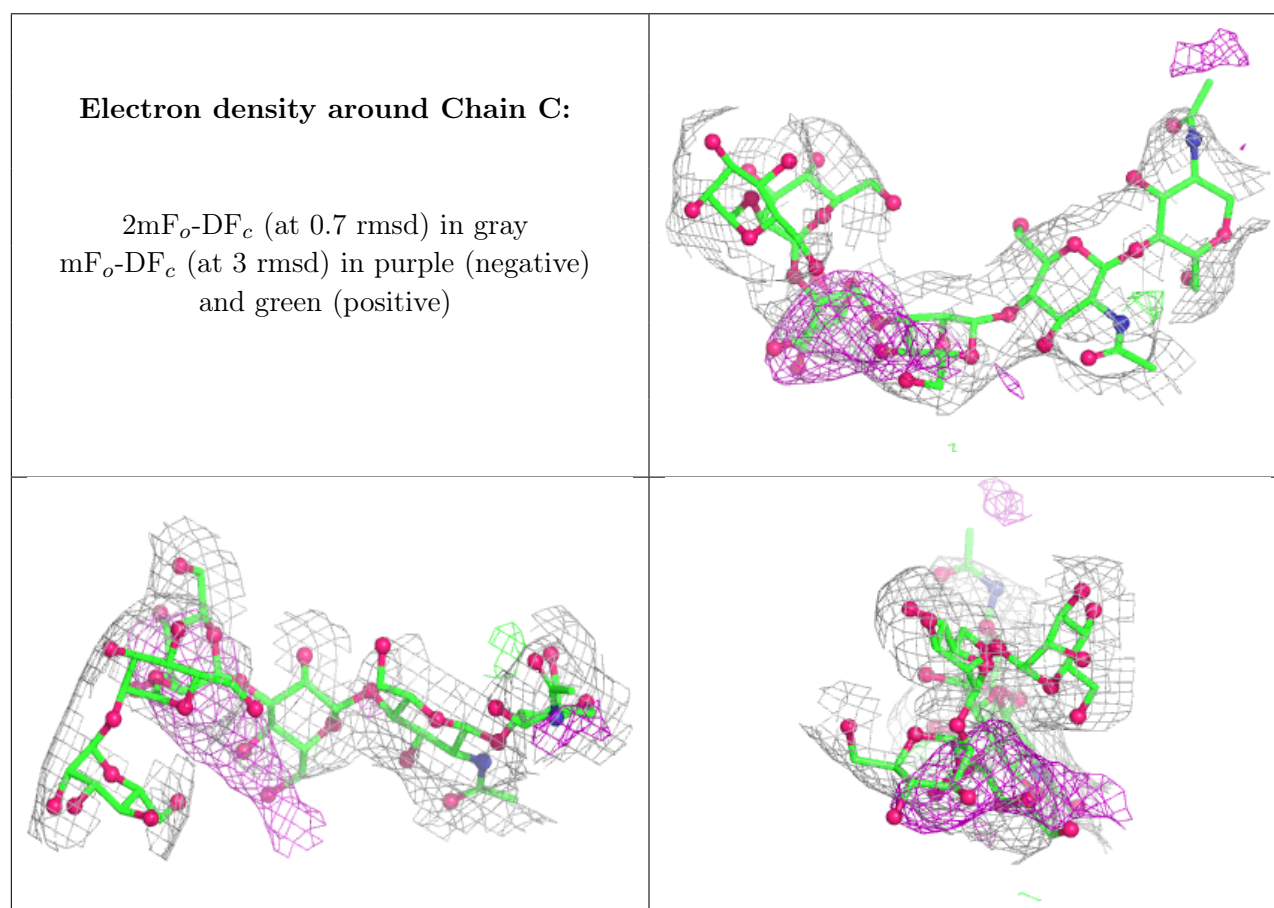
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	D	4	11/12	0.45	0.11	192,207,222,248	0
2	MAN	C	4	11/12	0.52	0.10	174,198,211,232	0
2	BMA	D	3	11/12	0.56	0.10	154,166,197,204	0
2	NAG	D	2	14/15	0.71	0.07	179,233,251,269	0

