Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 03:03 pm GMT

PDB ID	:	8S4D
Title	:	Crystal structure of a peptidergic GPCR in complex with a small synthetic G protein-biased agonist
Authors	:	Verdon, G.; Currinn, H.; Solcan, N.; Schlenker, O.; Brown, A.J.H.
Deposited on	:	2024-02-21
Resolution	:	2.58 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

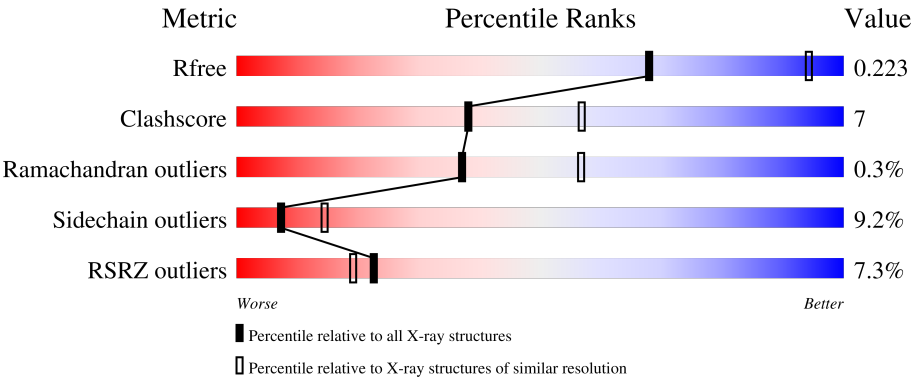
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.58 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}	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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	497	6% 61% 14% · 23%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3136 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 Apelin receptor,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	3029	1990	487	528	24	0	1	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP P35414
A	-16	LYS	-	expression tag	UNP P35414
A	-15	THR	-	expression tag	UNP P35414
A	-14	ILE	-	expression tag	UNP P35414
A	-13	ILE	-	expression tag	UNP P35414
A	-12	ALA	-	expression tag	UNP P35414
A	-11	LEU	-	expression tag	UNP P35414
A	-10	SER	-	expression tag	UNP P35414
A	-9	TYR	-	expression tag	UNP P35414
A	-8	ILE	-	expression tag	UNP P35414
A	-7	PHE	-	expression tag	UNP P35414
A	-6	CYS	-	expression tag	UNP P35414
A	-5	LEU	-	expression tag	UNP P35414
A	-4	VAL	-	expression tag	UNP P35414
A	-3	PHE	-	expression tag	UNP P35414
A	-2	ALA	-	expression tag	UNP P35414
A	-1	ASP	-	expression tag	UNP P35414
A	0	TYR	-	expression tag	UNP P35414
A	1	LYS	-	expression tag	UNP P35414
A	2	ASP	-	expression tag	UNP P35414
A	3	ASP	-	expression tag	UNP P35414
A	4	ASP	-	expression tag	UNP P35414
A	5	ASP	-	expression tag	UNP P35414
A	6	LYS	-	expression tag	UNP P35414
A	87	VAL	THR	engineered mutation	UNP P35414
A	112	ALA	ASN	engineered mutation	UNP P35414
A	177	ASN	THR	engineered mutation	UNP P35414

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Chain	Residue	Modelled	Actual	Comment	Reference
A	207	MET	THR	engineered mutation	UNP P35414
A	214	LEU	PHE	engineered mutation	UNP P35414
A	224	ALA	ILE	engineered mutation	UNP P35414
A	1007	TRP	MET	conflict	UNP A7ZVB5
A	1102	ILE	-	linker	UNP A7ZVB5
A	1103	GLN	-	linker	UNP A7ZVB5
A	1104	LYS	-	linker	UNP A7ZVB5
A	1105	TYR	-	linker	UNP A7ZVB5
A	1106	LEU	-	linker	UNP A7ZVB5
A	298	ALA	SER	engineered mutation	UNP P35414
A	325	LEU	-	expression tag	UNP P35414
A	326	MET	-	expression tag	UNP P35414
A	327	GLY	-	expression tag	UNP P35414
A	328	GLN	-	expression tag	UNP P35414
A	329	SER	-	expression tag	UNP P35414
A	330	ARG	-	expression tag	UNP P35414
A	331	LEU	-	expression tag	UNP P35414
A	332	GLU	-	expression tag	UNP P35414
A	333	VAL	-	expression tag	UNP P35414
A	334	LEU	-	expression tag	UNP P35414
A	335	PHE	-	expression tag	UNP P35414
A	336	GLN	-	expression tag	UNP P35414
A	337	GLY	-	expression tag	UNP P35414
A	338	PRO	-	expression tag	UNP P35414
A	339	ALA	-	expression tag	UNP P35414
A	340	SER	-	expression tag	UNP P35414
A	341	ALA	-	expression tag	UNP P35414
A	342	TRP	-	expression tag	UNP P35414
A	343	SER	-	expression tag	UNP P35414
A	344	HIS	-	expression tag	UNP P35414
A	345	PRO	-	expression tag	UNP P35414
A	346	GLN	-	expression tag	UNP P35414
A	347	PHE	-	expression tag	UNP P35414
A	348	GLU	-	expression tag	UNP P35414
A	349	LYS	-	expression tag	UNP P35414
A	350	GLY	-	expression tag	UNP P35414
A	351	SER	-	expression tag	UNP P35414
A	352	ALA	-	expression tag	UNP P35414
A	353	GLY	-	expression tag	UNP P35414
A	354	SER	-	expression tag	UNP P35414
A	355	ALA	-	expression tag	UNP P35414
A	356	ALA	-	expression tag	UNP P35414

