



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2020 – 12:14 PM JST

PDB ID : 7BVQ  
Title : Structure of human beta1 adrenergic receptor bound to carazolol  
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Deposited on : 2020-04-11  
Resolution : 2.50 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 : 2.14.6  
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) : 2.14.6

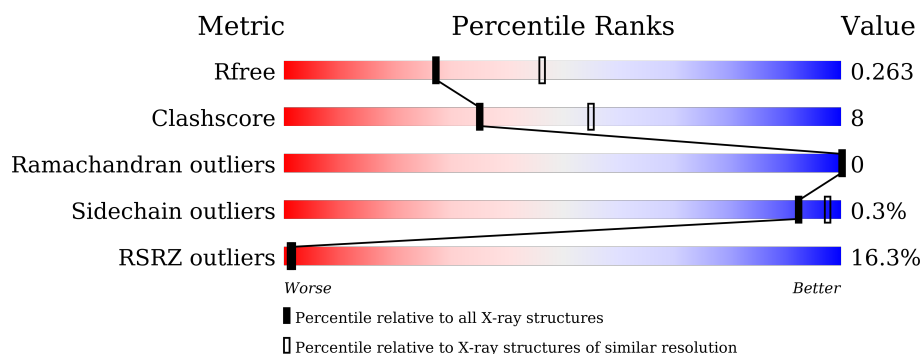
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	462	<div> <div>12%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	B	462	<div> <div>20%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
2	C	2	<div> <div>100%</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
8	CIT	A	1412	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7377 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 Endolysin,Beta-1 adrenergic receptor chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3588	2327	607	632	22			
1	B	451	Total	C	N	O	S	0	0	0
			3424	2221	575	607	21			

There are 24 discrepancies between the modelled and reference sequences:

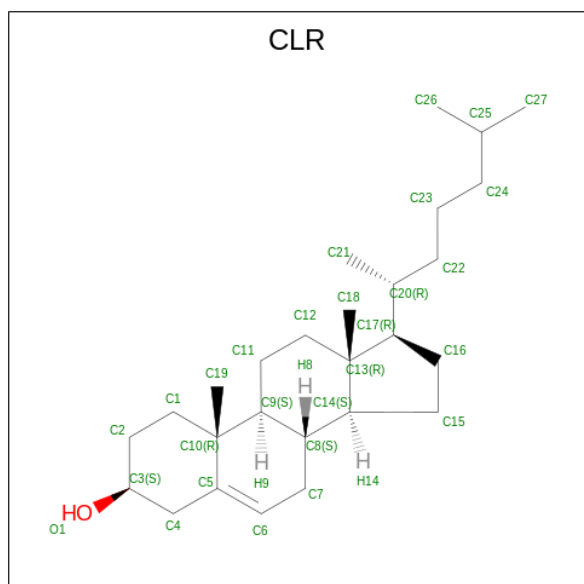
Chain	Residue	Modelled	Actual	Comment	Reference
A	884	ASP	-	expression tag	UNP D9IEF7
A	885	TYR	-	expression tag	UNP D9IEF7
A	886	LYS	-	expression tag	UNP D9IEF7
A	887	ASP	-	expression tag	UNP D9IEF7
A	888	ASP	-	expression tag	UNP D9IEF7
A	889	ASP	-	expression tag	UNP D9IEF7
A	890	ASP	-	expression tag	UNP D9IEF7
A	891	ALA	-	expression tag	UNP D9IEF7
A	944	THR	CYS	engineered mutation	UNP D9IEF7
A	987	ALA	CYS	engineered mutation	UNP D9IEF7
A	1052	ALA	-	linker	UNP D9IEF7
A	1053	ALA	-	linker	UNP D9IEF7
B	884	ASP	-	expression tag	UNP D9IEF7
B	885	TYR	-	expression tag	UNP D9IEF7
B	886	LYS	-	expression tag	UNP D9IEF7
B	887	ASP	-	expression tag	UNP D9IEF7
B	888	ASP	-	expression tag	UNP D9IEF7
B	889	ASP	-	expression tag	UNP D9IEF7
B	890	ASP	-	expression tag	UNP D9IEF7
B	891	ALA	-	expression tag	UNP D9IEF7
B	944	THR	CYS	engineered mutation	UNP D9IEF7
B	987	ALA	CYS	engineered mutation	UNP D9IEF7
B	1052	ALA	-	linker	UNP D9IEF7
B	1053	ALA	-	linker	UNP D9IEF7

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



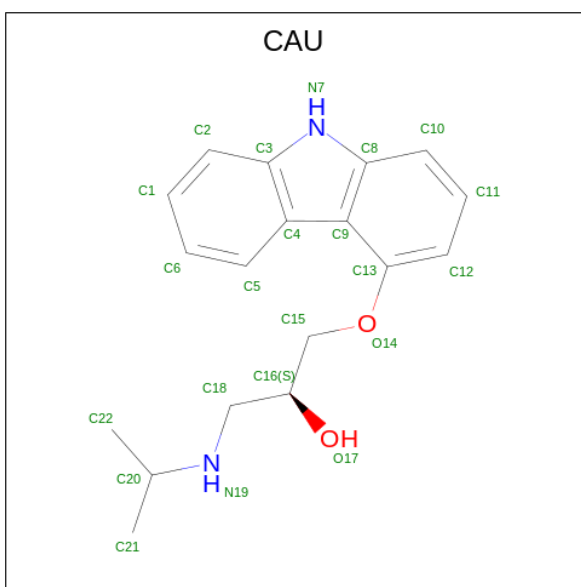
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



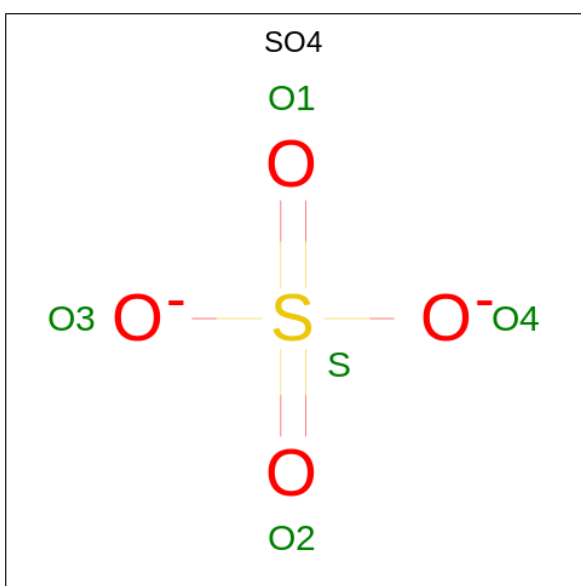
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 4 is (2S)-1-(9H-Carbazol-4-yloxy)-3-(isopropylamino)propan-2-ol (three-letter code: CAU) (formula: C<sub>18</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			22	18	2	2		
4	B	1	Total	C	N	O	0	0
			22	18	2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



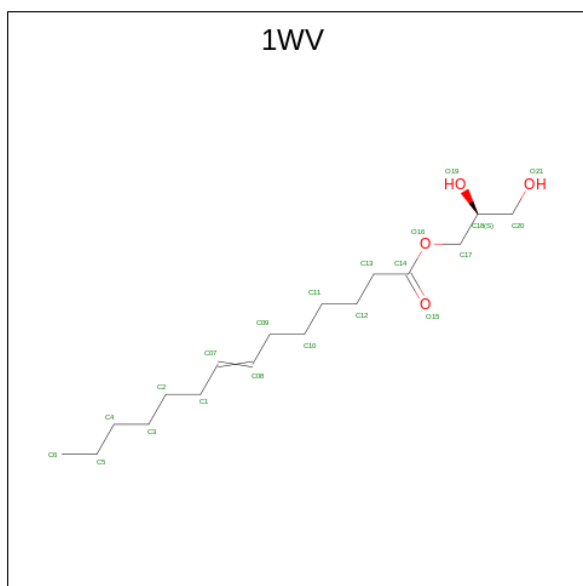
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 6 is (2S)-2,3-dihydroxypropyl (7Z)-tetradec-7-enoate (three-letter code: 1WV) (formula: C<sub>17</sub>H<sub>32</sub>O<sub>4</sub>).

