

## Full wwPDB X-ray Structure Validation Report (i)

#### Feb 3, 2022 – 12:13 pm GMT

PDB ID : 708Y

Title : Anomalous bromide substructure of NmHR under dark state conditions deter-

mined at 13.7 keV with serial crystallography

Authors: Mous, S.; Gotthard, G.; Ehrenberg, D.; Sen, S.; James, D.; Johnson, P.;

Weinert, T.; Nass, K.; Furrer, A.; Kekilli, D.; Ma, P.; Bruenle, S.; Casadei, C.; Martiel, I.; Dworkowski, F.; Gashi, D.; Skopintsev, P.; Wranik, M.; Knopp, G.; Panepucci, E.; Panneels, V.; Cirelli, C.; Ozerov, D.; Schertler, G.; Wang,

M.; Milne, C.; Standfuss, J.; Schapiro, I.; Heberle, J.; Nogly, P.

Deposited on : 2021-04-15

Resolution : 1.75 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 as 541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.26

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)

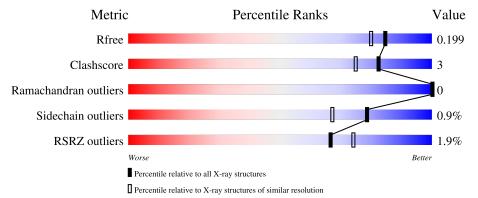
Validation Pipeline (wwPDB-VP) : 2.26

## 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 1.75 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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			
			2%			
1	A	296	84%	•	11%	



## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2376 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 Chloride pumping rhodopsin.

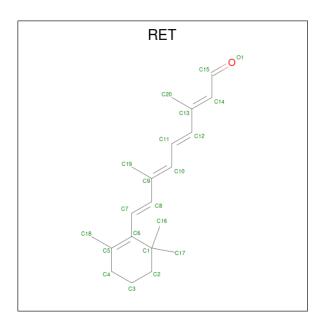
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	۸	262	Total	С	N	О	S	0	0	0
1	A	202	2099	1402	317	361	19	U	0	

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP W8VZW3
A	-14	ALA	-	expression tag	UNP W8VZW3
A	-13	SER	-	expression tag	UNP W8VZW3
A	-12	MET	-	expression tag	UNP W8VZW3
A	-11	THR	-	expression tag	UNP W8VZW3
A	-10	GLY	-	expression tag	UNP W8VZW3
A	-9	GLY	-	expression tag	UNP W8VZW3
A	-8	GLN	-	expression tag	UNP W8VZW3
A	-7	GLN	-	expression tag	UNP W8VZW3
A	-6	MET	-	expression tag	UNP W8VZW3
A	-5	GLY	-	expression tag	UNP W8VZW3
A	-4	ARG	-	expression tag	UNP W8VZW3
A	-3	ASP	-	expression tag	UNP W8VZW3
A	-2	PRO	-	expression tag	UNP W8VZW3
A	-1	ASN	-	expression tag	UNP W8VZW3
A	0	SER	-	expression tag	UNP W8VZW3
A	273	LEU	-	expression tag	UNP W8VZW3
A	274	GLU	-	expression tag	UNP W8VZW3
A	275	HIS	-	expression tag	UNP W8VZW3
A	276	HIS	-	expression tag	UNP W8VZW3
A	277	HIS	-	expression tag	UNP W8VZW3
A	278	HIS	-	expression tag	UNP W8VZW3
A	279	HIS	-	expression tag	UNP W8VZW3
A	280	HIS	_	expression tag	UNP W8VZW3

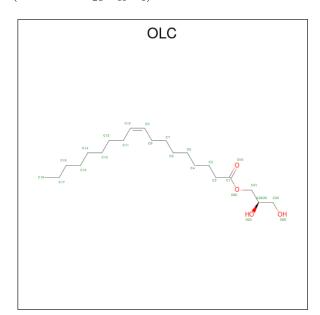
• Molecule 2 is RETINAL (three-letter code: RET) (formula:  $C_{20}H_{28}O$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 20 20	0	0

