Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 10:59 PM EDT

PDB ID	:	2VWA
Title	:	Crystal structure of a sporozoite protein essential for liver stage development of malaria parasite
Authors	:	Sharma, A.; Sharma, A.; Yogavel, M.; Gill, J.; Akhouri, R.R.
Deposited on	:	2008-06-20
Resolution	:	2.50 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:

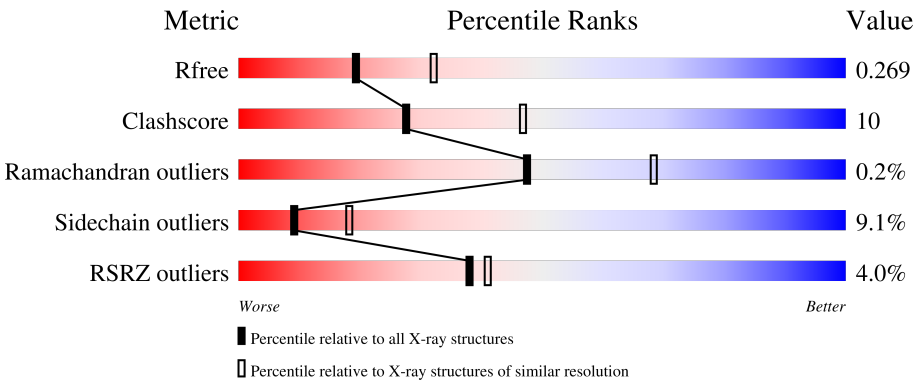
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	101	4% 68% 27%
1	B	101	3% 68% 27%
1	C	101	5% 74% 21%
1	D	101	3% 85% 14%
1	E	101	4% 65% 29%

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Mol	Chain	Length	Quality of chain
1	F	101	4% 81% 15%

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
2	PTY	A	1230	-	-	-	X
2	PTY	B	1230	-	-	-	X
2	PTY	D	1230	-	-	-	X
2	PTY	E	1230	-	-	-	X

2 Entry composition (i)

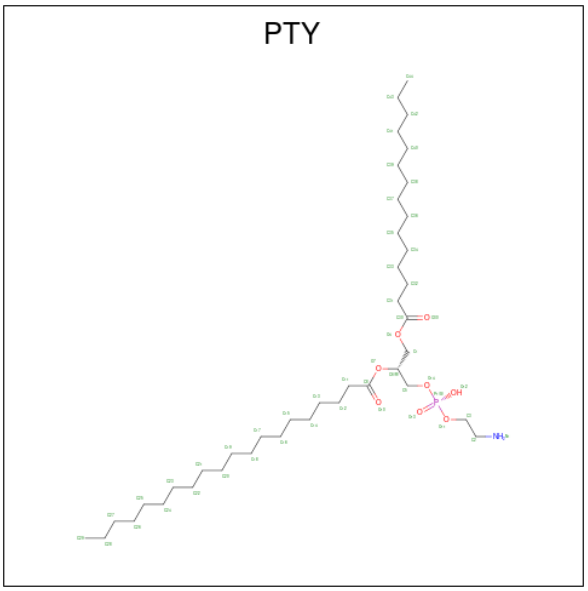
There are 3 unique types of molecules in this entry. The entry contains 5439 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PUTATIVE UNCHARACTERIZED PROTEIN PF13_0012.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	100	834	521	151	159	3	0	0	1
1	B	100	834	521	151	159	3	0	0	1
1	C	100	834	521	151	159	3	0	0	1
1	D	100	834	521	151	159	3	0	0	1
1	E	100	834	521	151	159	3	0	0	1
1	F	100	834	521	151	159	3	0	0	1

- Molecule 2 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	50	40	1	8	1	0	0
2	B	1	50	40	1	8	1	0	0
2	C	1	50	40	1	8	1	0	0
2	D	1	50	40	1	8	1	0	0
2	E	1	50	40	1	8	1	0	0
2	F	1	50	40	1	8	1	0	0

- Molecule 3 is water.

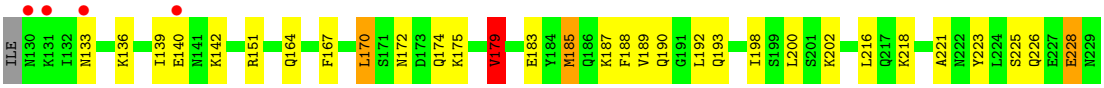
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	25	25	25	0	0
3	B	29	29	29	0	0
3	C	29	29	29	0	0
3	D	19	19	19	0	0
3	E	15	15	15	0	0
3	F	18	18	18	0	0

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.

