Full wwPDB X-ray Structure Validation Report (i)

Jun 6, 2022 – 03:47 pm BST

PDB ID	:	7P0I
Title	:	Crystal structure of a CGRP receptor ectodomain heterodimer bound to macrocyclic inhibitor Compound 13
Authors	:	Southall, S.M.
Deposited on	:	2021-06-29
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

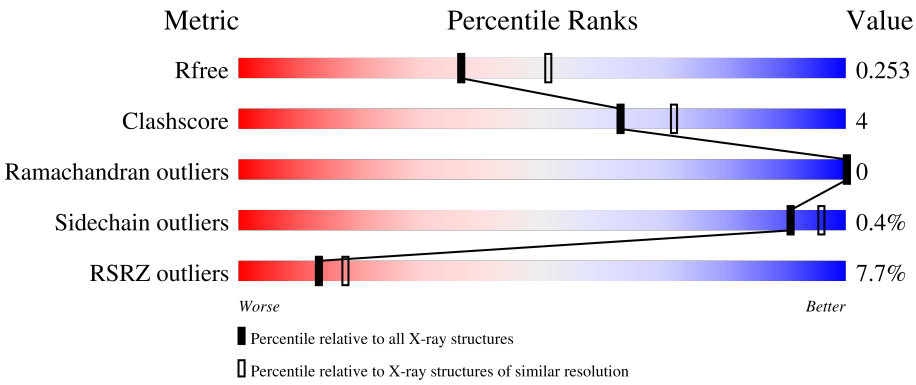
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	594	7% 85% 11% •
2	B	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4853 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 Maltose/maltodextrin-binding periplasmic protein,Receptor activity-modifying protein 1,Calcitonin gene-related peptide type 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	571	4569	2923	761	862	23	0	8	0

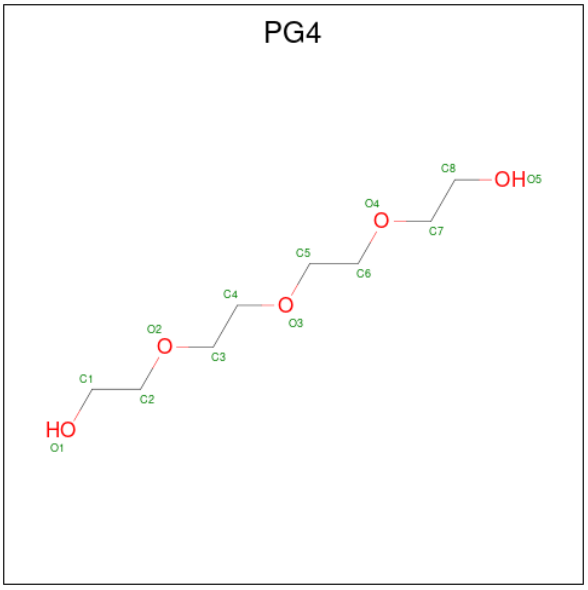
There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP P0AEX9
A	1	SER	-	expression tag	UNP P0AEX9
A	369	ASN	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
A	371	ALA	-	linker	UNP P0AEX9
A	372	ALA	-	linker	UNP P0AEX9
A	1022	GLU	-	linker	UNP P0AEX9
A	1023	PHE	-	linker	UNP P0AEX9
A	2026	GLY	-	linker	UNP O60894
A	2027	SER	-	linker	UNP O60894
A	2027A	ALA	-	linker	UNP O60894
A	2027B	GLY	-	linker	UNP O60894
A	2027C	SER	-	linker	UNP O60894
A	2027D	ALA	-	linker	UNP O60894
A	2027E	GLY	-	linker	UNP O60894
A	2027F	SER	-	linker	UNP O60894
A	2027G	ALA	-	linker	UNP O60894
A	2066	GLN	ASN	conflict	UNP Q16602
A	2118	GLN	ASN	conflict	UNP Q16602
A	2123	ASP	ASN	conflict	UNP Q16602
A	2145	HIS	-	expression tag	UNP Q16602
A	2146	HIS	-	expression tag	UNP Q16602
A	2147	HIS	-	expression tag	UNP Q16602
A	2148	HIS	-	expression tag	UNP Q16602
A	2149	HIS	-	expression tag	UNP Q16602
A	2150	HIS	-	expression tag	UNP Q16602