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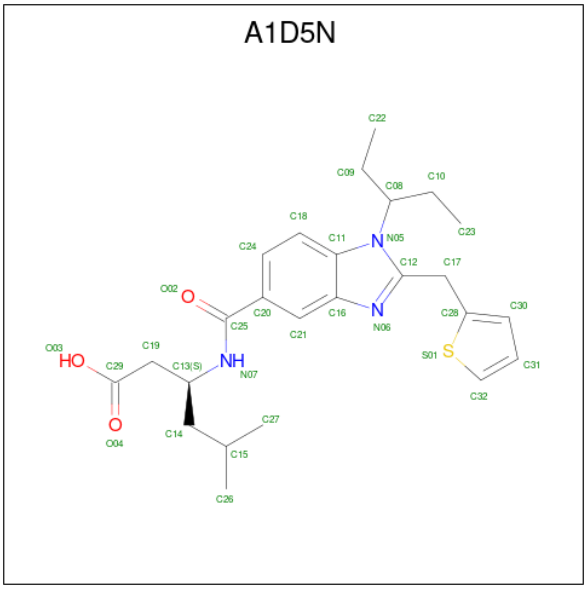
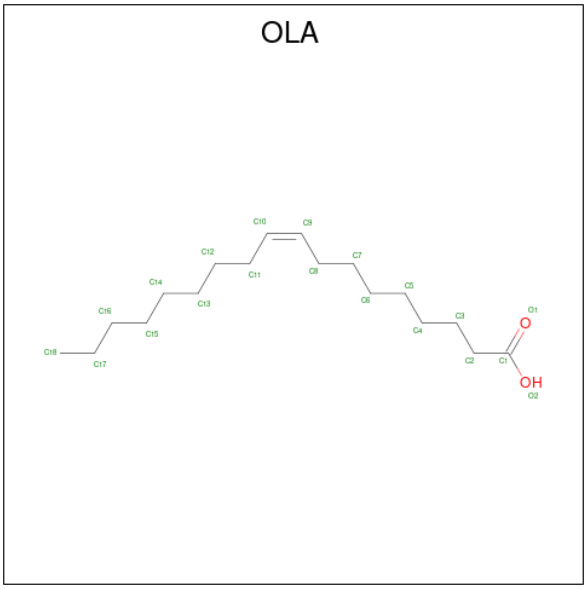
Chain	Residue	Modelled	Actual	Comment	Reference
A	357	GLY	-	expression tag	UNP P35414
A	358	SER	-	expression tag	UNP P35414
A	359	ALA	-	expression tag	UNP P35414
A	360	SER	-	expression tag	UNP P35414
A	361	ALA	-	expression tag	UNP P35414
A	362	TRP	-	expression tag	UNP P35414
A	363	SER	-	expression tag	UNP P35414
A	364	HIS	-	expression tag	UNP P35414
A	365	PRO	-	expression tag	UNP P35414
A	366	GLN	-	expression tag	UNP P35414
A	367	PHE	-	expression tag	UNP P35414
A	368	GLU	-	expression tag	UNP P35414
A	369	LYS	-	expression tag	UNP P35414
A	370	HIS	-	expression tag	UNP P35414
A	371	HIS	-	expression tag	UNP P35414
A	372	HIS	-	expression tag	UNP P35414
A	373	HIS	-	expression tag	UNP P35414
A	374	HIS	-	expression tag	UNP P35414
A	375	HIS	-	expression tag	UNP P35414
A	376	HIS	-	expression tag	UNP P35414
A	377	HIS	-	expression tag	UNP P35414
A	378	HIS	-	expression tag	UNP P35414
A	379	HIS	-	expression tag	UNP P35414

- Molecule 2 is (3 {S})-5-methyl-3-[[1-pentan-3-yl-2-(thiophen-2-ylmethyl)benzimidazol-5-yl] carbonylamino]hexanoic acid (three-letter code: A1D5N) (formula: $C_{25}H_{33}N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



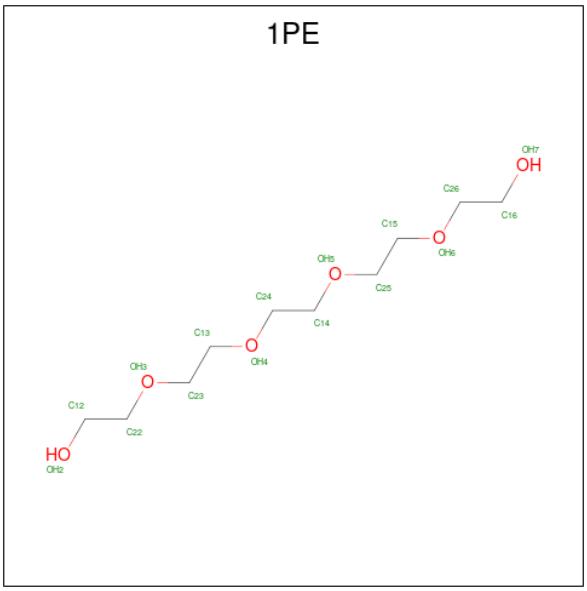
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O S 32 25 3 3 1	0	0

- Molecule 3 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 16 14 2	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 7 7	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 4 2	0	0

- Molecule 5 is water.

