



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2024 – 09:06 PM EDT

PDB ID : 3DDL
Title : Crystallographic Structure of Xanthorhodopsin, a Light-Driven Ion Pump with Dual Chromophore
Authors : Stagno, J.; Luecke, H.; Schobert, B.; Lanyi, J.K.; Imasheva, E.S.; Wang, J.M.; Balashov, S.P.
Deposited on : 2008-06-05
Resolution : 1.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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	:	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

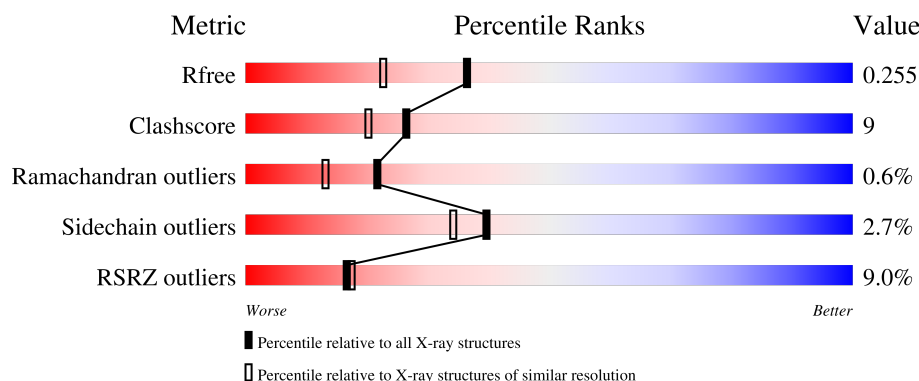
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	273	
1	B	273	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PX4	B	1415	X	-	-	-
6	PCW	B	1416	X	-	-	-

2 Entry composition [i](#)

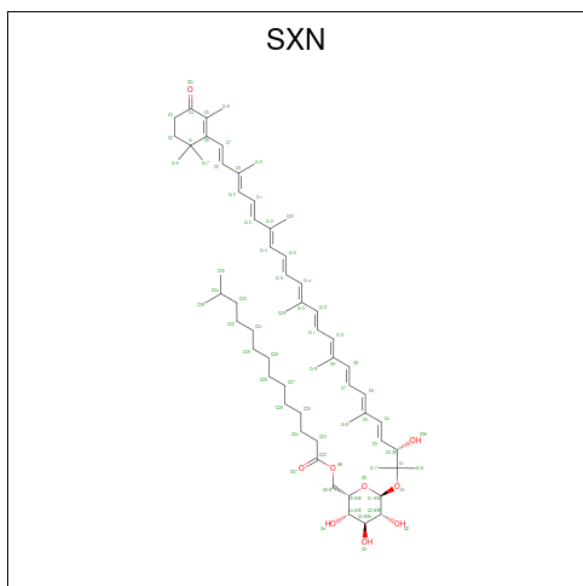
There are 7 unique types of molecules in this entry. The entry contains 4417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Xanthorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1971	1307	310	345	9			
1	B	250	Total	C	N	O	S	0	0	0
			1954	1297	308	340	9			

- Molecule 2 is Salinixanthin (three-letter code: SXN) (formula: $C_{61}H_{92}O_9$).

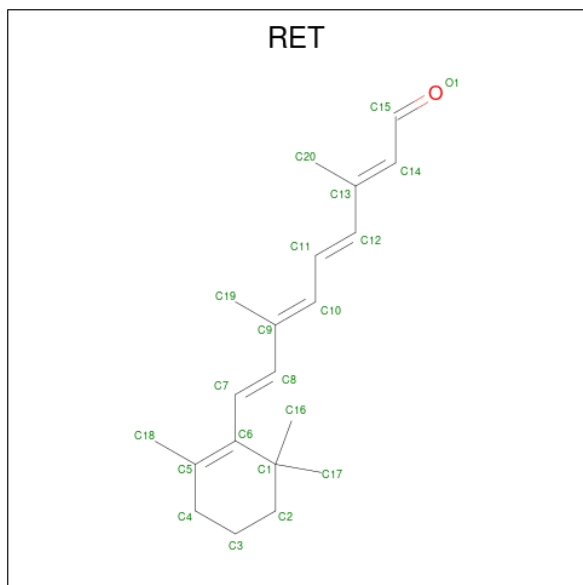


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			70	61	9		
2	B	1	Total	C	O	0	0
			70	61	9		

- Molecule 3 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

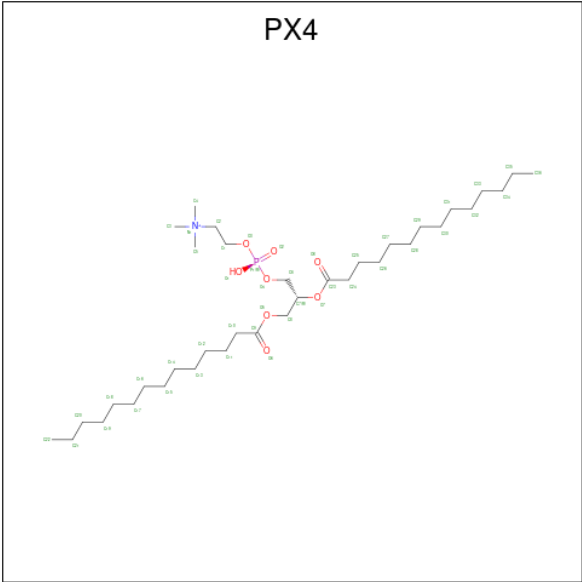
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total C 62 62	0	0
3	B	13	Total C 114 114	0	0

- Molecule 4 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



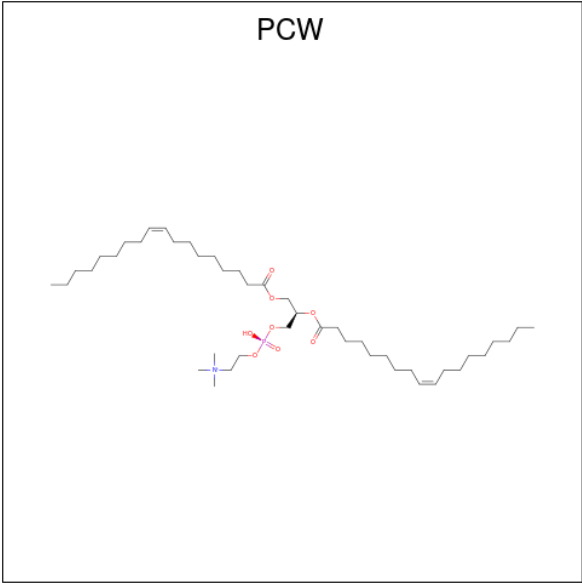
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 20 20	0	0
4	B	1	Total C 20 20	0	0

- Molecule 5 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: $C_{36}H_{73}NO_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
5	B	1	34	25	8	1	0	0

- Molecule 6 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
6	B	1	40	31	8	1	0	0

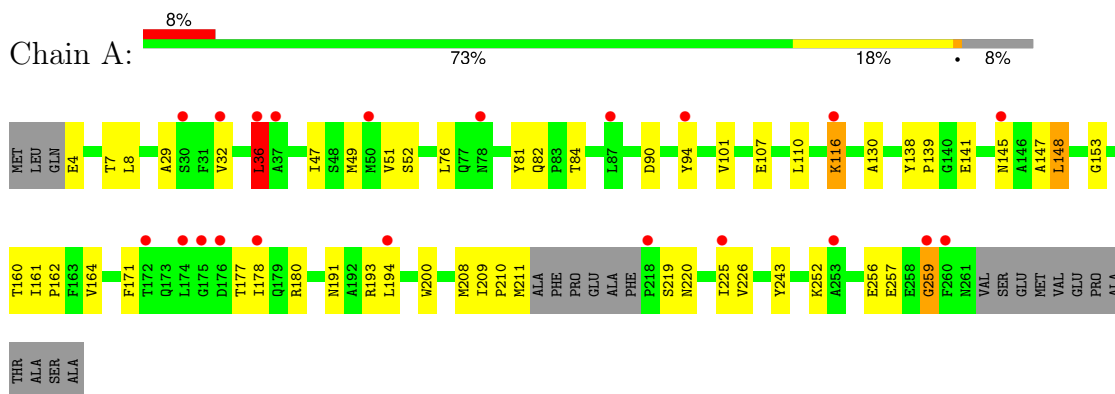
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	34	Total 34	O 34	0	0
7	B	28	Total 28	O 28	0	0