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

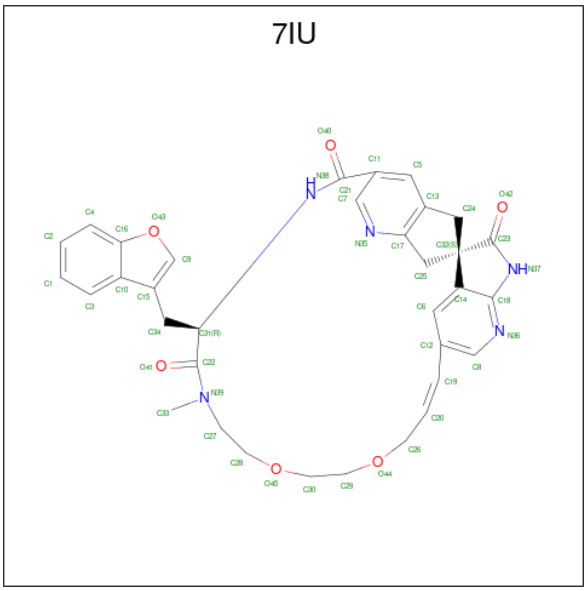
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	2	23	12	11	0	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 4 is (1S,20E)-10-(benzofuran-3-ylmethyl)-12-methyl-15,18-dioxa-5,9,12,24,26-pentazapentacyclo[20.5.2.11,4.13,7.025,28]hentriaconta-3(30),4,6,20,22(29),23,25(28)-heptaene-8,11,27-trione (three-letter code: 7IU) (formula: $C_{34}H_{33}N_5O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	45	34	5	6	0	0

- Molecule 5 is water.

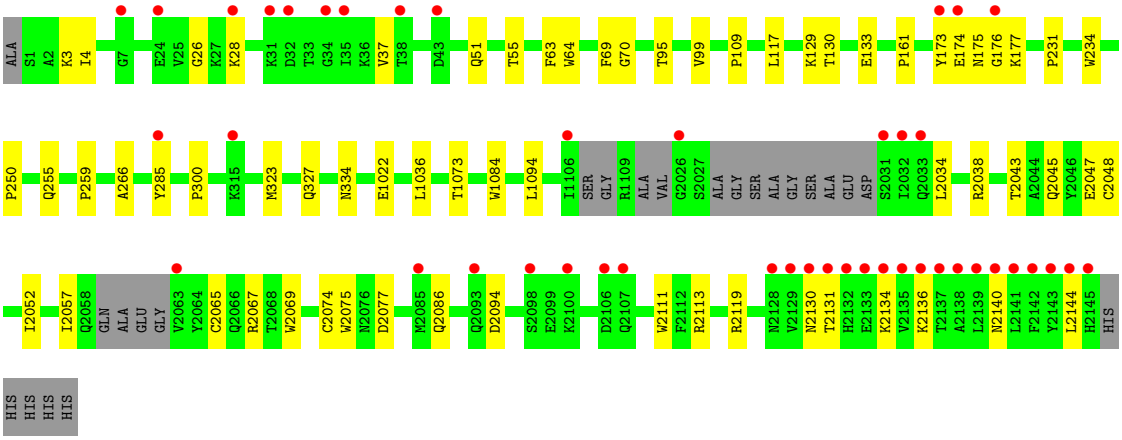
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	190	190	190	0	0

3 Residue-property plots (i)

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

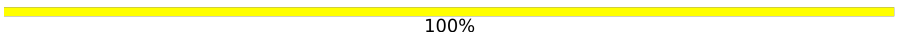
• Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Receptor activity-modifying protein 1,Calcitonin gene-related peptide type 1 receptor

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.19Å 77.63Å 97.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.69 – 2.30 41.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.69-2.30) 100.0 (41.43-2.30)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.197 , 0.251 0.201 , 0.253	Depositor DCC
R_{free} test set	1216 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4853	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GLC, 7IU, PG4

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	0.25	0/4706	0.45	0/6385

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

There are no bond length outliers.