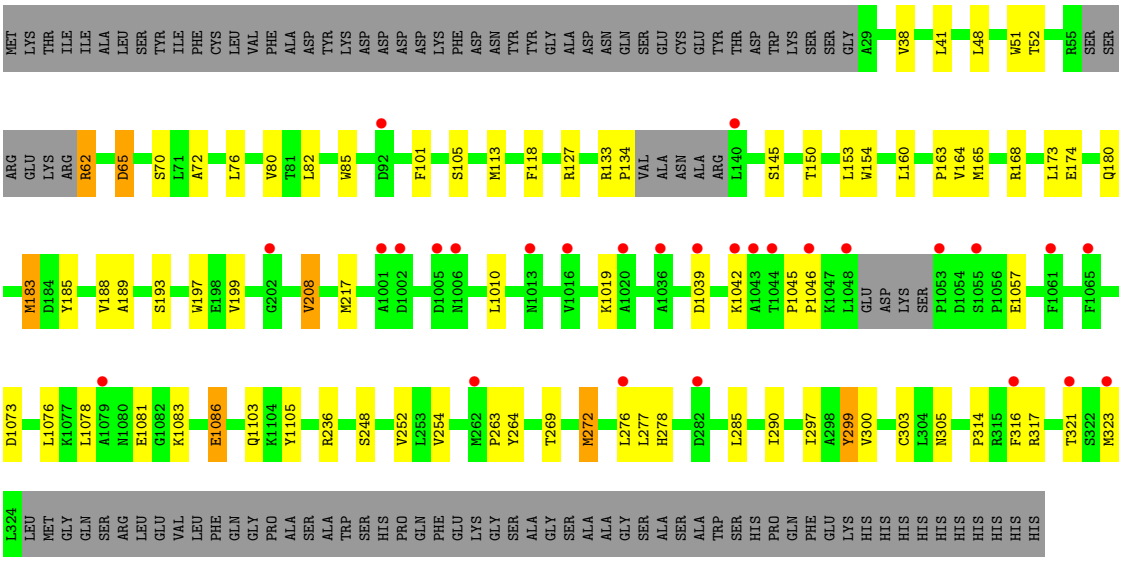
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0

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: Apelin receptor,Soluble cytochrome b562

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	65.82Å 153.95Å 111.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.97 – 2.58 76.97 – 2.58	Depositor EDS
% Data completeness (in resolution range)	53.4 (76.97-2.58) 53.4 (76.97-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.58Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.232 , 0.275 0.234 , 0.223	Depositor DCC
R_{free} test set	8963 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	3136	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, 1PE, A1D5N

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	0.40	0/3104	0.57	0/4224

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

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	3029	0	3082	43	0
2	A	32	0	0	2	0
3	A	67	0	104	2	0
4	A	6	0	7	1	0
5	A	2	0	0	0	0
All	All	3136	0	3193	43	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.

All (43) 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:314:PRO:HA	1:A:317:ARG:HG3	1.27	1.16
1:A:263:PRO:HG2	1:A:297:ILE:HD13	1.54	0.87
1:A:118:PHE:HB3	1:A:153[B]:LEU:HD13	1.67	0.75
1:A:51:TRP:CD1	1:A:323:MET:HE1	2.32	0.65
1:A:314:PRO:HA	1:A:317:ARG:CG	2.16	0.65
1:A:217:MET:HB3	1:A:254:VAL:HG22	1.83	0.61
1:A:314:PRO:CA	1:A:317:ARG:HG3	2.17	0.58
1:A:168:ARG:HE	1:A:183:MET:CE	2.20	0.55
1:A:269:THR:HA	1:A:272:MET:HE2	1.88	0.55
1:A:1105:TYR:HD1	1:A:236:ARG:NH2	2.05	0.55
1:A:189:ALA:HB1	1:A:193:SER:HB3	1.88	0.54
1:A:173:LEU:HG	1:A:174:GLU:HG2	1.89	0.54
1:A:38:VAL:HG23	1:A:303:CYS:SG	2.47	0.54
1:A:160:LEU:HD13	1:A:208:VAL:HG11	1.89	0.53
1:A:101:PHE:O	1:A:105:SER:HB3	2.10	0.50
1:A:164:VAL:HG12	3:A:1202:OLA:H72	1.94	0.49
1:A:52:THR:HG21	1:A:316:PHE:HD1	1.77	0.49
1:A:72:ALA:O	1:A:76:LEU:HB2	2.12	0.49
1:A:299:TYR:CE2	2:A:1201:A1D5N:C31	2.95	0.49
1:A:252:VAL:HG22	3:A:1204:OLA:H151	1.95	0.49
1:A:160:LEU:O	1:A:163:PRO:HD2	2.13	0.48
1:A:51:TRP:CD1	1:A:323:MET:CE	2.97	0.48
1:A:38:VAL:HG21	1:A:299:TYR:HB3	1.97	0.46
1:A:189:ALA:HB2	1:A:197:TRP:CD1	2.50	0.46
1:A:62:ARG:HG3	1:A:65:ASP:HB2	1.96	0.46
1:A:264:TYR:OH	2:A:1201:A1D5N:N06	2.48	0.46
1:A:164:VAL:HB	1:A:183:MET:HE1	1.99	0.44
1:A:1078:LEU:O	1:A:1081:GLU:HG2	2.17	0.44
1:A:118:PHE:HB2	1:A:153[A]:LEU:HD13	1.98	0.44
1:A:1045:PRO:HB2	1:A:1046:PRO:HD2	1.99	0.43
1:A:1083:LYS:HG3	1:A:1086:GLU:CB	2.49	0.43
1:A:1105:TYR:CD1	1:A:236:ARG:NH2	2.86	0.42
1:A:133:ARG:HB3	1:A:134:PRO:HD2	2.02	0.42
1:A:199:VAL:HG22	1:A:272:MET:HG2	2.01	0.42
1:A:70:SER:HB3	1:A:154:TRP:HE1	1.85	0.42
1:A:1039:ASP:HA	1:A:1042:LYS:HE3	2.02	0.41
1:A:52:THR:HG21	1:A:316:PHE:CD1	2.53	0.41
1:A:183:MET:HG2	1:A:185:TYR:CZ	2.56	0.41
1:A:85:TRP:NE1	1:A:105:SER:OG	2.51	0.41
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.87	0.41
1:A:1083:LYS:HG3	1:A:1086:GLU:HB3	2.02	0.41
1:A:305:ASN:HB3	4:A:1208:1PE:H221	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:TRP:NE1	1:A:323:MET:CE	2.84	0.40