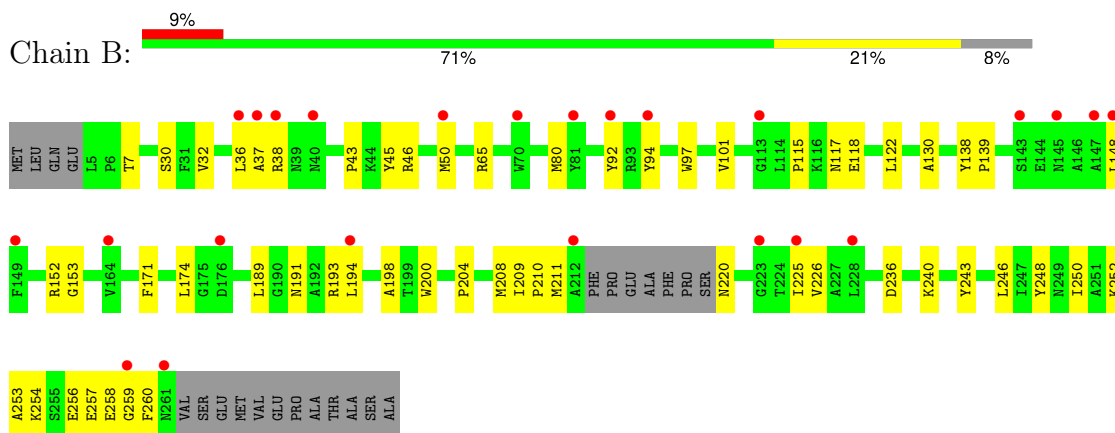
3 Residue-property plots

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: Xanthorhodopsin



• Molecule 1: Xanthorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.74Å 59.49Å 59.72Å 76.35° 74.93° 64.08°	Depositor
Resolution (Å)	45.10 – 1.90 45.10 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.1 (45.10-1.90) 94.0 (45.10-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.265 0.233 , 0.255	Depositor DCC
R_{free} test set	2333 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4417	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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: PX4, PCW, SXN, RET, UNL

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	0.54	0/2024	0.64	1/2761 (0.0%)
1	B	0.55	0/2006	0.62	0/2737
All	All	0.54	0/4030	0.63	1/5498 (0.0%)

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	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	36	LEU	CA-CB-CG	5.89	128.85	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	TYR	Sidechain
1	B	243	TYR	Sidechain

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	1971	0	1996	41	0
1	B	1954	0	1982	35	0
2	A	70	0	92	4	0
2	B	70	0	92	5	0
3	A	62	0	0	0	0
3	B	114	0	0	0	0
4	A	20	0	27	1	0
4	B	20	0	27	1	0
5	B	34	0	44	1	0
6	B	40	0	53	2	0
7	A	34	0	0	1	0
7	B	28	0	0	0	0
All	All	4417	0	4313	80	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 9.

All (80) 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:B:101:VAL:HG12	1:B:130:ALA:HB1	1.41	0.98
1:A:208:MET:HA	1:A:211:MET:HE3	1.50	0.93
1:A:101:VAL:HG12	1:A:130:ALA:HB1	1.49	0.91
1:A:8:LEU:HD21	1:A:225:ILE:HD11	1.68	0.75
1:A:194:LEU:HD21	2:A:1401:SNX:H8'	1.70	0.74
1:B:252:LYS:O	1:B:256:GLU:HG3	1.88	0.72
1:A:194:LEU:HD21	2:A:1401:SNX:H10'	1.74	0.70
1:A:101:VAL:HG13	1:A:200:TRP:CH2	2.30	0.67
1:A:138:TYR:HB3	1:A:139:PRO:HD3	1.76	0.66
1:B:32:VAL:O	1:B:36:LEU:HD13	1.94	0.66
1:B:198:ALA:HB1	2:B:1401:SNX:H31A	1.78	0.66
1:B:115:PRO:HD2	1:B:118:GLU:OE1	1.97	0.65
1:A:116:LYS:NZ	1:A:116:LYS:HB2	2.13	0.64
1:A:94:TYR:OH	1:A:138:TYR:HB2	1.98	0.64
1:B:101:VAL:HG13	1:B:200:TRP:CH2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:TYR:OH	1:B:138:TYR:HB2	2.00	0.62
1:B:38:ARG:O	1:B:46:ARG:HG2	2.00	0.61
1:A:76:LEU:HD13	1:A:81:TYR:CE1	2.35	0.61
1:B:101:VAL:CG1	1:B:130:ALA:HB1	2.24	0.61
1:B:253:ALA:O	1:B:257:GLU:HG3	2.03	0.59
1:A:194:LEU:HD23	1:A:194:LEU:O	2.03	0.58
1:B:236:ASP:O	1:B:240:LYS:HD2	2.02	0.58
1:B:138:TYR:HB3	1:B:139:PRO:HD3	1.86	0.57
1:B:46:ARG:O	1:B:50:MET:HG3	2.07	0.55
1:A:29:ALA:O	1:A:32:VAL:HG22	2.07	0.55
1:B:117:ASN:OD1	1:B:118:GLU:HG3	2.06	0.55
1:B:148:LEU:O	1:B:153:GLY:HA3	2.06	0.55
1:A:101:VAL:CG1	1:A:130:ALA:HB1	2.30	0.55
1:B:148:LEU:C	1:B:148:LEU:HD13	2.28	0.54
1:B:152:ARG:HG2	1:B:211:MET:CE	2.38	0.53
1:A:209:ILE:HB	1:A:210:PRO:HD3	1.89	0.53
1:A:145:ASN:HD21	1:A:147:ALA:HB3	1.75	0.52
1:A:171:PHE:CZ	1:A:193:ARG:HG2	2.46	0.51
1:A:180:ARG:O	1:A:180:ARG:HD2	2.11	0.51
1:A:84:THR:O	1:A:84:THR:HG22	2.10	0.51
1:A:178:ILE:H	1:A:178:ILE:HD12	1.76	0.51
1:B:122:LEU:HD21	1:B:174:LEU:HD11	1.92	0.50
1:B:258:GLU:OE2	1:B:260:PHE:HE2	1.94	0.50
1:A:52:SER:HA	1:A:107:GLU:OE2	2.12	0.50
5:B:1415:PX4:H20	5:B:1415:PX4:H47	1.94	0.50
1:A:145:ASN:HD21	1:A:147:ALA:CB	2.25	0.49
1:A:225:ILE:HG13	1:A:226:VAL:N	2.27	0.49
1:B:208:MET:O	1:B:211:MET:HG2	2.13	0.49
1:B:65:ARG:NH2	1:B:92:TYR:OH	2.47	0.48
1:A:178:ILE:HD12	1:A:178:ILE:N	2.28	0.48
1:B:171:PHE:CZ	1:B:193:ARG:HG2	2.49	0.47
1:B:209:ILE:N	1:B:210:PRO:HD2	2.29	0.47
1:A:252:LYS:O	1:A:256:GLU:HG3	2.15	0.47
1:A:47:ILE:HG23	1:A:110:LEU:HD13	1.96	0.47
1:A:116:LYS:HB2	1:A:116:LYS:HZ3	1.79	0.46
1:B:97:TRP:CD1	4:B:1301:RET:H14	2.49	0.46
1:B:37:ALA:HB1	1:B:248:TYR:CE1	2.51	0.46
1:A:180:ARG:HH21	1:A:180:ARG:HG3	1.82	0.45
1:B:152:ARG:HG2	1:B:211:MET:HE1	1.98	0.45
2:B:1401:SXN:O4'	6:B:1416:PCW:H283	2.17	0.45
1:A:49:MET:HA	1:A:49:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:TYR:OH	1:B:254:LYS:HE3	2.17	0.44
1:B:189:LEU:HD23	1:B:250:ILE:HD13	1.99	0.44
1:A:32:VAL:O	1:A:36:LEU:HB2	2.17	0.44
1:A:148:LEU:O	1:A:153:GLY:HA3	2.18	0.44
1:A:194:LEU:CD2	2:A:1401:SNX:H8'	2.43	0.43
1:A:47:ILE:O	1:A:51:VAL:HG23	2.18	0.43
1:A:7:THR:HB	1:A:82:GLN:OE1	2.18	0.43
2:B:1401:SNX:H7	2:B:1401:SNX:H19	1.79	0.43
1:A:191:ASN:ND2	2:A:1401:SNX:H5'	2.33	0.43
1:B:7:THR:HG22	1:B:80:MET:HE3	1.99	0.43
1:B:200:TRP:O	1:B:204:PRO:HD2	2.18	0.43
1:B:258:GLU:HB2	1:B:260:PHE:CD2	2.53	0.43
1:A:145:ASN:ND2	1:A:147:ALA:HB3	2.34	0.42
1:A:160:THR:O	1:A:164:VAL:HG13	2.20	0.42
1:B:246:LEU:CD2	6:B:1416:PCW:H261	2.49	0.42
1:A:180:ARG:HG3	1:A:180:ARG:NH2	2.35	0.41
1:A:194:LEU:HD23	1:A:194:LEU:C	2.41	0.41
4:A:1301:RET:H181	4:A:1301:RET:H7	1.78	0.41
1:B:191:ASN:ND2	2:B:1401:SNX:H5'	2.36	0.41
1:A:257:GLU:C	1:A:259:GLY:H	2.23	0.41
1:A:7:THR:HG22	7:A:430:HOH:O	2.21	0.41
1:A:161:ILE:HB	1:A:162:PRO:CD	2.51	0.41
1:B:194:LEU:CD2	2:B:1401:SNX:H6'	2.52	0.40
1:B:225:ILE:HG23	1:B:226:VAL:N	2.35	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	248/273 (91%)	237 (96%)	9 (4%)	2 (1%)	16 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	246/273 (90%)	241 (98%)	4 (2%)	1 (0%)	30	22
All	All	494/546 (90%)	478 (97%)	13 (3%)	3 (1%)	22	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	SER
1	A	259	GLY
1	B	259	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/223 (93%)	199 (96%)	8 (4%)	27	20
1	B	204/223 (92%)	201 (98%)	3 (2%)	60	59
All	All	411/446 (92%)	400 (97%)	11 (3%)	40	34

