Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2021 – 04:06 pm BST

PDB ID	:	6ZHO
Title	:	Crystal structure of a CGRP receptor ectodomain heterodimer with bound high affinity inhibitor
Authors	:	Southall, S.M.
Deposited on	:	2020-06-23
Resolution	:	1.60 Å(reported)

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

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

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

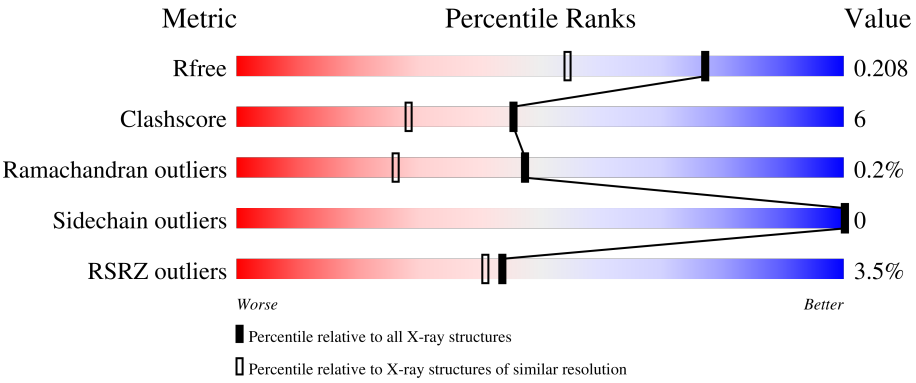
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	3% 86% 10%
2	B	2	50% 50%

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
4	PG4	A	2203	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5282 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	577	4650	2976	771	879	24	0	16	0

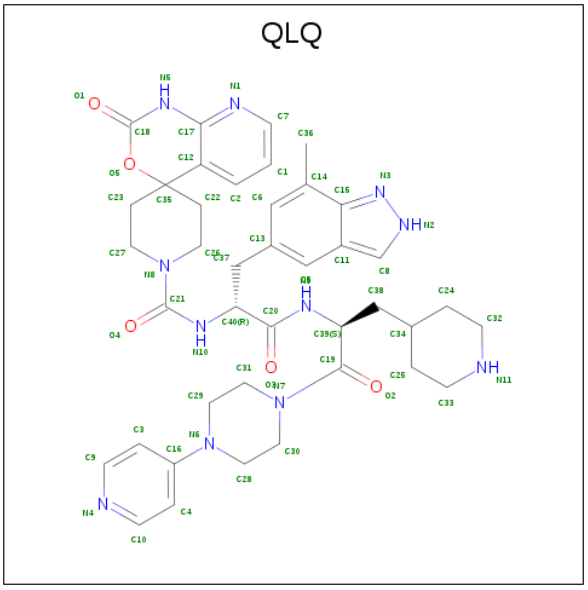
There are 25 discrepancies between the modelled and reference sequences:

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	2020	GLY	-	linker	UNP O60894
A	2021	SER	-	linker	UNP O60894
A	2022	ALA	-	linker	UNP O60894
A	2023	GLY	-	linker	UNP O60894
A	2024	SER	-	linker	UNP O60894
A	2025	ALA	-	linker	UNP O60894
A	2026	GLY	-	linker	UNP O60894
A	2027	SER	-	linker	UNP O60894
A	2028	ALA	-	linker	UNP O60894
A	2066	GLN	ASN	conflict	UNP Q16602
A	2118	GLN	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.

