Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 12:00 AM EDT

PDB ID	:	4Z34
Title	:	Crystal Structure of Human Lysophosphatidic Acid Receptor 1 in complex with ONO9780307
Authors	:	Chrencik, J.E.; Roth, C.B.; Terakado, M.; Kurata, H.; Omi, R.; Kihara, Y.; Warshaviak, D.; Nakade, S.; Asmar-Rovira, G.; Mileni, M.; Mizuno, H.; Griffith, M.T.; Rodgers, C.; Han, G.W.; Velasquez, J.; Chun, J.; Stevens, R.C.; Hanson, M.A.; GPCR Network (GPCR)
Deposited on	:	2015-03-30
Resolution	:	3.00 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 (i)) were used in the production of this report:

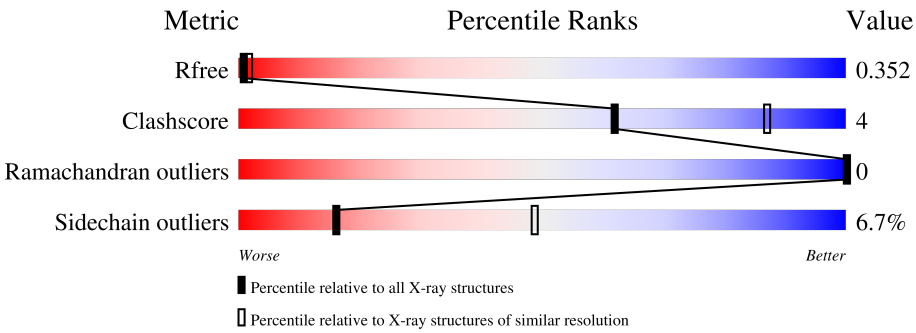
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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%

Mol	Chain	Length	Quality of chain
1	A	464	72% 10% • 17%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3047 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 Lysophosphatidic acid receptor 1, Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	2991	1945	492	529	25	0	0	0

There are 59 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q92633
A	-16	LYS	-	expression tag	UNP Q92633
A	-15	THR	-	expression tag	UNP Q92633
A	-14	ILE	-	expression tag	UNP Q92633
A	-13	ILE	-	expression tag	UNP Q92633
A	-12	ALA	-	expression tag	UNP Q92633
A	-11	LEU	-	expression tag	UNP Q92633
A	-10	SER	-	expression tag	UNP Q92633
A	-9	TYR	-	expression tag	UNP Q92633
A	-8	ILE	-	expression tag	UNP Q92633
A	-7	PHE	-	expression tag	UNP Q92633
A	-6	CYS	-	expression tag	UNP Q92633
A	-5	LEU	-	expression tag	UNP Q92633
A	-4	VAL	-	expression tag	UNP Q92633
A	-3	PHE	-	expression tag	UNP Q92633
A	-2	ALA	-	expression tag	UNP Q92633
A	-1	GLY	-	expression tag	UNP Q92633
A	0	ALA	-	expression tag	UNP Q92633
A	1	PRO	-	expression tag	UNP Q92633
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1043	ALA	-	linker	UNP P0ABE7
A	1044	THR	-	linker	UNP P0ABE7
A	1045	PRO	-	linker	UNP P0ABE7
A	1046	PRO	-	linker	UNP P0ABE7
A	1047	LYS	-	linker	UNP P0ABE7
A	1048	LEU	-	linker	UNP P0ABE7
A	1049	GLU	-	linker	UNP P0ABE7

