

Full wwPDB X-ray Structure Validation Report (i)

Feb 25, 2024 - 05:17 PM EST

PDB ID	:	6PH7
Title	:	Crystal structure of bovine opsin with nerol bound
Authors	:	Eger, B.T.; Morizumi, T.; Ernst, O.P.
Deposited on		
Resolution	:	2.90 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

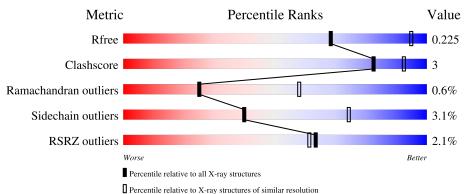
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	:::::::::::::::::::::::::::::::::::::::	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	А	348	2% 8 5%	7% • 6%
2	В	11	91%	9%
3	С	4	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
3	NAG	С	1	X	-	-	-
6	NZZ	А	407	-	-	-	Х



6PH7

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2790 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 Rhodopsin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	326	Total 2603	C 1735	N 401	0 441	S 26	0	1	0

• Molecule 2 is a protein called G protein CT2 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	В	11	Total 89	C 59	N 13	0 17	0	0	0

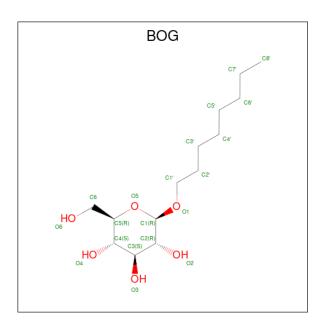
• Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose -(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucop yranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	С	4	Total 50	C 28	N 2	O 20	0	0	0

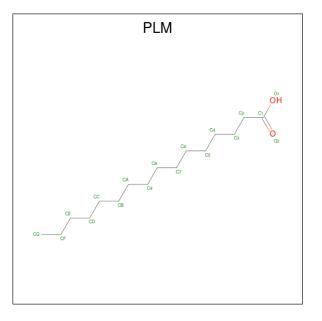
• Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).





Mol	Chain	Residues	At	\mathbf{oms}		ZeroOcc	AltConf
4	А	1	Total	С	Ο	0	0
		1	20	14	6		5

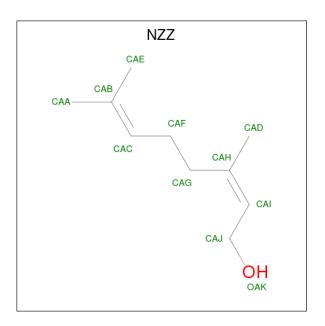
• Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
5	А	1	Total 17	C 16	0 1	0	0

• Molecule 6 is (2Z)-3,7-dimethylocta-2,6-dien-1-ol (three-letter code: NZZ) (formula: $C_{10}H_{18}O$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	At	oms		ZeroOcc	AltConf
6	А	1	Total	C	0	0	0
			11	10	T		



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.

Chain A:	85%	7% • 6%
H N2 F9 F9 F9 F9 F9 F9 F9 F9 F9 F1 F2 F1 F2 F1 F2 F1 F2 F1 F2 F1 F2 F1 F2 F1 F1 F2 F1 F1 F1 F1 F1 F1 F1 F1 F1 F1 F1 F1 F1	G90 H100 R145 F146 F146 F146 F147 F148 F148 F148 F135	H195 H196 E201 E201 E201 F203 F203 F203 F203 F203 F276 F276 F276 F276 F276 F276 F276
M317 M317 N326 N326 N326 CLV ALA ALA ALA ALA ALA ALA THR THR THR THR THR THR THR	GLU THR SER GLN VAL ALA ALA ALA	
• Molecule 2: G protei	n CT2 peptide	
Chain B:	91%	9%
F350		

• Molecule 1: Rhodopsin

 $\bullet \ Molecule \ 3: \ beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \\ ta-D-glucopyranose \\ (1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \\ \end{array}$

Chain C:	50%	50%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	243.14Å 243.14Å 108.43Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.26 - 2.90	Depositor
Resolution (A)	39.26 - 2.90	EDS
% Data completeness	99.0 (39.26-2.90)	Depositor
(in resolution range)	99.0 (39.26-2.90)	EDS
R _{merge}	0.05	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.24 (at 2.90\AA)	Xtriage
Refinement program	PHENIX (1.10_2155)	Depositor
D D.	0.214 , 0.225	Depositor
R, R_{free}	0.214 , 0.225	DCC
R_{free} test set	1364 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	84.0	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30, 61.8	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2790	wwPDB-VP
Average B, all atoms $(Å^2)$	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: NZZ, PLM, BMA, NAG, BOG

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		lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.26	0/2690	0.40	0/3666	
2	В	0.23	0/89	0.33	0/117	
All	All	0.26	0/2779	0.40	0/3783	

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	А	2603	0	2579	14	0
2	В	89	0	93	1	0
3	С	50	0	43	0	0
4	А	20	0	28	1	0
5	А	17	0	31	0	0
6	А	11	0	0	0	0
All	All	2790	0	2774	14	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 3.