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	36	LEU
1	A	90	ASP
1	A	116	LYS
1	A	141	GLU
1	A	148	LEU
1	A	177	THR
1	A	220	ASN
1	B	30	SER
1	B	43	PRO
1	B	220	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	77	GLN
1	A	145	ASN
1	A	220	ASN
1	B	39	ASN
1	B	77	GLN

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](#)

Of 27 ligands modelled in this entry, 21 are unknown - leaving 6 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	$\# Z > 2$
4	RET	A	1301	1	20,20,21	2.19	6 (30%)	27,27,28	2.30	10 (37%)
2	SXN	A	1401	-	69,71,71	2.12	17 (24%)	85,94,94	1.47	14 (16%)
6	PCW	B	1416	-	39,39,53	1.46	4 (10%)	42,44,61	1.27	5 (11%)
5	PX4	B	1415	-	33,33,45	1.42	3 (9%)	36,38,53	1.21	2 (5%)
2	SXN	B	1401	-	69,71,71	2.11	16 (23%)	85,94,94	1.44	13 (15%)
4	RET	B	1301	1	20,20,21	1.92	5 (25%)	27,27,28	2.44	13 (48%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	RET	A	1301	1	-	0/13/30/31	0/1/1/1
2	SXN	A	1401	-	-	20/65/105/105	0/2/2/2
6	PCW	B	1416	-	1/1/4/9	21/41/41/57	-
5	PX4	B	1415	-	1/1/4/5	16/35/35/49	-
2	SXN	B	1401	-	-	24/65/105/105	0/2/2/2
4	RET	B	1301	1	-	0/13/30/31	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	SXN	C2'-C3'	7.63	1.59	1.50
2	B	1401	SXN	C2'-C3'	7.33	1.58	1.50
4	A	1301	RET	C14-C13	5.79	1.37	1.33
2	A	1401	SXN	O6'-C22	5.53	1.49	1.33
2	B	1401	SXN	O6'-C22	5.35	1.48	1.33
2	B	1401	SXN	C1-C6	5.14	1.60	1.53
2	B	1401	SXN	C6-C5	5.12	1.42	1.35
2	A	1401	SXN	C6-C5	5.11	1.42	1.35
5	B	1415	PX4	O5-C9	4.98	1.47	1.33
6	B	1416	PCW	O2-C31	4.88	1.48	1.34
6	B	1416	PCW	O3-C11	4.76	1.47	1.33
5	B	1415	PX4	O7-C23	4.71	1.47	1.34
4	B	1301	RET	C1-C6	4.65	1.59	1.53
2	A	1401	SXN	C4'-C3'	4.23	1.41	1.32
2	B	1401	SXN	C4-C5	-4.11	1.39	1.47
2	A	1401	SXN	C4-C5	-3.93	1.39	1.47
4	A	1301	RET	C1-C6	3.89	1.58	1.53
6	B	1416	PCW	C20-C19	3.87	1.53	1.31
2	A	1401	SXN	C10'-C9'	3.85	1.44	1.35
5	B	1415	PX4	P1-O2	3.79	1.62	1.50
2	B	1401	SXN	C4'-C3'	3.78	1.40	1.32
2	A	1401	SXN	C1-C6	3.76	1.58	1.53
2	B	1401	SXN	C14'-C13'	3.74	1.44	1.35
6	B	1416	PCW	C40-C39	3.70	1.53	1.29
2	A	1401	SXN	C6'-C5'	3.68	1.44	1.35
4	A	1301	RET	C17-C1	3.66	1.60	1.53
2	B	1401	SXN	C10'-C9'	3.60	1.44	1.35
4	B	1301	RET	C17-C1	3.59	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1401	SXN	C6'-C5'	3.53	1.44	1.35
2	A	1401	SXN	C14'-C13'	3.47	1.43	1.35
2	B	1401	SXN	C14-C13	3.15	1.43	1.35
2	A	1401	SXN	C14-C13	3.13	1.43	1.35
2	A	1401	SXN	C7'-C8'	3.04	1.42	1.34
2	A	1401	SXN	C11'-C12'	3.01	1.42	1.34
2	B	1401	SXN	C11'-C12'	2.94	1.42	1.34
4	B	1301	RET	C14-C13	2.94	1.35	1.33
2	B	1401	SXN	C10-C9	2.82	1.42	1.35
2	A	1401	SXN	C10-C9	2.80	1.42	1.35
2	B	1401	SXN	C7-C8	2.77	1.41	1.33
2	A	1401	SXN	C7-C8	2.77	1.41	1.33
2	B	1401	SXN	C7'-C8'	2.74	1.41	1.34
4	A	1301	RET	C16-C1	2.70	1.58	1.53
4	B	1301	RET	C16-C1	2.61	1.58	1.53
4	A	1301	RET	C5-C6	2.60	1.38	1.34
2	A	1401	SXN	C11-C12	2.36	1.40	1.34
2	B	1401	SXN	C11-C12	2.30	1.40	1.34
2	A	1401	SXN	O1'-C1'A	2.29	1.50	1.40
4	A	1301	RET	C11-C12	2.23	1.40	1.34
4	B	1301	RET	C5-C6	2.19	1.38	1.34
2	B	1401	SXN	O1'-C1'A	2.18	1.49	1.40
2	A	1401	SXN	O5'-C1'A	2.10	1.47	1.41