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	374/497 (75%)	361 (96%)	12 (3%)	1 (0%)	37 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	LEU

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	326/422 (77%)	296 (91%)	30 (9%)	7 14

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	48	LEU

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Mol	Chain	Res	Type
1	A	62	ARG
1	A	65	ASP
1	A	80	VAL
1	A	113	MET
1	A	127	ARG
1	A	145	SER
1	A	150	THR
1	A	165	MET
1	A	180	GLN
1	A	183	MET
1	A	188	VAL
1	A	208	VAL
1	A	1010	LEU
1	A	1019	LYS
1	A	1057	GLU
1	A	1073	ASP
1	A	1076	LEU
1	A	1086	GLU
1	A	1103	GLN
1	A	248	SER
1	A	272	MET
1	A	277	LEU
1	A	278	HIS
1	A	285	LEU
1	A	290	ILE
1	A	299	TYR
1	A	300	VAL
1	A	321	THR

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	OLA	A	1203	-	15,15,19	0.61	0	15,15,19	0.79	0
3	OLA	A	1204	-	7,7,19	0.33	0	6,6,19	0.33	0
3	OLA	A	1202	-	19,19,19	0.50	0	19,19,19	0.78	0
3	OLA	A	1205	-	7,7,19	0.36	0	6,6,19	0.34	0
4	1PE	A	1208	-	5,5,15	0.36	0	4,4,14	0.24	0
2	A1D5N	A	1201	-	29,34,34	1.78	5 (17%)	30,47,47	2.31	3 (10%)
3	OLA	A	1206	-	7,7,19	0.31	0	6,6,19	0.37	0
3	OLA	A	1207	-	6,6,19	0.45	0	5,5,19	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
3	OLA	A	1203	-	-	7/13/13/17	-
3	OLA	A	1204	-	-	1/5/5/17	-
3	OLA	A	1202	-	-	8/17/17/17	-
3	OLA	A	1205	-	-	3/5/5/17	-
4	1PE	A	1208	-	-	0/3/3/13	-
2	A1D5N	A	1201	-	-	4/22/28/28	0/3/3/3
3	OLA	A	1206	-	-	0/5/5/17	-
3	OLA	A	1207	-	-	1/4/4/17	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	A1D5N	C25-N07	6.14	1.47	1.34
2	A	1201	A1D5N	C20-C25	3.91	1.58	1.50
2	A	1201	A1D5N	C17-C12	2.47	1.55	1.50
2	A	1201	A1D5N	O02-C25	-2.18	1.18	1.23
2	A	1201	A1D5N	C28-S01	-2.05	1.69	1.73

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	A1D5N	C31-C32-S01	-10.90	104.13	112.98
2	A	1201	A1D5N	C13-N07-C25	-2.88	118.56	122.55
2	A	1201	A1D5N	C12-C17-C28	-2.41	108.78	113.48

There are no chirality outliers.

All (24) torsion outliers are listed below:

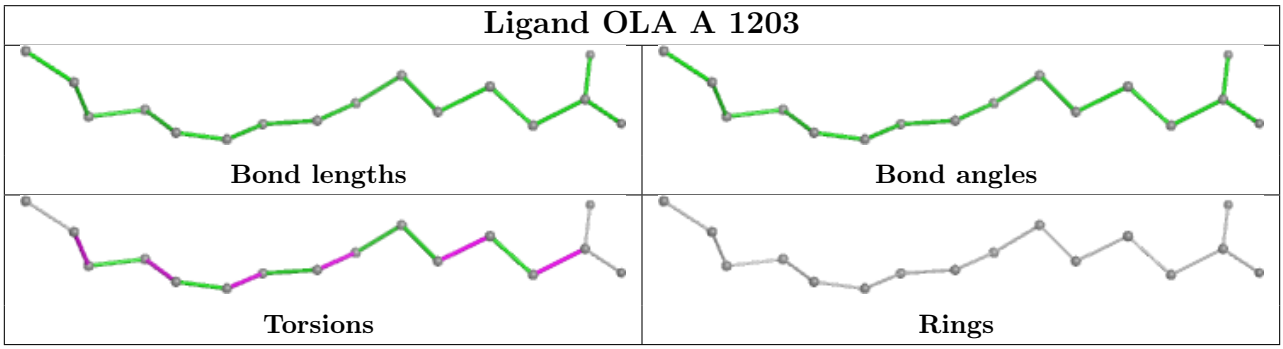
Mol	Chain	Res	Type	Atoms
3	A	1202	OLA	C1-C2-C3-C4
3	A	1202	OLA	C14-C15-C16-C17
3	A	1202	OLA	C3-C4-C5-C6
3	A	1202	OLA	C15-C16-C17-C18
3	A	1205	OLA	C10-C11-C12-C13
3	A	1203	OLA	C2-C3-C4-C5
3	A	1205	OLA	C11-C12-C13-C14
3	A	1203	OLA	C11-C12-C13-C14
3	A	1202	OLA	C13-C14-C15-C16
2	A	1201	A1D5N	C13-C19-C29-O03
2	A	1201	A1D5N	C13-C19-C29-O04
3	A	1207	OLA	C12-C13-C14-C15
3	A	1204	OLA	C13-C14-C15-C16
3	A	1202	OLA	O1-C1-C2-C3
3	A	1202	OLA	O2-C1-C2-C3
3	A	1203	OLA	C5-C6-C7-C8
3	A	1203	OLA	O1-C1-C2-C3
3	A	1202	OLA	C7-C8-C9-C10
3	A	1203	OLA	C9-C10-C11-C12
3	A	1203	OLA	O2-C1-C2-C3
3	A	1203	OLA	C7-C8-C9-C10
2	A	1201	A1D5N	N05-C08-C10-C23
3	A	1205	OLA	C14-C15-C16-C17
2	A	1201	A1D5N	C09-C08-C10-C23

