

wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2024 – 04:37 PM EDT

PDB ID : 8E0G

Title : Re-refined model of active mu-opioid receptor (PDB 5c1m) as an adduct with

BU72

Authors : Munro, T.A. Deposited on : 2022-08-09

Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

MolProbity : 4.02b-467

Mogul : 2022.3.0, CSD as543be (2022)

Xtriage (Phenix) : 1.20.1

EDS : 3.0

buster-report : 1.1.7 (2018)

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

CCP4 : 9.0.003 (Gargrove)

Density-Fitness : 1.0.11

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

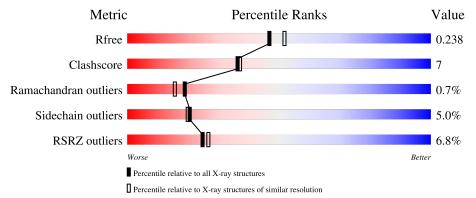
Validation Pipeline (wwPDB-VP) : 2.39

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 2.10 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	296	78%	20%	•
2	В	125	82%	10%	• 6%



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3509 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.

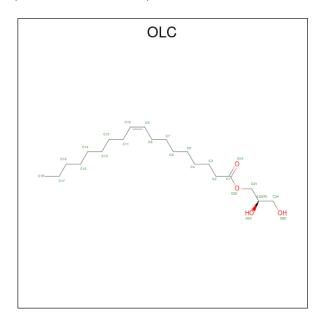
• Molecule 1 is a protein called Mu-type opioid receptor.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	296	Total	C	N	O 404	S	0	3	0
			2422	1605	387	404	26			

• Molecule 2 is a protein called Nanobody 39.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	118	Total 920	C 571	N 162	O 183	S 4	0	1	0

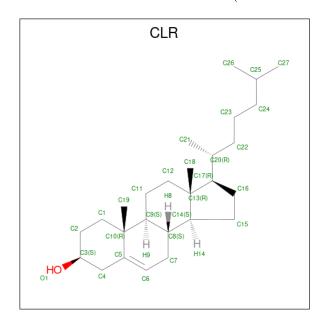
• Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 12 4	0	0
3	A	1	Total C O 18 14 4	0	0

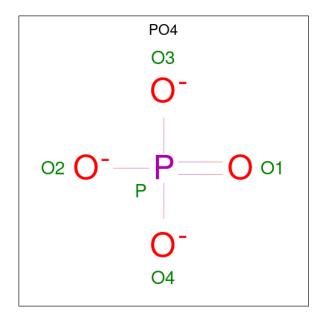


 \bullet Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $\mathrm{C_{27}H_{46}O}).$



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

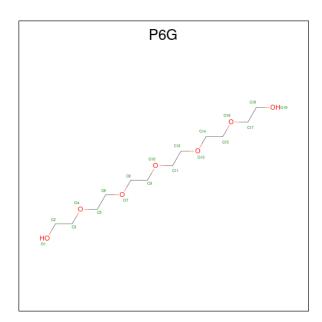
 \bullet Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: $\mathrm{O_4P}).$



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

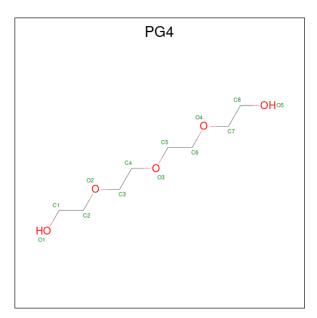
 \bullet Molecule 6 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $\mathrm{C}_{12}\mathrm{H}_{26}\mathrm{O}_{7}).$





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
6	A	1	Total 19	C 12	O 7	0	0

 \bullet Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $\mathrm{C_8H_{18}O_5}).$



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

• Molecule 8 is water.



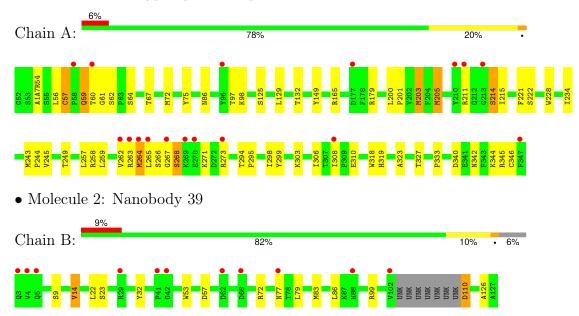
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	54	Total O 54 54	0	0
8	В	14	Total O 14 14	0	0



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: Mu-type opioid receptor





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants	44.43Å 144.00Å 209.90Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.50 - 2.10	Depositor
Resolution (A)	43.50 - 2.10	EDS
% Data completeness	99.8 (43.50-2.10)	Depositor
(in resolution range)	99.8 (43.50-2.10)	EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.89 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D D.	0.192 , 0.225	Depositor
R, R_{free}	0.211 , 0.238	DCC
R_{free} test set	2006 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 52.5	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3509	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: P6G, PO4, A1A7R, PG4, OLC, CLR, YCM

