



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 29, 2021 – 12:16 am BST

PDB ID : 6I44  
Title : Allosteric activation of human prekallikrein by apple domain disc rotation  
Authors : Li, C.; Pathak, M.; MacCrae, K.; Dreveny, I.; Emsley, J.  
Deposited on : 2018-11-09  
Resolution : 1.36 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](mailto: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.

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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 : 2.22  
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) : 2.22

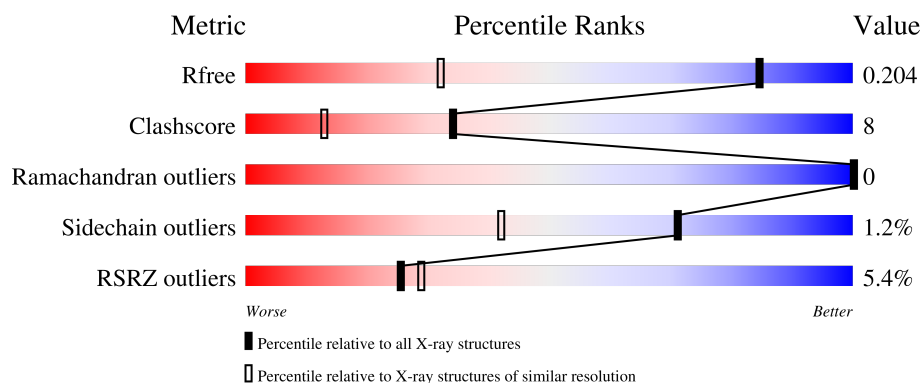
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.36 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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  $\geq 3$ , 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	627	<div> <div>5%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
2	B	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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	A	712	-	-	X	-
11	FMT	A	714	-	-	X	-
12	ACT	A	724	-	-	X	-
2	NAG	B	2	X	-	-	-

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 5669 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.

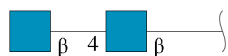
- Molecule 1 is a protein called Plasma kallikrein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	594	4817	3058	821	888	50	16	33	0

There are 16 discrepancies between the modelled and reference sequences:

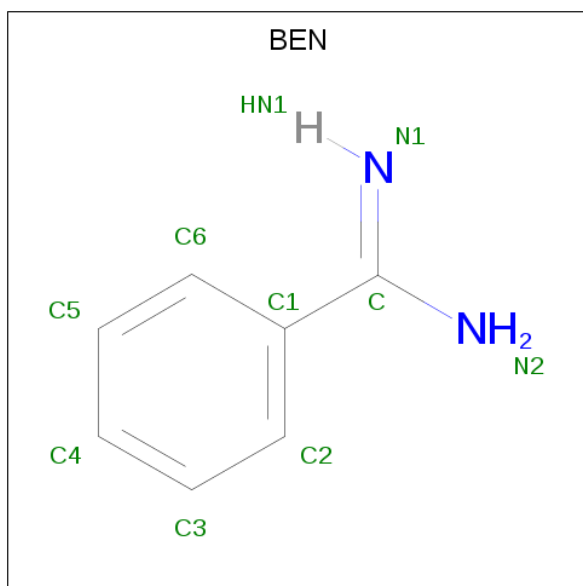
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ARG	-	expression tag	UNP P03952
A	-6	SER	-	expression tag	UNP P03952
A	-5	HIS	-	expression tag	UNP P03952
A	-4	HIS	-	expression tag	UNP P03952
A	-3	HIS	-	expression tag	UNP P03952
A	-2	HIS	-	expression tag	UNP P03952
A	-1	HIS	-	expression tag	UNP P03952
A	0	HIS	-	expression tag	UNP P03952
A	323	ALA	GLU	conflict	UNP P03952
A	325	ALA	LYS	conflict	UNP P03952
A	377	GLN	ASN	conflict	UNP P03952
A	434	GLN	ASN	conflict	UNP P03952
A	475	GLN	ASN	conflict	UNP P03952
A	507	ALA	LYS	conflict	UNP P03952
A	509	ALA	LYS	conflict	UNP P03952
A	559	ALA	SER	conflict	UNP P03952

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



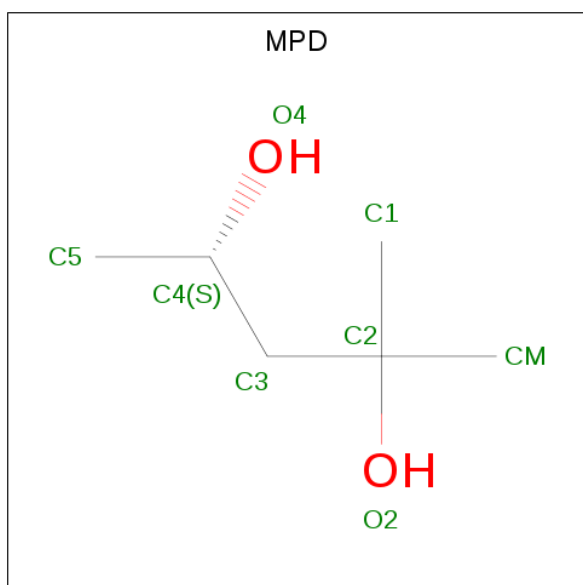
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			21	12	2	7			

- Molecule 3 is BENZAMIDINE (three-letter code: BEN) (formula:  $C_7H_8N_2$ ).



