



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 12:38 PM BST

PDB ID : 6RYF
Title : High-resolution crystal structure of ERAP1 in complex with 15mer phosphinic peptide
Authors : Giastas, P.; Stratikos, E.
Deposited on : 2019-06-10
Resolution : 1.72 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

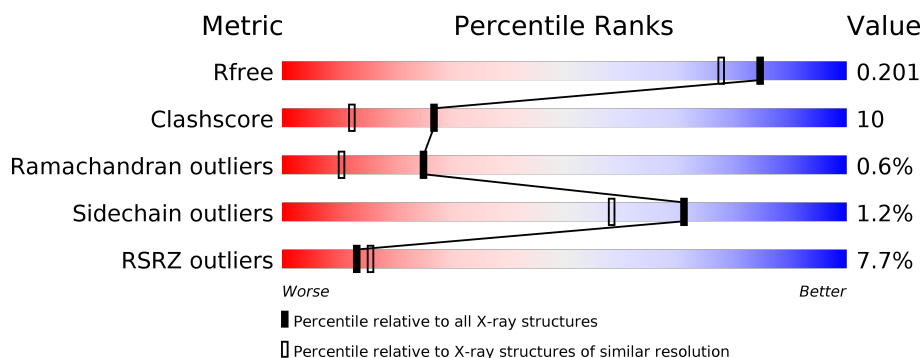
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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}	130704	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 on 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	894	<div> <div>7%</div> <div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>
2	G	14	<div> <div>43%</div> <div> <div>21%</div> <div>50%</div> <div>29%</div> </div> </div>
3	B	2	<div> <div>50%</div> <div>50%</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	2	-	-	-	X
3	NAG	C	2	-	-	-	X
6	EDO	A	1004	-	-	X	-
9	NAG	A	1033	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8020 atoms, of which 157 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 Endoplasmic reticulum aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	856	Total	C	N	O	S	0	15	0
			6943	4481	1144	1283	35			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	939	ARG	-	expression tag	UNP Q9NZ08

- Molecule 2 is a protein called PSE-ARG-ILE-GLN-ARG-ALA-PHE-VAL-THR-ILE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	10	Total	C	N	O	P	0	6	0
			134	91	21	21	1			

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

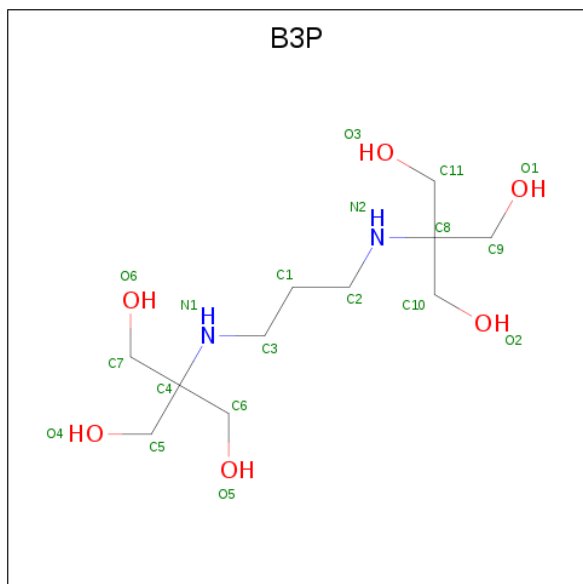


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

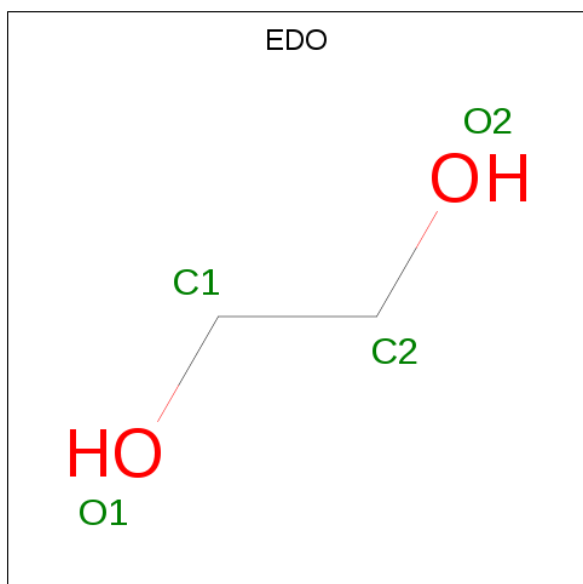
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			45	11	26	2	6		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			10	2	6	2		

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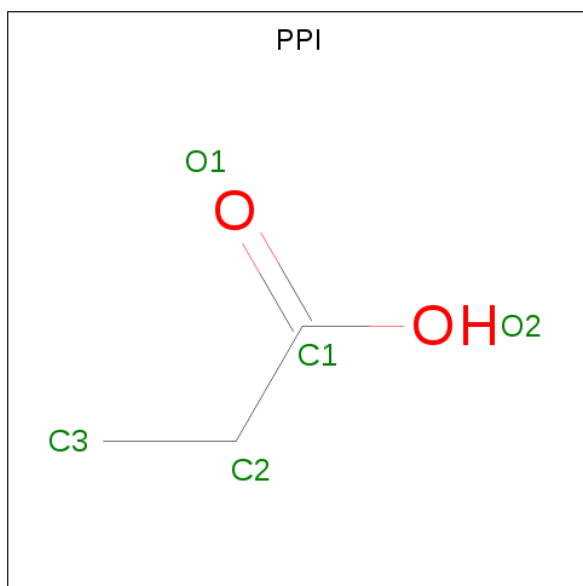
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

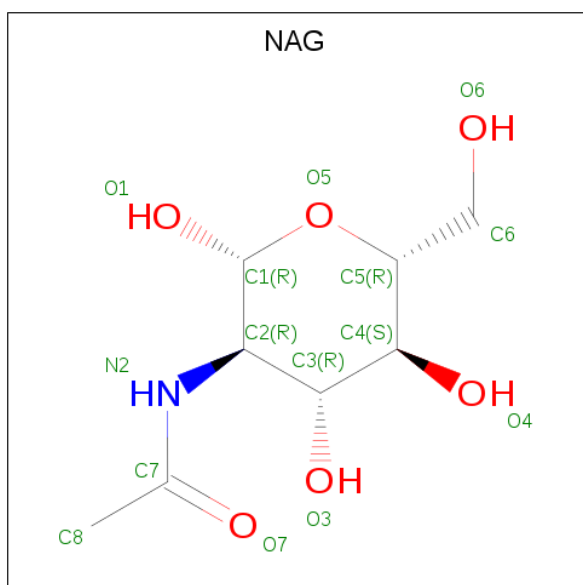
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Na	0	0
			4	4		