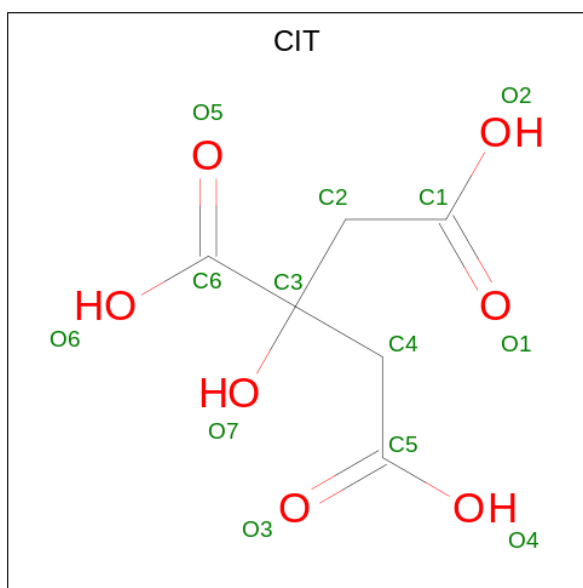


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 15 11 4	0	0
6	B	1	Total C O 15 11 4	0	0

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

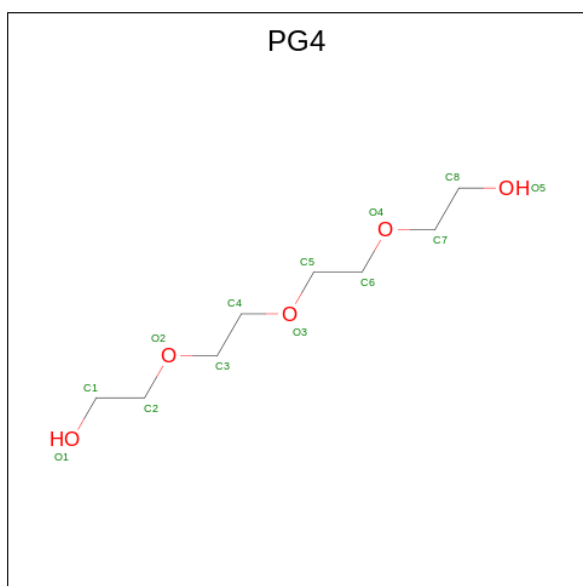
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0

- Molecule 8 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			13	6	7		
8	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			13	8	5		
9	A	1	Total	C	O	0	0
			13	8	5		
9	B	1	Total	C	O	0	0
			13	8	5		

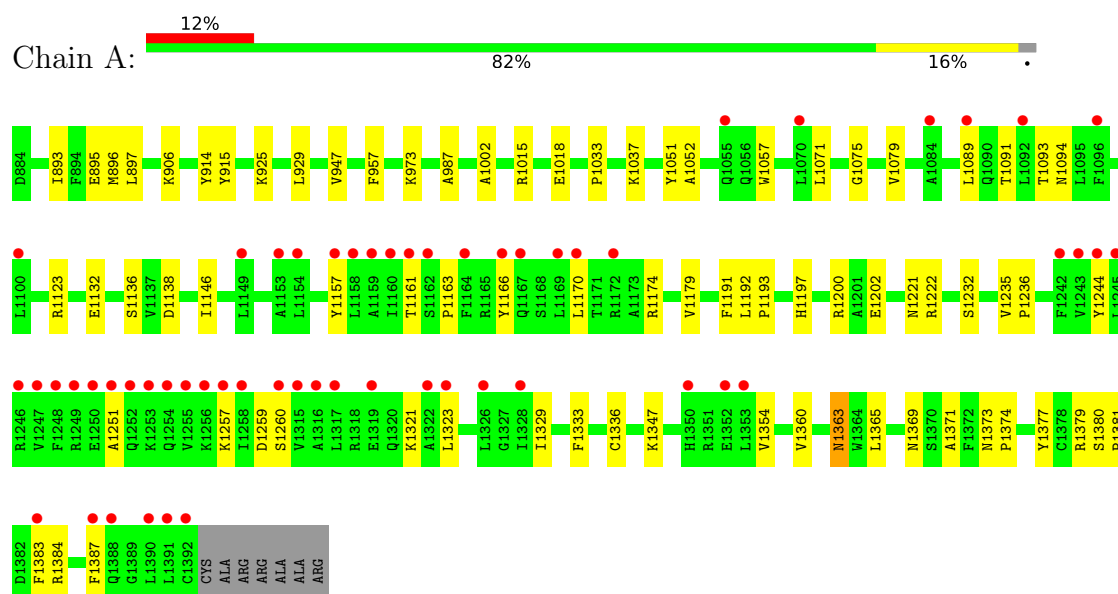
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	90	Total	O	0	0
			90	90		
10	B	31	Total	O	0	0
			31	31		

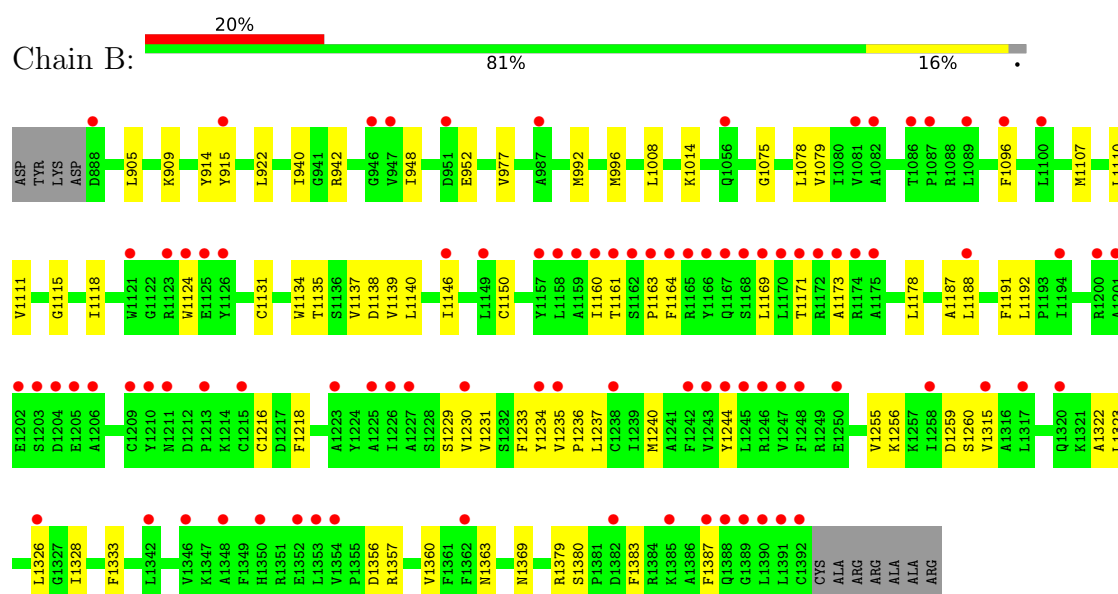
### 3 Residue-property plots

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: Endolysin,Beta-1 adrenergic receptor chimera



- Molecule 1: Endolysin,Beta-1 adrenergic receptor chimera



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

Chain C:  100%

GLU1  
GLU2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.13Å 52.83Å 142.75Å 92.14° 90.71° 116.65°	Depositor
Resolution (Å)	19.79 – 2.50 47.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.79-2.50) 99.9 (47.16-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.225 , 0.263 0.228 , 0.263	Depositor DCC
$R_{free}$ test set	2424 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.8	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.018 for k,h,-l 0.012 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7377	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GLC, CAU, PG4, SO4, CIT, 1WV, CLR

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	0.32	0/3668	0.49	0/4986
1	B	0.31	0/3497	0.49	0/4769
All	All	0.31	0/7165	0.49	0/9755