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



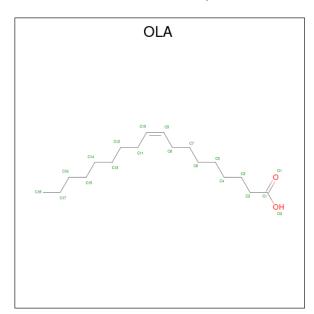
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0



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Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
3	A	1	Total 20	C 16	O 4	0	0

 $\bullet$  Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula:  $\mathrm{C_{18}H_{34}O_{2}}).$ 



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 19 17 2	0	0
4	A	1	Total C O 18 16 2	0	0
4	A	1	Total C O 13 11 2	0	0
4	A	1	Total C O 14 12 2	0	0
4	A	1	Total C O 20 18 2	0	0

 $\bullet$  Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total Br 5 5	0	5

• Molecule 6 is water.



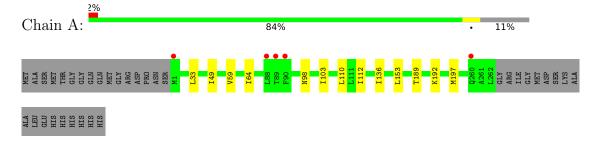
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	78	Total O 78 78	0	4



## 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: Chloride pumping rhodopsin





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	104.48Å 51.18Å 78.33Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $131.78^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	52.24 - 1.75	Depositor
Resolution (A)	52.24  -  1.75	EDS
% Data completeness	99.4 (52.24-1.75)	Depositor
(in resolution range)	99.4 (52.24-1.75)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.29 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D.D.	0.169 , 0.192	Depositor
$R, R_{free}$	0.174 , $0.199$	DCC
$R_{free}$ test set	1582 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$< L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2376	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 11.13% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: RET, OLA, BR, OLC

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
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.40	0/2173	0.50	0/2960

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2099	0	2153	8	0
2	A	20	0	27	2	0
3	A	70	0	107	1	1
4	A	104	0	154	0	0
5	A	5	0	0	3	1
6	A	78	0	0	2	0
All	All	2376	0	2441	12	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 3.

All (12) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$	
1:A:189:THR:OG1	5:A:314[B]:BR:BR	2.56	0.78	
1:A:49:ILE:HG23	1:A:112:ILE:HD13	1.67	0.76	
5:A:315[B]:BR:BR	6:A:476:HOH:O	2.58	0.76	
2:A:301:RET:H8	2:A:301:RET:H161	1.68	0.76	
3:A:302:OLC:O25	6:A:401[A]:HOH:O	1.99	0.73	
1:A:98:ASN:ND2	5:A:311[A]:BR:BR	2.78	0.72	
1:A:103:ILE:HD12	1:A:136:ILE:HD11	1.92	0.51	
1:A:49:ILE:CG2	1:A:112:ILE:HD13	2.38	0.49	
2:A:301:RET:H161	2:A:301:RET:C8	2.36	0.49	
1:A:33:LEU:HD22	1:A:59:VAL:HG22	1.96	0.47	
1:A:64:ILE:HG13	1:A:98:ASN:CG	2.41	0.41	
1:A:110:LEU:HD22	1:A:197[A]:MET:HE1	2.03	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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
3:A:302:OLC:O25	5:A:313[B]:BR:BR[4_445]	1.51	0.69

## 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	268/296 (90%)	266 (99%)	2 (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.

Mo	l Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	224/242 (93%)	222 (99%)	2 (1%)	78 67	

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

Mol	Chain	Res	Type
1	A	153	LEU
1	A	192	LYS

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)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 for Mogul analysis.