- Molecule 8 is PROPANOIC ACID (three-letter code: PPI) (formula: $C_3H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			10	3	5	2		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

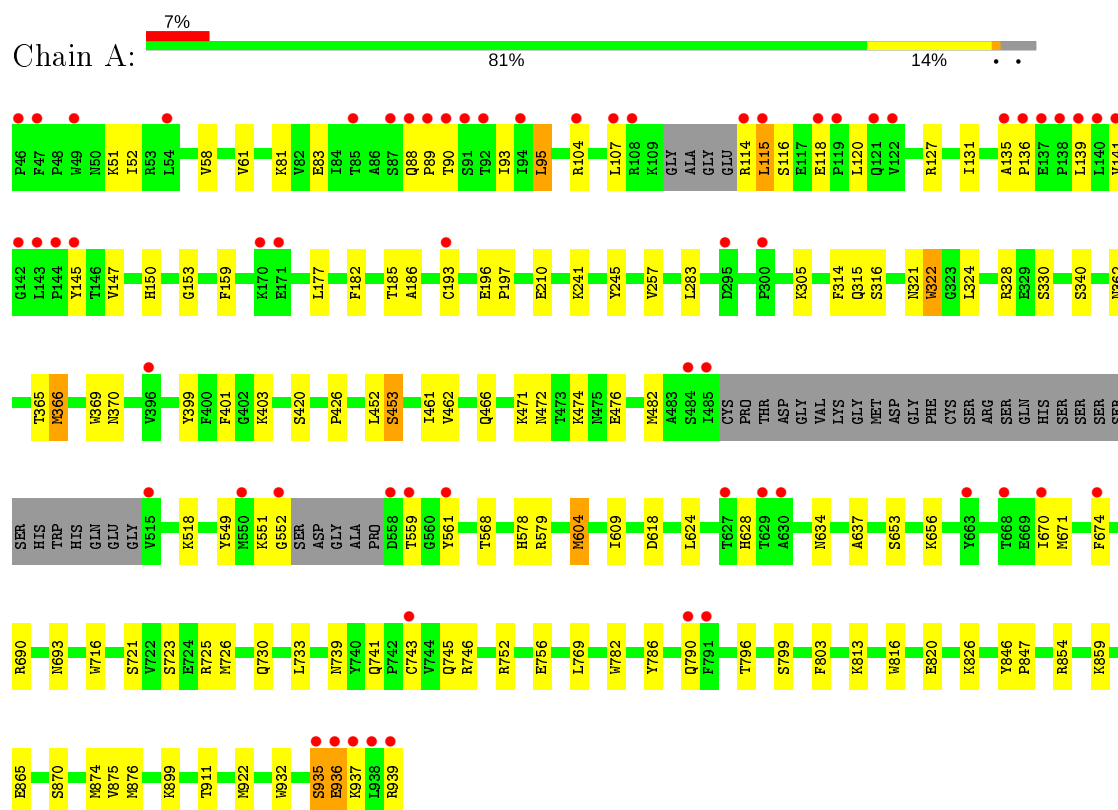
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	582	Total	O	0	0
			582	582		
10	G	7	Total	O	0	0
			7	7		

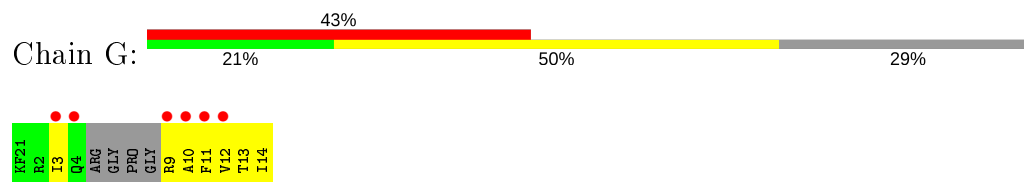
3 Residue-property plots

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: Endoplasmic reticulum aminopeptidase 1



- Molecule 2: PSE-ARG-ILE-GLN-ARG-ALA-PHE-VAL-THR-ILE



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





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

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	57.69Å 117.16Å 146.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.52 – 1.72 91.52 – 1.72	Depositor EDS
% Data completeness (in resolution range)	100.0 (91.52-1.72) 100.0 (91.52-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.72Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.176 , 0.201 0.176 , 0.201	Depositor DCC
R_{free} test set	1498 reflections (1.41%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8020	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, KF2, NAG, NA, PPI, B3P, EDO

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	0.40	3/7159 (0.0%)	0.54	0/9706
2	G	0.53	0/111	0.57	0/142
All	All	0.40	3/7270 (0.0%)	0.54	0/9848

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	CYS	CB-SG	-6.06	1.72	1.82
1	A	743[A]	CYS	CB-SG	5.43	1.91	1.82
1	A	743[B]	CYS	CB-SG	5.43	1.91	1.82

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	LEU	Peptide

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	6943	0	6871	138	0
2	G	134	0	120	24	0
3	B	28	0	25	1	0
3	C	28	0	25	1	0
4	A	1	0	0	0	0
5	A	19	26	26	0	0
6	A	84	126	126	20	0
7	A	4	0	0	0	0
8	A	5	5	5	3	0
9	A	28	0	26	0	0
10	A	582	0	0	9	2
10	G	7	0	0	1	0
All	All	7863	157	7224	148	2

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 10.