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3588	0	3622	59	0
1	B	3424	0	3378	57	0
2	C	23	0	21	5	0
3	A	28	0	46	4	0
4	A	22	0	22	2	0
4	B	22	0	22	4	0
5	A	30	0	0	1	0
5	B	10	0	0	0	0
6	A	15	0	18	1	0
6	B	15	0	18	1	0
7	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	26	0	10	5	0
9	A	39	0	54	4	0
9	B	13	0	18	0	0
10	A	90	0	0	1	0
10	B	31	0	0	1	0
All	All	7377	0	7229	118	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 (118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:GLC:H3	2:C:2:GLC:H5	1.41	1.02
2:C:1:GLC:H3	2:C:2:GLC:C5	2.11	0.80
1:A:1071:LEU:HD22	1:A:1371:ALA:HB1	1.68	0.75
1:B:1146:ILE:HG13	1:B:1236:PRO:HB2	1.75	0.69
1:A:1123:ARG:NH2	5:A:1403:SO4:O3	2.26	0.69
2:C:1:GLC:C3	2:C:2:GLC:H5	2.22	0.67
1:A:1015:ARG:NH2	1:A:1018:GLU:OE1	2.29	0.66
1:B:1255:VAL:HG23	1:B:1256:LYS:H	1.61	0.66
1:B:1110:LEU:HD11	1:B:1137:VAL:HG11	1.77	0.65
1:A:1363:ASN:HD22	1:A:1363:ASN:C	2.00	0.64
1:B:940:ILE:HG22	1:B:942:ARG:HG2	1.85	0.58
1:A:1132:GLU:OE2	1:A:1197:HIS:NE2	2.36	0.58
1:A:1136:SER:HB3	1:A:1191:PHE:CD1	2.38	0.58
1:A:1221:ASN:HB2	8:A:1411:CIT:H41	1.87	0.56
1:B:1110:LEU:HD12	1:B:1110:LEU:O	2.05	0.56
1:B:1235:VAL:HB	1:B:1236:PRO:HD3	1.87	0.56
1:A:897:LEU:HD12	1:A:957:PHE:CZ	2.42	0.55
1:A:1347:LYS:NZ	10:A:1504:HOH:O	2.40	0.55
1:A:1052:ALA:HA	9:A:1413:PG4:H12	1.88	0.55
1:B:1140:LEU:HD13	1:B:1187:ALA:HA	1.87	0.55
1:A:1075:GLY:O	1:A:1079:VAL:HG23	2.07	0.55
3:A:1401:CLR:H212	3:A:1401:CLR:H121	1.87	0.54
1:B:1131:CYS:O	1:B:1135:THR:N	2.39	0.54
1:B:1115:GLY:O	1:B:1118:ILE:HG22	2.07	0.54
1:B:1171:THR:HG22	1:B:1173:ALA:H	1.72	0.54
1:B:1111:VAL:HG11	1:B:1138:ASP:OD1	2.07	0.54
1:A:893:ILE:HG13	1:A:896:MET:HE2	1.89	0.54
1:B:1107:MET:HA	1:B:1111:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1187:ALA:O	1:B:1191:PHE:N	2.38	0.53
1:B:1244:TYR:OH	1:B:1323:LEU:O	2.26	0.53
1:A:1257:LYS:NZ	1:B:1169:LEU:HD21	2.22	0.53
1:A:1221:ASN:HB2	8:A:1411:CIT:C4	2.39	0.53
1:A:1336:CYS:HA	1:A:1365:LEU:HG	1.91	0.52
1:A:897:LEU:HD12	1:A:957:PHE:HZ	1.73	0.52
1:B:1259:ASP:OD1	1:B:1260:SER:N	2.42	0.52
1:A:1235:VAL:HB	1:A:1236:PRO:HD3	1.92	0.51
3:A:1401:CLR:H121	3:A:1401:CLR:C21	2.40	0.51
1:A:1089:LEU:O	1:A:1094:ASN:ND2	2.38	0.51
1:A:1192:LEU:HB3	1:A:1193:PRO:HD3	1.93	0.51
1:A:1163:PRO:HG3	1:B:1163:PRO:HG3	1.91	0.51
1:A:1360:VAL:HG21	6:A:1409:1WV:H16	1.93	0.51
1:B:1160:ILE:HG23	1:B:1161:THR:HG23	1.92	0.50
1:A:1333:PHE:HD1	1:A:1369:ASN:OD1	1.93	0.50
1:B:1380:SER:HB2	1:B:1383:PHE:HD2	1.75	0.50
1:B:1229:SER:O	1:B:1233:PHE:HB3	2.12	0.50
1:A:1381:PRO:HA	1:A:1384:ARG:HD3	1.93	0.50
1:A:1157:TYR:O	1:A:1161:THR:HG22	2.12	0.49
1:B:1357:ARG:HH21	6:B:1405:1WV:H6	1.77	0.49
1:A:1257:LYS:HZ1	1:B:1169:LEU:HD11	1.78	0.48
1:A:1071:LEU:CD2	1:A:1371:ALA:HB1	2.40	0.48
1:A:1138:ASP:OD2	4:A:1402:CAU:N19	2.47	0.48
1:B:1134:TRP:CH2	4:B:1401:CAU:H222	2.50	0.47
1:A:1033:PRO:O	1:A:1037:LYS:HG3	2.15	0.47
1:B:1138:ASP:OD2	4:B:1401:CAU:C18	2.63	0.46
1:A:1079:VAL:HG22	1:A:1387:PHE:HZ	1.80	0.46
1:B:1146:ILE:HG23	1:B:1236:PRO:HG2	1.98	0.46
1:B:1150:CYS:HB2	1:B:1236:PRO:HB3	1.98	0.46
1:B:1333:PHE:HD1	1:B:1369:ASN:OD1	1.98	0.46
1:A:1146:ILE:HG13	1:A:1236:PRO:HB2	1.98	0.46
1:B:1230:VAL:O	1:B:1235:VAL:HG23	2.16	0.46
1:A:973:LYS:HE3	1:A:1002:ALA:HB1	1.98	0.45
1:B:1139:VAL:HG13	4:B:1401:CAU:C11	2.46	0.45
1:A:1259:ASP:OD1	1:A:1260:SER:N	2.50	0.45
1:A:1321:LYS:HE2	1:A:1379:ARG:O	2.17	0.45
1:A:1354:VAL:O	1:A:1354:VAL:HG23	2.16	0.45
1:B:1146:ILE:HD13	1:B:1333:PHE:CE2	2.51	0.45
2:C:1:GLC:H4	2:C:2:GLC:O2	2.15	0.45
1:A:1179:VAL:HG11	3:A:1401:CLR:H72	1.99	0.45
1:B:1138:ASP:OD2	4:B:1401:CAU:N19	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:TRP:CD1	8:A:1412:CIT:H41	2.52	0.45
1:B:1255:VAL:HG23	1:B:1256:LYS:N	2.31	0.45
1:B:940:ILE:HD12	1:B:952:GLU:HB3	1.99	0.44
1:B:992:MET:O	1:B:996:MET:HG2	2.17	0.44
1:A:1363:ASN:ND2	1:A:1363:ASN:C	2.70	0.44
1:B:1096:PHE:HE1	1:B:1178:LEU:HD22	1.83	0.44
1:A:1200:ARG:HH11	9:A:1415:PG4:H12	1.82	0.44
1:B:1135:THR:HG21	1:B:1218:PHE:CD1	2.52	0.44
1:A:1174:ARG:CZ	1:B:1315:VAL:HG21	2.48	0.43
1:B:1231:VAL:HG12	1:B:1231:VAL:O	2.19	0.43
2:C:1:GLC:H3	2:C:2:GLC:O5	2.18	0.43
1:A:1200:ARG:HD3	9:A:1415:PG4:C1	2.49	0.43
1:A:1166:TYR:CE1	1:A:1170:LEU:HD12	2.54	0.43
1:B:914:TYR:HB3	1:B:922:LEU:HD11	2.00	0.43
1:A:1329:ILE:HD13	1:A:1377:TYR:HE1	1.82	0.43
1:A:1222:ARG:NH1	8:A:1411:CIT:O5	2.51	0.43
1:A:1251:ALA:HB1	1:B:1164:PHE:CE2	2.53	0.43
1:A:1091:THR:HG22	1:A:1093:THR:H	1.84	0.43
1:B:1236:PRO:O	1:B:1240:MET:N	2.39	0.42
1:A:1244:TYR:OH	1:A:1323:LEU:O	2.37	0.42
1:B:1234:TYR:HA	1:B:1237:LEU:HB3	2.01	0.42
1:B:1356:ASP:O	1:B:1360:VAL:HG12	2.20	0.42
1:A:1197:HIS:HB3	1:A:1200:ARG:HD2	2.01	0.42
1:B:1328:ILE:HD12	1:B:1379:ARG:NH1	2.34	0.42
1:B:1124:TRP:CB	1:B:1216:CYS:SG	3.08	0.42
1:A:1174:ARG:NH1	1:B:1315:VAL:HG21	2.34	0.42
1:A:906:LYS:HG2	1:A:947:VAL:HG22	2.02	0.42
1:A:896:MET:HE1	1:A:987:ALA:O	2.20	0.42
1:A:895:GLU:HB3	9:A:1413:PG4:H31	2.01	0.41
1:B:1383:PHE:HB3	1:B:1387:PHE:CE2	2.54	0.41
1:B:909:LYS:HG2	1:B:915:TYR:CD1	2.55	0.41
1:B:977:VAL:HG21	1:B:1008:LEU:HB3	2.01	0.41
1:A:1202:GLU:H	8:A:1411:CIT:C1	2.33	0.41
1:B:1146:ILE:HD13	1:B:1333:PHE:HE2	1.85	0.41
1:A:1373:ASN:HB2	1:A:1374:PRO:HD3	2.03	0.41
1:A:915:TYR:CE1	1:A:929:LEU:HD13	2.55	0.41
1:B:905:LEU:HD23	1:B:948:ILE:O	2.20	0.41
1:B:1014:LYS:NZ	10:B:1510:HOH:O	2.53	0.41
1:A:1347:LYS:HB2	1:A:1354:VAL:HG21	2.03	0.41
1:A:1380:SER:OG	1:A:1383:PHE:HD2	2.03	0.41
1:B:1078:LEU:HG	1:B:1387:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1322:ALA:O	1:B:1326:LEU:HD13	2.21	0.41
1:B:1111:VAL:CG1	1:B:1138:ASP:OD1	2.69	0.41
1:A:1232:SER:HB2	4:A:1402:CAU:H10	2.03	0.40
1:B:1075:GLY:O	1:B:1079:VAL:N	2.52	0.40
1:A:914:TYR:CD1	1:A:925:LYS:HA	2.56	0.40
3:A:1401:CLR:C12	3:A:1401:CLR:C21	3.00	0.40
1:B:1188:LEU:HD22	1:B:1192:LEU:HD12	2.04	0.40
1:A:896:MET:HG3	1:A:1051:TYR:CZ	2.56	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	453/462 (98%)	447 (99%)	6 (1%)	0	100	100
1	B	449/462 (97%)	434 (97%)	15 (3%)	0	100	100
All	All	902/924 (98%)	881 (98%)	21 (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	378/388 (97%)	377 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	346/388 (89%)	345 (100%)	1 (0%)	92	97
All	All	724/776 (93%)	722 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1363	ASN
1	B	1363	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

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	GLC	C	1	2	12,12,12	1.35	1 (8%)	17,17,17	0.88	0
2	GLC	C	2	2	11,11,12	2.11	3 (27%)	15,15,17	1.99	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GLC	O5-C1	5.31	1.52	1.43
2	C	1	GLC	O5-C1	2.98	1.50	1.42
2	C	2	GLC	C2-C3	-2.87	1.48	1.52
2	C	2	GLC	O5-C5	2.10	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	GLC	C1-C2-C3	4.60	115.32	109.67
2	C	2	GLC	O5-C1-C2	3.77	116.59	110.77
2	C	2	GLC	C1-O5-C5	3.20	116.52	112.19
2	C	2	GLC	C6-C5-C4	-2.14	107.98	113.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