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	2130	ASN	Peptide

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	4569	0	4439	39	1
2	B	23	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	26	0	36	0	0
4	A	45	0	0	0	0
5	A	190	0	0	2	0
All	All	4853	0	4495	39	1

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 4.

All (39) 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:129:LYS:NZ	5:A:2302:HOH:O	2.28	0.65
1:A:1084:TRP:O	1:A:2119:ARG:NH2	2.29	0.65
1:A:26:GLY:HA3	1:A:37:VAL:HG21	1.84	0.59
1:A:99:VAL:HG21	1:A:109:PRO:HD3	1.83	0.59
1:A:2043:THR:O	1:A:2047:GLU:HG3	2.03	0.59
1:A:28:LYS:HE3	1:A:285:TYR:HD2	1.71	0.56
1:A:234:TRP:HB2	1:A:300:PRO:HG2	1.87	0.56
1:A:174[B]:GLU:OE1	1:A:175:ASN:ND2	2.40	0.55
1:A:55:THR:HG22	1:A:1094:LEU:HD22	1.90	0.54
1:A:51:GLN:NE2	1:A:2057:ILE:HD12	2.26	0.51
1:A:51:GLN:HE21	1:A:2057:ILE:HD12	1.76	0.50
1:A:255[B]:GLN:OE1	5:A:2301:HOH:O	2.20	0.50
1:A:173:TYR:CZ	1:A:176:GLY:HA2	2.47	0.50
1:A:2067:ARG:N	1:A:2077:ASP:OD1	2.46	0.49
1:A:64:TRP:HB3	1:A:69:PHE:HE1	1.78	0.48
1:A:323:MET:O	1:A:327:GLN:HG3	2.13	0.48
1:A:2131:THR:HG23	1:A:2134:LYS:HE2	1.96	0.48
1:A:2074:CYS:O	1:A:2086:GLN:NE2	2.43	0.47
1:A:231:PRO:HA	1:A:234:TRP:CE2	2.50	0.47
1:A:2048:CYS:SG	1:A:2069:TRP:HB2	2.54	0.46
1:A:2131:THR:O	1:A:2131:THR:HG22	2.15	0.46
1:A:117:LEU:HD22	1:A:250:PRO:HD3	1.98	0.46
1:A:2052:ILE:HG23	1:A:2067:ARG:HD2	1.96	0.45
1:A:2065:CYS:HB3	1:A:2111:TRP:CE2	2.51	0.45
1:A:2140:ASN:O	1:A:2144:LEU:HB2	2.16	0.45
1:A:70:GLY:HA3	1:A:334:ASN:O	2.17	0.45
1:A:2045:GLN:HB2	1:A:2069:TRP:CZ2	2.52	0.44
1:A:63:PHE:CE1	1:A:266:ALA:HB2	2.53	0.44
1:A:2034:LEU:O	1:A:2038:ARG:HG3	2.16	0.44
1:A:130:THR:OG1	1:A:133:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2131:THR:CG2	1:A:2134:LYS:HE2	2.48	0.43
1:A:1022[B]:GLU:HG2	1:A:2113:ARG:NH2	2.33	0.43
1:A:1036:LEU:HD22	1:A:1073:THR:HG22	2.00	0.42
1:A:2136:LYS:O	1:A:2140:ASN:HB2	2.19	0.42
1:A:4:ILE:H	1:A:4:ILE:HD12	1.85	0.41
1:A:2075:TRP:CH2	1:A:2086:GLN:HG3	2.55	0.41
1:A:161:PRO:HG3	1:A:259:PRO:HA	2.01	0.41
1:A:95:THR:HB	1:A:109:PRO:HB2	2.04	0.40

All (1) 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)
1:A:28:LYS:NZ	1:A:175:ASN:OD1[4_445]	2.19	0.01