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			nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.93	$1/2427 \ (0.0\%)$	0.92	4/3302 (0.1%)	
2	В	0.93	1/940 (0.1%)	0.94	$2/1277 \ (0.2\%)$	
All	All	0.93	$2/3367 \ (0.1\%)$	0.92	6/4579 (0.1%)	

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	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
2	В	53	TRP	CB-CG	-7.82	1.36	1.50
1	A	228	TRP	CD2-CE2	-5.77	1.34	1.41

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	A	205	MET	CG-SD-CE	-6.70	89.48	100.20
2	В	72	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	179	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	179	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	165	ARG	NE-CZ-NH1	5.29	122.95	120.30

All (1) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
1	A	60	THR	CA

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	2422	0	2466	43	0
2	В	920	0	865	7	0
3	A	34	0	44	0	0
4	A	28	0	46	1	0
5	A	5	0	0	0	0
6	A	19	0	26	0	0
7	A	13	0	18	0	0
8	A	54	0	0	2	0
8	В	14	0	0	0	0
All	All	3509	0	3465	49	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 7.

The worst 5 of 49 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
2:B:32:TYR:HD1	2:B:77[A]:ASN:HD21	1.10	0.97
1:A:60:THR:HB	1:A:61:GLY:HA2	1.68	0.74
2:B:99:ARG:NH1	2:B:110:ASP:O	2.20	0.72
1:A:340:ASP:O	1:A:344:LYS:HB2	1.98	0.64
1:A:132:THR:HG23	1:A:215:ILE:HB	1.80	0.64

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	Perce	ntiles
1	A	295/296 (100%)	277 (94%)	16 (5%)	2 (1%)	19	16
2	В	115/125~(92%)	113 (98%)	1 (1%)	1 (1%)	14	11
All	All	410/421 (97%)	390 (95%)	17 (4%)	3 (1%)	19	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	SER
1	A	265	LEU
2	В	126	ALA

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	Percer	ntiles
1	A	$269/266 \ (101\%)$	254 (94%)	15 (6%)	17	16
2	В	97/96 (101%)	94 (97%)	3 (3%)	35	39
All	All	366/362 (101%)	348 (95%)	18 (5%)	20	20

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	346	CYS
2	В	110	ASP
2	В	14	VAL

Continued on next page...



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Mol	Chain	Res	Type
1	A	264	MET
1	A	308	ILE

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	127	ASN
1	A	171	HIS
1	A	319	HIS
1	A	342	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)

2 non-standard protein/DNA/RNA residues 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 C	Tuno	Chain	Res	Link	Bond lengths			Bond angles		
	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
1	YCM	A	57	1	7,9,10	0.49	0	5,10,12	1.08	1 (20%)
1	A1A7R	A	54	1	45,50,51	1.55	5 (11%)	45,81,83	1.19	3 (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
1	YCM	A	57	1	-	4/6/8/10	-
1	A1A7R	A	54	1	-	1/12/109/111	0/2/8/8



All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	54	A1A7R	C4-C3	-7.19	1.32	1.53
1	A	54	A1A7R	CE1-ND1	-3.96	1.40	1.44
1	A	54	A1A7R	O2-CE1	2.96	1.46	1.38
1	A	54	A1A7R	C4-C5	-2.64	1.49	1.53
1	A	54	A1A7R	C5-C23	2.06	1.57	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	${f Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^o)$
1	A	54	A1A7R	C3-C2-C7	-4.74	107.09	114.75
1	A	54	A1A7R	C24-C23-C22	-3.43	110.13	114.93
1	A	54	A1A7R	C8-C7-C6	2.20	112.89	109.62
1	A	57	YCM	CB-CA-C	-2.07	105.19	110.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	57	YCM	N-CA-CB-SG
1	A	57	YCM	CA-CB-SG-CD
1	A	57	YCM	SG-CD-CE-OZ1
1	A	57	YCM	SG-CD-CE-NZ2
1	A	54	A1A7R	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	57	YCM	5	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	Mol Type Chain R		Dog	Res Link	Во	Bond lengths			Bond angles		
Moi Type C	Chain	nes	Counts		RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
7	PG4	A	406	-	12,12,12	0.17	0	11,11,11	0.18	0	
5	PO4	A	404	-	4,4,4	0.76	0	6,6,6	0.48	0	
4	CLR	A	403	-	31,31,31	0.31	0	48,48,48	0.47	0	
3	OLC	A	402	-	17,17,24	0.25	0	18,18,25	0.31	0	
3	OLC	A	401	-	15,15,24	0.23	0	16,16,25	0.28	0	
6	P6G	A	405	-	18,18,18	0.26	0	17,17,17	0.15	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
7	PG4	A	406	-	-	4/10/10/10	-
4	CLR	A	403	-	-	0/10/68/68	0/4/4/4
3	OLC	A	402	-	-	7/17/17/24	-
3	OLC	A	401	-	-	4/15/15/24	_
6	P6G	A	405	-	-	12/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	406	PG4	O2-C3-C4-O3
6	A	405	P6G	O4-C5-C6-O7
6	A	405	P6G	O13-C14-C15-O16
3	A	402	OLC	C2-C1-O20-C21
3	A	402	OLC	O19-C1-O20-C21