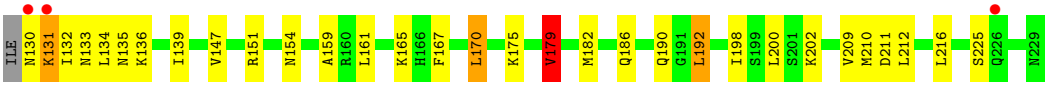
• Molecule 1: PUTATIVE UNCHARACTERIZED PROTEIN PF13_0012

Chain A:



• Molecule 1: PUTATIVE UNCHARACTERIZED PROTEIN PF13_0012

Chain B:

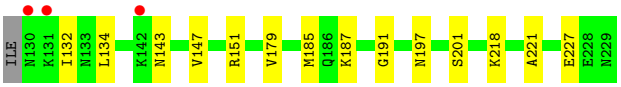


• Molecule 1: PUTATIVE UNCHARACTERIZED PROTEIN PF13_0012

Chain C:

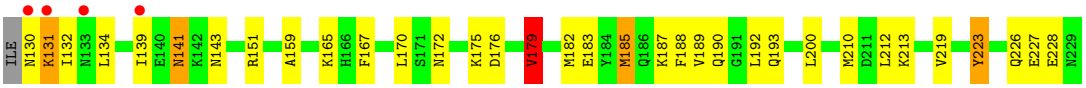
• Molecule 1: PUTATIVE UNCHARACTERIZED PROTEIN PF13_0012

Chain D:



• Molecule 1: PUTATIVE UNCHARACTERIZED PROTEIN PF13_0012

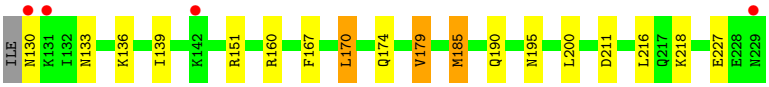
Chain E:



• Molecule 1: PUTATIVE UNCHARACTERIZED PROTEIN PF13_0012

Chain F:

4%
81%
15%


ILE
N130
K131
I132
N133
K136
I139
K142
R151
R160
F167
L170
Q174
V179
M185
Q190
N195
L200
D211
L216
Q217
K218
E227
E228
N229

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.54Å 38.27Å 145.70Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.00-2.50) 99.4 (24.33-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.19 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.271 0.218 , 0.269	Depositor DCC
R_{free} test set	1619 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5439	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.0522e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: PTY

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	0.71	1/844 (0.1%)	0.72	1/1128 (0.1%)
1	B	0.66	0/844	0.78	2/1128 (0.2%)
1	C	0.68	0/844	0.72	0/1128
1	D	0.70	0/844	0.71	0/1128
1	E	0.73	0/844	0.77	1/1128 (0.1%)
1	F	0.68	0/844	0.75	1/1128 (0.1%)
All	All	0.70	1/5064 (0.0%)	0.74	5/6768 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	GLU	C-N	-5.06	1.22	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	179	VAL	CB-CA-C	-6.92	98.25	111.40
1	A	179	VAL	CB-CA-C	-6.01	99.98	111.40
1	B	179	VAL	CB-CA-C	-5.50	100.96	111.40
1	E	179	VAL	CB-CA-C	-5.38	101.17	111.40
1	B	192	LEU	CA-CB-CG	5.21	127.30	115.30

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	834	0	821	23	0
1	B	834	0	821	17	0
1	C	834	0	821	21	0
1	D	834	0	821	6	0
1	E	834	0	821	20	0
1	F	834	0	821	13	0
2	A	50	0	79	5	0
2	B	50	0	79	1	0
2	C	50	0	79	8	0
2	D	50	0	79	1	0
2	E	50	0	79	3	0
2	F	50	0	79	6	0
3	A	25	0	0	2	0
3	B	29	0	0	1	0
3	C	29	0	0	2	0
3	D	19	0	0	1	0
3	E	15	0	0	0	0
3	F	18	0	0	1	0
All	All	5439	0	5400	107	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 10.