All (14) close contacts within the same asymmetric unit are listed below, sorted by their clash



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLU:HA	1:A:276:PHE:HZ	1.59	0.67
1:A:231:LYS:NZ	1:A:247:GLU:OE2	2.33	0.62
1:A:135:ARG:HG2	2:B:347:VAL:HB	1.84	0.60
1:A:62:THR:HG21	1:A:77:LEU:HD11	1.85	0.58
1:A:181:GLU:HB3	1:A:192:TYR:OH	2.10	0.52
1:A:189:ILE:HD13	1:A:203:PHE:HE2	1.74	0.52
1:A:61:VAL:HG11	1:A:317:MET:HG2	1.96	0.47
1:A:201:GLU:HA	1:A:276:PHE:CZ	2.46	0.47
1:A:20:VAL:HA	1:A:30:TYR:CZ	2.50	0.46
1:A:147:ARG:HE	1:A:147:ARG:HB3	1.49	0.45
1:A:100:HIS:CE1	4:A:401:BOG:H1'1	2.53	0.43
1:A:6:GLY:HA3	1:A:9:PHE:CZ	2.55	0.41
1:A:192:TYR:CE2	1:A:288:MET:HE1	2.56	0.41
1:A:181:GLU:HG3	1:A:186:SER:O	2.21	0.40

magnitude.

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	Percer	ntiles
1	А	325/348~(93%)	311 (96%)	12~(4%)	2(1%)	25	58
2	В	9/11~(82%)	9 (100%)	0	0	100	100
All	All	334/359~(93%)	320 (96%)	12~(4%)	2(1%)	25	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	195	HIS
1	А	90	GLY



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Analysed Rotameric Outliers		Percentiles		
1	А	279/296~(94%)	270~(97%)	9~(3%)	39 73		
2	В	10/10~(100%)	10 (100%)	0	100 100		
All	All	289/306~(94%)	280~(97%)	9~(3%)	40 74		

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

Mol	Chain	Res	Type
1	А	2	ASN
1	А	25	GLU
1	А	147	ARG
1	А	181	GLU
1	А	192	TYR
1	А	226	LEU
1	А	252	ARG
1	А	289	THR
1	А	326	ASN

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

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)

4 monosaccharides are modelled in this entry.



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

Mol	al Tuna Chain Bag		Dec	es Link	Bond lengths			Bond angles		
IVIOI	Type Chain Res	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2		
3	NAG	С	1	1,3	14,14,15	0.72	0	17,19,21	1.68	1 (5%)
3	NAG	С	2	3	14,14,15	0.62	0	17,19,21	1.00	0
3	BMA	С	3	3	11,11,12	0.50	0	15,15,17	0.72	0
3	BMA	С	4	3	11,11,12	1.08	1 (9%)	15,15,17	1.90	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	С	1	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	С	2	3	-	0/6/23/26	0/1/1/1
3	BMA	С	3	3	-	2/2/19/22	0/1/1/1
3	BMA	С	4	3	-	2/2/19/22	1/1/1/1

All (1)	bond	length	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	С	4	BMA	O5-C1	2.63	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
3	С	1	NAG	O5-C5-C6	6.03	116.65	107.20
3	С	4	BMA	O5-C5-C6	4.76	114.66	107.20
3	С	4	BMA	C1-O5-C5	4.38	118.13	112.19
3	С	4	BMA	C1-C2-C3	-2.38	106.75	109.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	С	1	NAG	C1



Mol	Chain	Res	Type	Atoms
3	С	3	BMA	O5-C5-C6-O6
3	С	3	BMA	C4-C5-C6-O6
3	С	4	BMA	C4-C5-C6-O6
3	С	4	BMA	O5-C5-C6-O6

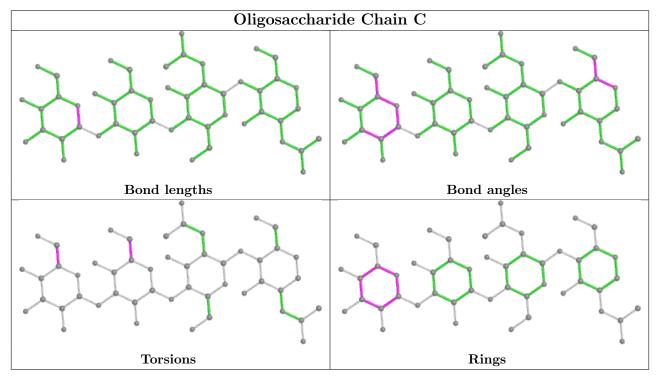
All (4) torsion outliers are listed below:

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	4	BMA	C1-C2-C3-C4-C5-O5

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



					Bo	Bond lengths			Bond angles		
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
4	BOG	А	401	-	20,20,20	0.88	0	$25,\!25,\!25$	1.19	3 (12%)	
6	NZZ	А	407	-	10,10,10	1.18	1 (10%)	11,11,11	2.82	4 (36%)	
5	PLM	А	406	-	16,16,17	0.31	0	15,15,17	0.50	0	

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).