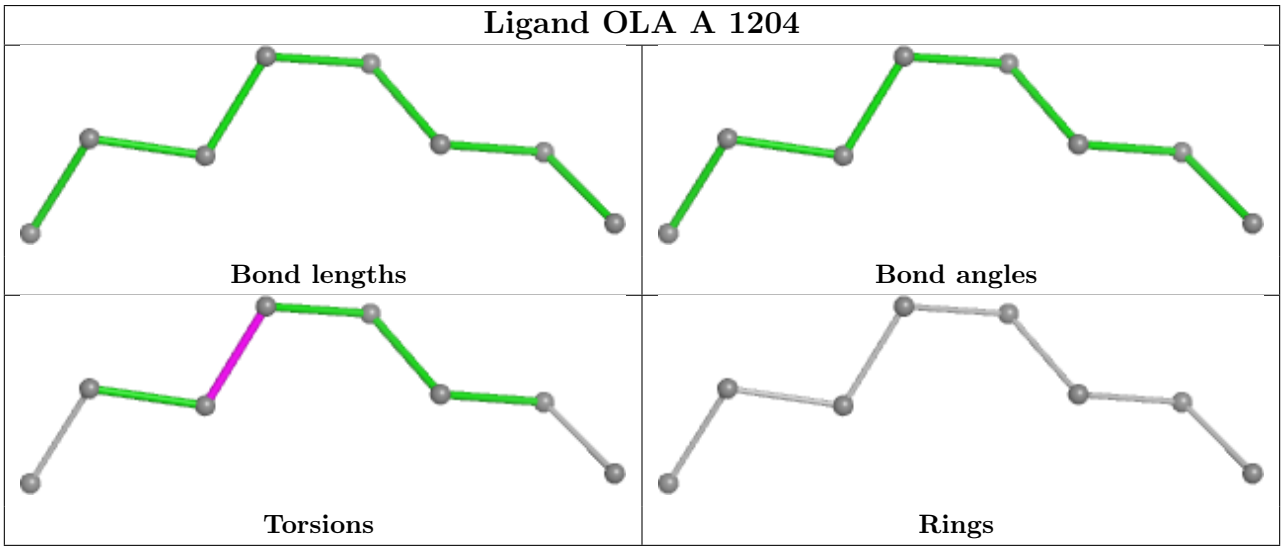
There are no ring outliers.

4 monomers are involved in 5 short contacts:

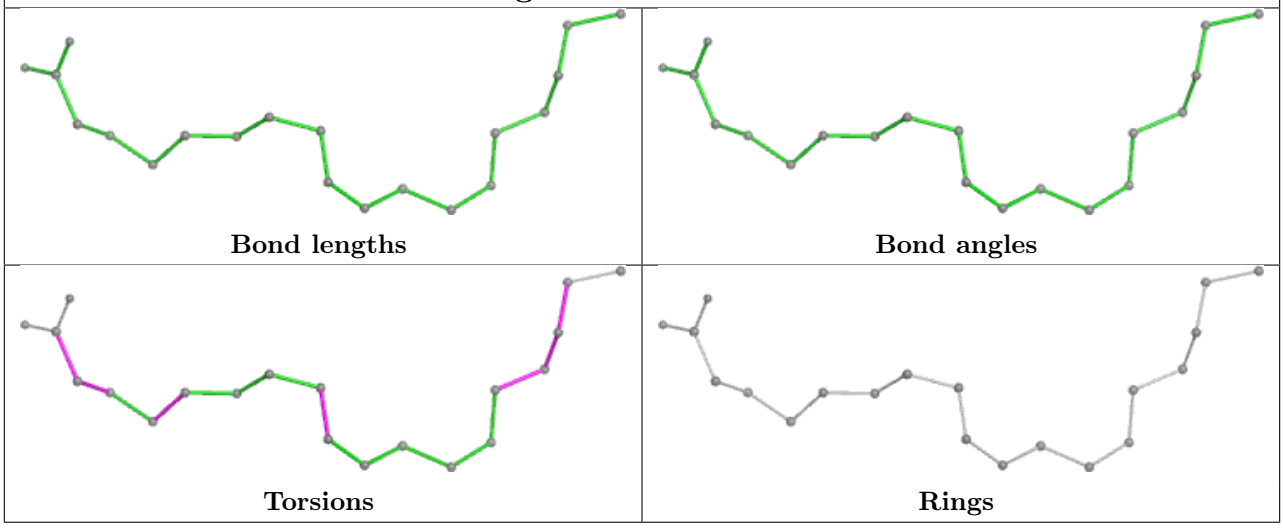
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1204	OLA	1	0
3	A	1202	OLA	1	0
4	A	1208	1PE	1	0
2	A	1201	A1D5N	2	0

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.