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1301	RET	C11-C10-C9	-5.69	119.31	127.28
4	B	1301	RET	C18-C5-C6	5.41	130.38	124.48
4	A	1301	RET	C18-C5-C6	4.88	129.81	124.48
4	A	1301	RET	C11-C10-C9	-4.84	120.49	127.28
2	A	1401	SXN	C11-C10-C9	-4.24	121.34	127.28
4	A	1301	RET	C8-C9-C10	-3.85	112.95	119.01
2	B	1401	SXN	C11-C10-C9	-3.77	122.00	127.28
2	A	1401	SXN	C7-C8-C9	-3.75	120.69	126.23
4	A	1301	RET	C7-C6-C5	-3.74	112.94	121.56
5	B	1415	PX4	O7-C23-C24	3.71	119.51	111.48
4	B	1301	RET	C8-C9-C10	-3.70	113.18	119.01
6	B	1416	PCW	O2-C31-C32	3.64	119.36	111.48
2	B	1401	SXN	C7-C8-C9	-3.61	120.90	126.23
2	A	1401	SXN	C1'A-O5'-C5'A	3.58	120.70	113.72
4	B	1301	RET	C7-C6-C5	-3.53	113.42	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1401	SXN	C3-C4-C5	3.44	121.74	118.64
2	B	1401	SXN	C1'A-O5'-C5'A	3.38	120.33	113.72
4	A	1301	RET	C1-C6-C7	3.32	124.65	115.65
2	A	1401	SXN	C15-C14-C13	-3.29	122.67	127.28
4	B	1301	RET	C1-C6-C7	3.19	124.30	115.65
2	A	1401	SXN	C3-C4-C5	3.11	121.44	118.64
2	B	1401	SXN	C15-C14-C13	-3.03	123.03	127.28
2	A	1401	SXN	C15'-C14'-C13'	-2.99	123.08	127.28
4	B	1301	RET	C20-C13-C12	2.96	122.61	118.09
2	B	1401	SXN	C15'-C14'-C13'	-2.93	123.17	127.28
4	A	1301	RET	C10-C11-C12	-2.83	115.00	123.20
4	A	1301	RET	C20-C13-C12	2.80	122.36	118.09
4	B	1301	RET	C10-C11-C12	-2.72	115.32	123.20
2	A	1401	SXN	O6'-C22-C23	2.69	120.03	111.83
5	B	1415	PX4	O5-C9-C10	2.68	120.02	111.83
2	B	1401	SXN	O6'-C22-C23	2.65	119.93	111.83
6	B	1416	PCW	O3-C11-C12	2.64	119.90	111.83
4	B	1301	RET	C12-C13-C14	-2.55	111.77	118.55
4	B	1301	RET	C19-C9-C8	2.50	121.90	118.09
4	B	1301	RET	C17-C1-C6	2.48	114.14	110.24
4	A	1301	RET	C12-C13-C14	-2.41	112.15	118.55
2	B	1401	SXN	C18'-C5'-C4'	2.39	121.74	118.09
2	B	1401	SXN	C19'-C9'-C8'	2.39	121.74	118.09
6	B	1416	PCW	C38-C39-C40	-2.38	109.31	126.65
2	A	1401	SXN	C19'-C9'-C8'	2.34	121.67	118.09
4	A	1301	RET	C19-C9-C8	2.32	121.62	118.09
2	A	1401	SXN	C18-C5-C6	-2.30	120.42	124.11
2	A	1401	SXN	C6'-C7'-C8'	-2.28	116.60	123.20
2	B	1401	SXN	C18-C5-C6	-2.27	120.46	124.11
2	B	1401	SXN	C6'-C7'-C8'	-2.26	116.64	123.20
2	A	1401	SXN	C18'-C5'-C4'	2.22	121.48	118.09
4	A	1301	RET	C17-C1-C6	2.18	113.67	110.24
6	B	1416	PCW	C2-O2-C31	2.15	122.94	117.80
2	A	1401	SXN	C15-C15'-C14'	-2.13	119.16	123.52
4	B	1301	RET	C11-C12-C13	-2.12	120.55	126.36
2	B	1401	SXN	O21-C4-C3	-2.12	117.40	120.87
2	B	1401	SXN	C10'-C11'-C12'	-2.10	117.10	123.20
2	A	1401	SXN	O5'-C5'A-C6'A	2.09	110.84	106.69
4	B	1301	RET	C2-C1-C6	2.07	113.45	110.44
6	B	1416	PCW	C18-C19-C20	-2.06	109.39	124.83
4	B	1301	RET	C18-C5-C4	-2.05	109.23	113.60
2	A	1401	SXN	C11'-C10'-C9'	-2.04	124.42	127.28

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1415	PX4	C7
6	B	1416	PCW	C2

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	SXN	O1'-C1'-C2'-O36
2	A	1401	SXN	O1'-C1'-C2'-C3'
2	A	1401	SXN	C17'-C1'-C2'-O36
2	A	1401	SXN	C17'-C1'-C2'-C3'
2	A	1401	SXN	C16'-C1'-C2'-O36
2	A	1401	SXN	C16'-C1'-C2'-C3'
2	A	1401	SXN	O36-C2'-C3'-C4'
2	B	1401	SXN	O1'-C1'-C2'-O36
2	B	1401	SXN	O1'-C1'-C2'-C3'
2	B	1401	SXN	C17'-C1'-C2'-O36
2	B	1401	SXN	C17'-C1'-C2'-C3'
2	B	1401	SXN	C16'-C1'-C2'-O36
2	B	1401	SXN	C16'-C1'-C2'-C3'
2	B	1401	SXN	O36-C2'-C3'-C4'
5	B	1415	PX4	O7-C7-C8-O5
5	B	1415	PX4	C24-C23-O7-C7
5	B	1415	PX4	O8-C23-O7-C7
2	A	1401	SXN	O5'-C5'A-C6'A-O6'
5	B	1415	PX4	C10-C9-O5-C8
2	B	1401	SXN	O5'-C5'A-C6'A-O6'
2	B	1401	SXN	C4'A-C5'A-C6'A-O6'
5	B	1415	PX4	O6-C9-O5-C8
2	A	1401	SXN	C4'A-C5'A-C6'A-O6'
6	B	1416	PCW	C11-C12-C13-C14
2	B	1401	SXN	C31-C32-C33-C34
2	B	1401	SXN	C32-C33-C34-C35
5	B	1415	PX4	C9-C10-C11-C12
2	A	1401	SXN	C32-C33-C34-C38
2	A	1401	SXN	C32-C33-C34-C35
2	B	1401	SXN	C32-C33-C34-C38
2	B	1401	SXN	C28-C29-C30-C31
2	A	1401	SXN	C29-C30-C31-C32
5	B	1415	PX4	C32-C33-C34-C35
2	B	1401	SXN	C22-C23-C24-C25
2	A	1401	SXN	C28-C29-C30-C31
6	B	1416	PCW	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
6	B	1416	PCW	C18-C19-C20-C21
2	A	1401	SXN	C24-C25-C26-C27
6	B	1416	PCW	C22-C23-C24-C25
2	B	1401	SXN	C23-C24-C25-C26
2	A	1401	SXN	C31-C32-C33-C34
5	B	1415	PX4	C23-C24-C25-C26
6	B	1416	PCW	C31-C32-C33-C34
6	B	1416	PCW	O2-C2-C3-O3
2	B	1401	SXN	C29-C30-C31-C32
5	B	1415	PX4	C28-C29-C30-C31
2	B	1401	SXN	C26-C27-C28-C29
6	B	1416	PCW	C32-C33-C34-C35
5	B	1415	PX4	C6-C7-C8-O5
6	B	1416	PCW	C1-C2-C3-O3
5	B	1415	PX4	C30-C31-C32-C33
2	A	1401	SXN	C22-C23-C24-C25
2	A	1401	SXN	C23-C24-C25-C26
6	B	1416	PCW	C23-C24-C25-C26
2	B	1401	SXN	C24-C25-C26-C27
5	B	1415	PX4	C25-C26-C27-C28
5	B	1415	PX4	C33-C34-C35-C36
6	B	1416	PCW	C36-C37-C38-C39
5	B	1415	PX4	C31-C32-C33-C34
2	B	1401	SXN	C1'-C2'-C3'-C4'
6	B	1416	PCW	C12-C11-O3-C3
6	B	1416	PCW	C15-C16-C17-C18
2	A	1401	SXN	C26-C27-C28-C29
6	B	1416	PCW	O11-C11-O3-C3
5	B	1415	PX4	C27-C28-C29-C30
6	B	1416	PCW	C33-C34-C35-C36
6	B	1416	PCW	C13-C14-C15-C16
2	B	1401	SXN	C30-C31-C32-C33
2	B	1401	SXN	C27-C28-C29-C30
6	B	1416	PCW	C14-C15-C16-C17
6	B	1416	PCW	C24-C25-C26-C27
2	A	1401	SXN	C5-C6-C7-C8
2	B	1401	SXN	C5-C6-C7-C8
6	B	1416	PCW	O2-C31-C32-C33
5	B	1415	PX4	O4-C6-C7-O7
6	B	1416	PCW	C34-C35-C36-C37
6	B	1416	PCW	O31-C31-C32-C33
2	A	1401	SXN	C30-C31-C32-C33