All (107) 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:C:130:ASN:HA	1:C:195:ASN:HD21	1.40	0.86
1:A:140:GLU:OE2	1:A:142:LYS:HE3	1.81	0.80
1:C:211:ASP:HA	2:C:1230:PTY:H271	1.66	0.77
1:C:222:ASN:HB2	3:C:2027:HOH:O	1.84	0.76
1:C:139:ILE:H	1:C:190:GLN:HE22	1.34	0.75
1:A:226:GLN:HA	1:A:226:GLN:OE1	1.84	0.75
1:F:167:PHE:HA	1:F:170:LEU:HD22	1.68	0.75
1:E:167:PHE:CZ	1:E:175:LYS:HB2	2.22	0.74
1:A:221:ALA:HB2	1:B:154:ASN:HD21	1.53	0.74
1:A:139:ILE:H	1:A:190:GLN:HE22	1.36	0.73
2:A:1230:PTY:H262	1:B:165:LYS:HE2	1.72	0.71
1:B:211:ASP:HA	2:B:1230:PTY:H271	1.73	0.71
1:A:172:ASN:ND2	1:A:223:TYR:OH	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LYS:HE2	1:B:132:ILE:O	1.93	0.69
1:E:183:GLU:O	1:E:187:LYS:HG2	1.94	0.68
1:B:139:ILE:H	1:B:190:GLN:HE22	1.41	0.68
1:C:167:PHE:HA	1:C:170:LEU:HD22	1.78	0.66
1:C:151:ARG:NH1	3:C:2005:HOH:O	2.29	0.64
1:A:167:PHE:CZ	1:A:175:LYS:HB2	2.34	0.63
1:E:141:ASN:HD21	1:E:143:ASN:HB3	1.64	0.63
1:C:154:ASN:HD21	1:D:221:ALA:HB2	1.64	0.62
1:D:143:ASN:HB3	1:D:201:SER:HA	1.82	0.61
1:E:185:MSE:CE	1:E:213:LYS:HB2	2.30	0.61
1:A:170:LEU:HG	1:A:174:GLN:HB3	1.83	0.60
1:B:159:ALA:HA	1:B:192:LEU:HD21	1.84	0.60
1:E:132:ILE:CG2	1:E:134:LEU:CD2	2.79	0.59
1:C:130:ASN:O	1:C:130:ASN:ND2	2.29	0.59
1:E:185:MSE:HE1	1:E:213:LYS:HB2	1.85	0.58
1:E:132:ILE:CG2	1:E:134:LEU:HD23	2.33	0.58
1:F:218:LYS:HE2	2:F:1230:PTY:C14	2.34	0.57
1:A:133:ASN:HD22	1:A:136:LYS:HG3	1.69	0.56
1:E:175:LYS:O	1:E:179:VAL:HG22	2.06	0.55
1:F:139:ILE:H	1:F:190:GLN:HE22	1.54	0.55
1:A:151:ARG:NH1	3:A:2005:HOH:O	2.39	0.55
1:B:182:MSE:HE1	1:B:210:MSE:SE	2.57	0.55
1:E:219:VAL:HA	2:E:1230:PTY:O10	2.07	0.55
1:F:151:ARG:NH1	3:F:2006:HOH:O	2.40	0.54
1:C:141:ASN:HD22	1:C:143:ASN:H	1.55	0.54
2:C:1230:PTY:H152	2:C:1230:PTY:H341	1.88	0.54
1:A:175:LYS:O	1:A:179:VAL:HG22	2.07	0.54
1:C:141:ASN:ND2	1:C:143:ASN:H	2.05	0.54
1:A:174:GLN:HG2	3:A:2014:HOH:O	2.07	0.54
1:C:218:LYS:HZ2	2:C:1230:PTY:H151	1.72	0.54
1:A:167:PHE:HA	1:A:170:LEU:HD22	1.91	0.53
1:F:211:ASP:HA	2:F:1230:PTY:H272	1.91	0.52
1:A:164:GLN:HE22	2:A:1230:PTY:HC6	1.74	0.52
2:A:1230:PTY:H172	1:B:130:ASN:HD21	1.73	0.51
1:B:151:ARG:NH2	1:B:198:ILE:HG13	2.24	0.51
1:F:218:LYS:HE2	2:F:1230:PTY:H142	1.92	0.51
2:D:1230:PTY:O13	2:D:1230:PTY:HC6	2.11	0.51
1:F:160:ARG:NH2	1:F:211:ASP:OD2	2.44	0.51
1:A:179:VAL:O	1:A:185:MSE:HE1	2.11	0.50
1:E:182:MSE:HE1	1:E:210:MSE:SE	2.62	0.50
2:F:1230:PTY:H342	2:F:1230:PTY:H132	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ARG:NH1	3:D:2003:HOH:O	2.41	0.50
2:F:1230:PTY:H132	2:F:1230:PTY:H322	1.93	0.49
1:A:172:ASN:CG	1:A:223:TYR:OH	2.51	0.49
1:E:139:ILE:H	1:E:190:GLN:HE22	1.61	0.49