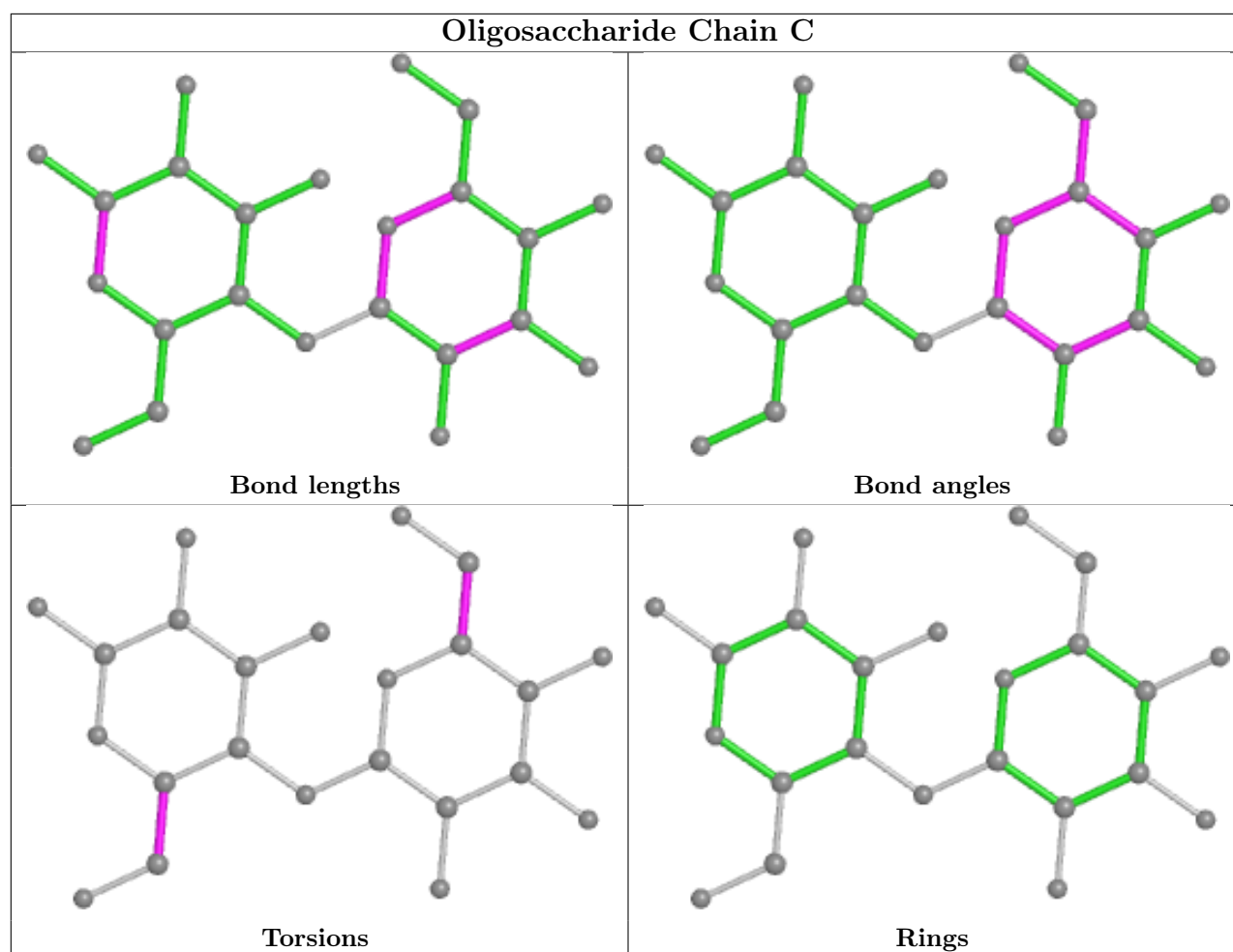
Mol	Chain	Res	Type	Atoms
2	C	1	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	5	0
2	C	2	GLC	5	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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\# Z  > 2$
5	SO4	A	1408	-	4,4,4	0.13	0	6,6,6	0.20	0
5	SO4	A	1403	-	4,4,4	0.15	0	6,6,6	0.21	0
9	PG4	A	1413	-	12,12,12	0.54	0	11,11,11	0.37	0
9	PG4	B	1406	-	12,12,12	0.52	0	11,11,11	0.72	0
5	SO4	A	1407	-	4,4,4	0.12	0	6,6,6	0.12	0
6	1WV	B	1405	-	14,14,20	2.14	3 (21%)	15,15,21	1.88	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	1WV	A	1409	-	14,14,20	2.15	3 (21%)	15,15,21	1.84	3 (20%)
8	CIT	A	1411	-	3,12,12	1.99	1 (33%)	3,17,17	2.00	1 (33%)
5	SO4	A	1404	-	4,4,4	0.19	0	6,6,6	0.14	0
3	CLR	A	1401	-	31,31,31	1.22	4 (12%)	48,48,48	1.45	8 (16%)
5	SO4	B	1404	-	4,4,4	0.19	0	6,6,6	0.18	0
8	CIT	A	1412	-	3,12,12	1.18	0	3,17,17	1.01	0
5	SO4	B	1403	-	4,4,4	0.13	0	6,6,6	0.33	0
4	CAU	B	1401	-	22,24,24	1.08	2 (9%)	31,33,33	1.33	4 (12%)
9	PG4	A	1414	-	12,12,12	0.54	0	11,11,11	0.28	0
4	CAU	A	1402	-	22,24,24	1.08	2 (9%)	31,33,33	1.33	4 (12%)
5	SO4	A	1406	-	4,4,4	0.15	0	6,6,6	0.16	0
5	SO4	A	1405	-	4,4,4	0.13	0	6,6,6	0.10	0
9	PG4	A	1415	-	12,12,12	0.54	0	11,11,11	0.50	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	PG4	A	1413	-	-	3/10/10/10	-
9	PG4	B	1406	-	-	4/10/10/10	-
9	PG4	A	1414	-	-	5/10/10/10	-
6	1WV	B	1405	-	-	6/14/14/20	-
6	1WV	A	1409	-	-	3/14/14/20	-
8	CIT	A	1411	-	-	2/6/16/16	-
3	CLR	A	1401	-	-	9/10/68/68	0/4/4/4
8	CIT	A	1412	-	-	3/6/16/16	-
4	CAU	B	1401	-	-	0/10/10/10	0/3/3/3
9	PG4	A	1415	-	-	4/10/10/10	-
4	CAU	A	1402	-	-	0/10/10/10	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1405	1WV	O15-C14	6.09	1.40	1.22
6	A	1409	1WV	O15-C14	6.04	1.40	1.22
6	A	1409	1WV	C07-C08	3.69	1.53	1.28
6	B	1405	1WV	C07-C08	3.64	1.53	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1402	CAU	C10-C8	-2.89	1.36	1.41
4	B	1401	CAU	C10-C8	-2.88	1.36	1.41
3	A	1401	CLR	C13-C14	-2.80	1.49	1.55
6	A	1409	1WV	O16-C14	2.61	1.40	1.33
6	B	1405	1WV	O16-C14	2.54	1.40	1.33
8	A	1411	CIT	C4-C3	-2.43	1.51	1.54
3	A	1401	CLR	C10-C9	-2.29	1.52	1.56
4	A	1402	CAU	C2-C3	-2.18	1.38	1.41
4	B	1401	CAU	C2-C3	-2.18	1.38	1.41
3	A	1401	CLR	C13-C17	-2.08	1.51	1.55
3	A	1401	CLR	C18-C13	-2.08	1.50	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1409	1WV	O16-C14-O15	-5.63	109.38	123.59
6	B	1405	1WV	O16-C14-O15	-5.57	109.53	123.59
3	A	1401	CLR	C3-C4-C5	-3.97	105.29	112.03
6	B	1405	1WV	O15-C14-C13	-3.74	109.14	123.73
3	A	1401	CLR	C2-C3-C4	-3.55	105.43	110.31
6	A	1409	1WV	O15-C14-C13	-3.55	109.90	123.73
8	A	1411	CIT	C3-C2-C1	-3.43	109.49	114.98
4	B	1401	CAU	C12-C13-C9	-3.38	117.48	121.58
4	A	1402	CAU	C12-C13-C9	-3.35	117.51	121.58
3	A	1401	CLR	C11-C12-C13	-2.87	107.86	112.78
3	A	1401	CLR	C7-C8-C14	-2.81	106.84	110.91
4	A	1402	CAU	O14-C13-C9	2.80	121.08	117.11
4	B	1401	CAU	O14-C13-C9	2.78	121.06	117.11
3	A	1401	CLR	C15-C14-C8	-2.73	114.58	119.08
4	B	1401	CAU	C5-C4-C3	2.30	121.22	118.17
4	A	1402	CAU	C5-C4-C3	2.29	121.21	118.17
3	A	1401	CLR	C4-C5-C10	2.19	119.33	116.42
4	A	1402	CAU	C18-N19-C20	2.18	121.40	114.44
4	B	1401	CAU	C18-N19-C20	2.17	121.38	114.44
6	B	1405	1WV	C09-C08-C07	-2.12	112.46	126.84
3	A	1401	CLR	C14-C8-C9	-2.10	106.28	109.09
6	A	1409	1WV	C09-C08-C07	-2.05	112.89	126.84
3	A	1401	CLR	C9-C10-C5	-2.03	106.46	109.65

There are no chirality outliers.