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	570/594 (96%)	563 (99%)	7 (1%)	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	479/484 (99%)	477 (100%)	2 (0%)	91 96

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

Mol	Chain	Res	Type
1	A	3	LYS
1	A	2094	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	284	ASN
1	A	327	GLN
1	A	2076	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 (i)

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	B	1	2	12,12,12	1.32	1 (8%)	17,17,17	0.90	0
2	GLC	B	2	2	11,11,12	1.75	3 (27%)	15,15,17	0.75	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	GLC	B	1	2	-	0/2/22/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	GLC	O5-C1	4.32	1.50	1.43
2	B	1	GLC	O5-C1	3.56	1.51	1.42
2	B	2	GLC	C2-C3	-2.27	1.49	1.52
2	B	2	GLC	O5-C5	2.08	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

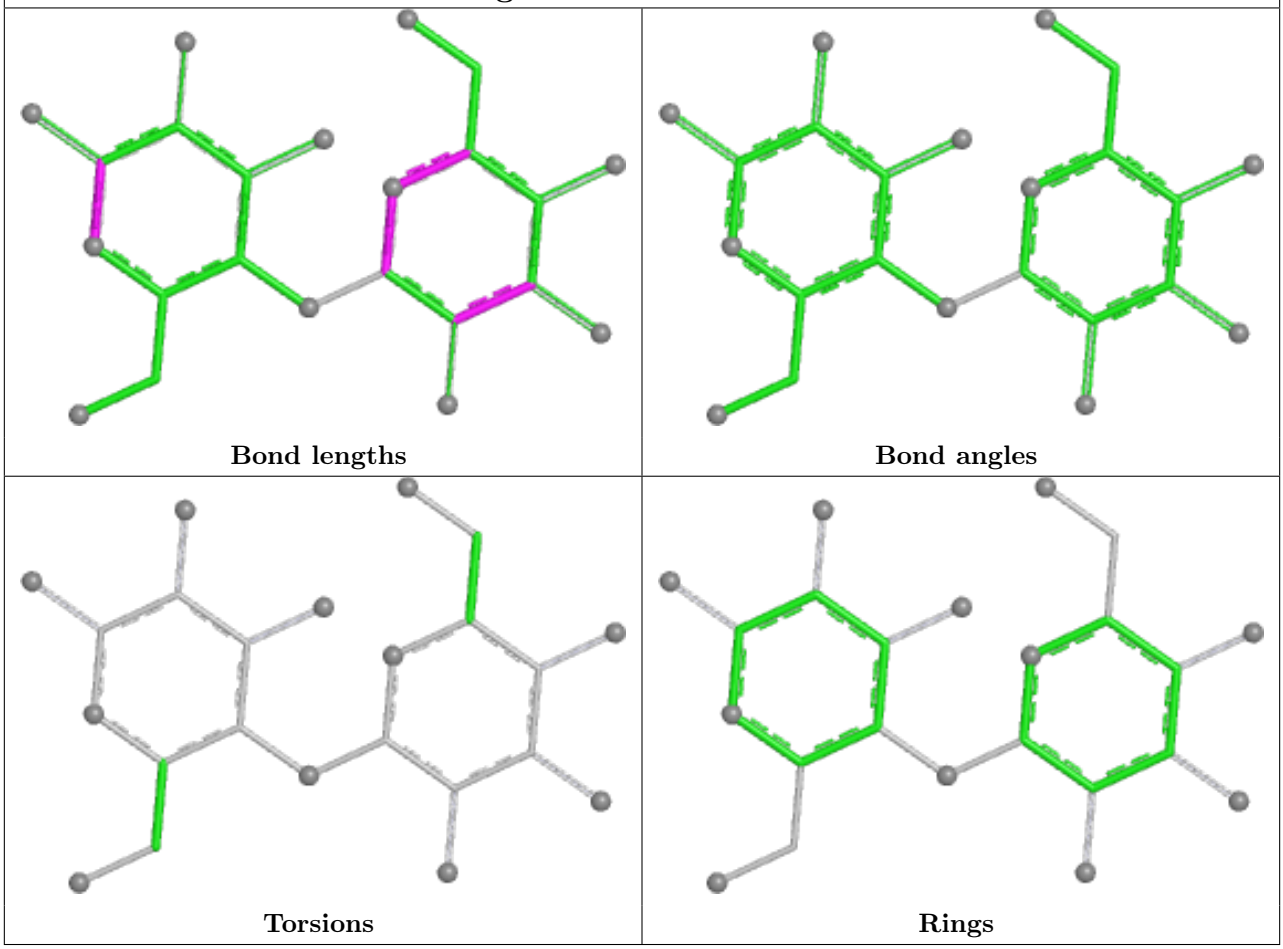
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain B