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

	Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
						Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
	2	RET	A	301	1	20,20,21	0.74	1 (5%)	27,27,28	1.37	4 (14%)



Mol	Trino	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OLC	A	302	-	24,24,24	0.80	2 (8%)	25,25,25	1.00	1 (4%)
4	OLA	A	310	-	16,19,19	0.73	1 (6%)	15,19,19	0.60	0
4	OLA	A	305	-	15,18,19	0.77	1 (6%)	14,18,19	0.50	0
4	OLA	A	306	-	14,17,19	0.77	1 (7%)	13,17,19	0.59	0
4	OLA	A	304	-	16,19,19	0.70	1 (6%)	15,19,19	0.62	0
4	OLA	A	309	-	10,13,19	0.93	1 (10%)	8,13,19	0.60	0
3	OLC	A	307	-	19,19,24	0.90	1 (5%)	20,20,25	0.93	1 (5%)
3	OLC	A	303	-	24,24,24	0.81	2 (8%)	25,25,25	0.89	1 (4%)
4	OLA	A	308	-	9,12,19	0.84	1 (11%)	8,12,19	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	RET	A	301	1	-	0/13/30/31	0/1/1/1
3	OLC	A	302	-	-	8/24/24/24	-
4	OLA	A	310	-	-	9/15/17/17	-
4	OLA	A	305	-	-	9/14/16/17	-
4	OLA	A	306	-	-	8/13/15/17	-
4	OLA	A	304	-	-	6/15/17/17	-
4	OLA	A	309	-	-	5/9/11/17	-
3	OLC	A	307	-	-	10/19/19/24	-
3	OLC	A	303	-	-	13/24/24/24	-
4	OLA	A	308	-	-	7/8/10/17	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
4	A	309	OLA	C10-C9	2.79	1.48	1.31
4	A	305	OLA	C10-C9	2.77	1.47	1.31
4	A	306	OLA	C10-C9	2.74	1.47	1.31
4	A	310	OLA	C10-C9	2.74	1.47	1.31
4	A	304	OLA	C10-C9	2.65	1.47	1.31
3	A	307	OLC	O20-C1	2.58	1.40	1.33
3	A	302	OLC	O20-C1	2.44	1.40	1.33
4	A	308	OLA	C9-C10	2.41	1.47	1.29



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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
3	A	303	OLC	O20-C1	2.40	1.40	1.33
2	A	301	RET	C14-C13	2.13	1.35	1.33
3	A	303	OLC	O20-C21	-2.10	1.40	1.45
3	A	302	OLC	O20-C21	-2.02	1.40	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	301	RET	C3-C4-C5	-2.98	108.75	114.08
2	A	301	RET	C7-C8-C9	-2.94	121.80	126.23
3	A	302	OLC	O20-C1-C2	2.86	120.87	111.91
3	A	307	OLC	O20-C1-C2	2.79	120.67	111.91
2	A	301	RET	C20-C13-C12	2.71	122.35	118.08
3	A	303	OLC	O20-C1-C2	2.60	120.07	111.91
2	A	301	RET	C10-C11-C12	-2.26	116.18	123.22

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	OLC	C21-C22-C24-O25
4	A	304	OLA	C1-C2-C3-C4
4	A	305	OLA	C1-C2-C3-C4
4	A	308	OLA	C1-C2-C3-C4
4	A	309	OLA	C9-C10-C11-C12
3	A	307	OLC	O19-C1-O20-C21
3	A	307	OLC	C2-C1-O20-C21
3	A	307	OLC	C1-C2-C3-C4
3	A	307	OLC	O20-C21-C22-O23
3	A	302	OLC	C2-C1-O20-C21
3	A	307	OLC	C4-C5-C6-C7
4	A	309	OLA	C5-C6-C7-C8
3	A	307	OLC	O20-C21-C22-C24
3	A	303	OLC	C12-C13-C14-C15
4	A	305	OLA	C2-C3-C4-C5
4	A	310	OLA	C12-C13-C14-C15
3	A	302	OLC	O19-C1-O20-C21
4	A	308	OLA	C4-C5-C6-C7
4	A	305	OLA	C11-C12-C13-C14
3	A	303	OLC	C4-C5-C6-C7
3	A	302	OLC	C11-C12-C13-C14
4	A	305	OLA	C12-C13-C14-C15