All (148) 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:604[B]:MET:HE2	1:A:634:ASN:O	1.57	1.04
1:A:340:SER:OG	2:G:9[B]:ARG:HB2	1.66	0.95
1:A:579[B]:ARG:H	8:A:1028:PPI:H33	1.36	0.89
1:A:579[A]:ARG:H	8:A:1028:PPI:H33	1.37	0.89
2:G:11[B]:PHE:CE2	2:G:13[B]:THR:HG22	2.08	0.89
1:A:716:TRP:H	6:A:1014:EDO:H11	1.38	0.88
1:A:114:ARG:N	10:A:1101:HOH:O	2.06	0.87
1:A:403:LYS:NZ	10:A:1103:HOH:O	2.08	0.86
2:G:11[B]:PHE:CZ	2:G:13[B]:THR:HG22	2.13	0.83
2:G:3:ILE:HD11	10:G:105:HOH:O	1.80	0.79
1:A:245:TYR:HB3	6:A:1015:EDO:H21	1.64	0.77
1:A:340:SER:HG	2:G:9[B]:ARG:HB2	1.48	0.77
1:A:107:LEU:HB2	1:A:120:LEU:HD11	1.69	0.75
1:A:401:PHE:CE1	1:A:604[B]:MET:HE1	2.24	0.72
1:A:769:LEU:HD21	2:G:10[B]:ALA:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:SER:O	1:A:328:ARG:HD2	1.90	0.71
1:A:752:ARG:O	1:A:756[A]:GLU:HG3	1.91	0.70
1:A:730:GLN:HG2	2:G:11[A]:PHE:CE1	2.26	0.70
1:A:89:PRO:HD3	1:A:141:VAL:HG11	1.74	0.69
1:A:674[A]:PHE:CZ	2:G:11[A]:PHE:HZ	2.12	0.68
1:A:114:ARG:O	1:A:115:LEU:HD13	1.95	0.67
1:A:936:GLU:OE2	1:A:939:ARG:HA	1.95	0.67
1:A:741:GLN:O	1:A:745:GLN:HG3	1.95	0.67
1:A:769:LEU:HD11	2:G:10[B]:ALA:HA	1.77	0.66
1:A:426:PRO:HD3	6:A:1016:EDO:H22	1.78	0.64
1:A:876:MET:HG2	1:A:911[A]:THR:CG2	2.27	0.64
1:A:670:ILE:HD11	1:A:674[A]:PHE:CE2	2.34	0.63
1:A:476:GLU:HG3	1:A:518:LYS:HE2	1.82	0.62
1:A:472:ASN:HB2	6:A:1010:EDO:H12	1.80	0.62
1:A:799[B]:SER:OG	2:G:10[B]:ALA:HB3	2.00	0.62
1:A:899:LYS:N	1:A:899:LYS:HD2	2.13	0.62
1:A:859:LYS:HD3	10:A:1164:HOH:O	2.01	0.60
1:A:366:MET:CE	1:A:369:TRP:CZ3	2.86	0.59
2:G:9[B]:ARG:O	2:G:10[B]:ALA:HB3	2.02	0.58
1:A:107:LEU:HD11	1:A:145:TYR:CD1	2.39	0.58
1:A:61:VAL:HG22	1:A:83:GLU:HB2	1.85	0.58
1:A:366:MET:HE3	1:A:369:TRP:CZ3	2.38	0.58
1:A:370:ASN:HD22	6:A:1004:EDO:H12	1.68	0.58
1:A:674[A]:PHE:CZ	2:G:11[A]:PHE:CZ	2.92	0.57
1:A:820:GLU:OE1	1:A:826:LYS:HG3	2.03	0.57
1:A:89:PRO:HD3	1:A:141:VAL:CG1	2.34	0.57
1:A:52:ILE:HG23	6:A:1016:EDO:H21	1.86	0.57
1:A:730:GLN:HG2	2:G:11[A]:PHE:CZ	2.39	0.57
1:A:670:ILE:HG13	1:A:674[A]:PHE:CE1	2.40	0.57
1:A:462:VAL:O	1:A:466:GLN:HG3	2.05	0.56
1:A:197:PRO:HD3	6:A:1015:EDO:H12	1.87	0.56
1:A:670:ILE:HG21	1:A:723[A]:SER:OG	2.05	0.56
2:G:3:ILE:O	2:G:3:ILE:HG12	2.05	0.56
1:A:399:TYR:OH	1:A:726:MET:HE1	2.05	0.55
1:A:401:PHE:CZ	1:A:604[B]:MET:HE1	2.41	0.55
1:A:932:TRP:O	1:A:936:GLU:HB2	2.08	0.54
1:A:670:ILE:HG13	1:A:674[A]:PHE:CZ	2.42	0.54
1:A:471:LYS:HB3	6:A:1010:EDO:O2	2.06	0.54
1:A:670:ILE:CG1	1:A:674[A]:PHE:CZ	2.90	0.54
1:A:104:ARG:HG3	1:A:150:HIS:HD2	1.70	0.54
1:A:366:MET:CE	1:A:369:TRP:CE3	2.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ASP:OD2	10:A:1105:HOH:O	2.18	0.54
1:A:120:LEU:HD23	1:A:135:ALA:HA	1.89	0.54
1:A:936:GLU:OE2	1:A:939:ARG:CA	2.56	0.53
1:A:670:ILE:HD11	1:A:674[A]:PHE:CZ	2.44	0.53
1:A:365:THR:O	1:A:472:ASN:HA	2.09	0.53
1:A:690:ARG:HE	6:A:1017:EDO:H12	1.74	0.52
1:A:107:LEU:HD11	1:A:145:TYR:HD1	1.74	0.52
1:A:935:SER:O	1:A:937:LYS:N	2.42	0.52
1:A:461:ILE:CG2	1:A:482:MET:HE2	2.39	0.52
1:A:769:LEU:HD11	2:G:10[B]:ALA:CA	2.39	0.52
1:A:89:PRO:CD	1:A:141:VAL:CG1	2.89	0.51
1:A:90:THR:O	1:A:139:LEU:HB2	2.10	0.51
1:A:153:GLY:HA2	3:B:1:NAG:H82	1.93	0.51
1:A:549:TYR:CD2	1:A:609:ILE:HD11	2.46	0.50
1:A:61:VAL:CG2	1:A:83:GLU:HB2	2.41	0.50
1:A:693:ASN:ND2	10:A:1102:HOH:O	2.08	0.49
1:A:370:ASN:ND2	6:A:1004:EDO:H12	2.27	0.49
1:A:870:SER:O	1:A:874:MET:HG3	2.13	0.49