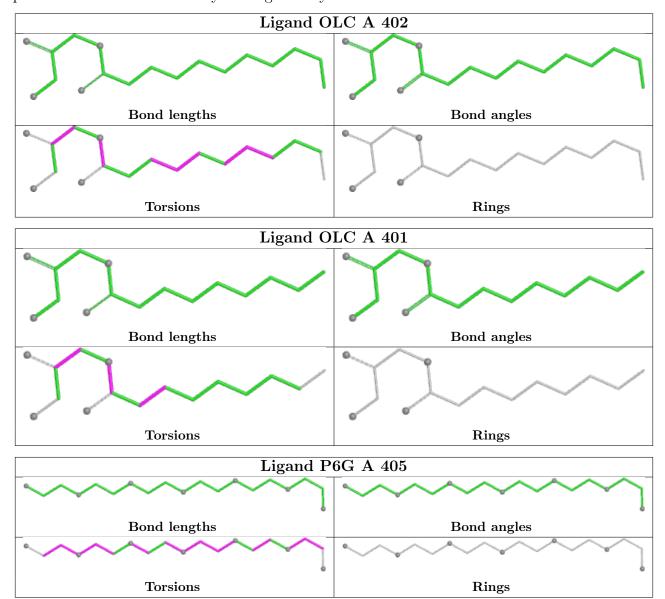
There are no ring outliers.

1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	CLR	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	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	294/296~(99%)	0.33	17 (5%) 30 32	20, 46, 104, 166	3 (1%)
2	В	118/125 (94%)	0.68	11 (9%) 16 17	25, 56, 92, 115	1 (0%)
All	All	412/421 (97%)	0.43	28 (6%) 25 27	20, 49, 101, 166	4 (0%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	102	VAL	8.5
2	В	3	GLN	4.6
1	A	210	TYR	4.4
1	A	265	LEU	4.4
1	A	347	PHE	4.2

6.2 Non-standard residues in protein, DNA, RNA chains (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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	YCM	A	57	10/11	0.83	0.13	89,105,110,114	0
1	A1A7R	A	54	43/44	0.96	0.07	34,38,67,83	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

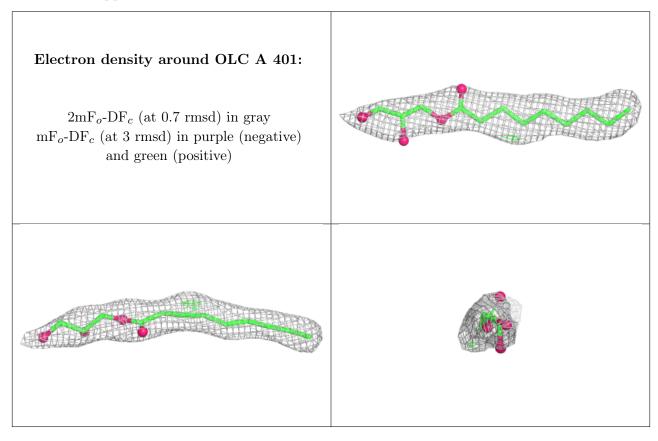


6.4 Ligands (i)

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
5	PO4	A	404	5/5	0.73	0.12	65,92,121,123	0
3	OLC	A	401	16/25	0.81	0.22	66,84,96,115	0
7	PG4	A	406	13/13	0.89	0.17	72,86,104,107	0
3	OLC	A	402	18/25	0.90	0.19	61,77,100,112	0
6	P6G	A	405	19/19	0.90	0.18	60,76,93,99	0
4	CLR	A	403	28/28	0.90	0.18	61,82,100,107	0

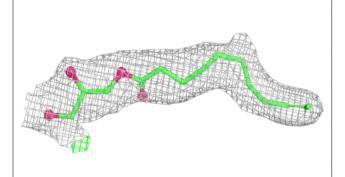
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

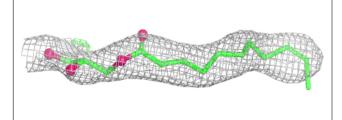


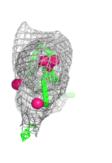


Electron density around OLC A 402:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

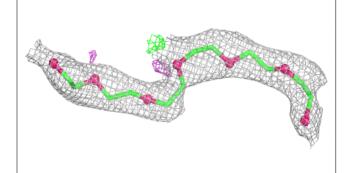


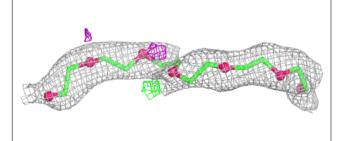


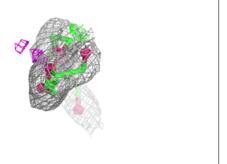


Electron density around P6G A 405:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