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Mol	Chain	m Res	Type	Atoms
3	A	303	OLC	O23-C22-C24-O25
4	A	308	OLA	C5-C6-C7-C8
4	A	310	OLA	C13-C14-C15-C16
4	A	305	OLA	C3-C4-C5-C6
3	A	302	OLC	C6-C7-C8-C9
4	A	308	OLA	C6-C7-C8-C9
4	A	304	OLA	C6-C7-C8-C9
4	A	306	OLA	C10-C11-C12-C13
3	A	303	OLC	O20-C21-C22-O23
3	A	303	OLC	C5-C6-C7-C8
3	A	307	OLC	C5-C6-C7-C8
4	A	304	OLA	C11-C10-C9-C8
4	A	305	OLA	C11-C10-C9-C8
4	A	306	OLA	C11-C10-C9-C8
4	A	309	OLA	C11-C10-C9-C8
4	A	305	OLA	C4-C5-C6-C7
3	A	303	OLC	C2-C3-C4-C5
3	A	303	OLC	O20-C21-C22-C24
4	A	308	OLA	C3-C4-C5-C6
4	A	308	OLA	C11-C10-C9-C8
4	A	305	OLA	C14-C15-C16-C17
3	A	307	OLC	O23-C22-C24-O25
4	A	310	OLA	C11-C12-C13-C14
4	A	305	OLA	C5-C6-C7-C8
4	A	306	OLA	C4-C5-C6-C7
4	A	306	OLA	C1-C2-C3-C4
3	A	302	OLC	C15-C16-C17-C18
3	A	303	OLC	C15-C16-C17-C18
3	A	303	OLC	C10-C11-C12-C13
4	A	310	OLA	C11-C10-C9-C8
4	A	310	OLA	C5-C6-C7-C8
4	A	304	OLA	C9-C10-C11-C12
4	A	309	OLA	C4-C5-C6-C7
4	A	308	OLA	C7-C8-C9-C10
4	A	310	OLA	C10-C11-C12-C13
4	A	306	OLA	C5-C6-C7-C8
4	A	310	OLA	C9-C10-C11-C12
4	A	304	OLA	C3-C4-C5-C6
3	A	302	OLC	C2-C3-C4-C5
3	A	303	OLC	C6-C7-C8-C9
3	A	302	OLC	C4-C5-C6-C7
4	A	306	OLA	C11-C12-C13-C14



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Mol	Chain	Res	Type	Atoms
3	A	307	OLC	C7-C8-C9-C10
4	A	306	OLA	C6-C7-C8-C9
4	A	306	OLA	C9-C10-C11-C12
4	A	309	OLA	C7-C8-C9-C10
4	A	304	OLA	C7-C8-C9-C10
3	A	307	OLC	C21-C22-C24-O25
3	A	303	OLC	C9-C10-C11-C12
3	A	303	OLC	C1-C2-C3-C4
4	A	310	OLA	C2-C3-C4-C5
3	A	302	OLC	C5-C6-C7-C8
4	A	310	OLA	C7-C8-C9-C10