All (39) torsion outliers are listed below:

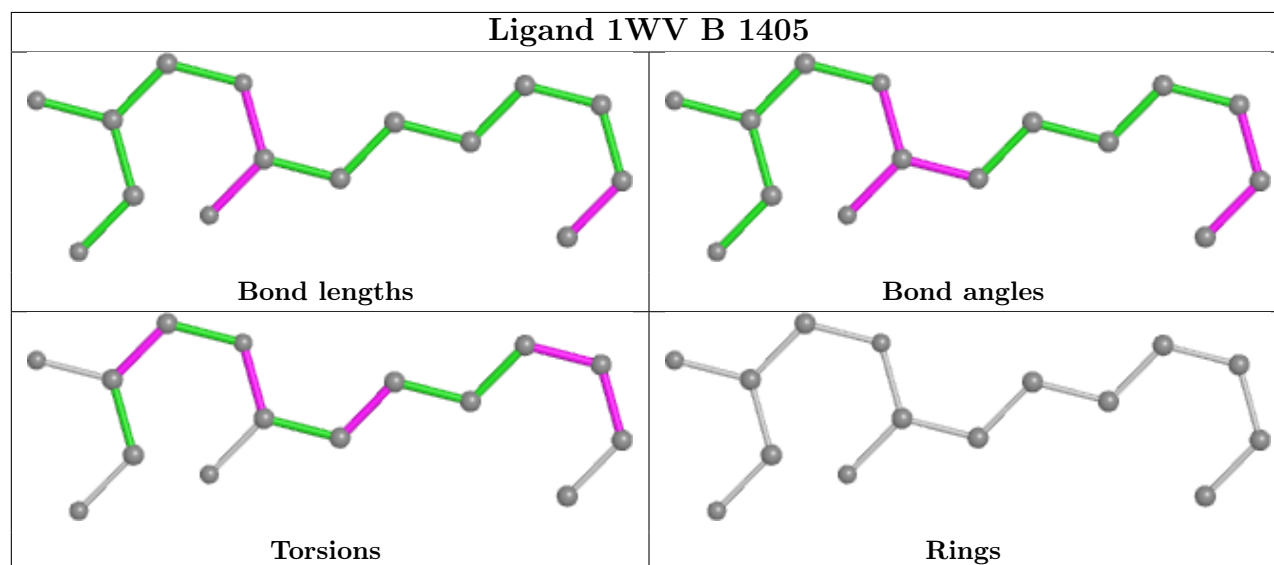
Mol	Chain	Res	Type	Atoms
6	B	1405	1WV	O16-C17-C18-C20
8	A	1412	CIT	C1-C2-C3-O7
8	A	1412	CIT	C1-C2-C3-C4
8	A	1412	CIT	C1-C2-C3-C6
9	B	1406	PG4	C6-C5-O3-C4
6	B	1405	1WV	O16-C17-C18-O19
9	A	1415	PG4	C1-C2-O2-C3
9	A	1414	PG4	O3-C5-C6-O4
9	A	1414	PG4	O2-C3-C4-O3
6	B	1405	1WV	O15-C14-O16-C17
3	A	1401	CLR	C21-C20-C22-C23
3	A	1401	CLR	C16-C17-C20-C22
3	A	1401	CLR	C17-C20-C22-C23
9	A	1414	PG4	O1-C1-C2-O2
3	A	1401	CLR	C23-C24-C25-C27
9	A	1415	PG4	O2-C3-C4-O3
3	A	1401	CLR	C23-C24-C25-C26
9	A	1414	PG4	O4-C7-C8-O5
6	A	1409	1WV	C13-C14-O16-C17
6	B	1405	1WV	C11-C12-C13-C14
6	B	1405	1WV	C07-C08-C09-C10
3	A	1401	CLR	C20-C22-C23-C24
9	B	1406	PG4	O1-C1-C2-O2
3	A	1401	CLR	C22-C23-C24-C25
9	A	1413	PG4	C1-C2-O2-C3
9	A	1415	PG4	O4-C7-C8-O5
9	A	1413	PG4	C3-C4-O3-C5
3	A	1401	CLR	C16-C17-C20-C21
8	A	1411	CIT	C6-C3-C4-C5
8	A	1411	CIT	C1-C2-C3-C4
9	A	1414	PG4	C3-C4-O3-C5
6	B	1405	1WV	C08-C09-C10-C11
3	A	1401	CLR	C13-C17-C20-C21
9	B	1406	PG4	C5-C6-O4-C7
6	A	1409	1WV	C07-C08-C09-C10
9	B	1406	PG4	O2-C3-C4-O3
6	A	1409	1WV	C11-C12-C13-C14
9	A	1413	PG4	C8-C7-O4-C6
9	A	1415	PG4	C8-C7-O4-C6

There are no ring outliers.

10 monomers are involved in 22 short contacts:

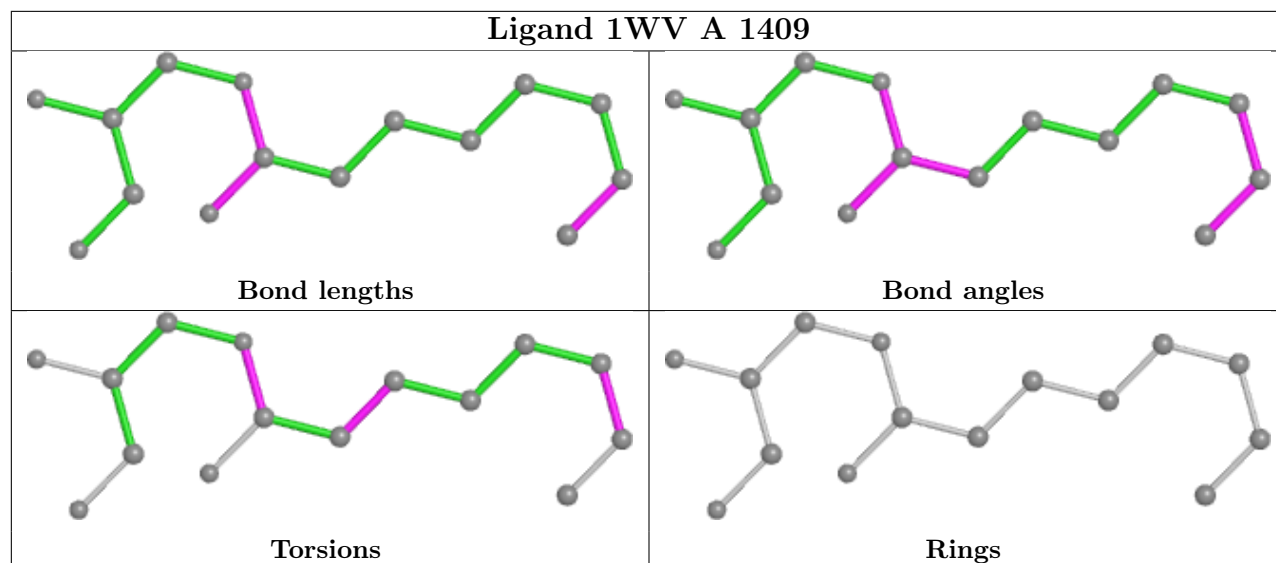
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1403	SO4	1	0
9	A	1413	PG4	2	0
6	B	1405	1WV	1	0
6	A	1409	1WV	1	0
8	A	1411	CIT	4	0
3	A	1401	CLR	4	0
8	A	1412	CIT	1	0
4	B	1401	CAU	4	0
4	A	1402	CAU	2	0
9	A	1415	PG4	2	0

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.