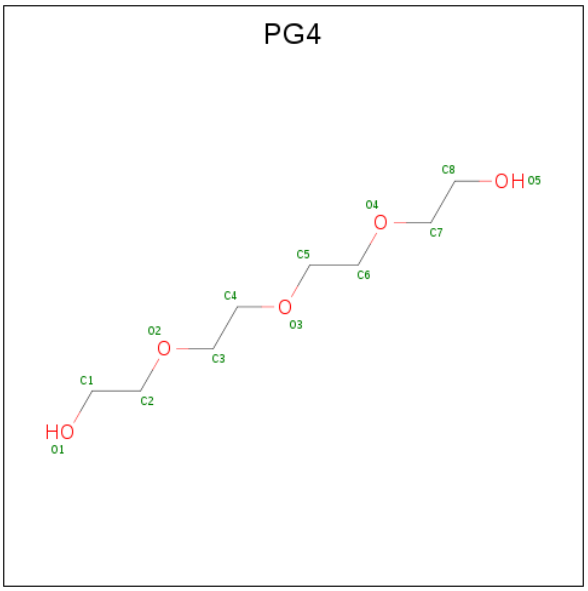
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	2	Total C O 23 12 11	0	0	0

- Molecule 3 is {N}-[(2 {R})-3-(7-methyl-2 {H}-indazol-5-yl)-1-oxidanylidene-1-[[(2 {S})-1-oxidanylidene-3-piperidin-4-yl-1-(4-pyridin-4-ylpiperazin-1-yl)propan-2-yl]amino]propan-2-yl]-2-oxidanylidene-spiro[1 {H}-pyrido[2,3-d][1,3]oxazine-4,4'-piperidine]-1'-carboxamide (three-letter code: QLQ) (formula: $C_{40}H_{49}N_{11}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 56 40 11 5	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

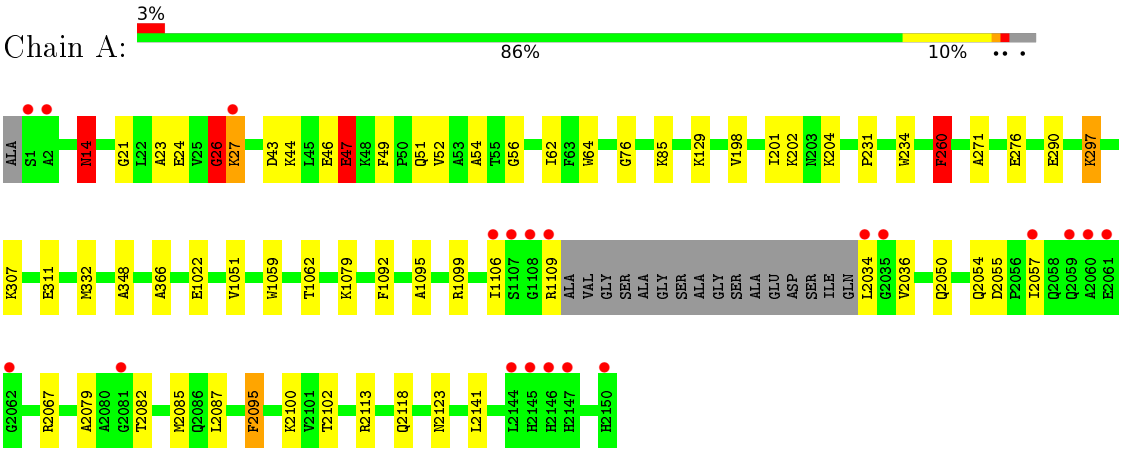
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	527	Total O 527 527	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



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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.72Å 76.96Å 97.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.48 – 1.60 38.48 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.48-1.60) 99.7 (38.48-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.179 , 0.214 0.175 , 0.208	Depositor DCC
R_{free} test set	3595 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	13.5	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.1	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	0.96	EDS
Total number of atoms	5282	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, QLQ, GLC

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	0.50	2/4819 (0.0%)	0.85	15/6543 (0.2%)