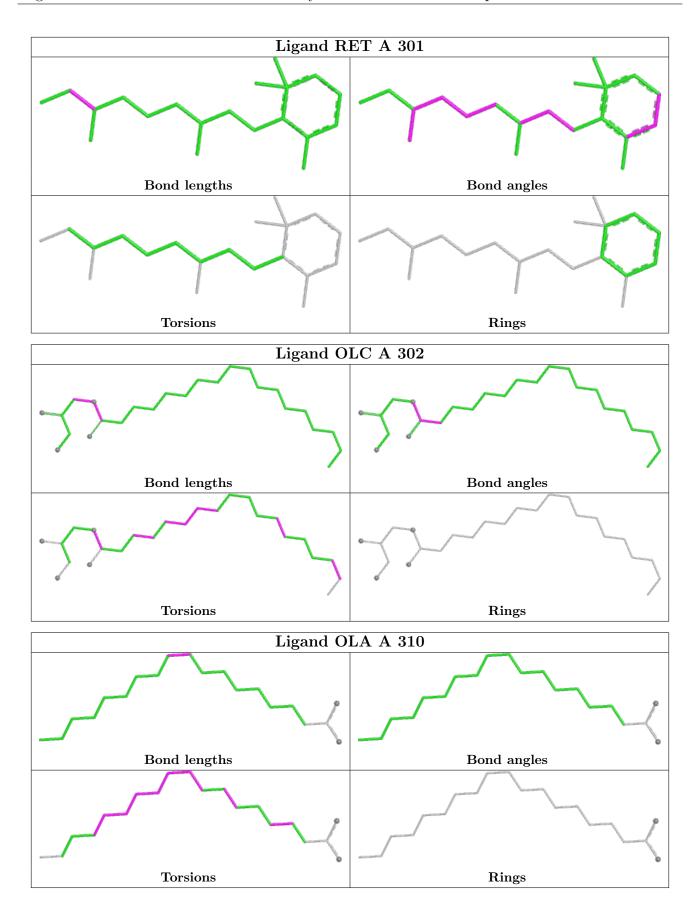
There are no ring outliers.

2 monomers are involved in 4 short contacts:

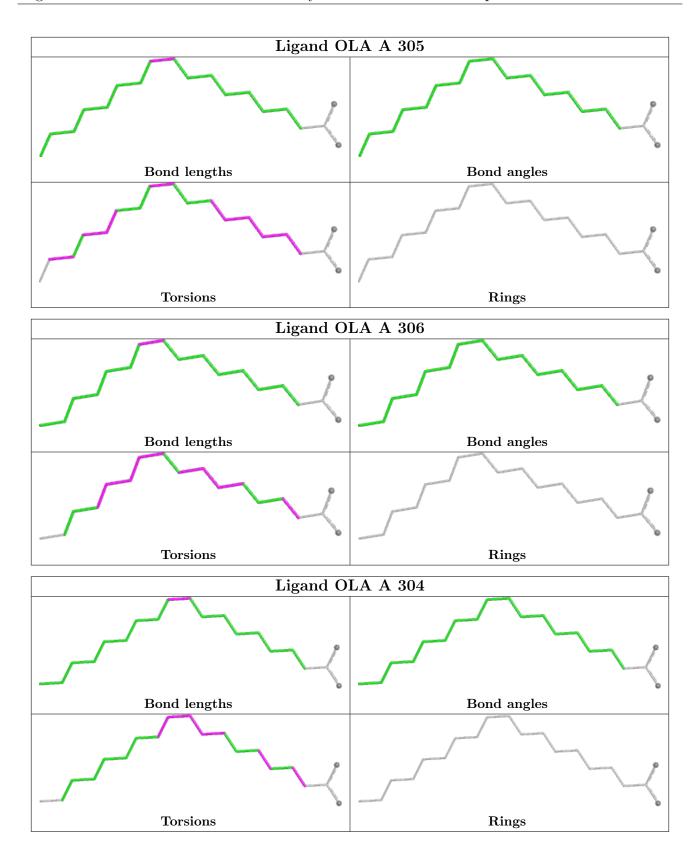
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RET	2	0
3	A	302	OLC	1	1

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.