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
4	BOG	А	401	-	-	7/11/31/31	0/1/1/1
6	NZZ	А	407	-	-	0/9/9/9	-
5	PLM	А	406	-	-	7/13/14/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
6	А	407	NZZ	CAJ-CAI	2.54	1.53	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
6	А	407	NZZ	CAJ-CAI-CAH	-7.48	115.55	127.21
6	А	407	NZZ	CAF-CAC-CAB	-3.48	115.86	127.75
4	А	401	BOG	C4-C3-C2	3.26	116.52	110.82
6	А	407	NZZ	CAD-CAH-CAG	2.63	119.70	115.27
4	А	401	BOG	C1-C2-C3	2.56	115.32	110.00
6	А	407	NZZ	CAE-CAB-CAA	2.42	119.94	114.60
4	А	401	BOG	C3-C4-C5	2.19	114.15	110.24

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	401	BOG	O5-C1-O1-C1'
5	А	406	PLM	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	А	401	BOG	O1-C1'-C2'-C3'
5	А	406	PLM	C4-C5-C6-C7
5	А	406	PLM	C2-C3-C4-C5
5	А	406	PLM	CA-CB-CC-CD
5	А	406	PLM	С7-С8-С9-СА
4	А	401	BOG	C2-C1-O1-C1'
4	А	401	BOG	C4'-C5'-C6'-C7'
5	А	406	PLM	C5-C6-C7-C8
5	А	406	PLM	C6-C7-C8-C9
4	А	401	BOG	C3'-C4'-C5'-C6'
4	А	401	BOG	C1'-C2'-C3'-C4'
4	А	401	BOG	C2'-C3'-C4'-C5'

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There are no ring outliers.

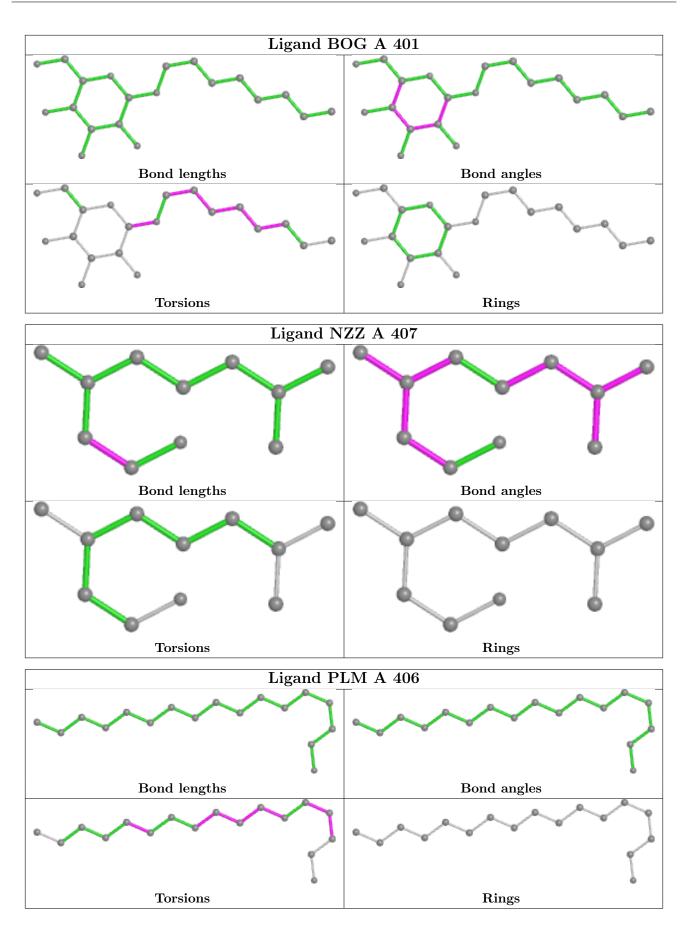
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	401	BOG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.