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	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	LYS	CE-NZ	6.65	1.65	1.49
1	A	27	LYS	CB-CG	6.32	1.69	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	GLU	OE1-CD-OE2	-27.84	89.89	123.30
1	A	47	GLU	CG-CD-OE1	15.68	149.67	118.30
1	A	27	LYS	CD-CE-NZ	-10.14	88.39	111.70
1	A	27	LYS	N-CA-CB	-10.02	92.56	110.60
1	A	47	GLU	CG-CD-OE2	-9.94	98.43	118.30
1	A	27	LYS	CB-CA-C	8.87	128.13	110.40
1	A	27	LYS	CA-CB-CG	-8.58	94.52	113.40
1	A	260	PHE	CB-CG-CD1	-8.04	115.17	120.80
1	A	46	GLU	C-N-CA	-6.25	106.09	121.70
1	A	14	ASN	CB-CA-C	5.97	122.35	110.40
1	A	14	ASN	CB-CG-ND2	-5.92	102.48	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1079	LYS	CD-CE-NZ	-5.84	98.27	111.70
1	A	2141	LEU	CB-CG-CD2	-5.78	101.17	111.00
1	A	2095	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	A	297	LYS	CB-CG-CD	-5.20	98.08	111.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ASN	Sidechain
1	A	2095	PHE	Sidechain
1	A	26	GLY	Mainchain,Peptide
1	A	260	PHE	Sidechain
1	A	47	GLU	Sidechain

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	4650	0	4518	56	1
2	B	23	0	21	0	0
3	A	56	0	0	0	0
4	A	26	0	36	14	0
5	A	527	0	0	15	3
All	All	5282	0	4575	60	3

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 6.