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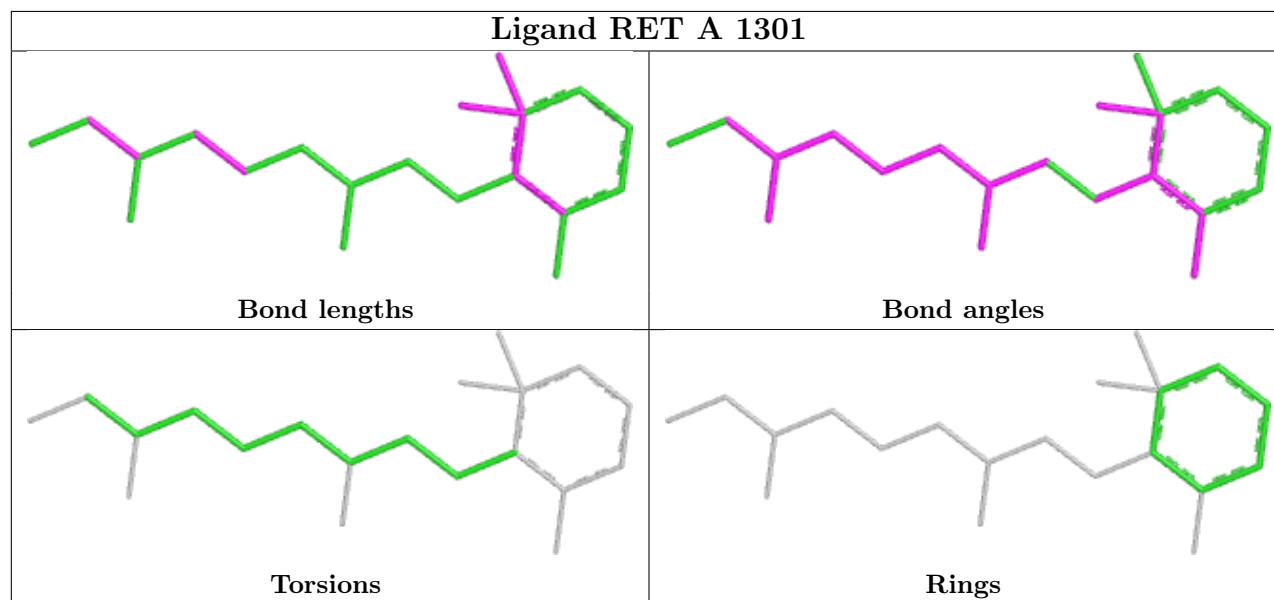
Mol	Chain	Res	Type	Atoms
2	B	1401	SXN	O6'-C22-C23-C24
6	B	1416	PCW	O3-C11-C12-C13
2	B	1401	SXN	O37-C22-C23-C24