5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PG4	A	2201	-	12,12,12	0.53	0	11,11,11	0.24	0
4	7IU	A	2203	-	44,51,51	0.76	0	55,74,74	1.26	7 (12%)
3	PG4	A	2202	-	12,12,12	0.52	0	11,11,11	0.22	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	PG4	A	2201	-	-	4/10/10/10	-
4	7IU	A	2203	-	-	4/31/58/58	0/6/7/7
3	PG4	A	2202	-	-	3/10/10/10	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2203	7IU	C32-C25-C17	-4.68	99.58	103.61
4	A	2203	7IU	C32-C24-C13	-3.80	100.02	104.10
4	A	2203	7IU	C24-C32-C25	-2.58	101.90	105.31
4	A	2203	7IU	C24-C13-C17	-2.42	108.57	110.69
4	A	2203	7IU	C3-C10-C16	-2.26	118.95	120.38
4	A	2203	7IU	C24-C13-C5	2.06	132.62	129.05
4	A	2203	7IU	C11-C5-C13	-2.03	118.39	121.47

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2201	PG4	O3-C5-C6-O4
3	A	2201	PG4	O1-C1-C2-O2
3	A	2201	PG4	C1-C2-O2-C3
4	A	2203	7IU	C20-C26-O44-C29
4	A	2203	7IU	C27-C28-O45-C30
3	A	2202	PG4	C8-C7-O4-C6
3	A	2201	PG4	C3-C4-O3-C5
4	A	2203	7IU	C29-C30-O45-C28
4	A	2203	7IU	C30-C29-O44-C26
3	A	2202	PG4	O2-C3-C4-O3
3	A	2202	PG4	C3-C4-O3-C5