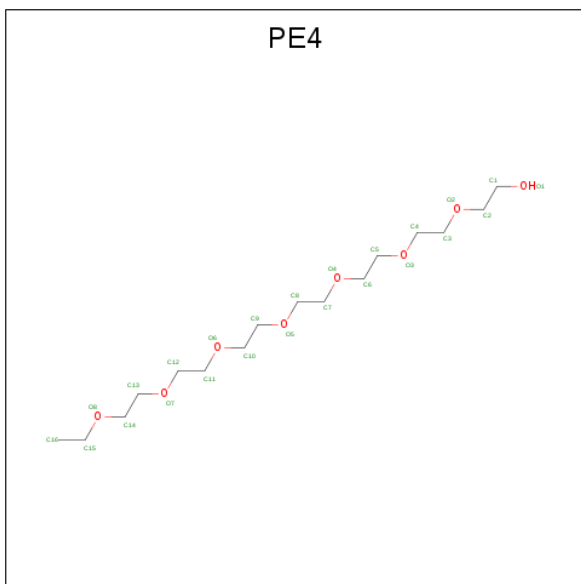
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	7	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



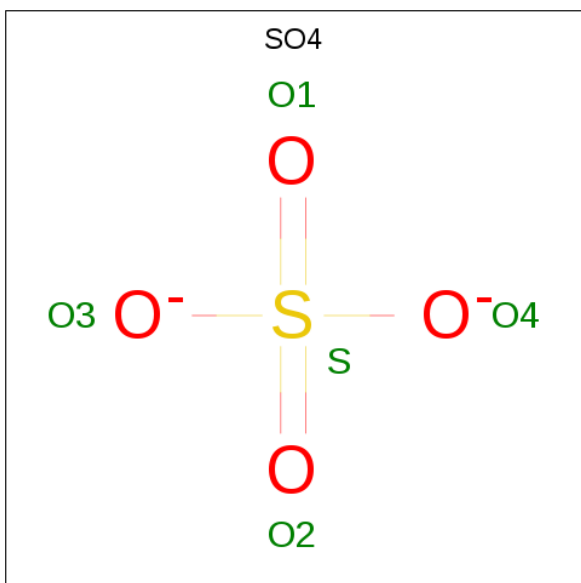
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			24	16	8		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

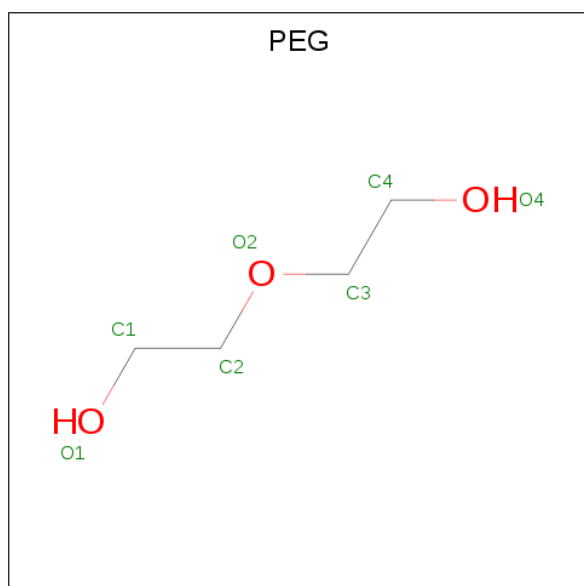
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



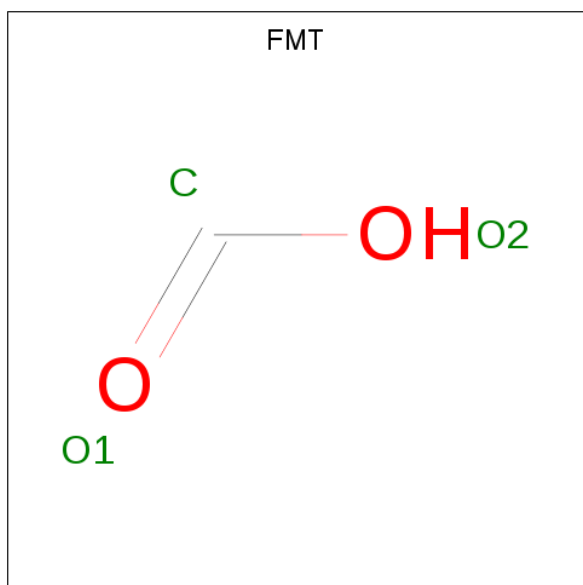
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		