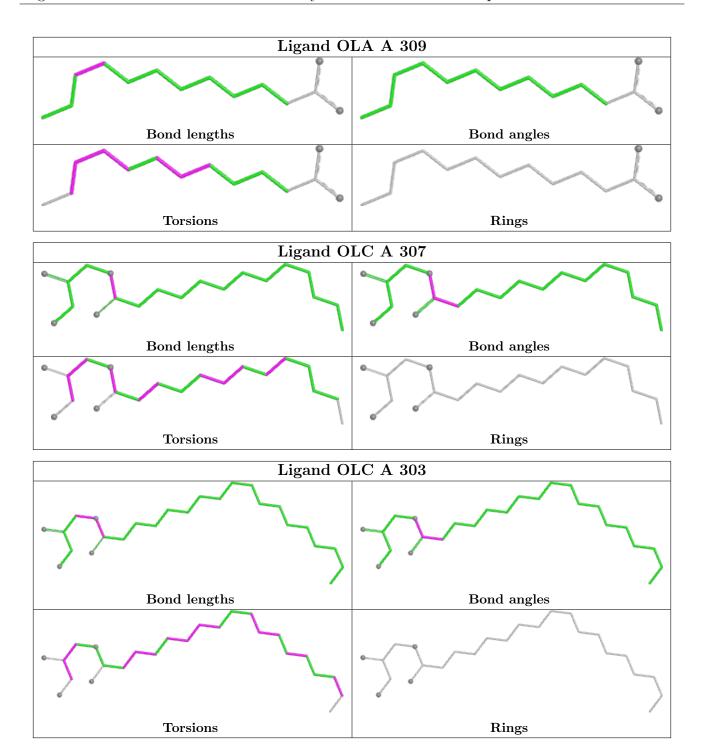




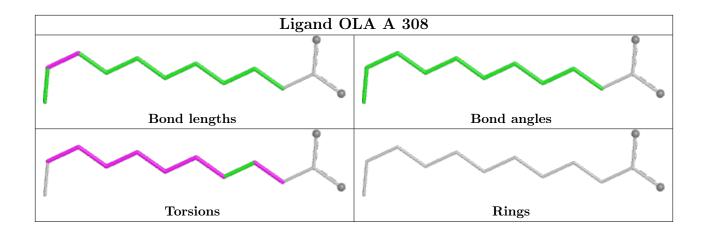












## 5.7 Other polymers (i)

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></rsrz>	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
1	A	262/296 (88%)	-0.26	5 (1%) 66 74	19, 30, 50, 72	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	LEU	3.9
1	A	1	MET	3.8
1	A	260	GLN	2.8
1	A	89	THR	2.4
1	A	90	PHE	2.4

## 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)

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.

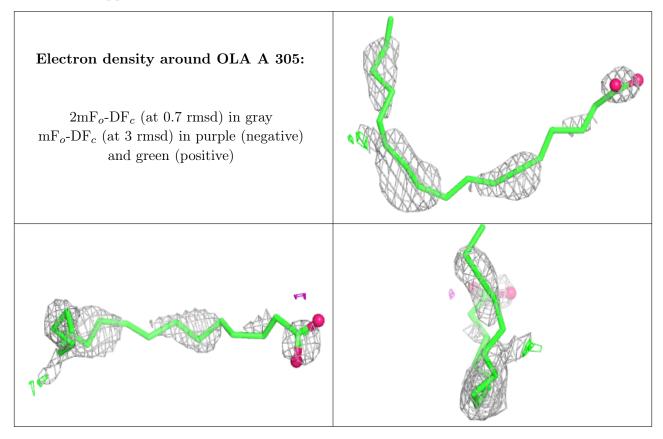
Mol	Type	Chain	$\operatorname{Res}$	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	OLA	A	305	19/20	0.64	0.29	57,73,86,90	0
4	OLA	A	306	18/20	0.68	0.21	45,62,79,79	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	OLA	A	308	13/20	0.70	0.22	64,78,89,94	0
4	OLA	A	310	20/20	0.72	0.20	55,66,91,98	0
3	OLC	A	307	20/25	0.75	0.25	62,76,91,98	0
5	BR	A	312[B]	1/1	0.75	0.15	56,56,56,56	1
4	OLA	A	304	20/20	0.77	0.17	47,65,86,87	0
3	OLC	A	303	25/25	0.82	0.17	52,67,79,83	0
4	OLA	A	309	14/20	0.83	0.23	52,59,79,84	0
3	OLC	A	302	25/25	0.84	0.16	43,61,74,78	0
5	BR	A	314[B]	1/1	0.88	0.25	71,71,71,71	1
5	BR	A	313[B]	1/1	0.92	0.08	57,57,57,57	1
5	BR	A	315[B]	1/1	0.94	0.11	55,55,55,55	1
2	RET	A	301	20/21	0.96	0.08	19,22,25,26	0
5	BR	A	311[A]	1/1	0.98	0.03	27,27,27,27	1