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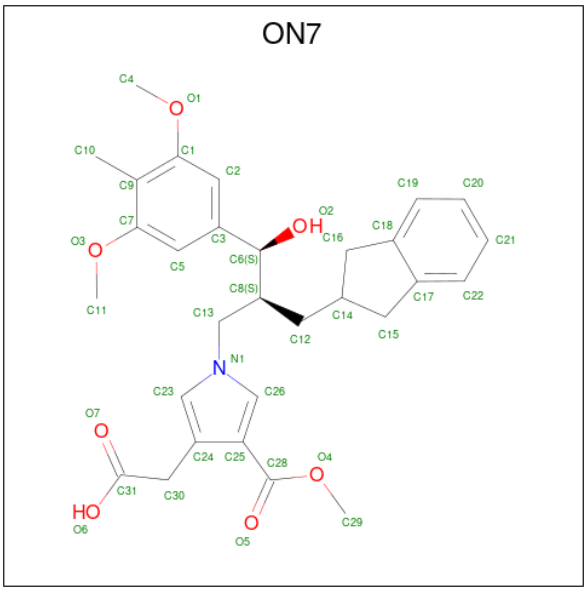
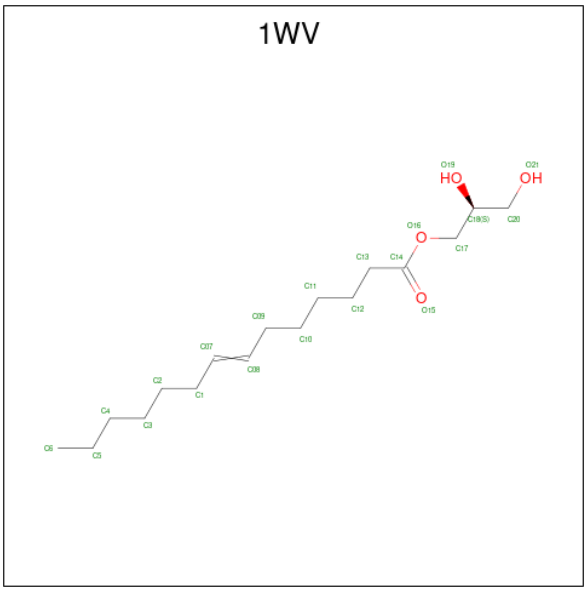
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	ASP	-	linker	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	-	linker	UNP P0ABE7
A	327	GLY	-	expression tag	UNP Q92633
A	328	ARG	-	expression tag	UNP Q92633
A	329	PRO	-	expression tag	UNP Q92633
A	330	LEU	-	expression tag	UNP Q92633
A	331	GLU	-	expression tag	UNP Q92633
A	332	VAL	-	expression tag	UNP Q92633
A	333	LEU	-	expression tag	UNP Q92633
A	334	PHE	-	expression tag	UNP Q92633
A	335	GLN	-	expression tag	UNP Q92633
A	336	GLY	-	expression tag	UNP Q92633
A	337	PRO	-	expression tag	UNP Q92633
A	338	HIS	-	expression tag	UNP Q92633
A	339	HIS	-	expression tag	UNP Q92633
A	340	HIS	-	expression tag	UNP Q92633
A	341	HIS	-	expression tag	UNP Q92633
A	342	HIS	-	expression tag	UNP Q92633
A	343	HIS	-	expression tag	UNP Q92633
A	344	HIS	-	expression tag	UNP Q92633
A	345	HIS	-	expression tag	UNP Q92633
A	346	HIS	-	expression tag	UNP Q92633
A	347	HIS	-	expression tag	UNP Q92633
A	348	ASP	-	expression tag	UNP Q92633
A	349	TYR	-	expression tag	UNP Q92633
A	350	LYS	-	expression tag	UNP Q92633
A	351	ASP	-	expression tag	UNP Q92633
A	352	ASP	-	expression tag	UNP Q92633
A	353	ASP	-	expression tag	UNP Q92633
A	354	ASP	-	expression tag	UNP Q92633
A	355	LYS	-	expression tag	UNP Q92633

- Molecule 2 is {1-[(2S,3S)-2-(2,3-dihydro-1H-inden-2-ylmethyl)-3-(3,5-dimethoxy-4-methylphenyl)-3-hydroxypropyl]-4-(methoxycarbonyl)-1 H-pyrrol-3-yl}acetic acid (three-letter code: ON7) (formula: $C_{30}H_{35}NO_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	38	30	1	7	0	0

- Molecule 3 is (2S)-2,3-dihydroxypropyl (7Z)-tetradec-7-enoate (three-letter code: 1WV) (formula: $C_{17}H_{32}O_4$).