1:C:170:LEU:HG	1:C:174:GLN:HB3	1.95	0.48
1:B:186:GLN:HG2	1:B:209:VAL:HG21	1.95	0.48
1:F:133:ASN:ND2	1:F:136:LYS:HD2	2.28	0.48
1:E:141:ASN:C	1:E:141:ASN:HD22	2.17	0.48
1:B:167:PHE:HA	1:B:170:LEU:HD22	1.95	0.48
1:C:132:ILE:H	1:C:132:ILE:HD13	1.79	0.47
1:D:134:LEU:O	1:D:187:LYS:HD3	2.14	0.47
1:B:133:ASN:ND2	1:B:136:LYS:H	2.13	0.47
2:E:1230:PTY:HC6	2:E:1230:PTY:O12	2.14	0.47
1:A:151:ARG:NH2	1:A:198:ILE:HG13	2.29	0.47
2:E:1230:PTY:H141	2:E:1230:PTY:H332	1.97	0.46
1:F:218:LYS:HE2	2:F:1230:PTY:H141	1.96	0.46
1:C:141:ASN:HD22	1:C:141:ASN:C	2.18	0.46
1:E:226:GLN:C	1:E:228:GLU:H	2.19	0.46
1:C:211:ASP:CA	2:C:1230:PTY:H271	2.42	0.45
1:E:132:ILE:HG21	1:E:134:LEU:HD21	1.98	0.45
1:C:141:ASN:HD22	1:C:142:LYS:N	2.15	0.45
1:C:185:MSE:HE1	1:C:213:LYS:HG3	1.99	0.44
1:C:186:GLN:HG2	1:C:209:VAL:HG21	2.00	0.44
1:F:170:LEU:HG	1:F:174:GLN:HB3	2.00	0.44
1:F:185:MSE:HE2	1:F:185:MSE:HB2	1.96	0.44
1:A:226:GLN:OE1	1:A:226:GLN:CA	2.61	0.44
1:B:133:ASN:ND2	1:B:136:LYS:HG3	2.33	0.44
1:A:133:ASN:ND2	1:A:136:LYS:H	2.15	0.43
2:C:1230:PTY:H351	2:C:1230:PTY:H382	1.52	0.43
1:A:185:MSE:H	1:A:185:MSE:HG2	1.52	0.43
1:B:151:ARG:NH1	3:B:2004:HOH:O	2.49	0.43
1:F:167:PHE:O	1:F:170:LEU:HB2	2.18	0.43
1:B:175:LYS:O	1:B:179:VAL:HG22	2.19	0.42
1:E:172:ASN:CG	1:E:223:TYR:OH	2.58	0.42
1:E:226:GLN:O	1:E:228:GLU:N	2.52	0.42
1:C:218:LYS:NZ	2:C:1230:PTY:H151	2.35	0.42
1:C:227:GLU:OE1	1:C:227:GLU:HA	2.20	0.42
1:E:189:VAL:HG12	1:E:193:GLN:HE21	1.85	0.42
1:A:189:VAL:HG12	1:A:193:GLN:HE21	1.84	0.42
2:C:1230:PTY:H342	2:C:1230:PTY:H311	1.77	0.42
1:E:159:ALA:HA	1:E:192:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ASN:HD21	1:B:135:ASN:HB3	1.85	0.41
1:B:133:ASN:HD22	1:B:136:LYS:H	1.67	0.41
1:A:183:GLU:HG2	1:A:187:LYS:HE2	2.02	0.41
1:E:131:LYS:HG3	1:E:132:ILE:N	2.36	0.41
1:E:132:ILE:HG21	1:E:134:LEU:CD2	2.49	0.41
1:D:218:LYS:HB2	1:D:218:LYS:HE3	1.84	0.41
2:C:1230:PTY:H341	2:C:1230:PTY:H132	2.02	0.41
1:D:132:ILE:HG23	1:D:191:GLY:HA3	2.03	0.41
1:F:130:ASN:HD22	1:F:195:ASN:HD21	1.67	0.41
1:C:224:LEU:HD23	1:C:224:LEU:HA	1.96	0.40
1:A:164:GLN:NE2	2:A:1230:PTY:HC6	2.37	0.40
1:A:218:LYS:HB3	2:A:1230:PTY:H131	2.03	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	98/101 (97%)	98 (100%)	0	0	100	100
1	B	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
1	C	98/101 (97%)	98 (100%)	0	0	100	100
1	D	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
1	E	98/101 (97%)	97 (99%)	0	1 (1%)	15	28
1	F	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
All	All	588/606 (97%)	580 (99%)	7 (1%)	1 (0%)	47	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	227	GLU