All (60) 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:2301:HOH:O	1.87	1.03
1:A:297:LYS:NZ	5:A:2302:HOH:O	1.92	1.00
1:A:204:LYS:HZ1	4:A:2202:PG4:H21	1.28	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2055:ASP:O	1:A:2067:ARG:NH2	2.02	0.93
1:A:1059:TRP:HB2	1:A:1109:ARG:HH11	1.41	0.85
1:A:260:PHE:HB3	1:A:332:MET:HG3	1.61	0.81
1:A:24:GLU:OE1	5:A:2302:HOH:O	2.00	0.80
1:A:276:GLU:OE2	5:A:2303:HOH:O	2.00	0.79
1:A:204:LYS:NZ	4:A:2202:PG4:H21	1.98	0.77
1:A:2118:GLN:OE1	5:A:2304:HOH:O	2.05	0.75
1:A:52:VAL:HG13	1:A:2057:ILE:HD11	1.70	0.73
1:A:24:GLU:O	1:A:27:LYS:HB3	1.90	0.72
1:A:44:LYS:HE2	1:A:47:GLU:OE2	1.92	0.69
1:A:14:ASN:HD22	1:A:64:TRP:HZ3	1.41	0.68
1:A:2085:MET:HG2	1:A:2102:THR:HG22	1.74	0.68
1:A:2123:ASN:ND2	5:A:2310:HOH:O	2.28	0.66
1:A:2118:GLN:NE2	5:A:2309:HOH:O	2.26	0.66
1:A:23:ALA:O	1:A:27:LYS:HB2	2.01	0.61
1:A:21:GLY:HA2	5:A:2302:HOH:O	2.02	0.60
1:A:201:ILE:HG22	4:A:2202:PG4:H52	1.85	0.57
1:A:271:ALA:HB2	4:A:2203:PG4:H31	1.87	0.57
1:A:1059:TRP:HB2	1:A:1109:ARG:NH1	2.14	0.57
1:A:2050:GLN:O	1:A:2054:GLN:HG3	2.06	0.55
1:A:1051:VAL:HG11	1:A:1062[A]:THR:HG22	1.90	0.54
1:A:14:ASN:ND2	1:A:64:TRP:CZ3	2.67	0.53
1:A:2087:LEU:HD23	1:A:2100:LYS:HD3	1.91	0.53
1:A:2079:ALA:O	1:A:2082:THR:HG23	2.10	0.52
1:A:26:GLY:CA	1:A:27:LYS:HB2	2.39	0.51
1:A:24:GLU:O	1:A:27:LYS:CB	2.59	0.49
1:A:76:GLY:O	4:A:2203:PG4:H61	2.14	0.48
1:A:2034:LEU:HD23	1:A:2036:VAL:N	2.30	0.47
1:A:43[B]:ASP:OD1	1:A:44:LYS:N	2.49	0.46
1:A:297:LYS:HD2	1:A:297:LYS:C	2.35	0.46
1:A:348:ALA:HB2	1:A:366:ALA:HB2	1.98	0.46
1:A:198:VAL:O	1:A:202:LYS:HG3	2.16	0.45
1:A:307:LYS:O	1:A:311[B]:GLU:HG3	2.15	0.45
1:A:26:GLY:HA3	5:A:2379:HOH:O	2.16	0.45
1:A:56:GLY:HA3	4:A:2203:PG4:H21	1.98	0.45
4:A:2203:PG4:H41	5:A:2305:HOH:O	2.17	0.45
1:A:54:ALA:O	1:A:1095:ALA:HA	2.17	0.44
1:A:14:ASN:ND2	1:A:64:TRP:HZ3	2.10	0.44
1:A:1095:ALA:CB	4:A:2203:PG4:H82	2.47	0.44
4:A:2203:PG4:O2	5:A:2305:HOH:O	2.20	0.44
1:A:1106:ILE:HD12	1:A:2054:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2202:PG4:H41	5:A:2715:HOH:O	2.18	0.44
1:A:23:ALA:O	1:A:27:LYS:HD2	2.19	0.43
1:A:1092:PHE:HD1	4:A:2203:PG4:HO5	1.67	0.43
1:A:231:PRO:HA	1:A:234:TRP:CE2	2.53	0.43
4:A:2203:PG4:H72	5:A:2749:HOH:O	2.19	0.43
1:A:271:ALA:CB	4:A:2203:PG4:H31	2.49	0.42
1:A:1099:ARG:NH1	5:A:2318:HOH:O	2.51	0.42
1:A:1106:ILE:HD11	1:A:2050:GLN:HB3	2.02	0.42
1:A:1095:ALA:HB3	4:A:2203:PG4:H82	2.01	0.42
1:A:51:GLN:HB2	1:A:2057:ILE:CD1	2.50	0.42
1:A:297:LYS:HB3	1:A:297:LYS:HE3	1.58	0.41
1:A:1022[B]:GLU:HG2	1:A:2113:ARG:NH2	2.35	0.41
1:A:49:PHE:HB2	1:A:62:ILE:HD12	2.03	0.41
1:A:85:LYS:NZ	5:A:2339:HOH:O	2.53	0.41
1:A:129:LYS:HE2	1:A:129:LYS:HA	2.03	0.40
1:A:2034:LEU:HD23	1:A:2036:VAL:H	1.86	0.40

All (3) 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:290[B]:GLU:OE2	5:A:2732:HOH:O[4_445]	2.12	0.08
5:A:2691:HOH:O	5:A:2694:HOH:O[4_545]	2.14	0.06
5:A:2514:HOH:O	5:A:2681:HOH:O[2_554]	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	589/594 (99%)	578 (98%)	10 (2%)	1 (0%)	47 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	491/484 (101%)	491 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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	1075	HIS
1	A	2054	GLN
1	A	2107	GLN
1	A	2118	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	0.57	0	17,17,17	0.78	0
2	GLC	B	2	2	11,11,12	0.53	0	15,15,17	0.84	1 (6%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	GLC	C1-O5-C5	2.02	114.94	112.19