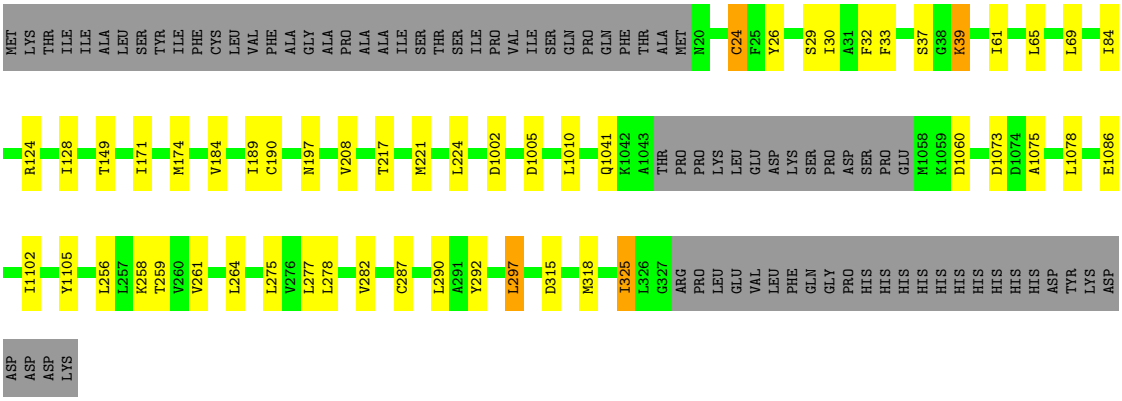
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	18	14	4	0	0

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. 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. 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: Lysophosphatidic acid receptor 1, Soluble cytochrome b562

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	34.28Å 112.15Å 154.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.81 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.6 (30.00-3.00) 83.6 (29.81-3.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 3.00Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.254 , 0.281 0.323 , 0.352	Depositor DCC
R_{free} test set	531 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 6.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	3047	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1WV, ON7

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	0.49	0/3052	0.65	1/4152 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	32	PHE	CA-CB-CG	5.35	126.74	113.90

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	2991	0	2987	26	0
2	A	38	0	34	4	0
3	A	18	0	23	0	0
All	All	3047	0	3044	27	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 4.

All (27) 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:84:ILE:HD13	1:A:256:LEU:HD21	1.53	0.90
1:A:124:ARG:O	1:A:128:ILE:HD12	1.87	0.75
1:A:208:VAL:CG2	1:A:282:VAL:HG21	2.21	0.70
1:A:84:ILE:HD13	1:A:256:LEU:CD2	2.21	0.69
1:A:61:ILE:O	1:A:65:LEU:HD13	2.00	0.62
1:A:208:VAL:HG23	1:A:282:VAL:HG21	1.81	0.61
1:A:184:VAL:HG12	1:A:184:VAL:O	2.02	0.60
1:A:69:LEU:HD22	1:A:325:ILE:HG21	1.86	0.56
1:A:1075:ALA:HA	1:A:1078:LEU:HD12	1.88	0.56
1:A:297:LEU:HD23	2:A:2001:ON7:H24	1.88	0.55
1:A:29:SER:O	1:A:33:PHE:CD2	2.66	0.48
1:A:26:TYR:O	1:A:29:SER:HB2	2.14	0.48
1:A:258:LYS:O	1:A:261:VAL:HG22	2.13	0.48
1:A:278:LEU:HD11	2:A:2001:ON7:H30	1.94	0.47
1:A:29:SER:HB3	1:A:33:PHE:HE2	1.78	0.47
1:A:84:ILE:CD1	1:A:256:LEU:HD21	2.36	0.47
1:A:297:LEU:CD2	2:A:2001:ON7:H24	2.45	0.46
1:A:221:MET:HA	1:A:224:LEU:HD12	1.98	0.45
1:A:1078:LEU:HD13	1:A:1086:GLU:HB3	1.99	0.45
2:A:2001:ON7:C21	2:A:2001:ON7:H23	2.47	0.44
1:A:277:LEU:HG	1:A:290:LEU:HD23	2.00	0.43
1:A:39:LYS:HG3	1:A:197:ASN:O	2.19	0.42
1:A:171:ILE:O	1:A:174:MET:HG2	2.19	0.41
1:A:24:CYS:O	1:A:189:ILE:HD11	2.21	0.41
1:A:275:LEU:HA	1:A:278:LEU:HD12	2.03	0.41
1:A:37:SER:HB3	1:A:197:ASN:HA	2.03	0.41
1:A:258:LYS:HG3	1:A:259:THR:N	2.35	0.41