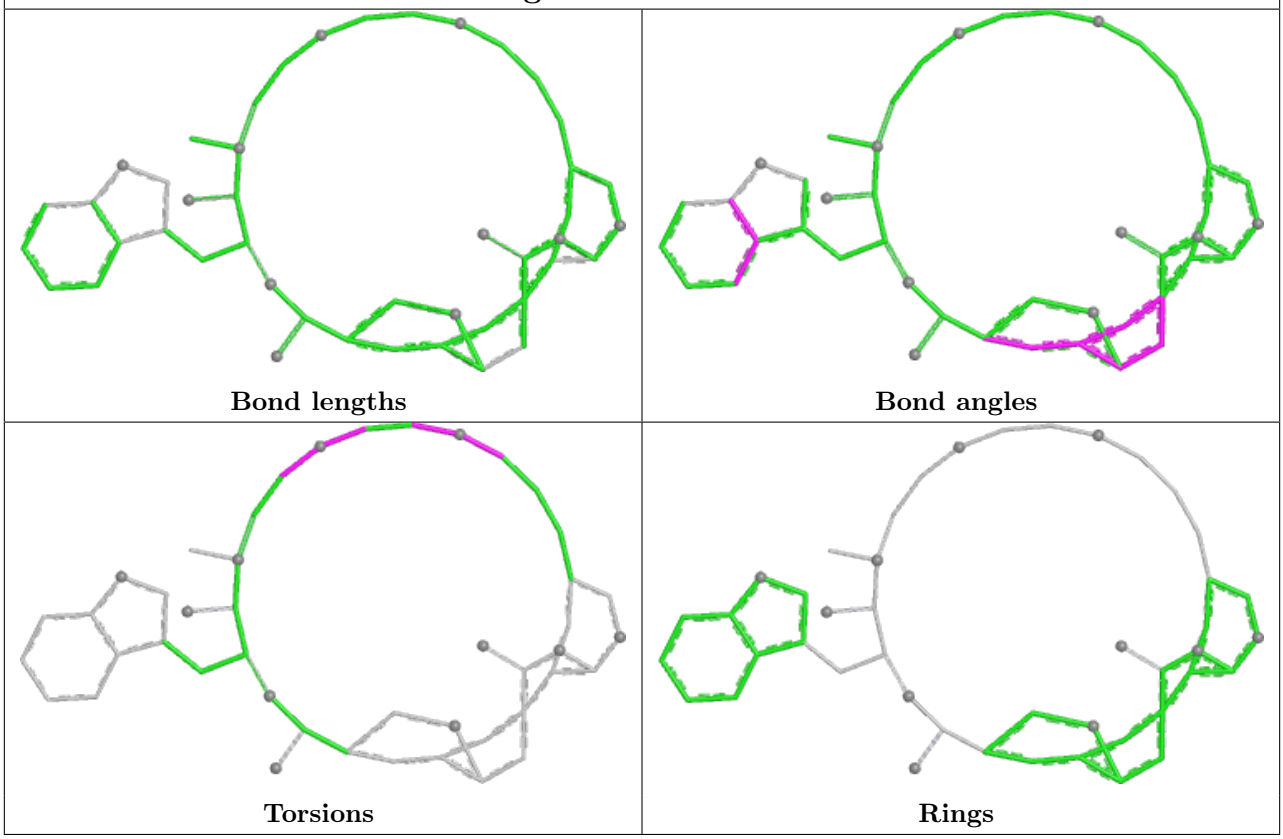
There are no ring outliers.

No monomer is involved in short contacts.

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 then 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 7IU A 2203



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	571/594 (96%)	0.47	44 (7%) 13 17	24, 35, 73, 145	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2135	VAL	10.5
1	A	2026	GLY	9.6
1	A	2144	LEU	7.3
1	A	2145	HIS	6.3
1	A	2063	VAL	5.6
1	A	2130	ASN	5.4
1	A	2032	ILE	5.1
1	A	2136	LYS	5.0
1	A	43	ASP	4.3
1	A	2033	GLN	4.2
1	A	2132	HIS	4.1
1	A	2131	THR	3.7
1	A	176	GLY	3.7
1	A	38	THR	3.7
1	A	285	TYR	3.6
1	A	2134	LYS	3.6
1	A	28	LYS	3.5
1	A	2129	VAL	3.4
1	A	173	TYR	3.3
1	A	2098	SER	3.3
1	A	35	ILE	3.3
1	A	2093	GLN	3.3
1	A	2133	GLU	3.2
1	A	32	ASP	3.1
1	A	174[A]	GLU	3.1
1	A	2137	THR	3.0
1	A	2140	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	2100	LYS	2.7
1	A	1106	ILE	2.7
1	A	2107	GLN	2.7
1	A	2085	MET	2.7
1	A	2031	SER	2.5
1	A	31	LYS	2.5
1	A	2139	LEU	2.5
1	A	7	GLY	2.4
1	A	2128	ASN	2.4
1	A	315	LYS	2.4
1	A	2142	PHE	2.4
1	A	2143	TYR	2.3
1	A	24	GLU	2.3
1	A	34	GLY	2.2
1	A	2138	ALA	2.2
1	A	2106	ASP	2.1
1	A	2141	LEU	2.1