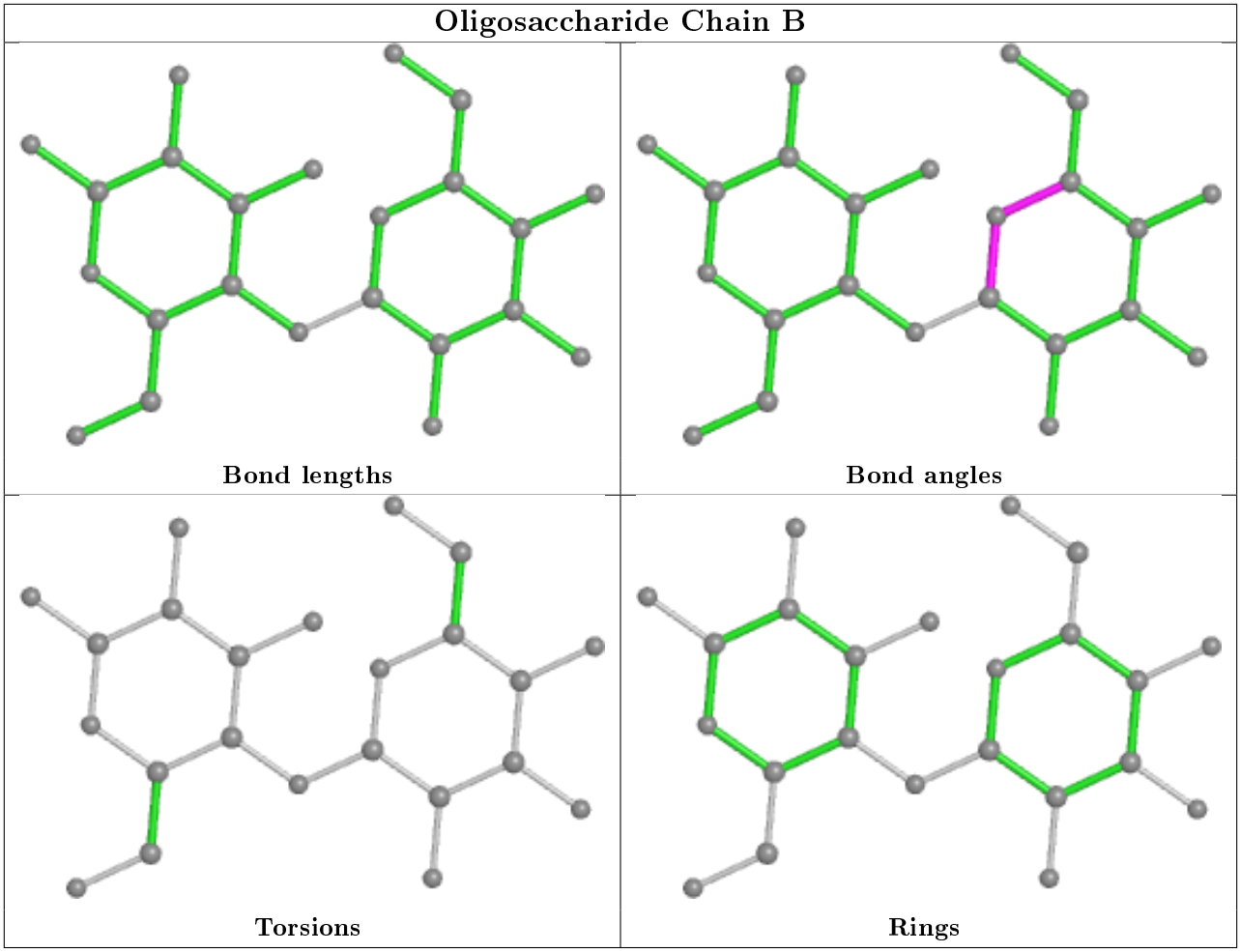
There are no chirality outliers.

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.