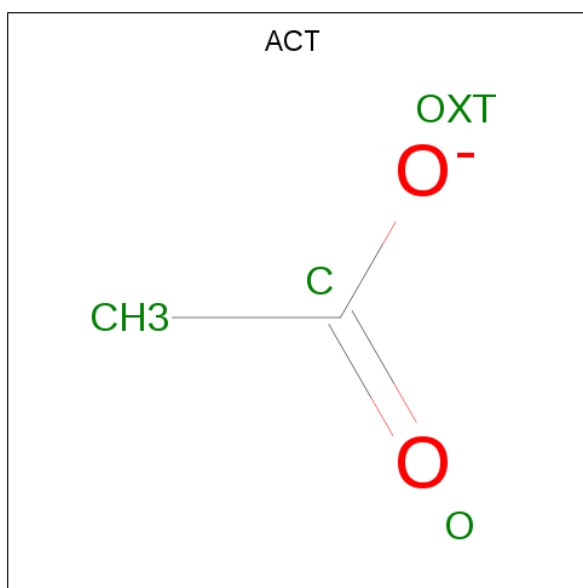
- Molecule 11 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 3 1 2	0	0
11	A	1	Total C O 3 1 2	0	0
11	A	1	Total C O 3 1 2	0	0
11	A	1	Total C O 3 1 2	0	0
11	A	1	Total C O 3 1 2	0	0
11	A	1	Total C O 3 1 2	0	0
11	A	1	Total C O 3 1 2	0	0
11	A	1	Total C O 3 1 2	0	0

- Molecule 12 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



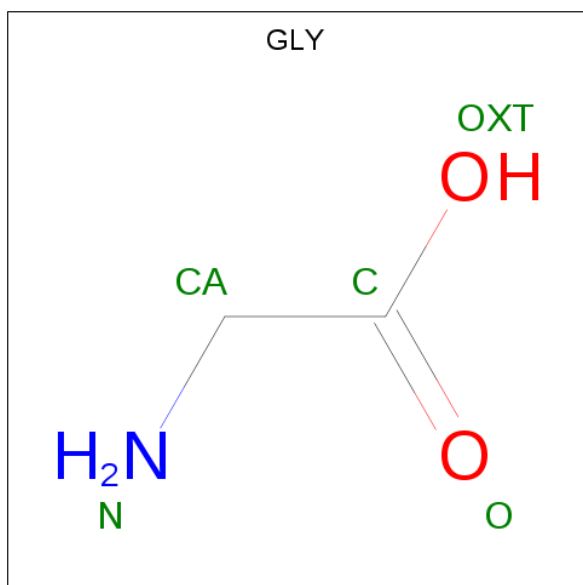
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 4 2 2	0	0
12	A	1	Total C O 4 2 2	0	0
12	A	1	Total C O 4 2 2	0	0
12	A	1	Total C O 4 2 2	0	0

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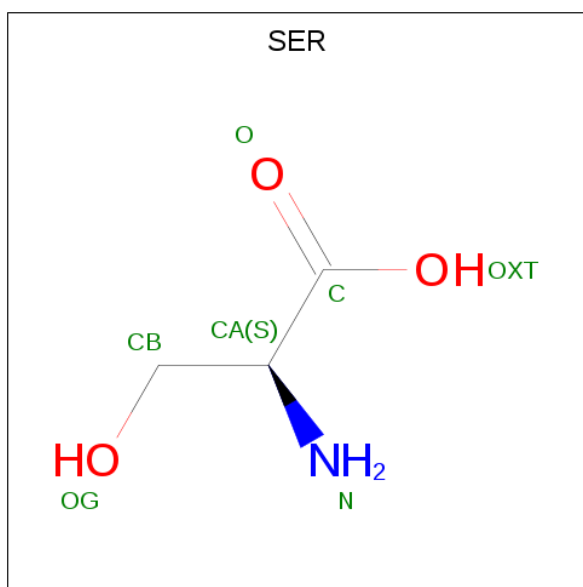
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	1
			8	4	4		
12	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 13 is GLYCINE (three-letter code: GLY) (formula:  $C_2H_5NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 14 is SERINE (three-letter code: SER) (formula:  $C_3H_7NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	N	O	0	0
			7	3	1	3		

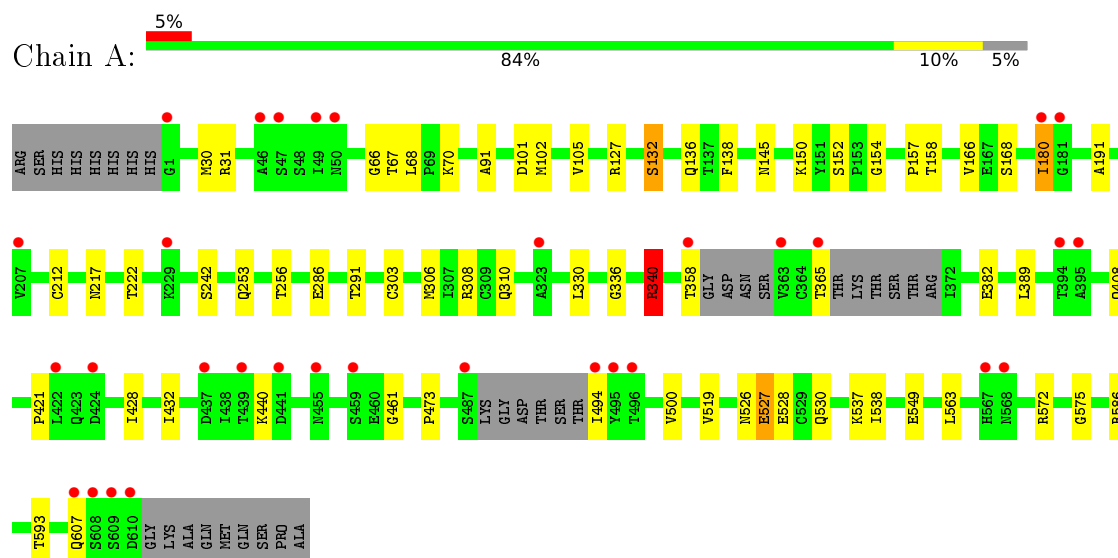
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	637	Total	O	0	44
			681	681		