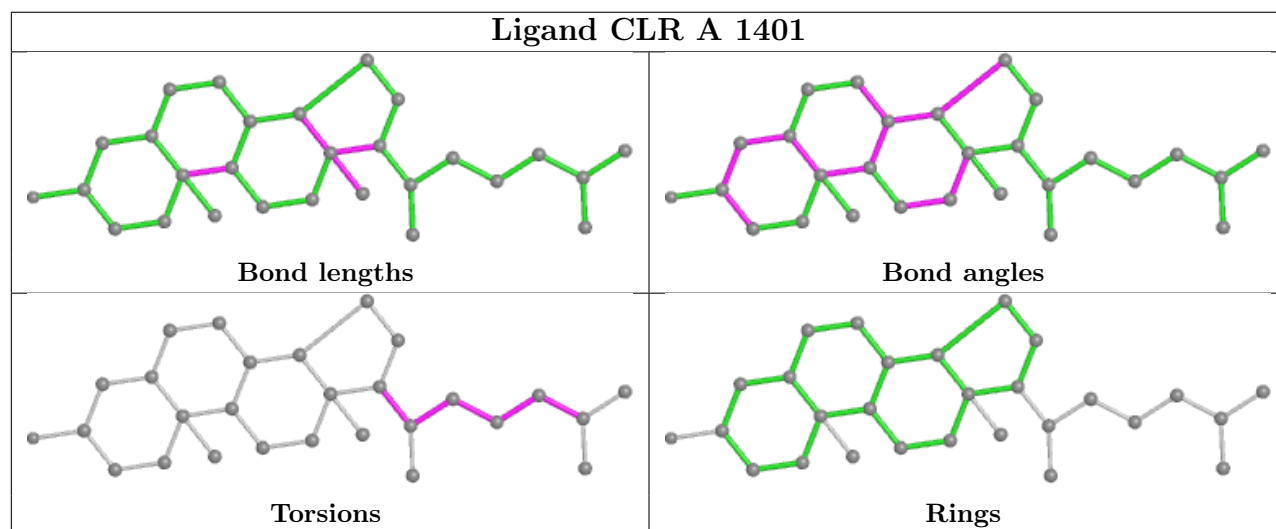


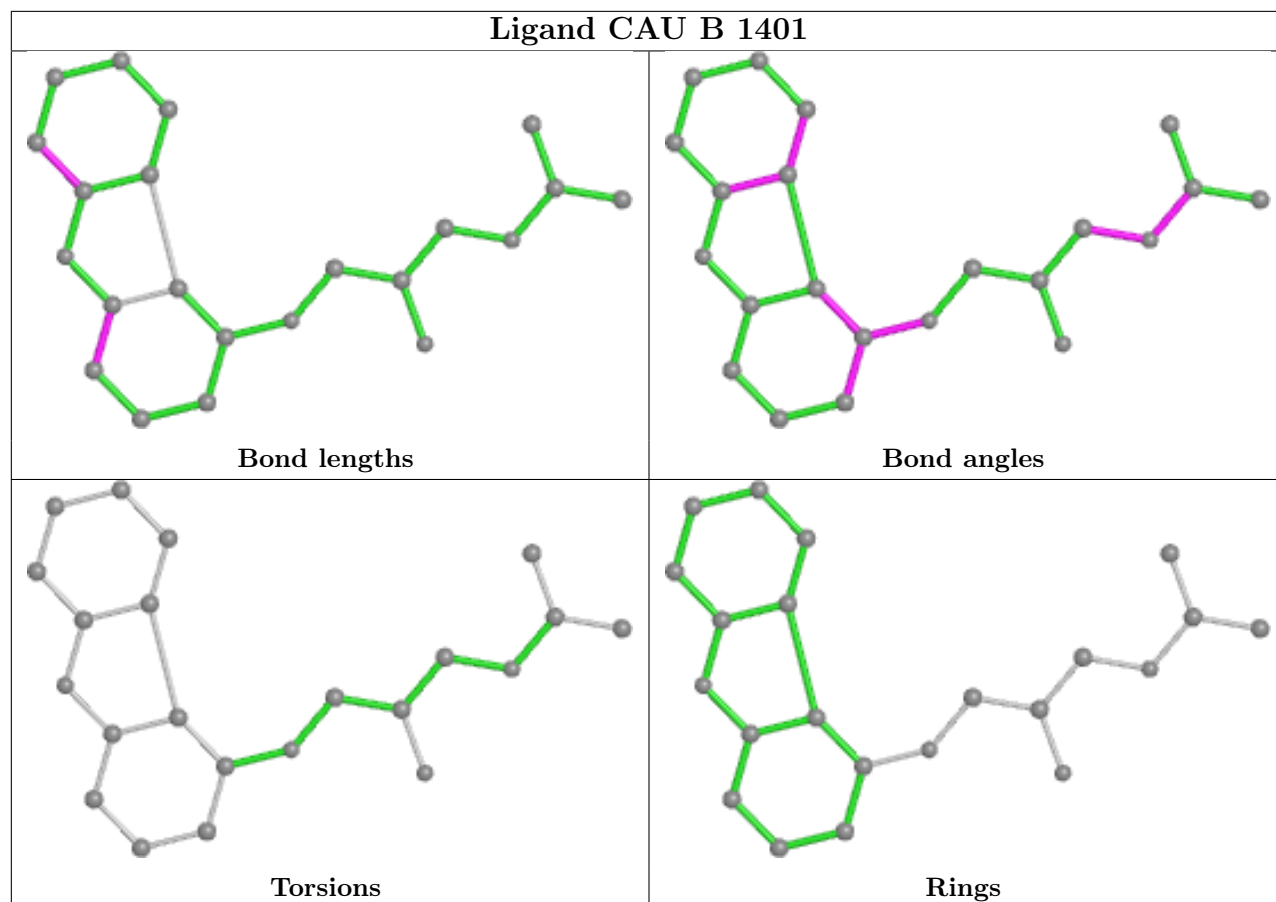


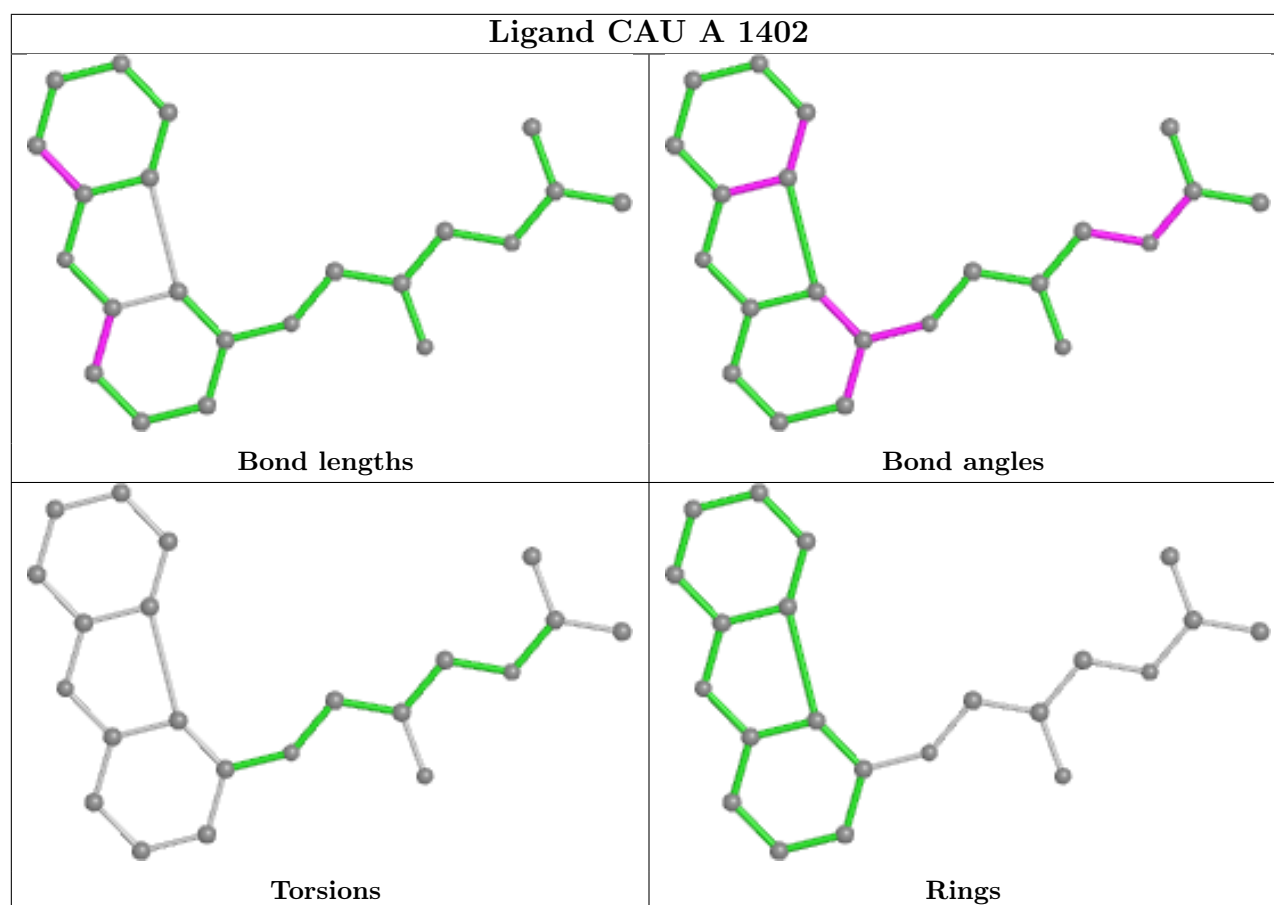
## Ligand 1WV A 1409



## Ligand CLR A 1401







## 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, 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	455/462 (98%)	0.88	57 (12%) <b>3</b> <b>3</b>	29, 59, 113, 141	0
1	B	451/462 (97%)	1.29	91 (20%) <b>1</b> <b>0</b>	30, 90, 134, 153	0
All	All	906/924 (98%)	1.09	148 (16%) <b>1</b> <b>1</b>	29, 70, 127, 153	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1392	CYS	12.6
1	B	1164	PHE	12.0
1	B	1391	LEU	11.0
1	B	1170	LEU	9.0
1	A	1257	LYS	8.5
1	B	1352	GLU	8.3
1	B	1166	TYR	8.2
1	B	1169	LEU	8.1
1	B	1210	TYR	7.0
1	A	1258	ILE	7.0
1	B	1089	LEU	7.0
1	B	1390	LEU	6.5
1	A	1255	VAL	6.5
1	B	1204	ASP	6.2
1	A	1254	GLN	6.1
1	B	1158	LEU	5.8
1	B	1159	ALA	5.8
1	B	1123	ARG	5.7
1	A	1387	PHE	5.6
1	A	1390	LEU	5.6
1	B	1124	TRP	5.6
1	B	1168	SER	5.5
1	B	1353	LEU	5.5
1	B	1086	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	1201	ALA	5.4
1	A	1315	VAL	5.4
1	A	1249	ARG	5.2
1	A	1326	LEU	5.2
1	A	1256	LYS	5.2
1	B	1172	ARG	5.1
1	A	1248	PHE	4.9
1	B	1165	ARG	4.9
1	B	1206	ALA	4.8
1	B	1354	VAL	4.8
1	B	1242	PHE	4.8
1	A	1160	ILE	4.7
1	B	1202	GLU	4.7
1	B	1387	PHE	4.5
1	B	1223	ALA	4.5
1	B	1342	LEU	4.4
1	B	1346	VAL	4.3
1	B	1082	ALA	4.2
1	A	1245	LEU	4.2
1	A	1089	LEU	4.2
1	A	1246	ARG	4.1
1	B	1087	PRO	4.1
1	A	1316	ALA	4.0
1	A	1242	PHE	4.0
1	A	1391	LEU	3.9
1	A	1159	ALA	3.9
1	A	1317	LEU	3.9
1	B	1160	ILE	3.9
1	B	1382	ASP	3.8
1	B	1121	TRP	3.8
1	B	1163	PRO	3.7
1	B	1245	LEU	3.7
1	B	1389	GLY	3.6
1	B	1247	VAL	3.6
1	B	1320	GLN	3.6
1	B	1157	TYR	3.6
1	B	1161	THR	3.6
1	B	915	TYR	3.5
1	B	1173	ALA	3.5
1	B	1167	GLN	3.5
1	A	1164	PHE	3.5
1	A	1253	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1383	PHE	3.4
1	B	1226	ILE	3.4
1	A	1158	LEU	3.4
1	B	1315	VAL	3.4
1	B	1248	PHE	3.4
1	B	1243	VAL	3.3
1	B	1385	LYS	3.3
1	B	1175	ALA	3.2
1	B	1225	ALA	3.2
1	A	1252	GLN	3.2
1	A	1247	VAL	3.2
1	A	1154	LEU	3.2
1	A	1055	GLN	3.2
1	A	1353	LEU	3.2
1	B	888	ASP	3.1
1	B	1246	ARG	3.1
1	A	1250	GLU	3.1
1	A	1251	ALA	3.1
1	A	1172	ARG	3.0
1	B	1205	GLU	3.0
1	A	1243	VAL	3.0
1	B	1146	ILE	2.9
1	B	1149	LEU	2.9
1	B	1200	ARG	2.9
1	A	1169	LEU	2.9
1	A	1157	TYR	2.9
1	B	1317	LEU	2.9
1	B	1234	TYR	2.9
1	A	1162	SER	2.8
1	A	1352	GLU	2.8
1	B	1162	SER	2.8
1	B	1081	VAL	2.7