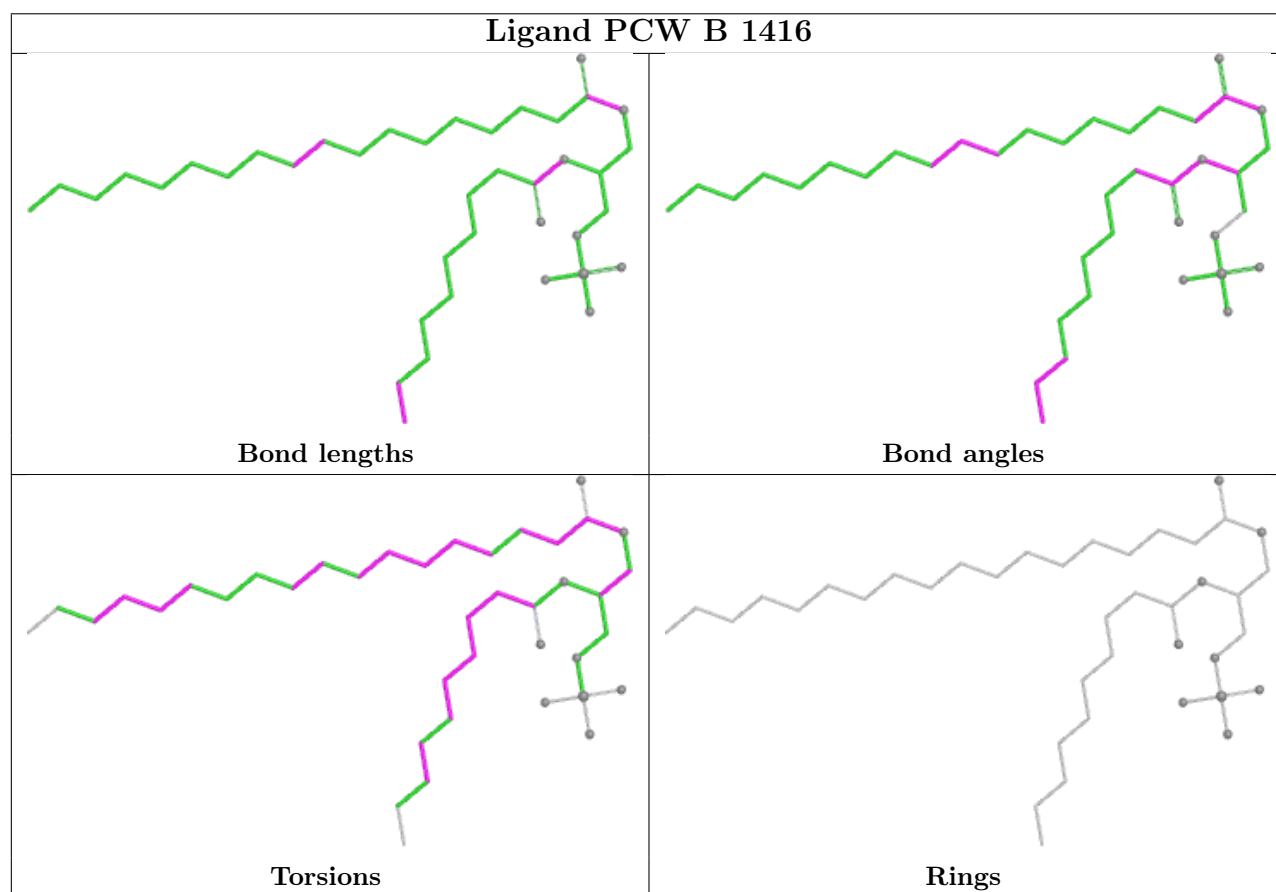
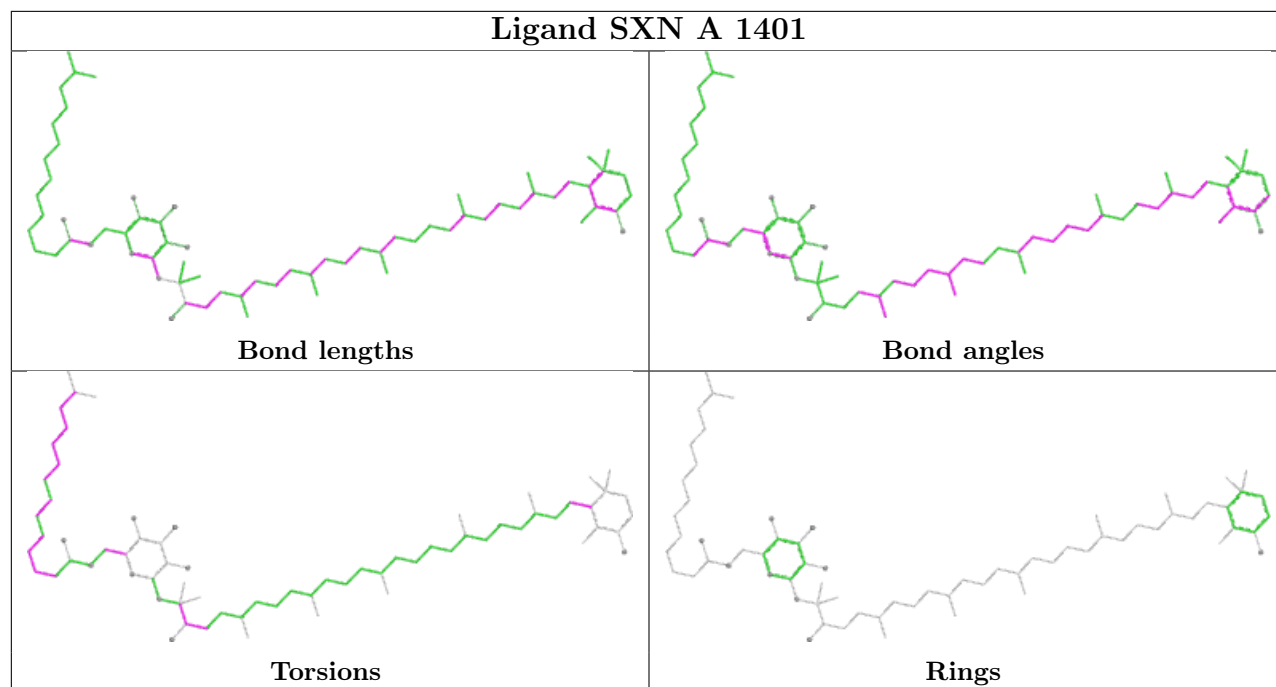
There are no ring outliers.

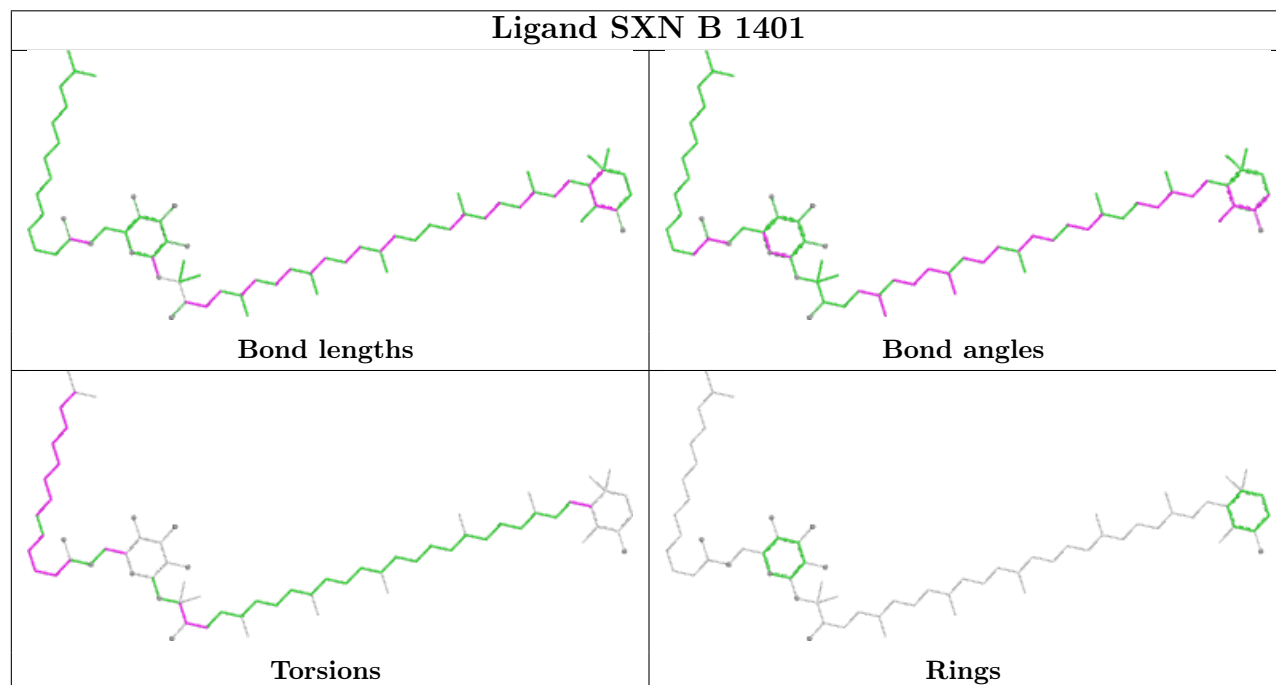
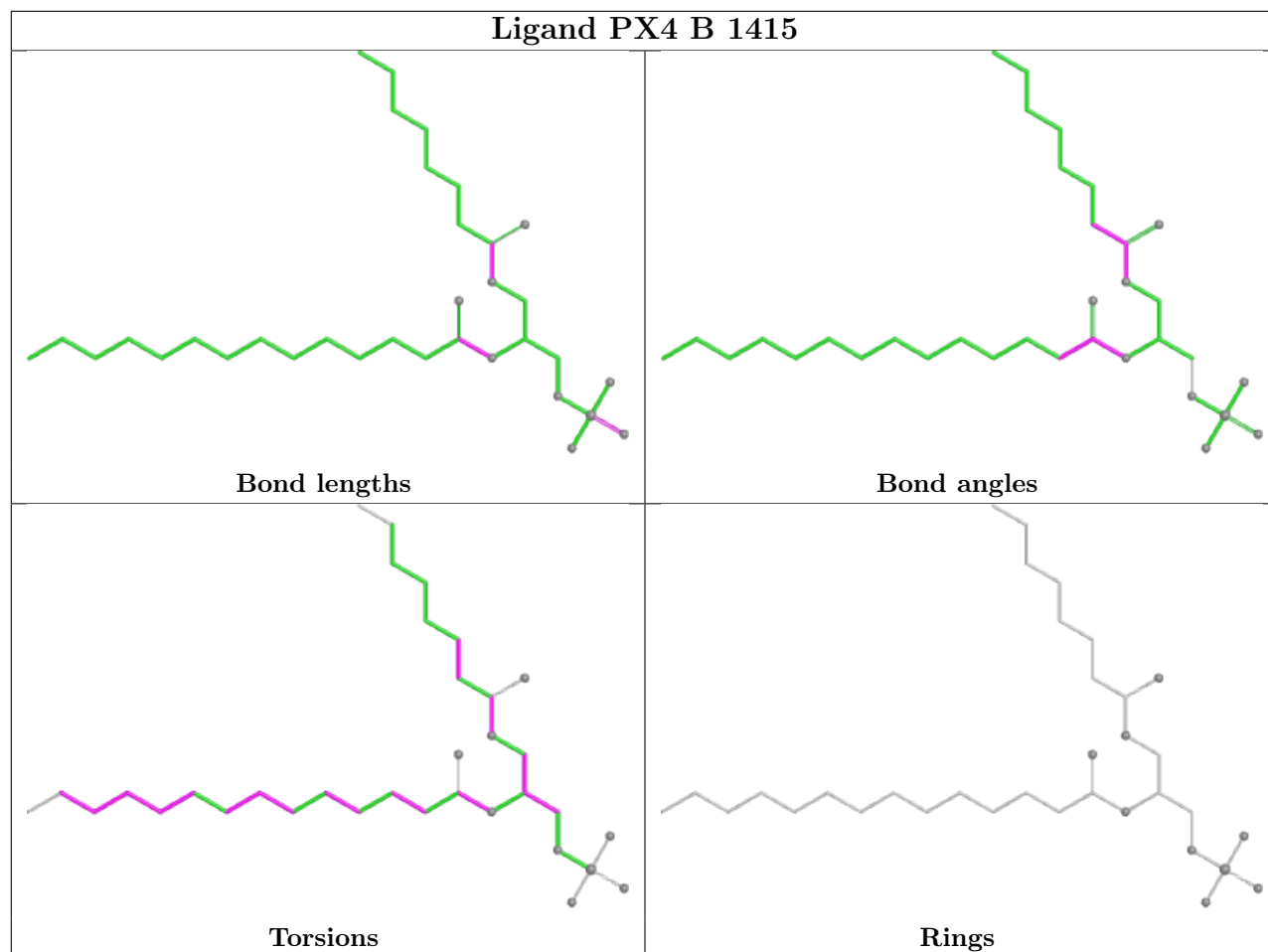
6 monomers are involved in 13 short contacts:

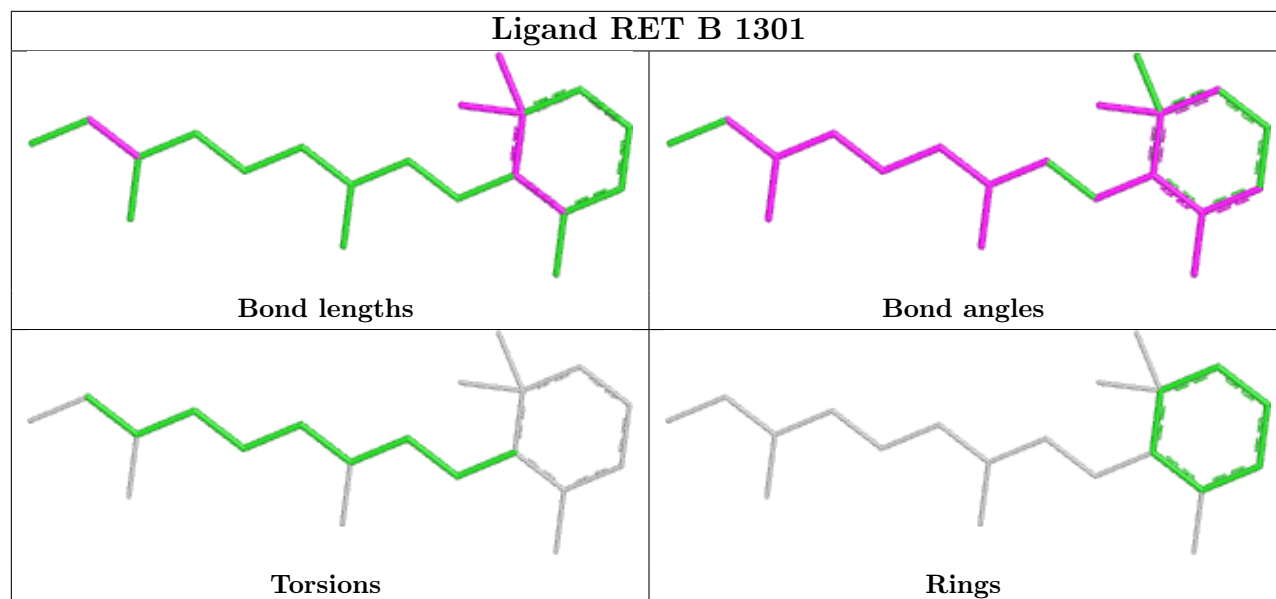
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	RET	1	0
2	A	1401	SXN	4	0
6	B	1416	PCW	2	0
5	B	1415	PX4	1	0
2	B	1401	SXN	5	0
4	B	1301	RET	1	0

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 than 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

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, 95th 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	252/273 (92%)	0.79	21 (8%) 19 20	28, 41, 68, 76	0
1	B	250/273 (91%)	0.72	24 (9%) 15 15	29, 40, 63, 76	0
All	All	502/546 (91%)	0.75	45 (8%) 17 17	28, 40, 65, 76	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	TYR	5.2
1	A	225	ILE	4.8
1	B	259	GLY	4.6
1	B	94	TYR	4.6
1	B	145	ASN	4.4
1	B	223	GLY	3.7
1	A	253	ALA	3.5
1	A	37	ALA	3.5
1	B	149	PHE	3.5
1	A	145	ASN	3.4
1	A	30	SER	3.2
1	A	174	LEU	3.2
1	B	92	TYR	3.2
1	B	212	ALA	3.2
1	A	78	ASN	3.1
1	A	36	LEU	3.0
1	B	36	LEU	2.8
1	B	148	LEU	2.8
1	A	176	ASP	2.7
1	A	260	PHE	2.6
1	B	228	LEU	2.6
1	A	194	LEU	2.6
1	B	147	ALA	2.6
1	A	32	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	225	ILE	2.6
1	B	70	TRP	2.5
1	B	38	ARG	2.4
1	A	218	PRO	2.4
1	A	172	THR	2.4
1	A	259	GLY	2.4
1	B	40	ASN	2.3
1	A	87	LEU	2.3
1	A	175	GLY	2.2
1	A	116	LYS	2.2
1	B	143	SER	2.2
1	B	50	MET	2.2
1	B	261	ASN	2.2
1	B	81	TYR	2.2
1	B	37	ALA	2.1
1	A	50	MET	2.1
1	B	164	VAL	2.1
1	A	178	ILE	2.1
1	B	113	GLY	2.0
1	B	176	ASP	2.0
1	B	194	LEU	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, 95th 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(\AA^2)	Q<0.9
3	UNL	A	1404	9/-	0.63	0.20	74,74,75,76	0
6	PCW	B	1416	40/54	0.70	0.14	56,77,91,92	0