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, 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	326/348~(93%)	-0.00	7 (2%) 63 61	68, 89, 135, 165	0
2	В	11/11 (100%)	-0.18	0 100 100	86, 104, 121, 132	0
All	All	337/359~(93%)	-0.01	7 (2%) 63 61	68, 89, 135, 165	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	144	SER	3.7
1	А	1	MET	3.6
1	А	143	MET	2.9
1	А	145	ASN	2.9
1	А	198	THR	2.8
1	А	148	PHE	2.5
1	A	147	ARG	2.5

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^{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
3	BMA	С	4	11/12	0.86	0.22	137,144,148,153	0
3	BMA	С	3	11/12	0.90	0.24	100,121,136,148	0

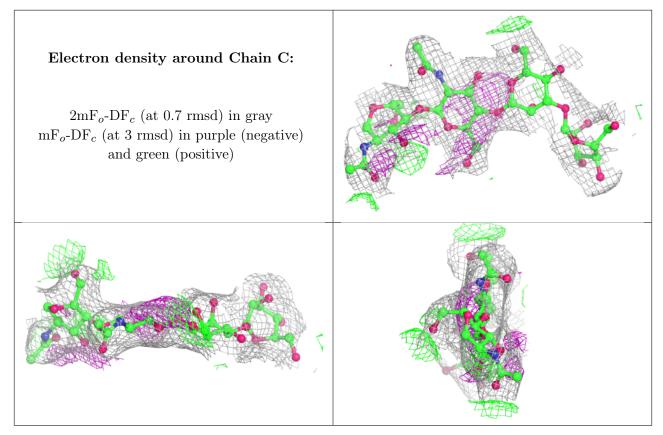
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
3	NAG	С	1	14/15	0.93	0.14	59,69,92,102	0
3	NAG	С	2	14/15	0.96	0.18	43,57,79,102	0

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



6.4 Ligands (i)

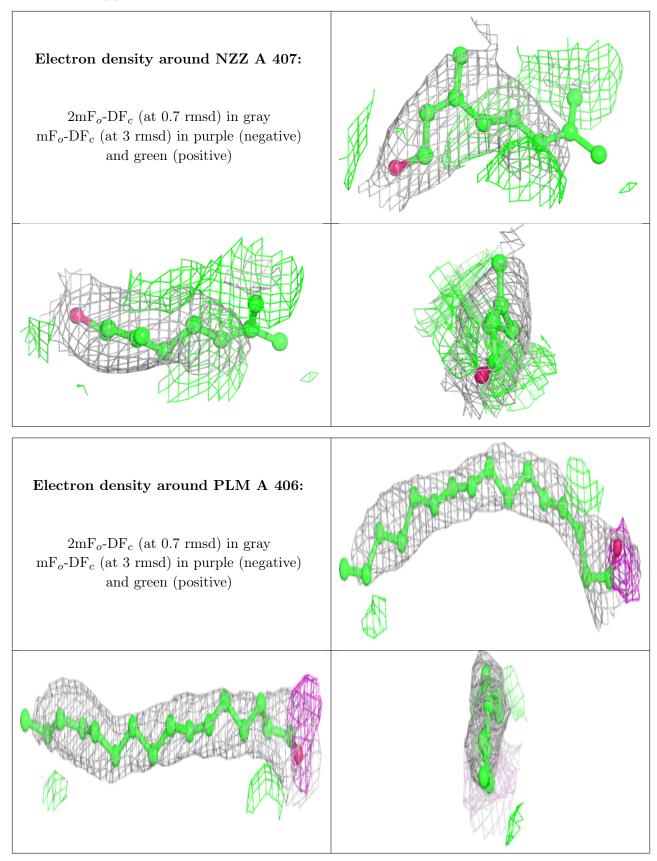
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	NZZ	А	407	11/11	0.78	0.42	$94,\!113,\!161,\!162$	0
5	PLM	А	406	17/18	0.82	0.30	95,100,111,123	0
4	BOG	А	401	20/20	0.85	0.42	100,125,136,136	0

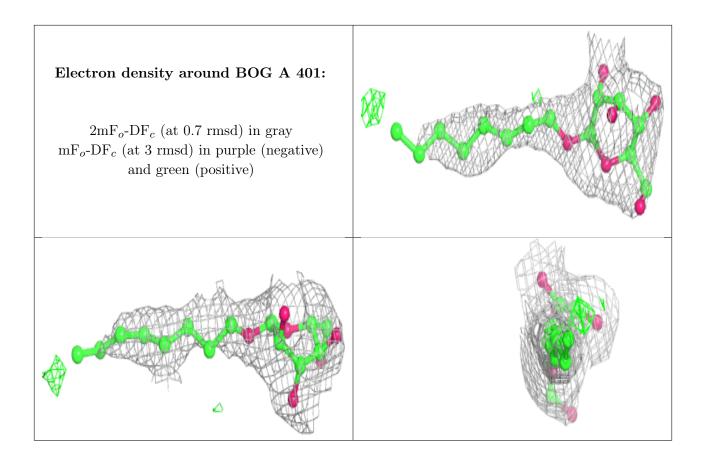
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different



orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

There are no such residues in this entry.