1:A:876:MET:HG2	1:A:911[A]:THR:HG22	1.94	0.49
1:A:159:PHE:CB	1:A:315:GLN:HB2	2.43	0.49
1:A:58:VAL:HG11	1:A:93:ILE:HG23	1.94	0.49
1:A:399:TYR:CZ	1:A:726:MET:HE1	2.48	0.48
1:A:461:ILE:HG22	1:A:482:MET:HE2	1.96	0.48
1:A:81:LYS:HA	1:A:147:VAL:O	2.13	0.48
1:A:846:TYR:CG	1:A:847:PRO:HD3	2.48	0.48
1:A:88:GLN:HA	1:A:141:VAL:CG1	2.43	0.47
1:A:95:LEU:HD12	1:A:131:ILE:HG13	1.96	0.47
1:A:899:LYS:H	1:A:899:LYS:HD2	1.79	0.47
1:A:114:ARG:C	1:A:115:LEU:HD22	2.35	0.47
1:A:716:TRP:N	6:A:1014:EDO:H11	2.18	0.47
1:A:330:SER:HB2	2:G:9[B]:ARG:NH2	2.30	0.47
1:A:401:PHE:CE2	1:A:671:MET:HE2	2.50	0.47
2:G:14[B]:ILE:OXT	2:G:14[B]:ILE:HD12	2.14	0.47
1:A:210:GLU:HG3	3:C:1:NAG:H83	1.96	0.47
1:A:568:THR:HA	1:A:578:HIS:O	2.15	0.47
1:A:721:SER:O	1:A:725:ARG:HG3	2.14	0.47
1:A:875:VAL:HG12	1:A:911[A]:THR:HG21	1.97	0.47
1:A:401:PHE:CD1	1:A:604[B]:MET:HE1	2.49	0.47
1:A:803:PHE:HZ	2:G:14[B]:ILE:HD11	1.79	0.46
1:A:104:ARG:NH1	10:A:1129:HOH:O	2.48	0.46
1:A:340:SER:OG	2:G:9[B]:ARG:CB	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:LEU:O	1:A:628:HIS:HB3	2.15	0.46
1:A:196:GLU:CA	6:A:1015:EDO:H11	2.47	0.45
1:A:51:LYS:HD3	6:A:1011:EDO:H11	1.98	0.45
1:A:399:TYR:CE1	1:A:726:MET:HE1	2.51	0.45
1:A:674[A]:PHE:CE1	2:G:11[A]:PHE:HZ	2.34	0.45
6:A:1008:EDO:O2	10:A:1107:HOH:O	2.21	0.45
1:A:733:LEU:HD22	1:A:769:LEU:HD13	1.98	0.45
1:A:653:SER:OG	1:A:656:LYS:HG2	2.17	0.45
1:A:89:PRO:CD	1:A:141:VAL:HG13	2.46	0.45
1:A:674[A]:PHE:CE2	2:G:11[A]:PHE:CZ	3.05	0.45
1:A:118:GLU:OE2	1:A:136:PRO:HG2	2.16	0.45
1:A:604[B]:MET:CE	1:A:637:ALA:HB3	2.47	0.44
1:A:739:ASN:OD1	1:A:741:GLN:NE2	2.51	0.44
1:A:854:ARG:HB3	6:A:1008:EDO:H21	1.98	0.44
1:A:95:LEU:HD11	1:A:131:ILE:HD11	1.99	0.44
1:A:322:TRP:CD2	1:A:362:ASN:HB3	2.53	0.44
1:A:182:PHE:HA	1:A:186:ALA:HB3	1.99	0.44
1:A:452:LEU:O	1:A:453:SER:CB	2.65	0.44
1:A:782:TRP:CD2	1:A:813:LYS:HD2	2.52	0.43
1:A:88:GLN:HA	1:A:141:VAL:HG11	2.00	0.43
1:A:401:PHE:CD1	1:A:604[B]:MET:CE	3.01	0.43
1:A:559:THR:HG23	1:A:561:TYR:H	1.84	0.43
1:A:314:PHE:HB3	1:A:328:ARG:HG3	2.01	0.43
1:A:461:ILE:CG2	1:A:482:MET:CE	2.97	0.43
1:A:796:THR:HA	2:G:9[B]:ARG:HE	1.84	0.43
1:A:241:LYS:HB3	1:A:241:LYS:HE3	1.74	0.43
1:A:604[B]:MET:HE1	1:A:637:ALA:HB3	2.01	0.43
1:A:670:ILE:HB	10:A:1117:HOH:O	2.17	0.43
1:A:786:TYR:O	1:A:790:GLN:OE1	2.36	0.43
2:G:9[B]:ARG:O	2:G:10[B]:ALA:CB	2.67	0.43
1:A:551:LYS:HA	1:A:552:GLY:HA2	1.61	0.42
1:A:366:MET:HE2	1:A:369:TRP:CE3	2.54	0.42
1:A:604[B]:MET:HE2	1:A:634:ASN:C	2.34	0.42
1:A:876:MET:HG2	1:A:911[A]:THR:HG23	2.01	0.42
1:A:321:ASN:HB2	1:A:324:LEU:O	2.20	0.42
1:A:474:LYS:HE2	10:A:1381:HOH:O	2.20	0.42
1:A:88:GLN:CA	1:A:141:VAL:HG12	2.50	0.42
1:A:420[B]:SER:HB3	6:A:1004:EDO:H11	2.02	0.42
1:A:257:VAL:HG23	1:A:283:LEU:HD22	2.02	0.41
2:G:11[B]:PHE:HE2	2:G:13[B]:THR:HG22	1.78	0.41
1:A:185:THR:O	6:A:1003:EDO:H21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:LYS:HE3	1:A:899:LYS:HA	2.03	0.41
1:A:52:ILE:HB	6:A:1011:EDO:H22	2.02	0.41
1:A:401:PHE:CD2	1:A:604[B]:MET:HE3	2.55	0.41
1:A:816:TRP:CZ2	1:A:820:GLU:HG3	2.56	0.41
1:A:420[A]:SER:OG	6:A:1004:EDO:H11	2.21	0.41
1:A:127:ARG:HD2	1:A:127:ARG:HA	1.93	0.40
1:A:716:TRP:HB2	6:A:1014:EDO:H22	2.02	0.40
1:A:104:ARG:HG2	1:A:150:HIS:HB2	2.04	0.40
1:A:786:TYR:CZ	1:A:790:GLN:NE2	2.89	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1403:HOH:O	10:A:1403:HOH:O[2_51111]	2.18	0.02
10:A:1676:HOH:O	10:A:1682:HOH:O[4_-16115]	2.18	0.02