### 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: Plasma kallikrein



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.61Å 129.63Å 55.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.05 – 1.36 28.03 – 1.36	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.05-1.36) 99.7 (28.03-1.36)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 1.36Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.167 , 0.196 0.177 , 0.204	Depositor DCC
$R_{free}$ test set	7196 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.9	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5669	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, NA, FMT, ACT, BEN, SO4, PEG, NAG, PE4, MPD, CL

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	0.89	6/5022 (0.1%)	0.97	3/6796 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132[A]	SER	CA-CB	-6.09	1.43	1.52
1	A	132[B]	SER	CA-CB	-6.09	1.43	1.52
1	A	382	GLU	CD-OE2	-5.68	1.19	1.25
1	A	242[A]	SER	C-O	5.19	1.33	1.23
1	A	242[B]	SER	C-O	5.19	1.33	1.23
1	A	440	LYS	CB-CG	5.19	1.66	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340[A]	ARG	CB-CA-C	5.83	122.05	110.40
1	A	340[B]	ARG	CB-CA-C	5.83	122.05	110.40
1	A	31	ARG	NE-CZ-NH2	-5.76	117.42	120.30

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	4817	0	4779	74	0
2	B	21	0	15	1	0
3	A	9	0	7	0	0
4	A	8	0	14	0	0
5	A	24	0	34	8	0
6	A	5	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	14	0	20	3	0
10	A	24	0	32	6	0
11	A	24	0	9	4	0
12	A	28	0	21	6	0
13	A	5	0	2	0	0
14	A	7	0	4	0	0
15	A	681	0	0	22	0
All	All	5669	0	4937	83	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 8.