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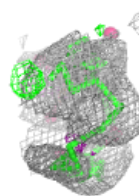
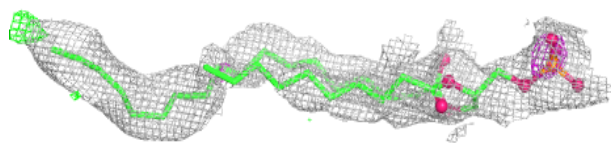
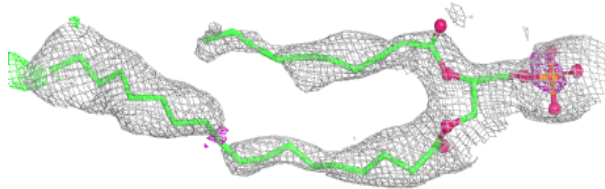
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UNL	A	1408	7/-	0.71	0.15	62,62,64,65	0
3	UNL	B	1414	8/-	0.74	0.24	63,65,67,69	0
3	UNL	B	1409	7/-	0.74	0.19	68,68,69,70	0
3	UNL	B	1405	7/-	0.76	0.20	66,67,69,69	0
2	SXN	A	1401	70/70	0.76	0.17	53,79,92,94	0
3	UNL	A	1407	7/-	0.77	0.17	65,66,66,66	0
3	UNL	A	1406	12/-	0.77	0.13	65,67,68,68	0
3	UNL	B	1411	6/-	0.78	0.20	54,56,60,60	0
3	UNL	B	1404	7/-	0.79	0.19	66,69,74,74	0
3	UNL	A	1405	7/-	0.79	0.25	67,68,68,69	0
5	PX4	B	1415	34/46	0.80	0.17	57,70,81,83	0
2	SXN	B	1401	70/70	0.81	0.15	43,76,90,91	0
3	UNL	B	1407	8/-	0.82	0.12	71,72,73,73	0
3	UNL	A	1403	7/-	0.82	0.14	54,58,60,60	0
3	UNL	B	1412	11/-	0.83	0.19	63,65,67,68	0
3	UNL	B	1408	7/-	0.84	0.25	73,73,74,75	0
3	UNL	B	1413	7/-	0.85	0.19	71,73,74,76	0
3	UNL	B	1410	8/-	0.85	0.14	61,62,63,63	0
3	UNL	B	1406	12/-	0.85	0.16	70,72,74,75	0
3	UNL	B	1403	16/-	0.85	0.16	47,50,52,53	0
3	UNL	A	1402	7/-	0.87	0.17	53,53,55,57	0
3	UNL	A	1409	6/-	0.87	0.21	57,57,58,59	0
3	UNL	B	1402	10/-	0.91	0.15	51,54,57,58	0
4	RET	A	1301	20/21	0.92	0.09	29,33,36,37	0
4	RET	B	1301	20/21	0.93	0.08	30,32,35,35	0

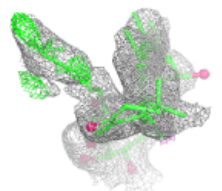
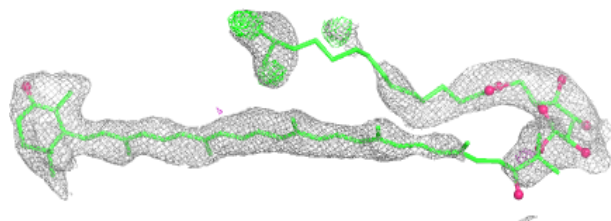
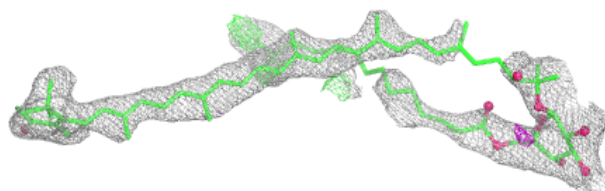
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PCW B 1416:

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

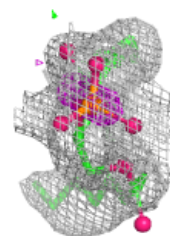
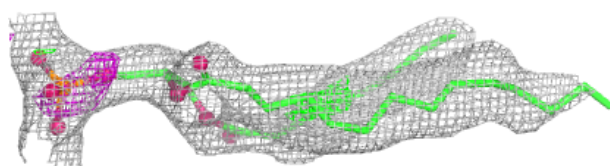
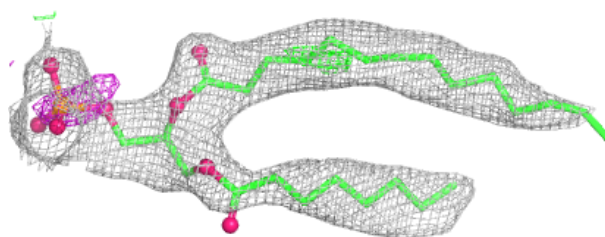
**Electron density around SXN A 1401:**

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

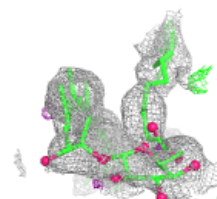
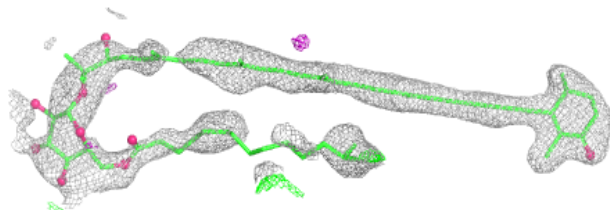
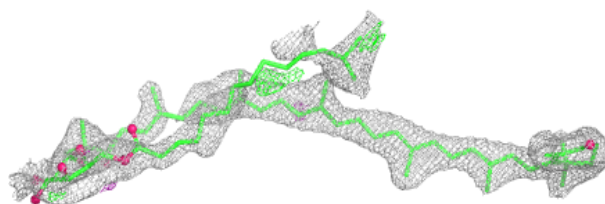


Electron density around PX4 B 1415:

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

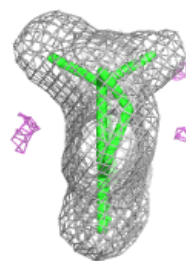
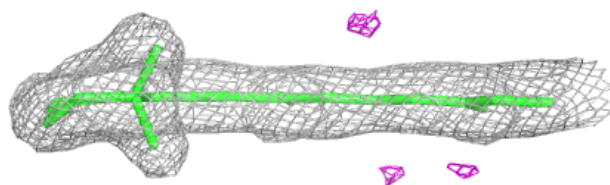
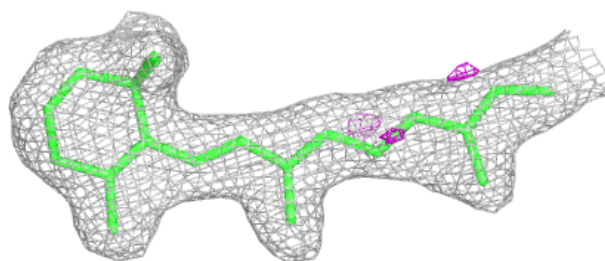
**Electron density around SXN B 1401:**

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

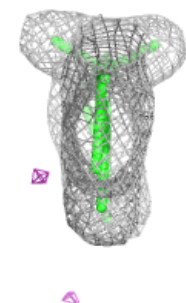
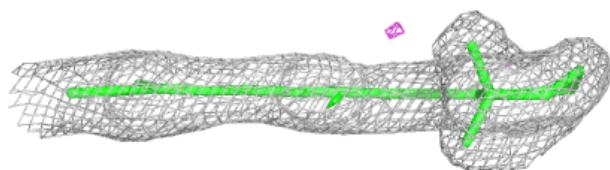
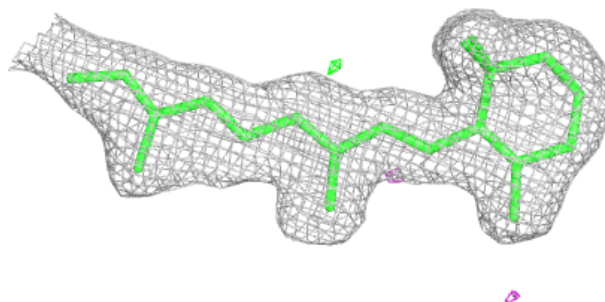


Electron density around RET A 1301:

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

**Electron density around RET B 1301:**

$2mF_o-DF_c$ (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.