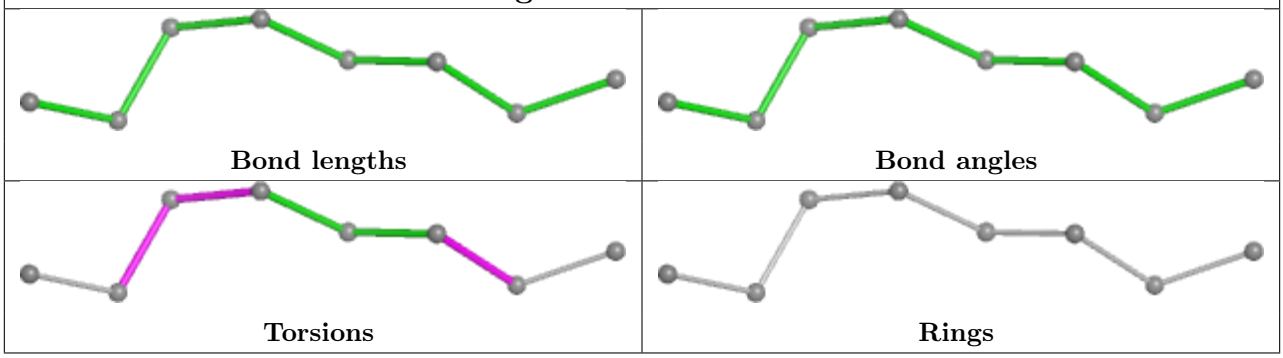


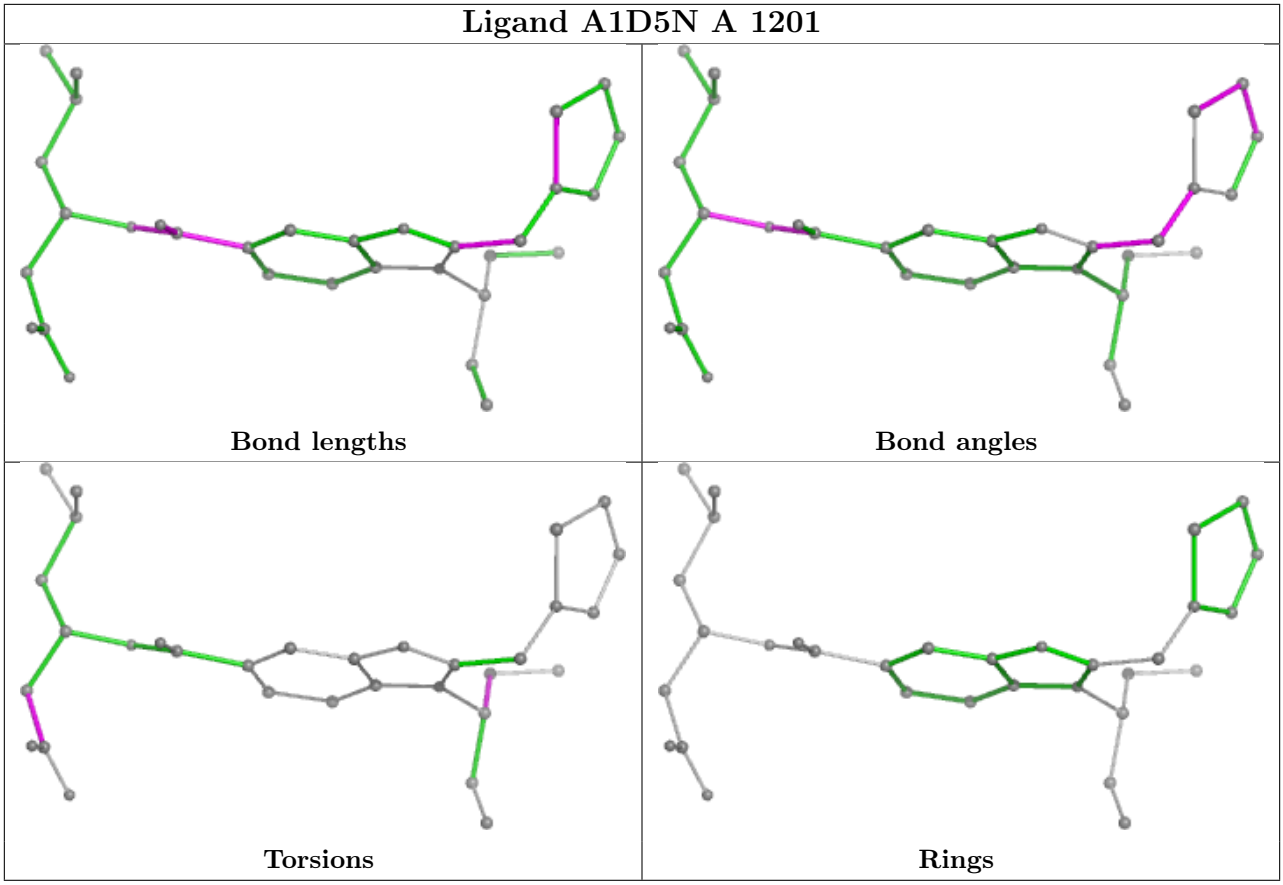


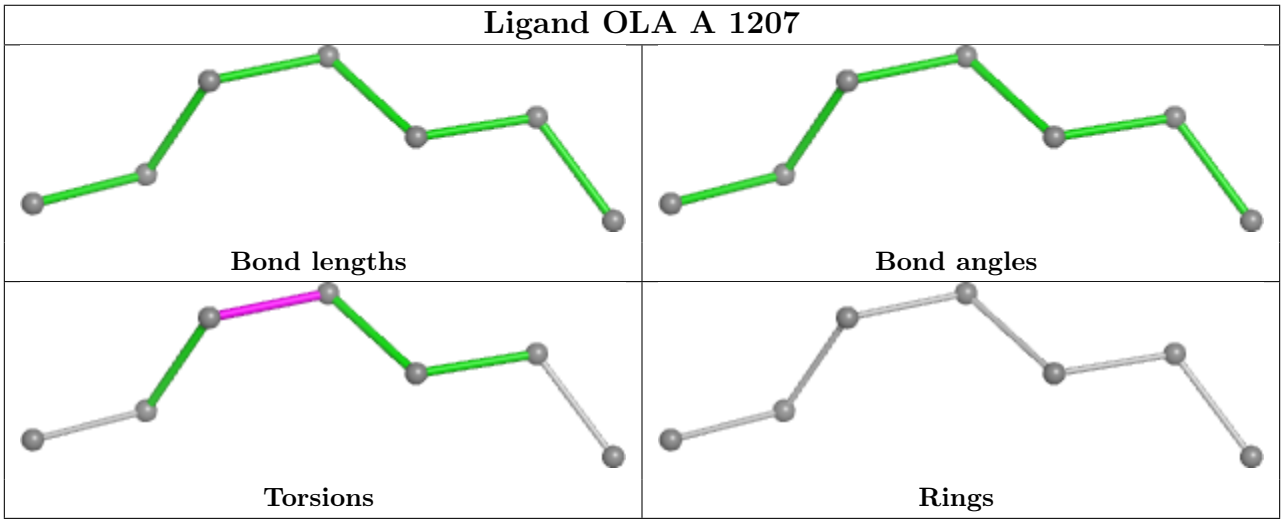
Ligand OLA A 1202



Ligand OLA A 1205







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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	381/497 (76%)	0.66	28 (7%)	22	19	26, 64, 98, 121	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1043	ALA	5.1
1	A	1006	ASN	4.5
1	A	1016	VAL	4.2
1	A	323	MET	4.1
1	A	1048	LEU	4.1
1	A	1044	THR	3.8
1	A	1013	ASN	3.8
1	A	1039	ASP	3.4
1	A	276	LEU	3.3
1	A	1053	PRO	3.2
1	A	1005	ASP	3.2
1	A	1001	ALA	3.1
1	A	1061	PHE	2.9
1	A	1036	ALA	2.7
1	A	1020	ALA	2.6
1	A	1079	ALA	2.6
1	A	140	LEU	2.5
1	A	321	THR	2.2
1	A	316	PHE	2.2
1	A	202	GLY	2.1
1	A	1046	PRO	2.1
1	A	1055	SER	2.1
1	A	1002	ASP	2.1
1	A	262	MET	2.1
1	A	92	ASP	2.1
1	A	1042	LYS	2.0
1	A	1065	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	282	ASP	2.0