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	QLQ	A	2201	-	62,63,63	1.08	5 (8%)	76,90,90	1.72	11 (14%)
4	PG4	A	2202	-	12,12,12	0.55	0	11,11,11	0.67	0
4	PG4	A	2203	-	12,12,12	0.39	0	11,11,11	0.69	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	QLQ	A	2201	-	-	2/36/81/81	0/8/8/8
4	PG4	A	2202	-	-	7/10/10/10	-
4	PG4	A	2203	-	-	4/10/10/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2201	QLQ	C23-C35	3.31	1.56	1.53
3	A	2201	QLQ	C19-N7	2.99	1.39	1.34
3	A	2201	QLQ	C6-C14	2.72	1.41	1.37
3	A	2201	QLQ	C20-N9	2.17	1.38	1.34
3	A	2201	QLQ	C11-C15	-2.04	1.40	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2201	QLQ	C27-C23-C35	5.93	117.06	111.84
3	A	2201	QLQ	C29-N6-C28	5.58	123.85	111.52
3	A	2201	QLQ	C26-C22-C35	-4.77	107.64	111.84
3	A	2201	QLQ	C23-C27-N8	-4.05	102.93	110.92
3	A	2201	QLQ	C34-C38-C39	3.87	119.73	114.52
3	A	2201	QLQ	C38-C39-C19	-2.66	104.35	109.35
3	A	2201	QLQ	C9-N4-C10	2.64	123.06	116.85
3	A	2201	QLQ	C4-C10-N4	-2.58	119.14	123.62
3	A	2201	QLQ	C33-C25-C34	2.21	115.56	112.14
3	A	2201	QLQ	C36-C14-C15	2.07	122.04	120.03
3	A	2201	QLQ	C22-C35-C12	2.04	115.37	110.99

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2201	QLQ	C24-C34-C38-C39
4	A	2203	PG4	O2-C3-C4-O3
4	A	2202	PG4	O2-C3-C4-O3
4	A	2203	PG4	O4-C7-C8-O5
4	A	2203	PG4	O1-C1-C2-O2
4	A	2202	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	2202	PG4	O3-C5-C6-O4
4	A	2203	PG4	C3-C4-O3-C5
4	A	2202	PG4	C6-C5-O3-C4
3	A	2201	QLQ	C25-C34-C38-C39
4	A	2202	PG4	C5-C6-O4-C7
4	A	2202	PG4	C3-C4-O3-C5
4	A	2202	PG4	C4-C3-O2-C2

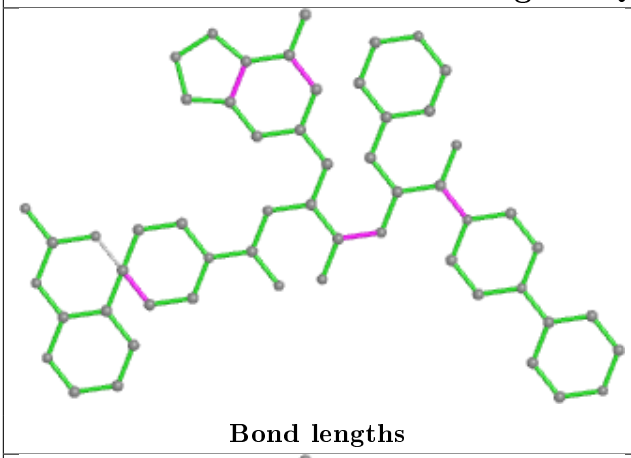
There are no ring outliers.

2 monomers are involved in 14 short contacts:

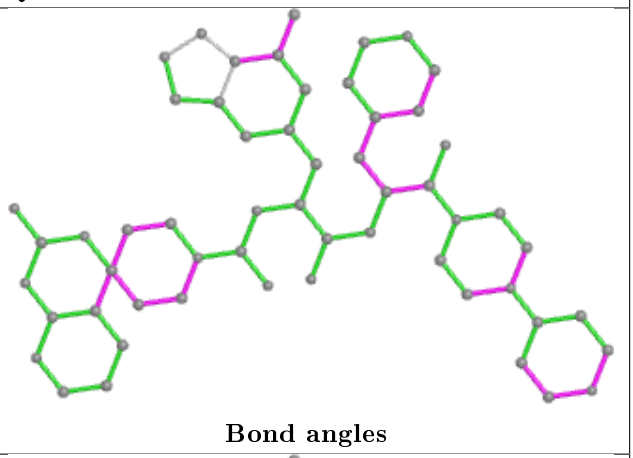
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2202	PG4	4	0
4	A	2203	PG4	10	0

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 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.