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

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

6.3 Carbohydrates (i)

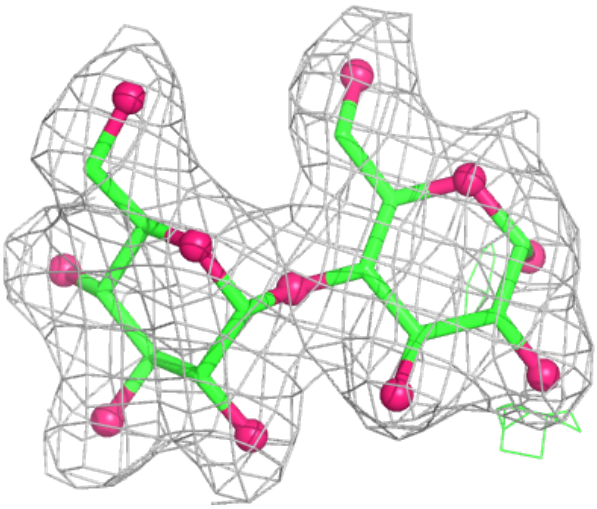
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

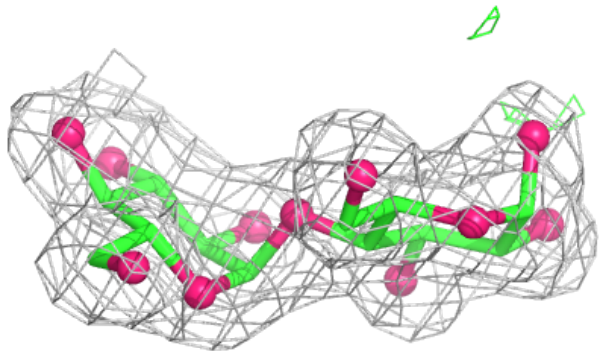
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	B	1	12/12	0.94	0.13	23,28,32,33	0
2	GLC	B	2	11/12	0.96	0.15	23,26,29,33	0

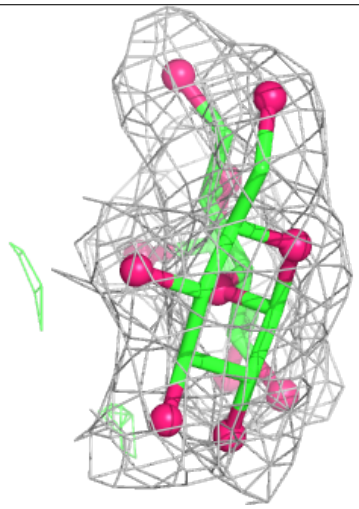
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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





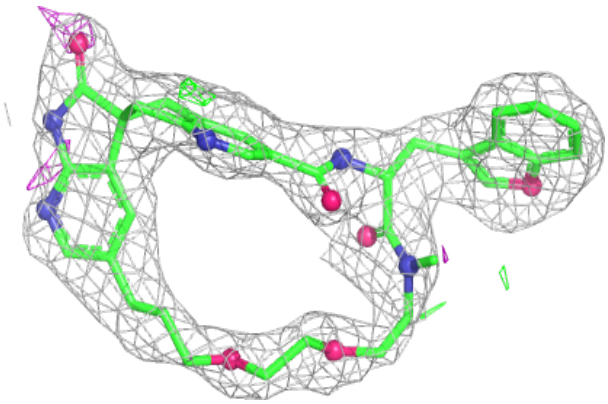
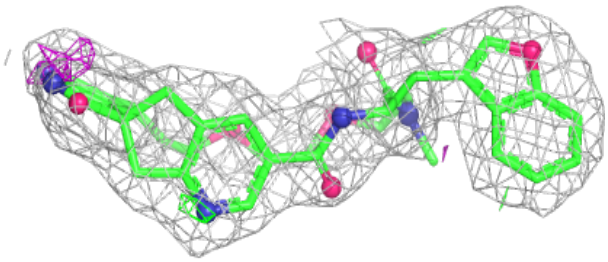


6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PG4	A	2202	13/13	0.57	0.29	66,73,85,86	0
3	PG4	A	2201	13/13	0.77	0.20	44,48,54,55	13
4	7IU	A	2203	45/45	0.90	0.17	25,32,49,53	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 7IU A 2203: $2mF_o$-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.