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	863/894 (96%)	837 (97%)	22 (2%)	4 (0%)	29	13
2	G	10/14 (71%)	6 (60%)	2 (20%)	2 (20%)	0	0
All	All	873/908 (96%)	843 (97%)	24 (3%)	6 (1%)	25	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	936	GLU
1	A	116	SER
1	A	453	SER

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Mol	Chain	Res	Type
1	A	865	GLU
2	G	12[A]	VAL
2	G	12[B]	VAL

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	768/796 (96%)	757 (99%)	11 (1%)	67	52
2	G	11/10 (110%)	11 (100%)	0	100	100
All	All	779/806 (97%)	768 (99%)	11 (1%)	71	52

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	A	177	LEU
1	A	305	LYS
1	A	322	TRP
1	A	366	MET
1	A	604[A]	MET
1	A	604[B]	MET
1	A	746[A]	ARG
1	A	746[B]	ARG
1	A	922	MET
1	A	935	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	605	ASN
1	A	642	ASN
1	A	741	GLN
1	A	790	GLN

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Mol	Chain	Res	Type
1	A	934	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 ⓘ

4 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	$\# Z > 2$
3	NAG	B	1	1,3	14,14,15	0.41	0	17,19,21	0.65	0
3	NAG	B	2	3	14,14,15	0.36	0	17,19,21	0.49	0
3	NAG	C	1	1,3	14,14,15	0.35	0	17,19,21	0.36	0
3	NAG	C	2	3	14,14,15	0.33	0	17,19,21	0.53	0

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
3	NAG	B	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

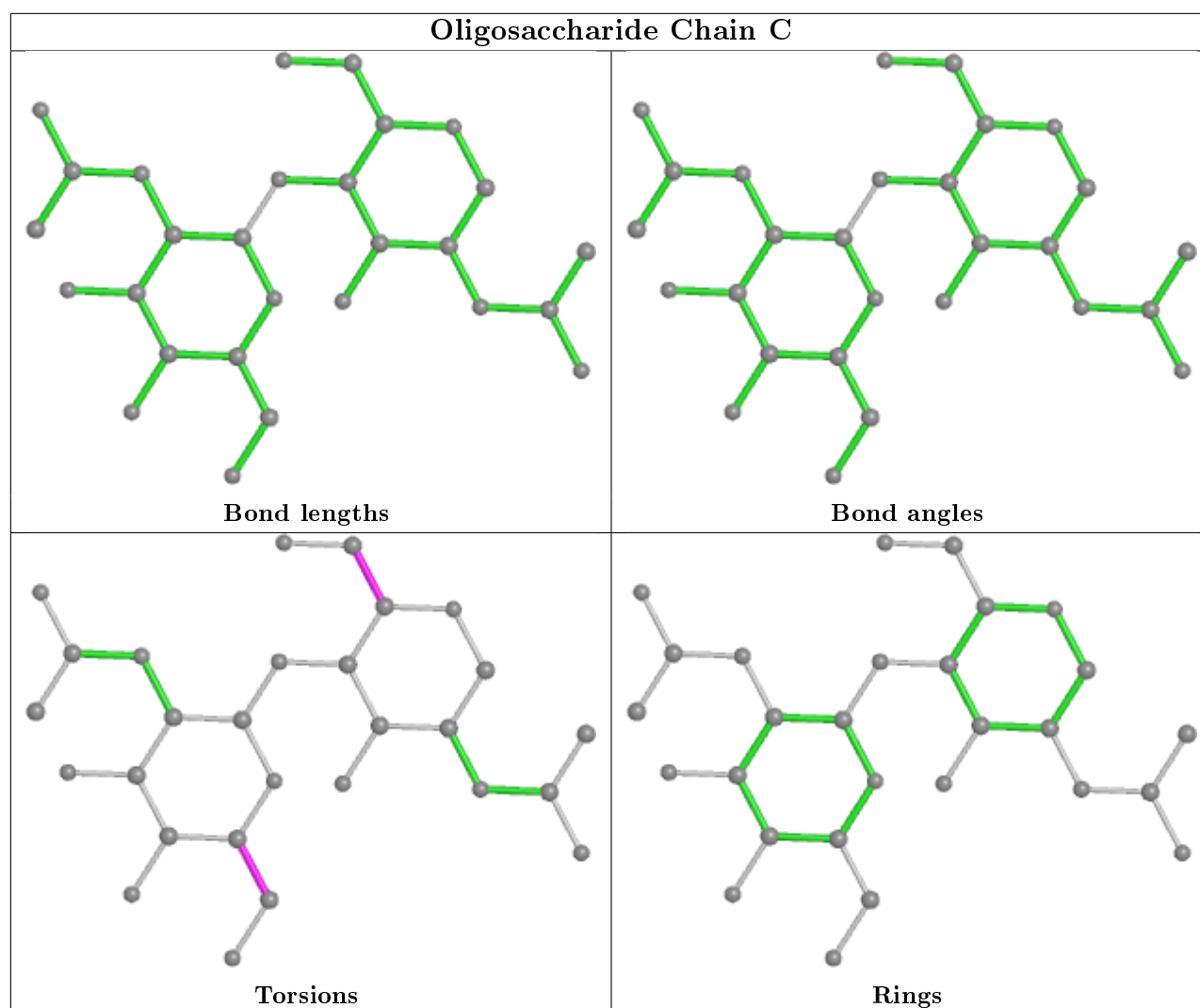
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
3	B	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 5 are monoatomic - leaving 25 for Mogul analysis.