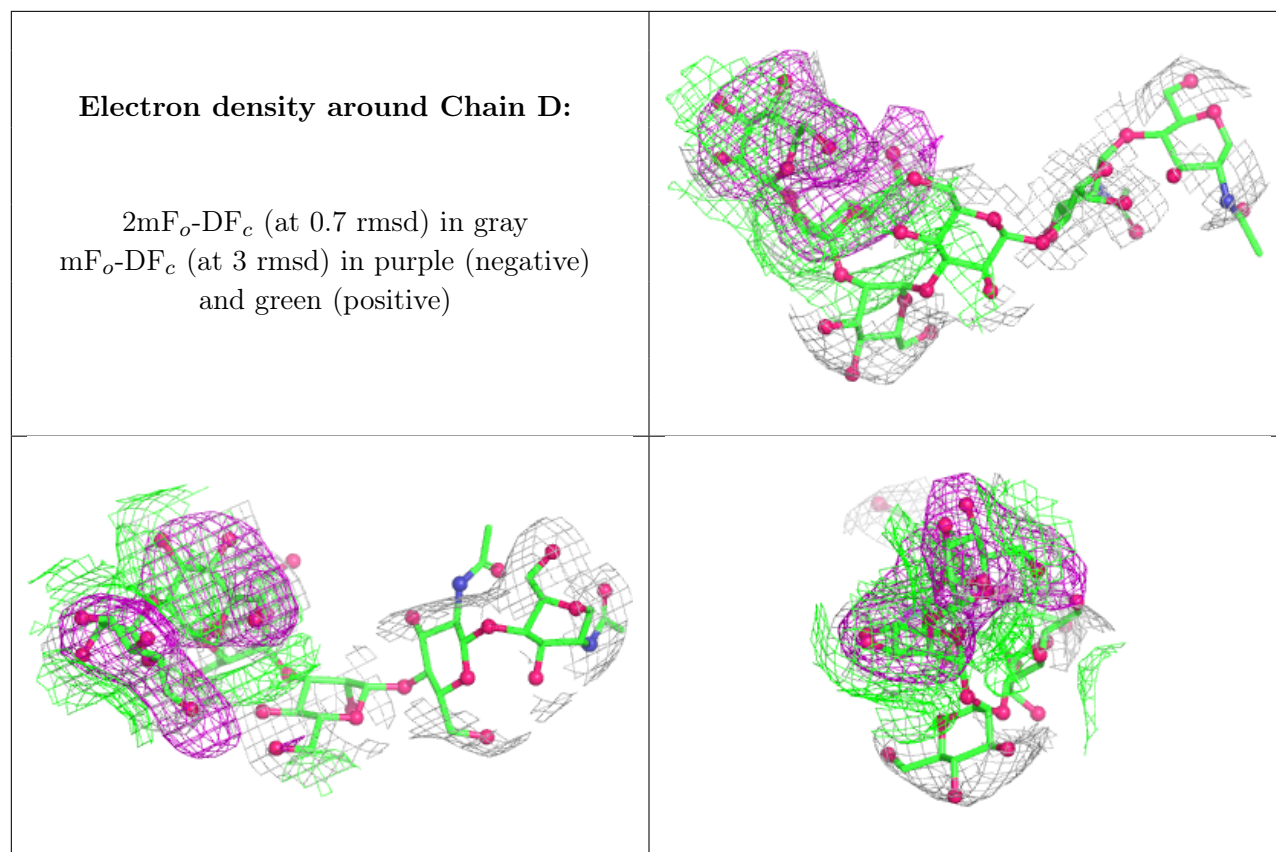
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	2	14/15	0.77	0.08	185,230,255,258	0
2	BMA	C	3	11/12	0.83	0.10	144,158,181,199	0
2	MAN	D	5	11/12	0.84	0.20	30,30,30,30	0
2	NAG	C	1	14/15	0.87	0.10	161,192,236,244	0
2	MAN	D	6	11/12	0.89	0.19	30,30,30,30	0
2	NAG	D	1	14/15	0.91	0.07	119,162,218,225	0
2	MAN	C	5	11/12	0.93	0.05	152,163,183,183	0
2	MAN	C	6	11/12	0.94	0.05	149,180,211,224	0

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





6.4 Ligands [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
4	NAG	B	1702	14/15	0.50	0.13	155,179,210,226	0
4	NAG	A	1702	14/15	0.74	0.07	155,179,185,185	0
4	NAG	B	1701	14/15	0.75	0.07	192,209,231,234	0
3	SO4	A	1701	5/5	0.83	0.05	157,173,190,198	0

6.5 Other polymers [i](#)

There are no such residues in this entry.