All (83) 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:127:ARG:HG2	12:A:724:ACT:H1	1.31	1.10
1:A:526[B]:ASN:HD21	1:A:538:ILE:HG22	1.18	1.04
1:A:154:GLY:H	1:A:217[A]:ASN:HD21	1.10	0.98
1:A:526[B]:ASN:ND2	1:A:538:ILE:HG22	1.81	0.94
1:A:154:GLY:H	1:A:217[B]:ASN:HD21	1.18	0.91
1:A:138:PHE:CE1	1:A:166[B]:VAL:CG1	2.56	0.88
11:A:719:FMT:H	15:A:941:HOH:O	1.74	0.86
1:A:127:ARG:HG2	12:A:724:ACT:CH3	2.08	0.84
1:A:421:PRO:HG3	15:A:1178:HOH:O	1.87	0.75
5:A:703:PE4:H11	15:A:1304:HOH:O	1.87	0.74
1:A:494:ILE:HD11	15:A:1352:HOH:O	1.88	0.74
5:A:703:PE4:H142	15:A:1324:HOH:O	1.86	0.73
1:A:132[B]:SER:OG	10:A:712:GOL:H12	1.89	0.73
1:A:494:ILE:HG22	15:A:1250:HOH:O	1.88	0.73
10:A:712:GOL:H31	15:A:874:HOH:O	1.89	0.71
5:A:703:PE4:H162	15:A:1324:HOH:O	1.92	0.70
1:A:180[A]:ILE:HD12	1:A:180[A]:ILE:O	1.93	0.69
1:A:526[B]:ASN:ND2	1:A:538:ILE:CG2	2.57	0.68
1:A:127:ARG:CG	12:A:724:ACT:H1	2.19	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:CE1	1:A:166[B]:VAL:HG11	2.30	0.66
1:A:138:PHE:CE1	1:A:166[A]:VAL:HG22	2.33	0.64
1:A:138:PHE:CD1	1:A:166[B]:VAL:CG1	2.82	0.62
1:A:461:GLY:HA3	9:A:707:PEG:H11	1.81	0.62
1:A:306[B]:MET:HG2	15:A:1115:HOH:O	1.99	0.61
1:A:500[B]:VAL:HG23	1:A:519:VAL:HG12	1.83	0.61
1:A:67:THR:HA	5:A:703:PE4:H161	1.83	0.61
10:A:712:GOL:C3	15:A:874:HOH:O	2.48	0.59
1:A:138:PHE:HE1	1:A:166[B]:VAL:CG1	2.12	0.59
1:A:66:GLY:HA3	12:A:725[B]:ACT:H3	1.86	0.56
1:A:340[A]:ARG:HG2	15:A:816:HOH:O	2.05	0.56
1:A:180[A]:ILE:HD12	1:A:180[A]:ILE:C	2.25	0.56
1:A:102[A]:MET:HE3	1:A:157:PRO:HG2	1.87	0.55
1:A:68:LEU:H	5:A:703:PE4:H161	1.71	0.55
1:A:586:ARG:HD2	15:A:1338:HOH:O	2.07	0.55
1:A:138:PHE:CD1	1:A:166[B]:VAL:HG12	2.42	0.54
1:A:154:GLY:N	1:A:217[B]:ASN:HD21	1.99	0.54
1:A:138:PHE:CE1	1:A:166[A]:VAL:CG2	2.92	0.53
1:A:212:CYS:O	11:A:720:FMT:H	2.10	0.52
1:A:152[B]:SER:OG	1:A:158:THR:HG23	2.10	0.52
12:A:721:ACT:H2	15:A:1361:HOH:O	2.10	0.51
1:A:222:THR:CG2	1:A:256[A]:THR:CG2	2.88	0.51
1:A:102[B]:MET:HE2	1:A:168:SER:HB3	1.93	0.51
1:A:527[A]:GLU:HG2	1:A:528:GLU:N	2.26	0.50
1:A:138:PHE:CE1	1:A:166[B]:VAL:HG12	2.46	0.49
1:A:138:PHE:HE1	1:A:166[B]:VAL:HG11	1.72	0.49
1:A:461:GLY:CA	9:A:707:PEG:H32	2.43	0.49
1:A:432[A]:ILE:HG13	15:A:1039[A]:HOH:O	2.12	0.49
1:A:101:ASP:OD1	10:A:712:GOL:H11	2.13	0.48
1:A:494:ILE:CG2	15:A:1250:HOH:O	2.52	0.48
1:A:30[B]:MET:SD	1:A:91:ALA:HA	2.53	0.48
1:A:308:ARG:HH22	11:A:714:FMT:C	2.27	0.48
1:A:67:THR:CA	5:A:703:PE4:H161	2.43	0.47
1:A:306[A]:MET:SD	1:A:330[A]:LEU:HD12	2.54	0.47
1:A:138:PHE:HE1	1:A:166[A]:VAL:CG2	2.28	0.47
1:A:500[B]:VAL:CG2	1:A:519:VAL:CG1	2.93	0.47
1:A:136:GLN:HG3	1:A:145:ASN:HD21	1.80	0.47
1:A:340[A]:ARG:NH2	15:A:816:HOH:O	2.49	0.46
1:A:191:ALA:HB2	1:A:256[A]:THR:HG21	1.97	0.45
1:A:530:GLN:OE1	1:A:537:LYS:HD2	2.16	0.45
10:A:709:GOL:H31	15:A:833[B]:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:THR:HB	15:A:1128:HOH:O	2.18	0.44
1:A:70:LYS:HE3	5:A:703:PE4:H122	1.99	0.44
1:A:537:LYS:HD2	1:A:537:LYS:HA	1.73	0.44
1:A:500[B]:VAL:HG23	1:A:519:VAL:CG1	2.47	0.43
1:A:389:LEU:HD22	1:A:428:ILE:HG12	2.00	0.43
1:A:408:GLN:HG3	1:A:473:PRO:HA	2.01	0.43
1:A:105:VAL:O	1:A:150:LYS:HA	2.17	0.43
1:A:138:PHE:CE1	1:A:166[B]:VAL:HG13	2.50	0.43
1:A:310:GLN:OE1	1:A:336:GLY:HA2	2.18	0.43
1:A:127:ARG:CG	12:A:724:ACT:CH3	2.89	0.42
1:A:461:GLY:HA3	9:A:707:PEG:H32	2.01	0.42
15:A:1109[B]:HOH:O	2:B:1:NAG:H83	2.19	0.42
1:A:365:THR:C	15:A:1270[B]:HOH:O	2.57	0.42
1:A:526[B]:ASN:HD21	1:A:538:ILE:CG2	2.05	0.42
1:A:253:GLN:NE2	15:A:801:HOH:O	2.31	0.42
1:A:222:THR:HG23	1:A:256[A]:THR:CG2	2.50	0.41
1:A:70:LYS:CE	5:A:703:PE4:H122	2.50	0.41
1:A:303:CYS:HB2	1:A:330[B]:LEU:HD12	2.03	0.41
1:A:291[B]:THR:HG21	15:A:1138:HOH:O	2.21	0.41
1:A:286[A]:GLU:OE1	11:A:714:FMT:C	2.68	0.41
1:A:575:GLY:HA2	1:A:593:THR:O	2.21	0.41
1:A:500[A]:VAL:HG22	1:A:563:LEU:HD13	2.04	0.40
1:A:101:ASP:OD1	10:A:712:GOL:C1	2.69	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	619/627 (99%)	606 (98%)	13 (2%)	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	552/547 (101%)	543 (98%)	9 (2%)	62 30