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	$\# Z > 2$
9	NAG	A	1033	1	14,14,15	0.17	0	17,19,21	0.46	0
5	B3P	A	1002	-	18,18,18	0.57	0	21,23,23	1.07	1 (4%)
6	EDO	A	1009	-	3,3,3	0.47	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	1011	-	3,3,3	0.49	0	2,2,2	0.25	0
6	EDO	A	1023	-	3,3,3	0.45	0	2,2,2	0.33	0
6	EDO	A	1007	-	3,3,3	0.51	0	2,2,2	0.31	0
6	EDO	A	1022	-	3,3,3	0.48	0	2,2,2	0.25	0
6	EDO	A	1010	-	3,3,3	0.44	0	2,2,2	0.32	0
6	EDO	A	1006	-	3,3,3	0.46	0	2,2,2	0.07	0
6	EDO	A	1005	-	3,3,3	0.49	0	2,2,2	0.52	0
6	EDO	A	1017	-	3,3,3	0.50	0	2,2,2	0.24	0
6	EDO	A	1012	-	3,3,3	0.49	0	2,2,2	0.20	0
6	EDO	A	1020	-	3,3,3	0.37	0	2,2,2	0.61	0
6	EDO	A	1008	-	3,3,3	0.39	0	2,2,2	0.39	0
6	EDO	A	1018	-	3,3,3	0.50	0	2,2,2	0.27	0
8	PPI	A	1028	-	1,4,4	0.36	0	1,4,4	0.62	0
6	EDO	A	1014	-	3,3,3	0.46	0	2,2,2	0.41	0
6	EDO	A	1003	-	3,3,3	0.46	0	2,2,2	0.09	0
6	EDO	A	1019	-	3,3,3	0.49	0	2,2,2	0.30	0
6	EDO	A	1015	-	3,3,3	0.31	0	2,2,2	0.57	0
6	EDO	A	1021	-	3,3,3	0.49	0	2,2,2	0.28	0
9	NAG	A	1034	1	14,14,15	0.58	0	17,19,21	0.53	0
6	EDO	A	1016	-	3,3,3	0.39	0	2,2,2	0.46	0
6	EDO	A	1004	-	3,3,3	0.49	0	2,2,2	0.32	0
6	EDO	A	1013	-	3,3,3	0.45	0	2,2,2	0.33	0

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
9	NAG	A	1033	1	-	2/6/23/26	0/1/1/1
5	B3P	A	1002	-	-	2/28/28/28	-
6	EDO	A	1009	-	-	1/1/1/1	-
6	EDO	A	1011	-	-	1/1/1/1	-
6	EDO	A	1023	-	-	0/1/1/1	-
6	EDO	A	1007	-	-	0/1/1/1	-
6	EDO	A	1022	-	-	1/1/1/1	-
6	EDO	A	1010	-	-	1/1/1/1	-
6	EDO	A	1006	-	-	0/1/1/1	-
6	EDO	A	1005	-	-	0/1/1/1	-
6	EDO	A	1017	-	-	1/1/1/1	-
6	EDO	A	1012	-	-	1/1/1/1	-
6	EDO	A	1020	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	1008	-	-	0/1/1/1	-
6	EDO	A	1018	-	-	1/1/1/1	-
8	PPI	A	1028	-	-	0/0/2/2	-
6	EDO	A	1014	-	-	1/1/1/1	-
6	EDO	A	1003	-	-	1/1/1/1	-
6	EDO	A	1019	-	-	0/1/1/1	-
6	EDO	A	1015	-	-	0/1/1/1	-
6	EDO	A	1021	-	-	0/1/1/1	-
9	NAG	A	1034	1	-	0/6/23/26	0/1/1/1
6	EDO	A	1016	-	-	0/1/1/1	-
6	EDO	A	1004	-	-	1/1/1/1	-
6	EDO	A	1013	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	B3P	C11-C8-C10	-3.16	103.37	110.04

There are no chirality outliers.

All (16) torsion outliers are listed below:

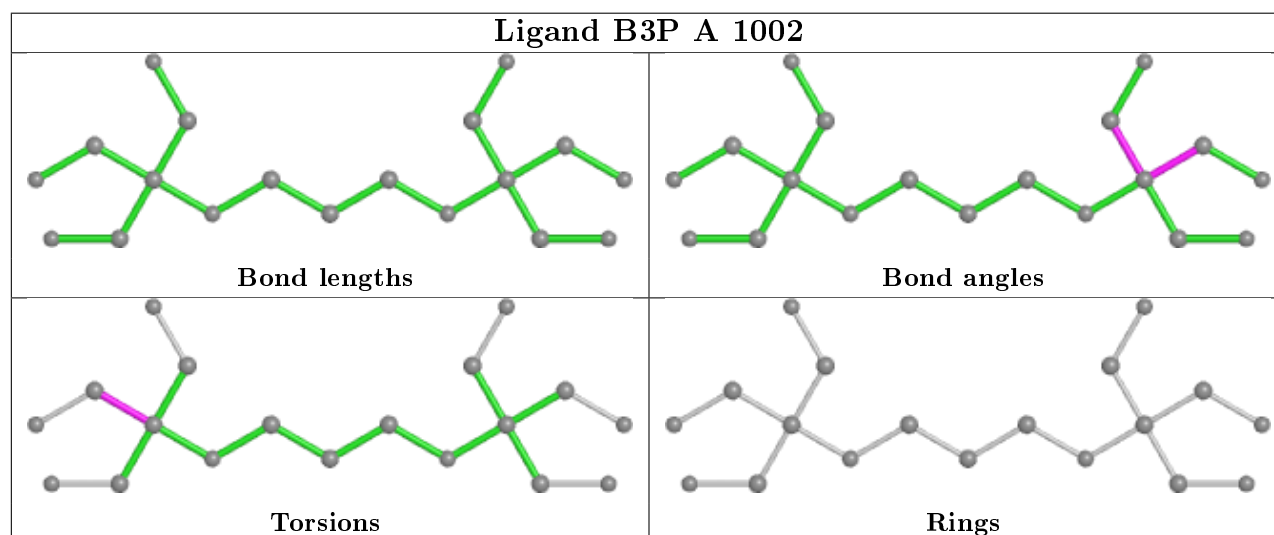
Mol	Chain	Res	Type	Atoms
9	A	1033	NAG	O5-C5-C6-O6
9	A	1033	NAG	C4-C5-C6-O6
5	A	1002	B3P	N1-C4-C6-O5
6	A	1009	EDO	O1-C1-C2-O2
6	A	1010	EDO	O1-C1-C2-O2
6	A	1018	EDO	O1-C1-C2-O2
6	A	1003	EDO	O1-C1-C2-O2
6	A	1011	EDO	O1-C1-C2-O2
6	A	1017	EDO	O1-C1-C2-O2
6	A	1012	EDO	O1-C1-C2-O2
6	A	1004	EDO	O1-C1-C2-O2
6	A	1020	EDO	O1-C1-C2-O2
6	A	1014	EDO	O1-C1-C2-O2
6	A	1013	EDO	O1-C1-C2-O2
6	A	1022	EDO	O1-C1-C2-O2
5	A	1002	B3P	C7-C4-C6-O5