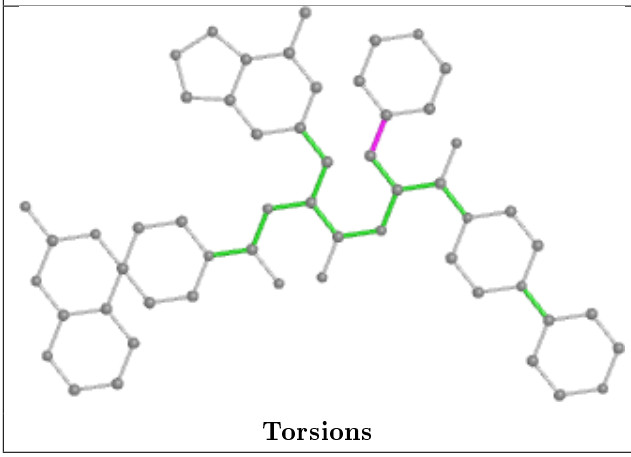
Ligand QLQ A 2201



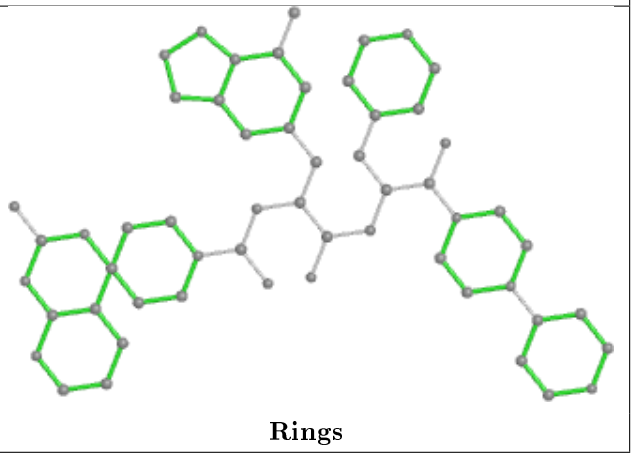
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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	577/594 (97%)	-0.22	20 (3%) 44 41	6, 15, 38, 96	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1108	GLY	9.4
1	A	1106	ILE	6.0
1	A	1107	SER	4.3
1	A	2059	GLN	4.2
1	A	2060	ALA	4.2
1	A	2144	LEU	4.2
1	A	27	LYS	4.0
1	A	2061	GLU	3.9
1	A	2034	LEU	3.7
1	A	2057	ILE	3.7
1	A	2147	HIS	3.6
1	A	1109	ARG	3.3
1	A	2150	HIS	3.3
1	A	2	ALA	3.1
1	A	2035	GLY	2.8
1	A	2081	GLY	2.6
1	A	2145	HIS	2.6
1	A	1	SER	2.2
1	A	2062	GLY	2.2
1	A	2146	HIS	2.1

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

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

6.3 Carbohydrates (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^{th} 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	0.96	0.11	8,13,18,24	0
2	GLC	B	2	11/12	0.98	0.11	7,9,10,11	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^{th} 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
4	PG4	A	2203	13/13	0.66	0.27	41,47,55,56	0
4	PG4	A	2202	13/13	0.84	0.11	14,25,36,38	0
3	QLQ	A	2201	56/56	0.97	0.07	7,12,25,27	0

6.5 Other polymers (i)

There are no such residues in this entry.