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180[A]	ILE
1	A	180[B]	ILE
1	A	340[A]	ARG
1	A	340[B]	ARG
1	A	527[A]	GLU
1	A	527[B]	GLU
1	A	549	GLU
1	A	572	ARG
1	A	607	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	145	ASN
1	A	455	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

2 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	B	1	1,2	14,14,15	0.63	0	17,19,21	1.69	5 (29%)
2	NAG	B	2	2	5,6,15	0.67	0	2,7,21	1.37	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
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	1/1/2/7	5/6/6/26	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	1	NAG	C1-C2-N2	-3.90	103.82	110.49
2	B	1	NAG	C6-C5-C4	3.17	120.42	113.00
2	B	1	NAG	O5-C5-C6	-2.68	103.01	107.20
2	B	1	NAG	C8-C7-N2	2.03	119.53	116.10
2	B	1	NAG	O7-C7-N2	-2.00	118.27	121.95

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2	NAG	C1

All (7) torsion outliers are listed below:

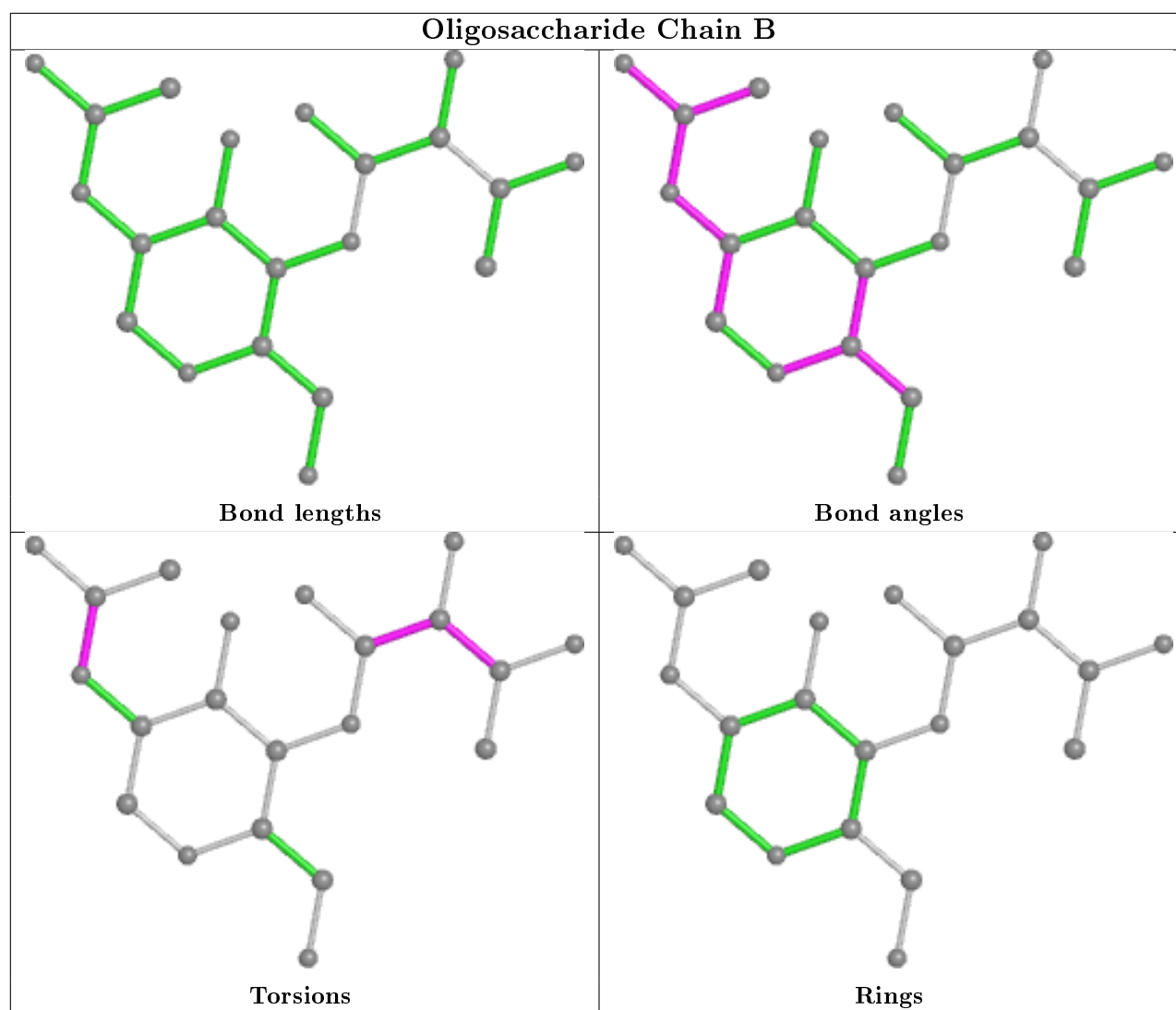
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C1-C2-C3
2	B	2	NAG	O5-C1-C2-N2
2	B	2	NAG	C1-C2-C3-C4
2	B	2	NAG	C1-C2-C3-O3
2	B	2	NAG	N2-C2-C3-C4
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	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 [i](#)