There are no ring outliers.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1011	EDO	2	0
6	A	1010	EDO	2	0
6	A	1017	EDO	1	0
6	A	1008	EDO	2	0
8	A	1028	PPI	3	0
6	A	1014	EDO	3	0
6	A	1003	EDO	1	0
6	A	1015	EDO	3	0
6	A	1016	EDO	2	0
6	A	1004	EDO	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	856/894 (95%)	0.68	61 (7%) 16 18	21, 34, 64, 107	0
2	G	9/14 (64%)	3.53	6 (66%) 0 0	33, 38, 73, 85	1 (11%)
All	All	865/908 (95%)	0.70	67 (7%) 13 16	21, 34, 65, 107	1 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	11[A]	PHE	8.1
1	A	89	PRO	7.8
1	A	938	LEU	7.3
2	G	10[A]	ALA	6.6
1	A	937	LYS	6.2
1	A	939	ARG	6.2
1	A	143	LEU	6.1
1	A	142	GLY	6.0
1	A	107	LEU	5.7
1	A	171	GLU	5.5
1	A	114	ARG	5.5
1	A	87	SER	5.4
1	A	629	THR	5.2
1	A	559	THR	5.1
1	A	627	THR	5.1
1	A	85	THR	5.1
1	A	936	GLU	5.0
1	A	791	PHE	5.0
1	A	115	LEU	5.0
1	A	515	VAL	4.9
1	A	145	TYR	4.9
1	A	135	ALA	4.7
1	A	170	LYS	4.5
1	A	46	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	137	GLU	4.3
1	A	670	ILE	4.2
2	G	3	ILE	4.2
1	A	558	ASP	4.1
1	A	136	PRO	4.0
1	A	630	ALA	4.0
1	A	144	PRO	3.9
2	G	9[B]	ARG	3.8
2	G	12[A]	VAL	3.8
1	A	935	SER	3.7
1	A	119	PRO	3.7
2	G	4	GLN	3.7
1	A	92	THR	3.7
1	A	140	LEU	3.7
1	A	674[A]	PHE	3.5
1	A	668	THR	3.5
1	A	91	SER	3.1
1	A	104	ARG	3.1
1	A	790	GLN	3.1
1	A	561	TYR	3.0
1	A	122	VAL	2.9
1	A	743[A]	CYS	2.8
1	A	90	THR	2.8
1	A	141	VAL	2.8
1	A	139	LEU	2.7
1	A	552	GLY	2.7
1	A	138	PRO	2.7
1	A	88	GLN	2.6
1	A	94	ILE	2.5
1	A	193	CYS	2.5
1	A	485	ILE	2.5
1	A	47	PHE	2.4
1	A	663	TYR	2.4
1	A	550	MET	2.3
1	A	49	TRP	2.2
1	A	108	ARG	2.2
1	A	118	GLU	2.2
1	A	121	GLN	2.2
1	A	54	LEU	2.2
1	A	396	VAL	2.1
1	A	300	PRO	2.1
1	A	484[A]	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	295	ASP	2.0

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

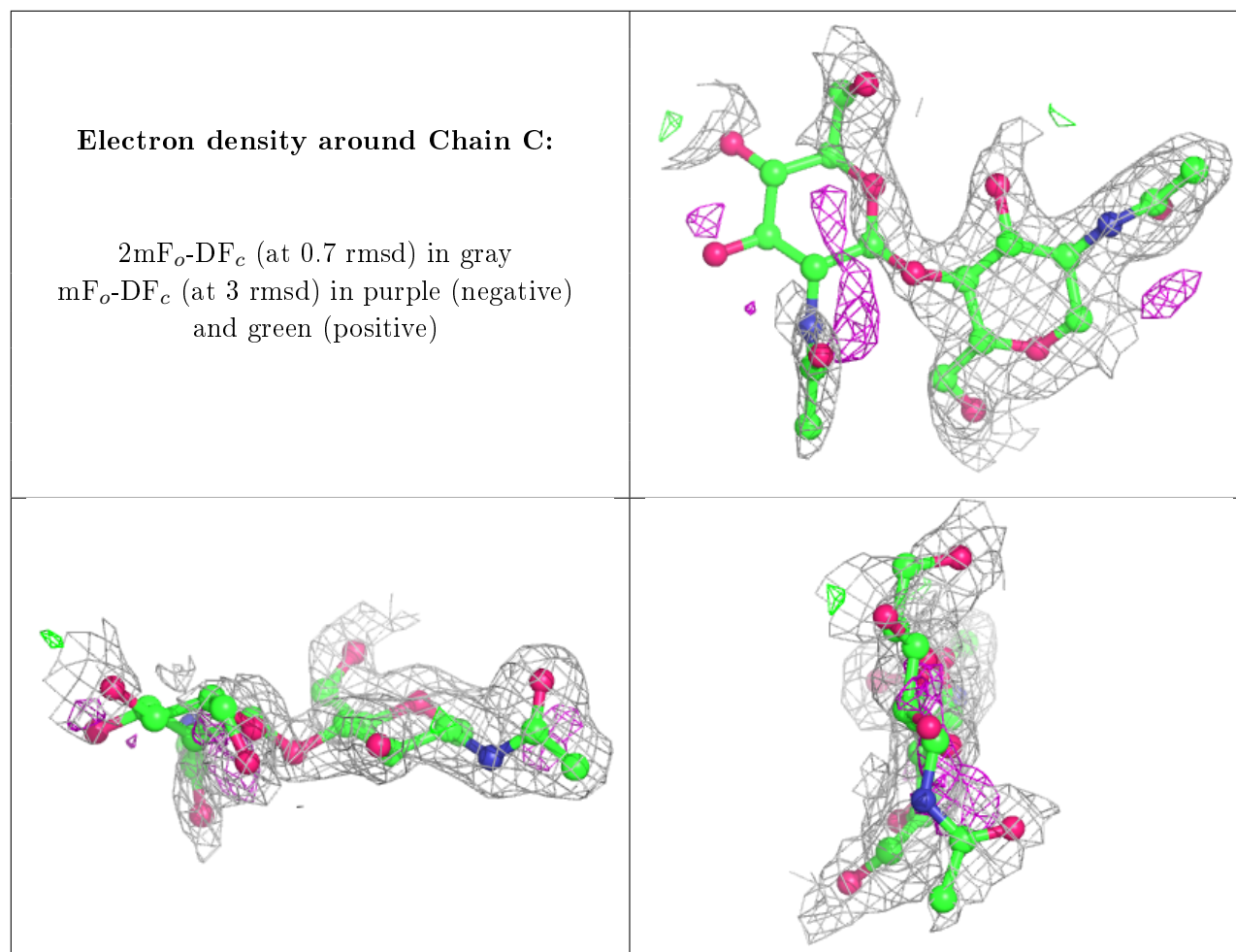
There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
3	NAG	C	2	14/15	0.26	0.56	60,77,90,91	0
3	NAG	B	1	14/15	0.44	0.27	51,61,72,79	0
3	NAG	B	2	14/15	0.46	0.52	74,85,90,91	0
3	NAG	C	1	14/15	0.85	0.19	35,46,62,71	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.