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)

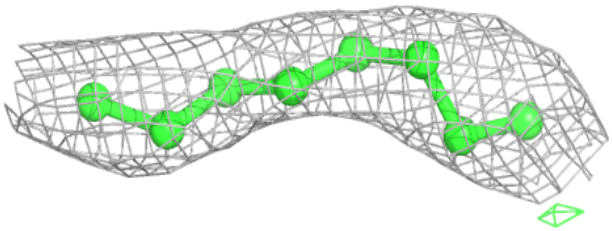
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

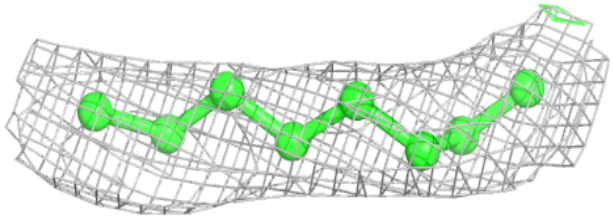
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OLA	A	1205	8/20	0.79	0.15	33,34,36,36	0
4	1PE	A	1208	6/16	0.80	0.17	47,47,48,48	0
3	OLA	A	1204	8/20	0.86	0.13	45,45,45,45	0
3	OLA	A	1207	7/20	0.87	0.08	23,24,25,26	0
3	OLA	A	1202	20/20	0.89	0.12	42,44,47,48	0
3	OLA	A	1203	16/20	0.89	0.12	40,45,51,52	0
3	OLA	A	1206	8/20	0.90	0.10	40,40,40,40	0
2	A1D5N	A	1201	32/32	0.91	0.11	40,44,49,50	0

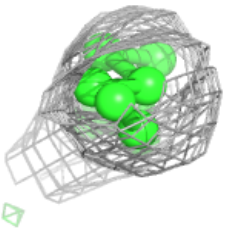
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 1205:

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

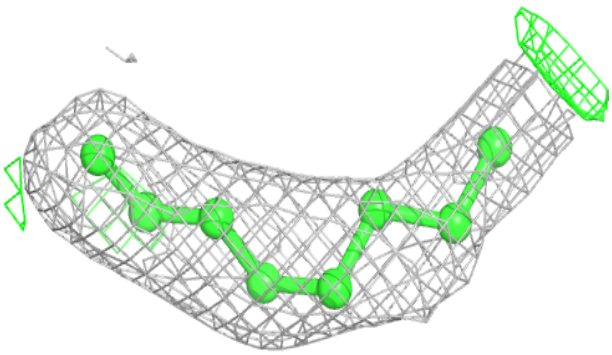


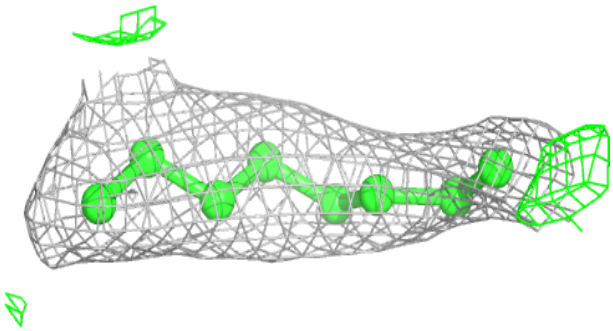


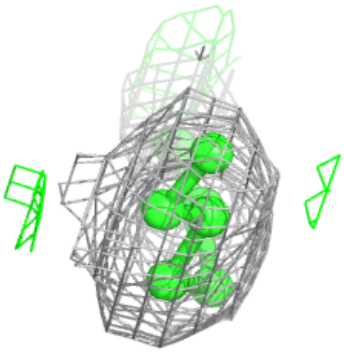


Electron density around OLA A 1204:

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

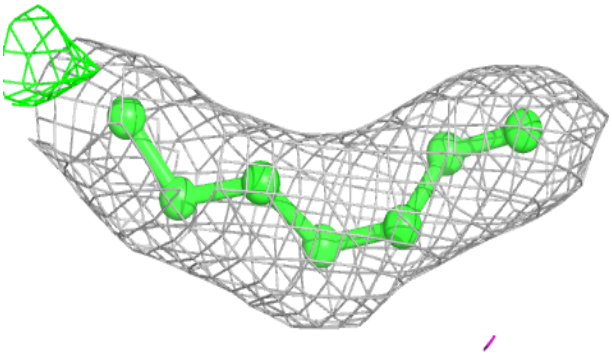


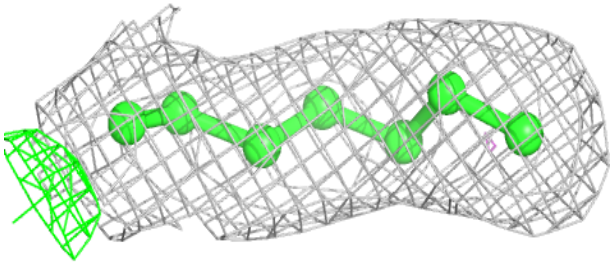


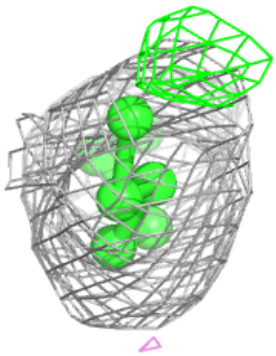


Electron density around OLA A 1207:

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

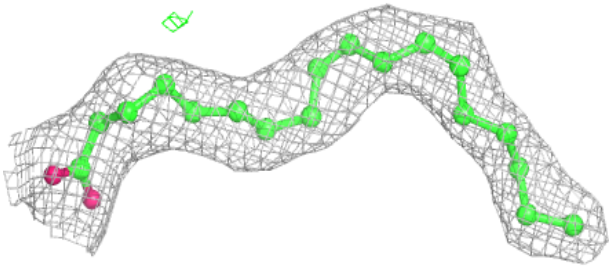


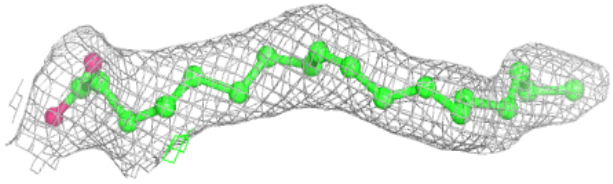


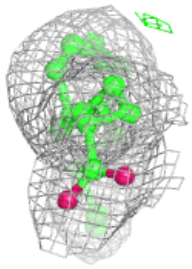


Electron density around OLA A 1202:

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

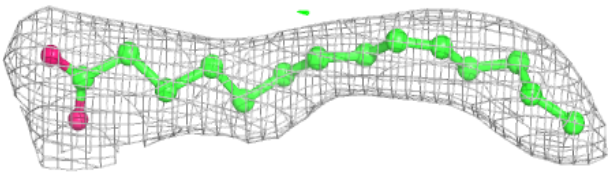


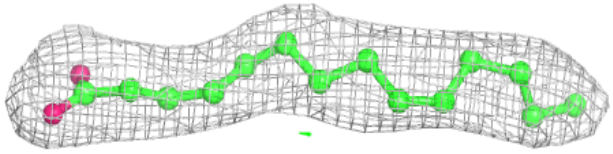


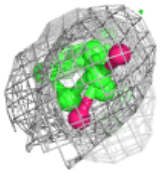


Electron density around OLA A 1203:

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

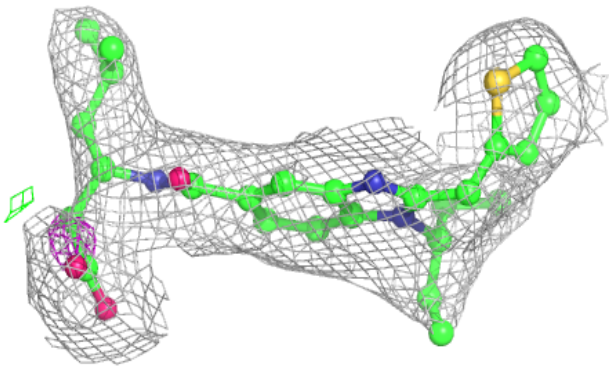


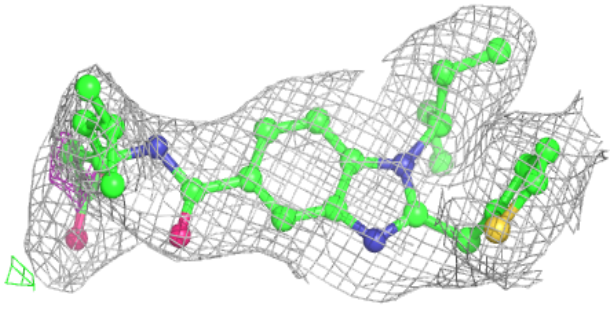


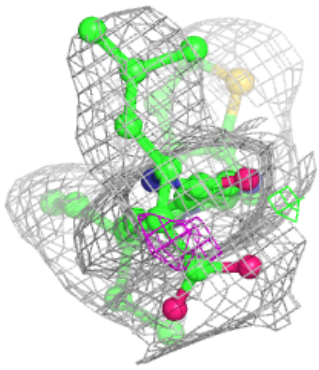


Electron density around A1D5N A 1201:

$2mF_o$-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)

There are no such residues in this entry.