1	A	1167	GLN	2.7
1	B	1203	SER	2.7
1	A	1153	ALA	2.6
1	A	1166	TYR	2.6
1	B	1235	VAL	2.6
1	A	1070	LEU	2.6
1	B	1056	GLN	2.6
1	B	946	GLY	2.6
1	B	1388	GLN	2.6
1	B	1238	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1084	ALA	2.6
1	A	1319	GLU	2.6
1	B	1350	HIS	2.5
1	B	1250	GLU	2.5
1	A	1244	TYR	2.5
1	B	1213	PRO	2.5
1	B	1227	ALA	2.5
1	B	1230	VAL	2.5
1	A	1350	HIS	2.4
1	B	1188	LEU	2.4
1	B	1211	ASN	2.4
1	B	1348	ALA	2.4
1	A	1100	LEU	2.4
1	B	951	ASP	2.4
1	B	1362	PHE	2.4
1	A	1092	LEU	2.4
1	B	1171	THR	2.3
1	B	1209	CYS	2.3
1	A	1323	LEU	2.3
1	B	1326	LEU	2.3
1	B	1174	ARG	2.3
1	B	1194	ILE	2.2
1	A	1161	THR	2.2
1	B	1126	TYR	2.2
1	B	1096	PHE	2.2
1	B	1244	TYR	2.2
1	A	1322	ALA	2.2
1	B	987	ALA	2.2
1	B	947	VAL	2.1
1	A	1392	CYS	2.1
1	A	1328	ILE	2.1
1	B	1125	GLU	2.1
1	A	1260	SER	2.1
1	A	1388	GLN	2.1
1	B	1258	ILE	2.1
1	B	1100	LEU	2.1
1	B	1215	CYS	2.0
1	A	1149	LEU	2.0
1	A	1096	PHE	2.0
1	A	1170	LEU	2.0

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

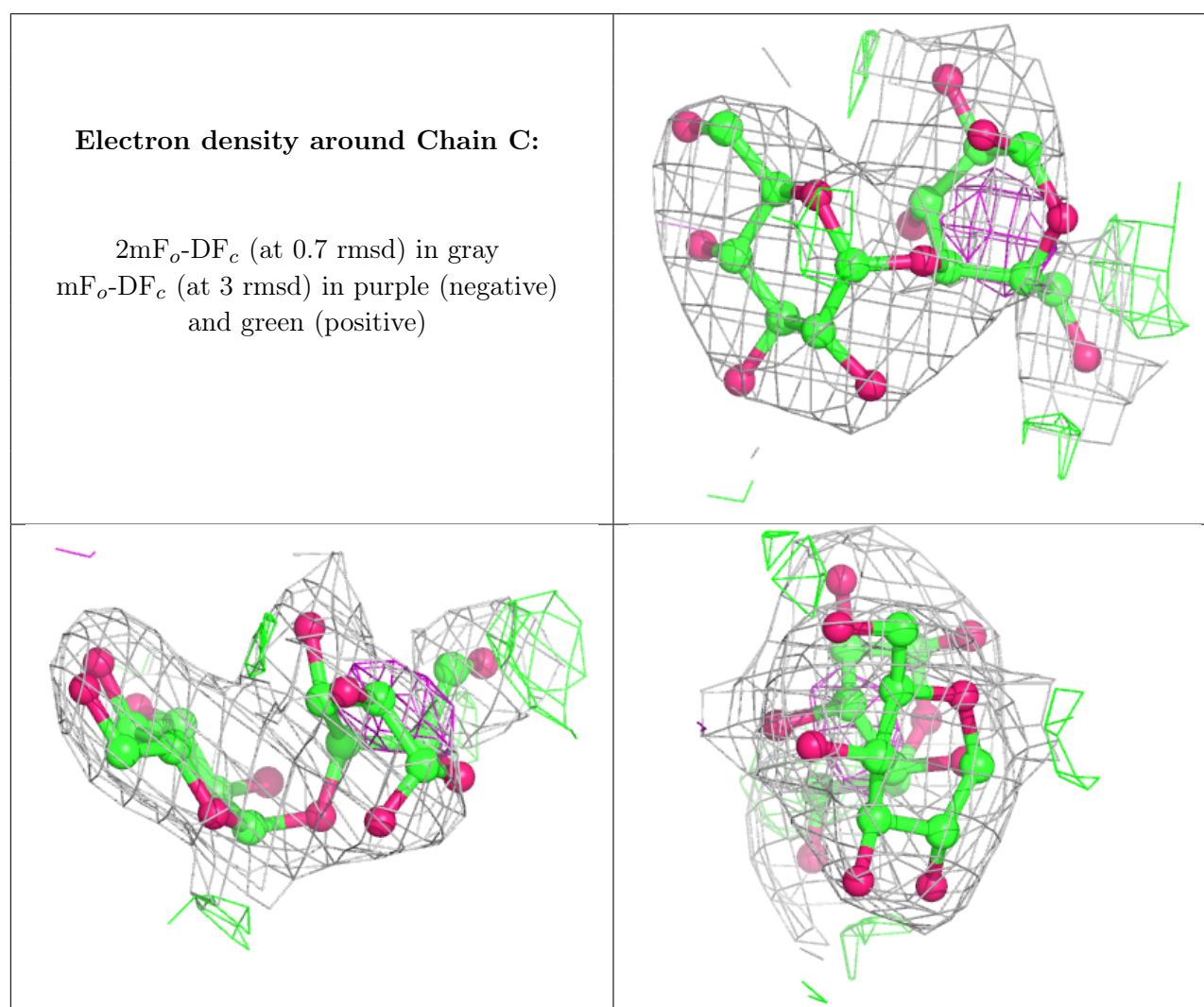
There are no non-standard protein/DNA/RNA residues in this entry.

## 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( $\text{\AA}^2$ )	Q<0.9
2	GLC	C	1	12/12	0.54	0.26	48,65,75,77	0
2	GLC	C	2	11/12	0.91	0.17	53,62,75,76	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 ⓘ

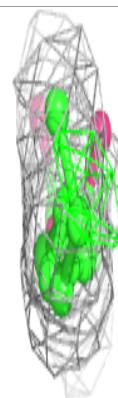
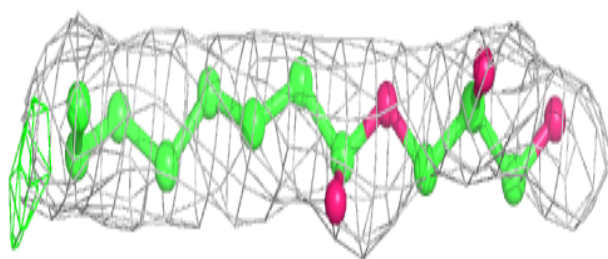
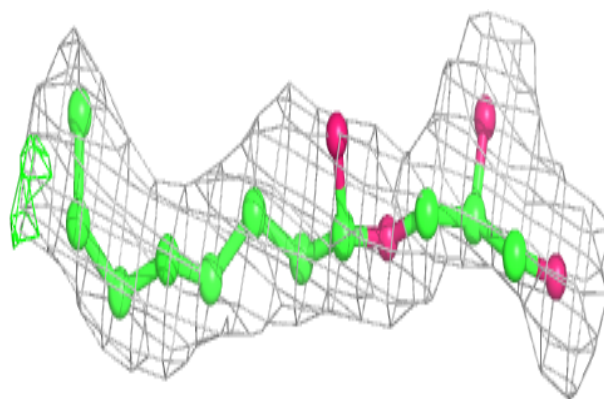
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
6	1WV	B	1405	15/21	0.67	0.24	78,89,106,107	0
8	CIT	A	1412	13/13	0.74	0.47	56,67,76,76	0
6	1WV	A	1409	15/21	0.79	0.22	58,71,86,86	0
4	CAU	B	1401	22/22	0.80	0.29	98,118,122,124	0
9	PG4	A	1415	13/13	0.80	0.23	65,71,75,77	0
8	CIT	A	1411	13/13	0.85	0.23	65,77,87,90	0
9	PG4	A	1414	13/13	0.87	0.32	58,65,72,75	0
5	SO4	A	1405	5/5	0.87	0.17	59,63,79,91	0
3	CLR	A	1401	28/28	0.89	0.33	77,86,96,98	0
9	PG4	B	1406	13/13	0.89	0.30	63,71,91,94	0
9	PG4	A	1413	13/13	0.92	0.26	46,60,66,70	0
5	SO4	A	1408	5/5	0.93	0.15	68,70,80,95	0
4	CAU	A	1402	22/22	0.94	0.16	52,60,66,66	0
5	SO4	A	1407	5/5	0.95	0.21	61,69,81,93	0
5	SO4	A	1406	5/5	0.97	0.14	52,57,59,65	0
5	SO4	B	1403	5/5	0.99	0.18	35,41,44,46	0
5	SO4	A	1403	5/5	0.99	0.18	41,43,51,56	0
5	SO4	B	1404	5/5	0.99	0.18	40,44,47,51	0
7	NA	A	1410	1/1	0.99	0.07	47,47,47,47	0
5	SO4	A	1404	5/5	1.00	0.23	33,33,35,37	0