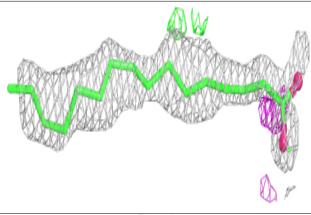
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

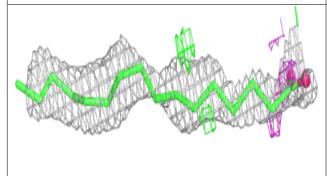


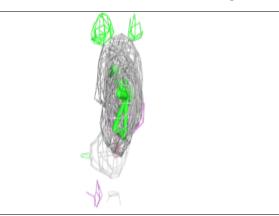


## Electron density around OLA A 306:

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

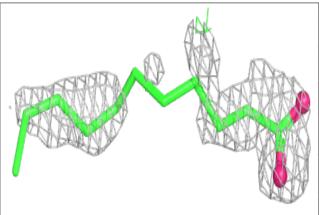


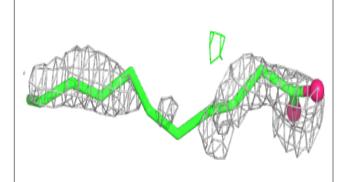


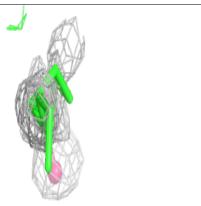


#### Electron density around OLA A 308:

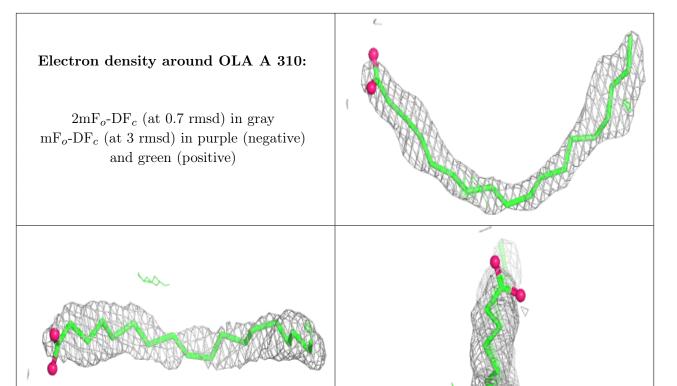
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