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	Percentiles	
1	A	381/464 (82%)	366 (96%)	15 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/400 (78%)	292 (93%)	21 (7%)	16	49

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	CYS
1	A	30	ILE
1	A	39	LYS
1	A	149	THR
1	A	190	CYS
1	A	217	THR
1	A	1002	ASP
1	A	1005	ASP
1	A	1010	LEU
1	A	1041	GLN
1	A	1060	ASP
1	A	1073	ASP
1	A	1102	ILE
1	A	1105	TYR
1	A	264	LEU
1	A	287	CYS
1	A	292	TYR
1	A	297	LEU
1	A	315	ASP
1	A	318	MET
1	A	325	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	1099	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	1WV	A	2002	-	17,17,20	1.35	2 (11%)	18,18,21	1.14	2 (11%)
2	ON7	A	2001	-	39,41,41	1.74	6 (15%)	46,58,58	1.45	7 (15%)

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	1WV	A	2002	-	-	10/17/17/20	-
2	ON7	A	2001	-	-	8/30/38/38	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	ON7	C8-C6	4.73	1.60	1.53
3	A	2002	1WV	C08-C07	3.99	1.54	1.31
2	A	2001	ON7	C25-C24	3.73	1.44	1.39
2	A	2001	ON7	C30-C31	3.51	1.58	1.51
2	A	2001	ON7	C1-C9	2.86	1.44	1.40
2	A	2001	ON7	O4-C28	2.57	1.39	1.33
2	A	2001	ON7	C25-C28	-2.45	1.45	1.50
3	A	2002	1WV	C2-C1	-2.26	1.35	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	ON7	C26-C25-C28	-4.09	121.71	127.78
2	A	2001	ON7	O3-C7-C9	3.71	117.87	115.01
2	A	2001	ON7	C29-O4-C28	2.88	121.39	115.83
2	A	2001	ON7	C12-C14-C15	-2.69	107.60	115.34
2	A	2001	ON7	O7-C31-C30	-2.48	115.96	123.04
3	A	2002	1WV	C3-C2-C1	2.39	126.98	112.35
3	A	2002	1WV	C2-C1-C07	2.31	127.55	112.55
2	A	2001	ON7	O3-C7-C5	-2.16	120.40	124.12
2	A	2001	ON7	O5-C28-C25	2.05	128.44	121.57

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	ON7	C26-C25-C28-O5
2	A	2001	ON7	C26-C25-C28-O4
3	A	2002	1WV	O16-C17-C18-O19
3	A	2002	1WV	C07-C1-C2-C3
3	A	2002	1WV	C1-C07-C08-C09
2	A	2001	ON7	C5-C7-O3-C11
3	A	2002	1WV	O15-C14-O16-C17
3	A	2002	1WV	C13-C14-O16-C17
2	A	2001	ON7	C2-C1-O1-C4
2	A	2001	ON7	C9-C7-O3-C11
2	A	2001	ON7	C9-C1-O1-C4
3	A	2002	1WV	O16-C17-C18-C20
2	A	2001	ON7	C14-C12-C8-C6
3	A	2002	1WV	C07-C08-C09-C10
3	A	2002	1WV	C12-C13-C14-O16