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	$\# Z  > 2$
11	FMT	A	716	-	0,2,2	0.00	-	0,1,1	0.00	-
4	MPD	A	702	-	7,7,7	0.49	0	9,10,10	0.50	0
11	FMT	A	719	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BEN	A	701	-	9,9,9	0.40	0	7,11,11	1.25	1 (14%)
14	SER	A	728	-	3,6,6	1.13	0	1,7,7	0.27	0
12	ACT	A	723	-	1,3,3	2.93	1 (100%)	0,3,3	0.00	-
10	GOL	A	712	-	5,5,5	0.10	0	5,5,5	0.56	0
13	GLY	A	727	-	1,4,4	0.06	0	0,4,4	0.00	-
12	ACT	A	726	-	1,3,3	3.50	1 (100%)	0,3,3	0.00	-
10	GOL	A	711	-	5,5,5	0.13	0	5,5,5	0.32	0
11	FMT	A	713	-	0,2,2	0.00	-	0,1,1	0.00	-
9	PEG	A	708	-	6,6,6	0.48	0	5,5,5	0.25	0
12	ACT	A	725[B]	-	1,3,3	4.63	1 (100%)	0,3,3	0.00	-
12	ACT	A	722	-	1,3,3	1.36	0	0,3,3	0.00	-
12	ACT	A	725[A]	-	1,3,3	4.60	1 (100%)	0,3,3	0.00	-
10	GOL	A	710	-	5,5,5	0.19	0	5,5,5	0.48	0
11	FMT	A	715	-	0,2,2	0.00	-	0,1,1	0.00	-
9	PEG	A	707	-	6,6,6	0.33	0	5,5,5	0.44	0
12	ACT	A	721	-	1,3,3	3.39	1 (100%)	0,3,3	0.00	-
12	ACT	A	724	-	1,3,3	3.02	1 (100%)	0,3,3	0.00	-
5	PE4	A	703	-	23,23,23	0.26	0	22,22,22	0.47	0
11	FMT	A	718	-	0,2,2	0.00	-	0,1,1	0.00	-
10	GOL	A	709	-	5,5,5	0.15	0	5,5,5	1.12	0
11	FMT	A	717	-	0,2,2	0.00	-	0,1,1	0.00	-
11	FMT	A	714	-	0,2,2	0.00	-	0,1,1	0.00	-
11	FMT	A	720	-	0,2,2	0.00	-	0,1,1	0.00	-
6	SO4	A	704	-	4,4,4	0.33	0	6,6,6	0.42	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
10	GOL	A	710	-	-	4/4/4/4	-
4	MPD	A	702	-	-	0/5/5/5	-
10	GOL	A	711	-	-	0/4/4/4	-
3	BEN	A	701	-	-	4/4/4/4	0/1/1/1
9	PEG	A	707	-	-	2/4/4/4	-
13	GLY	A	727	-	-	0/0/2/2	-
14	SER	A	728	-	-	0/2/6/6	-
5	PE4	A	703	-	-	6/21/21/21	-
9	PEG	A	708	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	A	709	-	-	2/4/4/4	-
10	GOL	A	712	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	725[B]	ACT	CH3-C	4.63	1.54	1.48
12	A	725[A]	ACT	CH3-C	4.60	1.54	1.48
12	A	726	ACT	CH3-C	3.50	1.53	1.48
12	A	721	ACT	CH3-C	3.39	1.53	1.48
12	A	724	ACT	CH3-C	3.02	1.52	1.48
12	A	723	ACT	CH3-C	2.93	1.52	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	BEN	C1-C-N2	2.86	122.37	118.05

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	710	GOL	O1-C1-C2-O2
10	A	710	GOL	O1-C1-C2-C3
10	A	710	GOL	C1-C2-C3-O3
10	A	712	GOL	C1-C2-C3-O3
10	A	712	GOL	O2-C2-C3-O3
5	A	703	PE4	O6-C11-C12-O7
9	A	707	PEG	O2-C3-C4-O4
10	A	709	GOL	C1-C2-C3-O3
9	A	708	PEG	O1-C1-C2-O2
10	A	710	GOL	O2-C2-C3-O3
5	A	703	PE4	O1-C1-C2-O2
9	A	707	PEG	O1-C1-C2-O2
10	A	709	GOL	O2-C2-C3-O3
5	A	703	PE4	O3-C5-C6-O4
5	A	703	PE4	C8-C7-O4-C6
5	A	703	PE4	C16-C15-O8-C14
3	A	701	BEN	N2-C-C1-C2
3	A	701	BEN	N2-C-C1-C6
9	A	708	PEG	C1-C2-O2-C3