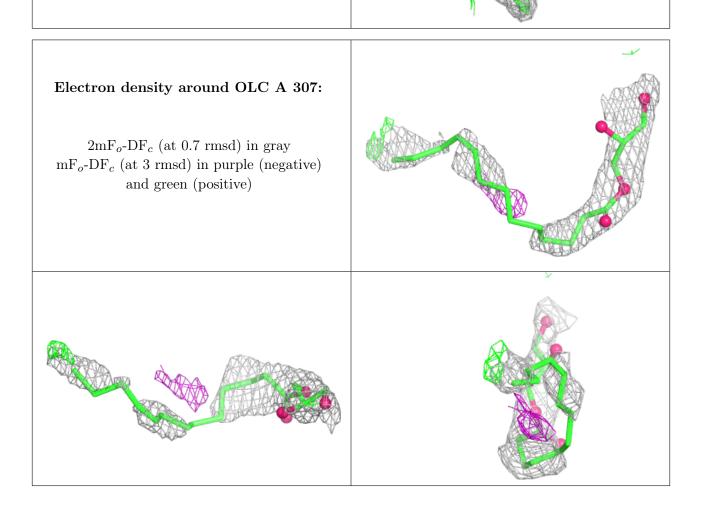






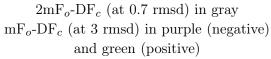


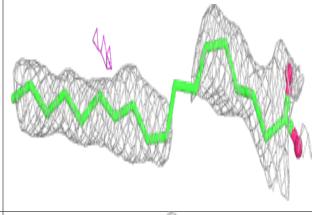


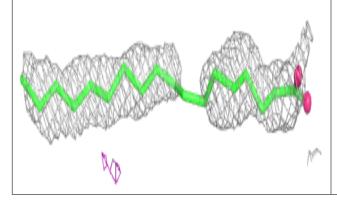


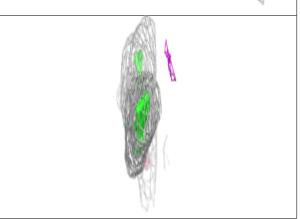


# Electron density around OLA A 304:



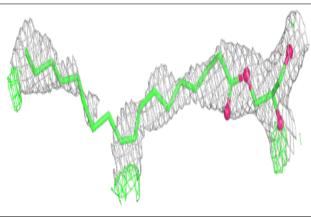


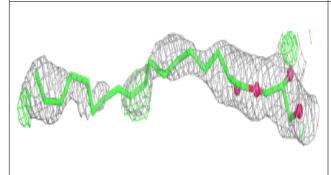


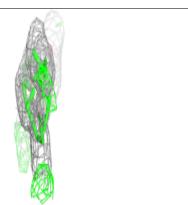


#### Electron density around OLC A 303:

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



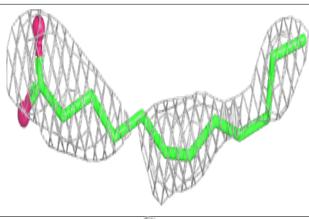


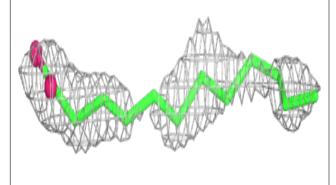


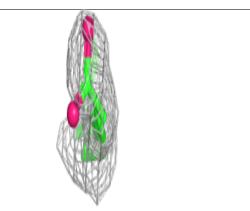


#### Electron density around OLA A 309:

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

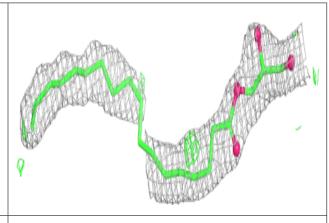


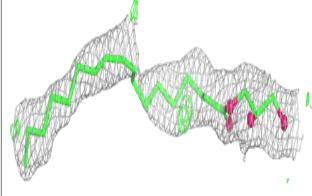


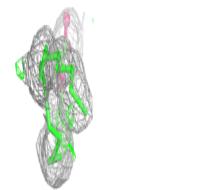


#### Electron density around OLC A 302:

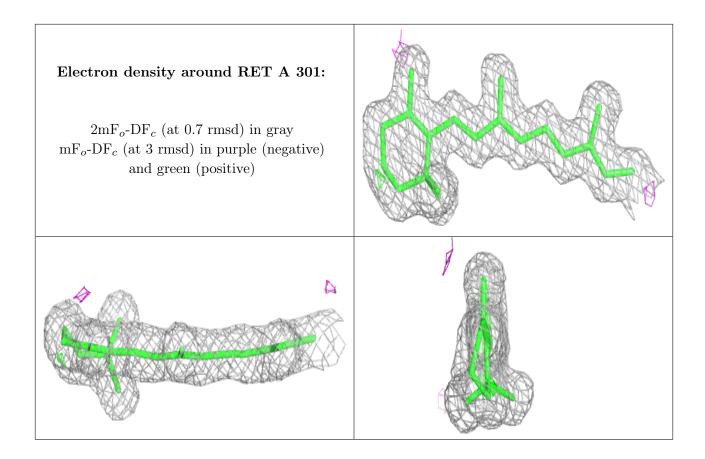
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)











## 6.5 Other polymers (i)

There are no such residues in this entry.