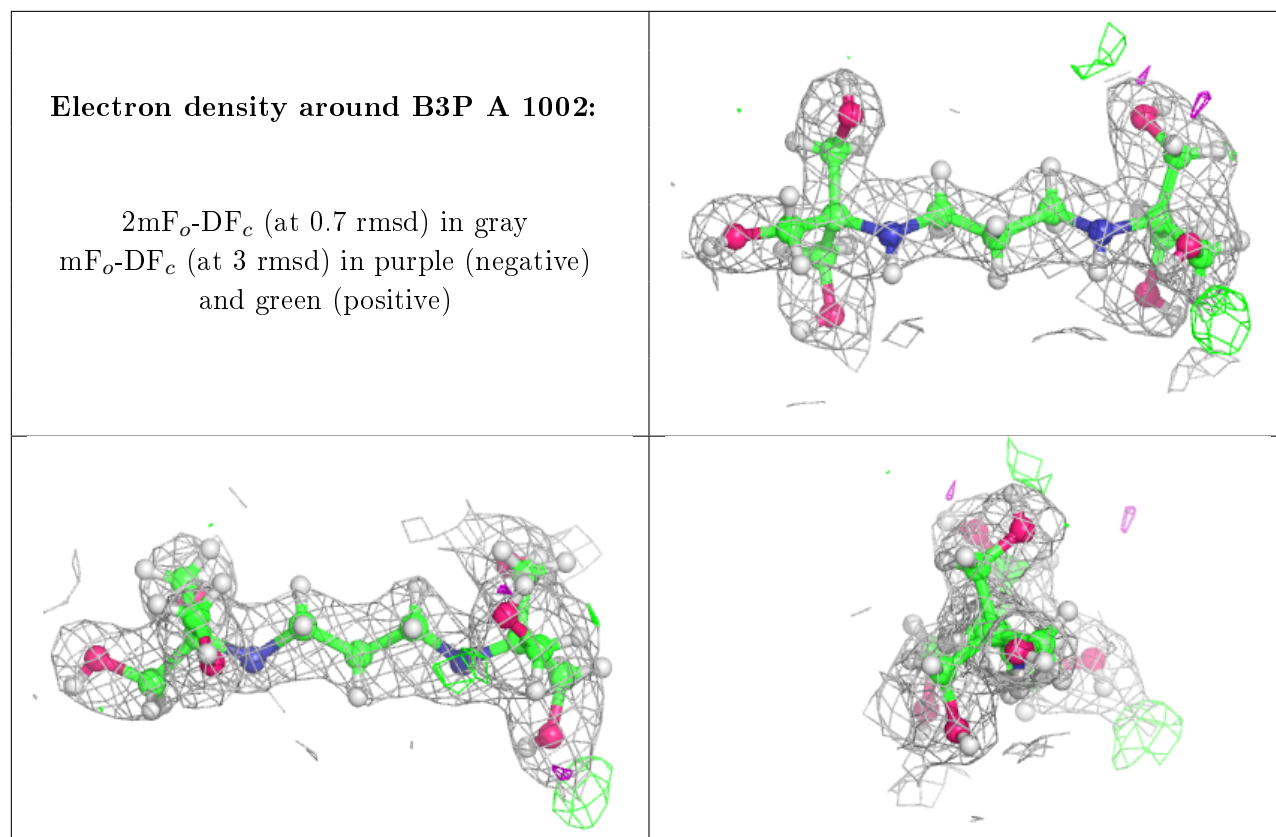
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	NAG	A	1033	14/15	0.52	0.46	78,93,98,101	0
9	NAG	A	1034	14/15	0.55	0.32	55,65,74,75	0
8	PPI	A	1028	5/5	0.62	0.23	28,46,62,62	0
6	EDO	A	1011	4/4	0.67	0.29	47,56,63,68	0
6	EDO	A	1019	4/4	0.70	0.14	64,77,81,82	0
6	EDO	A	1023	4/4	0.72	0.16	65,78,81,81	0
6	EDO	A	1009	4/4	0.72	0.14	44,53,59,65	0
6	EDO	A	1022	4/4	0.77	0.17	52,63,66,71	10
6	EDO	A	1018	4/4	0.79	0.21	52,63,68,69	0
6	EDO	A	1017	4/4	0.82	0.17	47,61,66,74	0
6	EDO	A	1004	4/4	0.83	0.13	38,56,64,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	A	1012	4/4	0.84	0.13	49,59,66,71	0
5	B3P	A	1002	19/19	0.84	0.17	32,42,57,61	0
6	EDO	A	1021	4/4	0.86	0.11	60,72,82,85	0
6	EDO	A	1006	4/4	0.87	0.17	33,48,58,58	0
6	EDO	A	1003	4/4	0.87	0.12	31,45,54,54	0
6	EDO	A	1013	4/4	0.87	0.15	46,60,72,79	0
6	EDO	A	1010	4/4	0.89	0.19	41,49,59,60	0
6	EDO	A	1005	4/4	0.89	0.10	33,40,43,49	0
6	EDO	A	1007	4/4	0.91	0.16	34,53,64,64	0
6	EDO	A	1015	4/4	0.92	0.22	35,43,57,57	0
6	EDO	A	1016	4/4	0.92	0.16	36,45,56,66	0
6	EDO	A	1020	4/4	0.93	0.31	40,50,72,87	0
6	EDO	A	1008	4/4	0.95	0.25	22,56,67,67	0
7	NA	A	1027	1/1	0.97	0.10	42,42,42,42	0
7	NA	A	1024	1/1	0.97	0.11	42,42,42,42	0
6	EDO	A	1014	4/4	0.97	0.12	23,36,47,57	0
4	ZN	A	1001	1/1	0.99	0.10	26,26,26,26	0
7	NA	A	1026	1/1	0.99	0.10	34,34,34,34	0
7	NA	A	1025	1/1	0.99	0.10	34,34,34,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.