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Mol	Chain	Res	Type	Atoms
3	A	2002	1WV	C08-C07-C1-C2
2	A	2001	ON7	C24-C30-C31-O7
3	A	2002	1WV	C12-C13-C14-O15

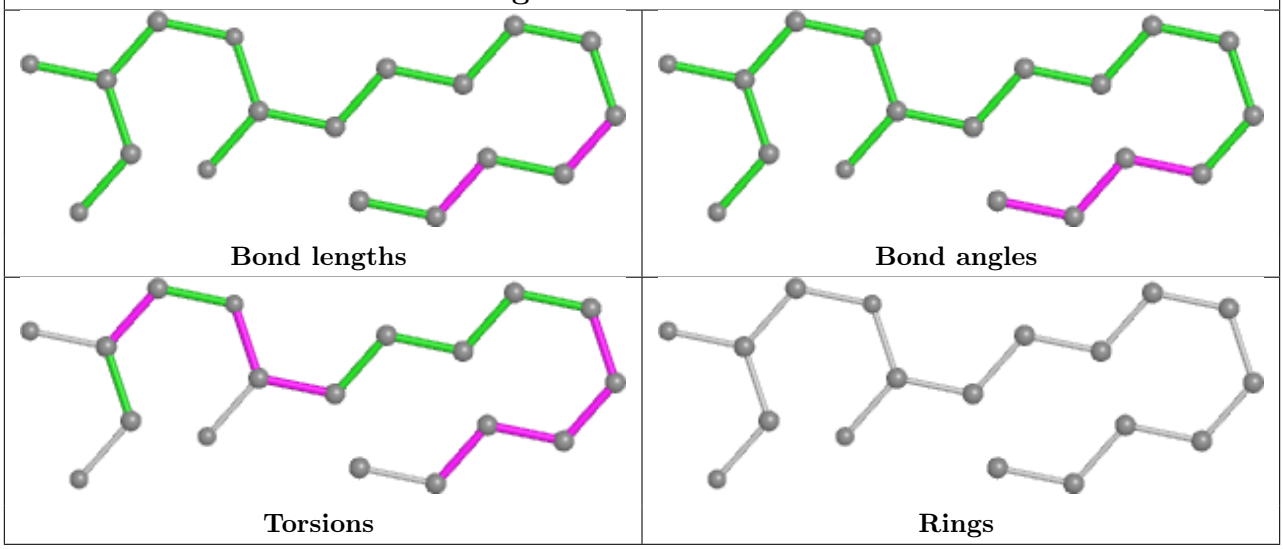
There are no ring outliers.

1 monomer is involved in 4 short contacts:

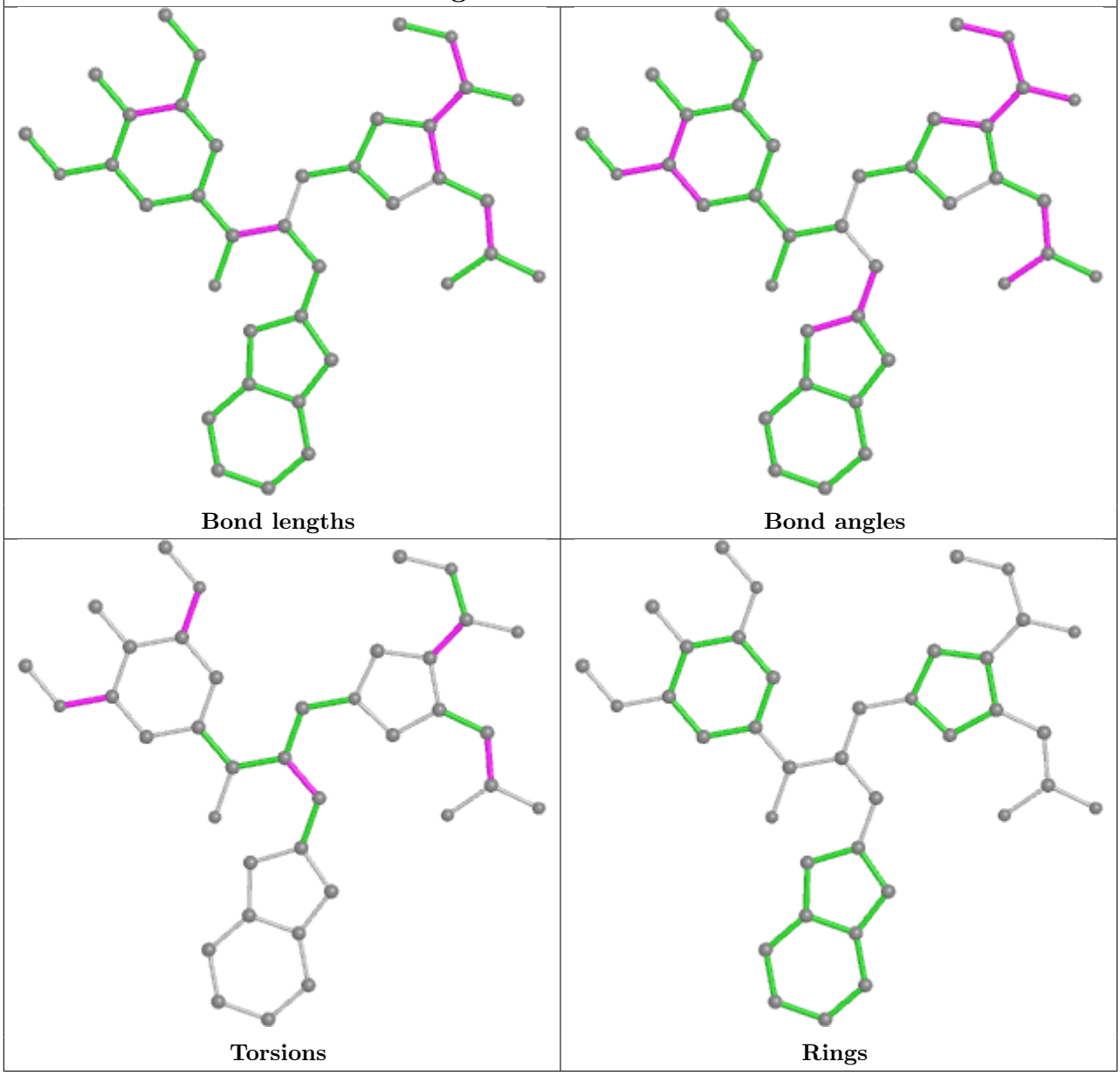
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	ON7	4	0

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 1WV A 2002



Ligand ON7 A 2001



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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

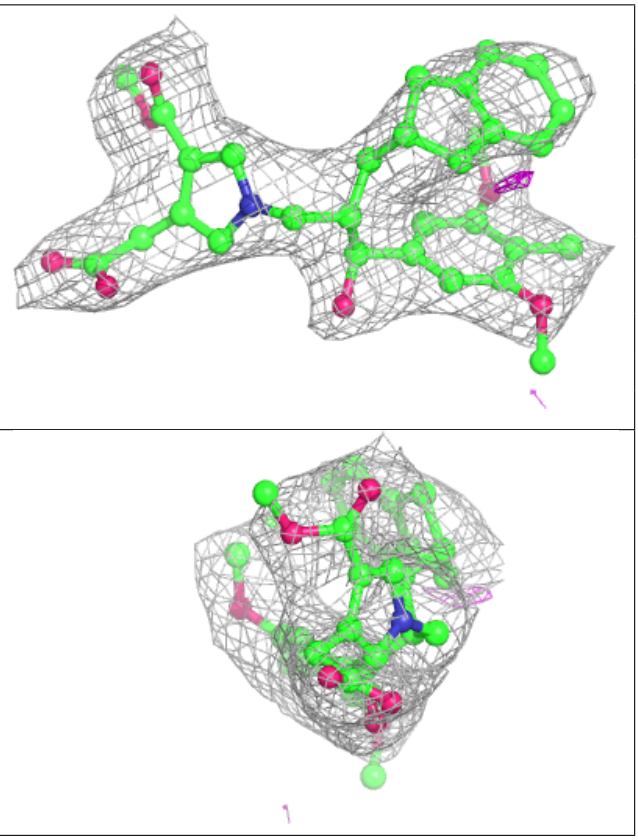
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