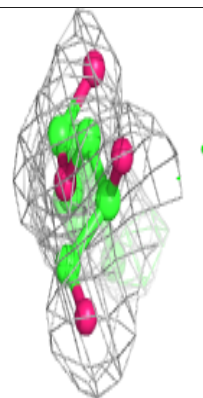
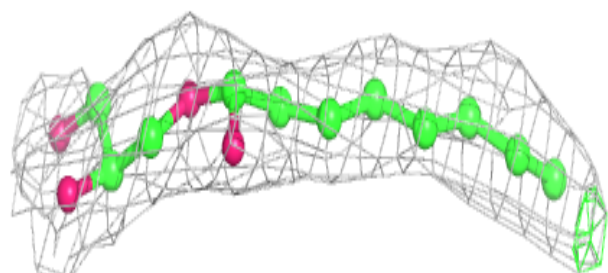
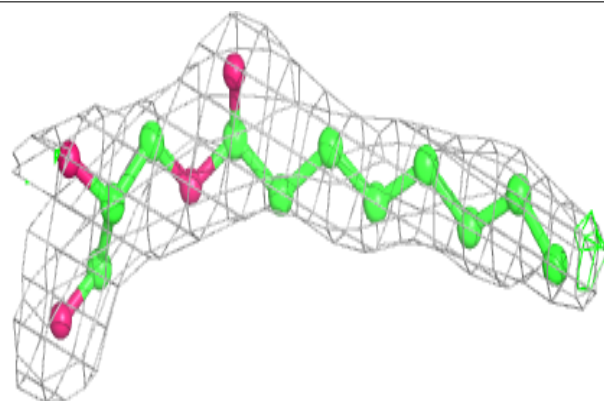
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 1WV B 1405:**

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

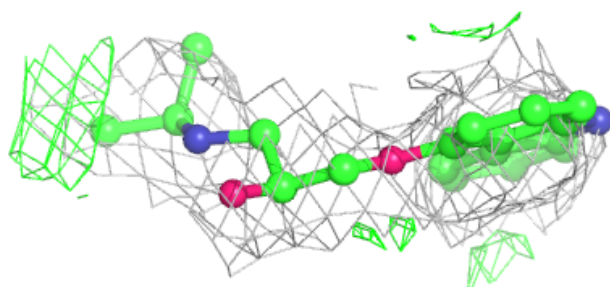
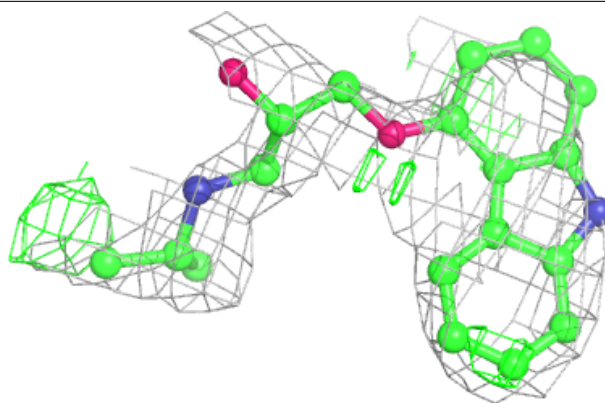
**Electron density around 1WV A 1409:**

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

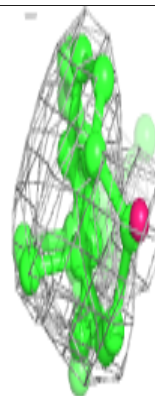
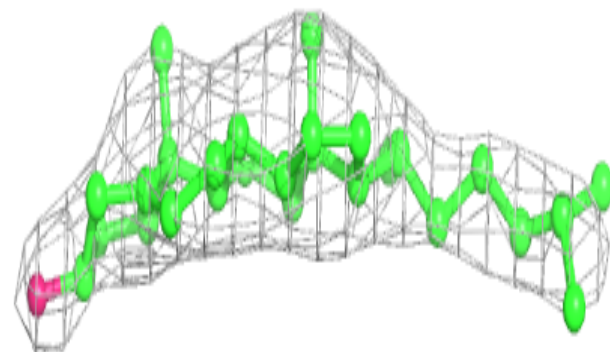
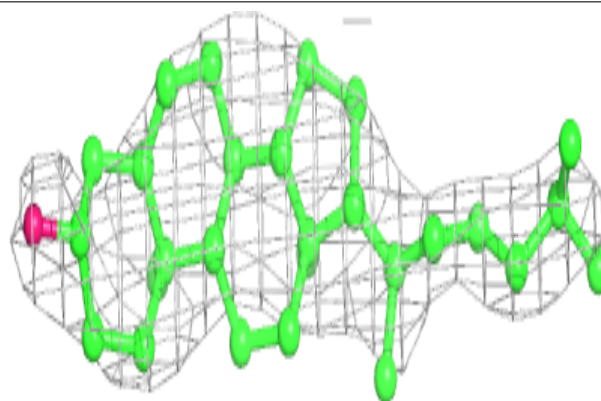


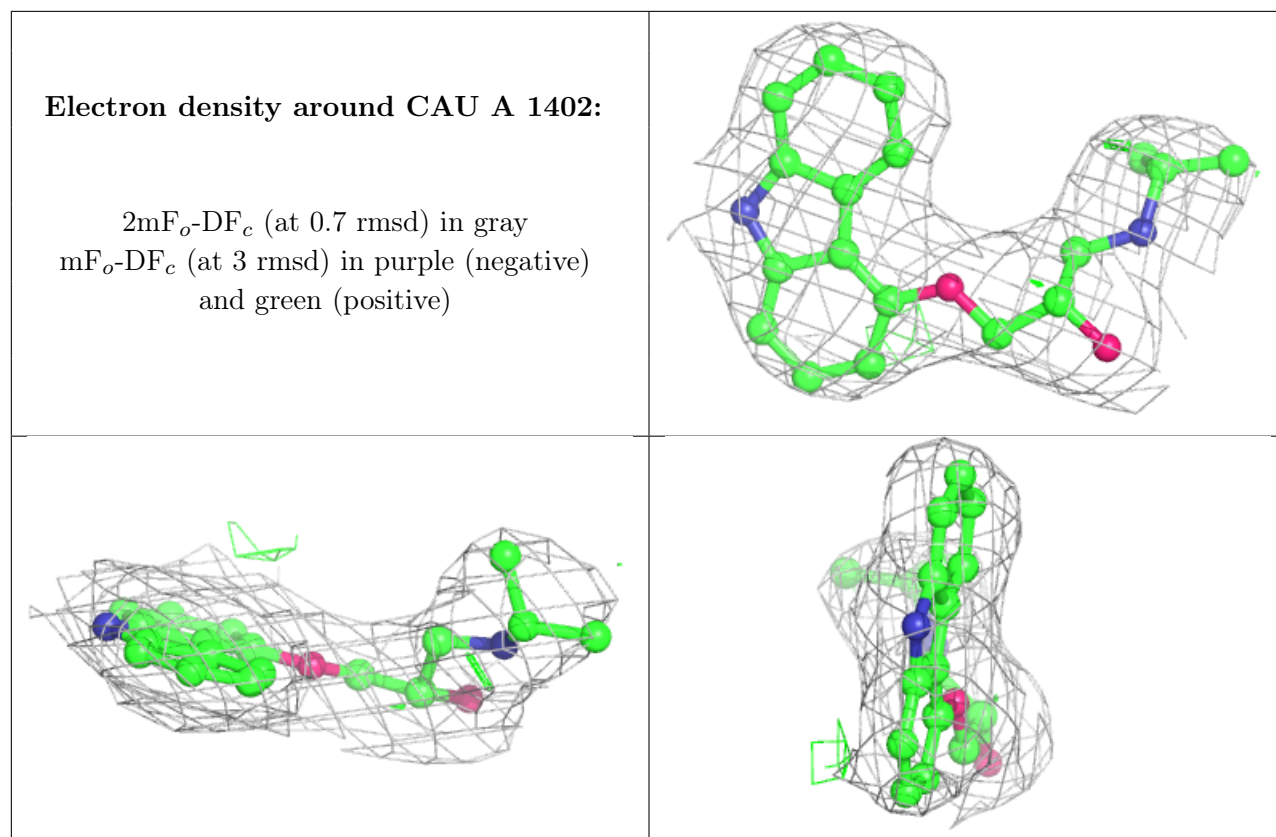
**Electron density around CAU B 1401:**

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

**Electron density around CLR A 1401:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.