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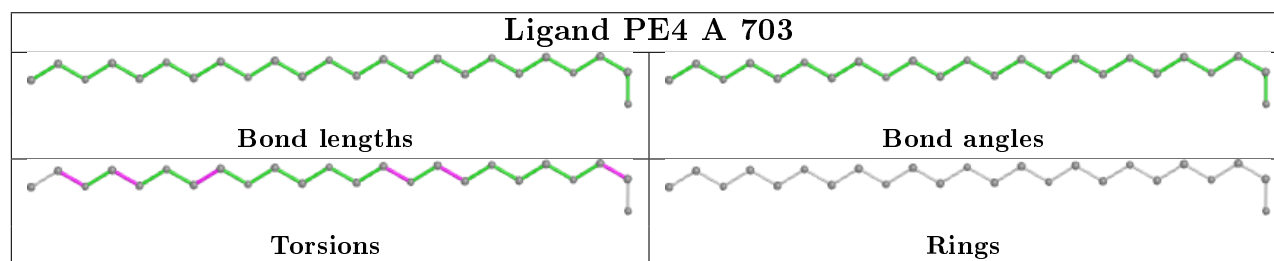
Mol	Chain	Res	Type	Atoms
3	A	701	BEN	N1-C-C1-C2
3	A	701	BEN	N1-C-C1-C6
5	A	703	PE4	O7-C13-C14-O8

There are no ring outliers.

10 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	719	FMT	1	0
10	A	712	GOL	5	0
12	A	725[B]	ACT	1	0
9	A	707	PEG	3	0
12	A	721	ACT	1	0
12	A	724	ACT	4	0
5	A	703	PE4	8	0
10	A	709	GOL	1	0
11	A	714	FMT	2	0
11	A	720	FMT	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	594/627 (94%)	0.29	32 (5%) 25 29	8, 16, 35, 53	22 (3%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	THR	6.2
1	A	180[A]	ILE	6.0
1	A	494	ILE	5.5
1	A	365	THR	5.2
1	A	487	SER	4.2
1	A	608	SER	4.1
1	A	395	ALA	4.0
1	A	422	LEU	3.9
1	A	609	SER	3.8
1	A	229	LYS	3.5
1	A	496	THR	3.1
1	A	363	VAL	3.0
1	A	49	ILE	2.9
1	A	323	ALA	2.8
1	A	439	THR	2.7
1	A	495	TYR	2.6
1	A	607	GLN	2.5
1	A	46	ALA	2.5
1	A	424[A]	ASP	2.4
1	A	441	ASP	2.4
1	A	358	THR	2.3
1	A	610	ASP	2.3
1	A	1	GLY	2.3
1	A	437	ASP	2.2
1	A	568	ASN	2.2
1	A	207	VAL	2.2
1	A	47	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	50	ASN	2.1
1	A	181	GLY	2.1
1	A	455	ASN	2.1
1	A	567	HIS	2.0
1	A	459	SER	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	B	2	7/15	0.78	0.27	28,32,34,36	3
2	NAG	B	1	14/15	0.86	0.17	21,30,43,47	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
9	PEG	A	707	7/7	0.64	0.14	45,47,49,49	2
11	FMT	A	715	3/3	0.65	0.24	51,51,52,52	0
10	GOL	A	710	6/6	0.66	0.13	49,51,52,53	0
12	ACT	A	725[A]	4/4	0.69	0.24	30,33,35,35	4
12	ACT	A	725[B]	4/4	0.69	0.24	33,33,37,38	4
12	ACT	A	721	4/4	0.73	0.18	58,63,64,66	0
10	GOL	A	711	6/6	0.74	0.13	37,44,45,49	0
12	ACT	A	724	4/4	0.75	0.17	49,52,54,55	0
5	PE4	A	703	24/24	0.77	0.14	16,24,26,29	0
11	FMT	A	714	3/3	0.79	0.24	31,31,34,34	0
10	GOL	A	712	6/6	0.80	0.12	31,38,46,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	ACT	A	723	4/4	0.81	0.13	40,43,44,48	0
9	PEG	A	708	7/7	0.81	0.19	33,37,43,45	2
11	FMT	A	717	3/3	0.82	0.14	29,29,30,32	3
11	FMT	A	713	3/3	0.83	0.23	36,36,36,37	0
11	FMT	A	718	3/3	0.85	0.11	37,37,43,45	0
13	GLY	A	727	5/5	0.85	0.13	20,27,29,31	3
11	FMT	A	716	3/3	0.86	0.15	20,20,30,39	0
12	ACT	A	726	4/4	0.87	0.14	47,49,51,55	0
6	SO4	A	704	5/5	0.88	0.14	23,24,32,32	4
12	ACT	A	722	4/4	0.89	0.11	21,22,24,28	0
11	FMT	A	720	3/3	0.91	0.12	10,10,19,22	2
14	SER	A	728	7/7	0.94	0.12	15,16,23,25	1
4	MPD	A	702	8/8	0.95	0.11	17,17,21,22	0
3	BEN	A	701	9/9	0.95	0.09	14,16,19,20	0
10	GOL	A	709	6/6	0.96	0.06	15,21,23,23	0
7	CL	A	705	1/1	0.97	0.05	30,30,30,30	0
11	FMT	A	719	3/3	0.97	0.16	11,11,11,14	3
8	NA	A	706	1/1	0.99	0.11	20,20,20,20	0

## 6.5 Other polymers

There are no such residues in this entry.