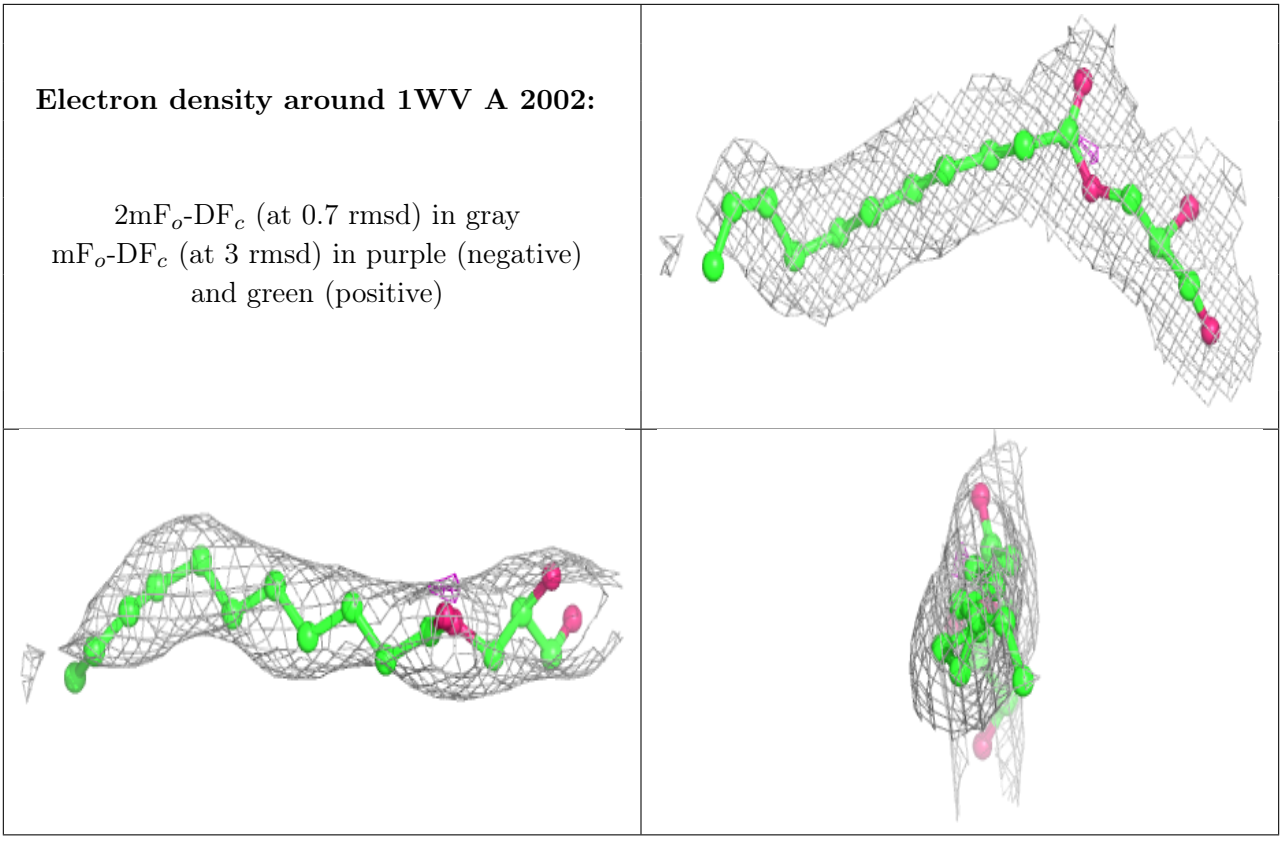
Electron density around ON7 A 2001:

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



Electron density around 1WV A 2002:

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



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.