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	95/94 (101%)	85 (90%)	10 (10%)	7 13
1	B	95/94 (101%)	84 (88%)	11 (12%)	5 10
1	C	95/94 (101%)	88 (93%)	7 (7%)	13 27
1	D	95/94 (101%)	90 (95%)	5 (5%)	22 43
1	E	95/94 (101%)	82 (86%)	13 (14%)	3 7
1	F	95/94 (101%)	89 (94%)	6 (6%)	18 34
All	All	570/564 (101%)	518 (91%)	52 (9%)	9 18

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LEU
1	A	179	VAL
1	A	185	MSE
1	A	188	PHE
1	A	192	LEU
1	A	200	LEU
1	A	202	LYS
1	A	216	LEU
1	A	225	SER
1	A	228	GLU
1	B	131	LYS
1	B	134	LEU
1	B	147	VAL
1	B	161	LEU
1	B	170	LEU
1	B	179	VAL
1	B	200	LEU
1	B	202	LYS
1	B	212	LEU
1	B	216	LEU
1	B	225	SER
1	C	130	ASN

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Mol	Chain	Res	Type
1	C	132	ILE
1	C	141	ASN
1	C	170	LEU
1	C	200	LEU
1	C	202	LYS
1	C	216	LEU
1	D	147	VAL
1	D	179	VAL
1	D	185	MSE
1	D	197	ASN
1	D	227	GLU
1	E	130	ASN
1	E	131	LYS
1	E	141	ASN
1	E	151	ARG
1	E	165	LYS
1	E	170	LEU
1	E	176	ASP
1	E	179	VAL
1	E	185	MSE
1	E	188	PHE
1	E	200	LEU
1	E	212	LEU
1	E	223	TYR
1	F	170	LEU
1	F	179	VAL
1	F	185	MSE
1	F	200	LEU
1	F	216	LEU
1	F	227	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	133	ASN
1	A	153	ASN
1	A	164	GLN
1	A	172	ASN
1	A	190	GLN
1	A	195	ASN
1	A	222	ASN

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Mol	Chain	Res	Type
1	B	130	ASN
1	B	133	ASN
1	B	153	ASN
1	B	154	ASN
1	B	172	ASN
1	B	190	GLN
1	B	217	GLN
1	B	226	GLN
1	C	141	ASN
1	C	153	ASN
1	C	154	ASN
1	C	172	ASN
1	C	190	GLN
1	C	195	ASN
1	C	217	GLN
1	E	133	ASN
1	E	135	ASN
1	E	141	ASN
1	E	144	ASN
1	E	186	GLN
1	E	190	GLN
1	E	195	ASN
1	E	217	GLN
1	F	130	ASN
1	F	153	ASN
1	F	164	GLN
1	F	190	GLN
1	F	217	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PTY	B	1230	-	49,49,49	1.02	2 (4%)	52,54,54	1.15	4 (7%)
2	PTY	C	1230	-	49,49,49	1.03	2 (4%)	52,54,54	1.01	3 (5%)
2	PTY	A	1230	-	49,49,49	1.00	2 (4%)	52,54,54	1.02	3 (5%)
2	PTY	E	1230	-	49,49,49	0.99	2 (4%)	52,54,54	1.10	4 (7%)
2	PTY	F	1230	-	49,49,49	0.95	2 (4%)	52,54,54	0.98	2 (3%)
2	PTY	D	1230	-	49,49,49	0.98	2 (4%)	52,54,54	1.02	3 (5%)

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	PTY	B	1230	-	-	36/53/53/53	-
2	PTY	C	1230	-	-	30/53/53/53	-
2	PTY	A	1230	-	-	32/53/53/53	-
2	PTY	E	1230	-	-	33/53/53/53	-
2	PTY	F	1230	-	-	30/53/53/53	-
2	PTY	D	1230	-	-	32/53/53/53	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1230	PTY	O4-C30	4.73	1.47	1.33
2	C	1230	PTY	O7-C8	4.62	1.47	1.34
2	E	1230	PTY	O4-C30	4.54	1.46	1.33
2	A	1230	PTY	O7-C8	4.53	1.47	1.34
2	B	1230	PTY	O7-C8	4.52	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1230	PTY	O7-C8	4.50	1.47	1.34
2	C	1230	PTY	O4-C30	4.46	1.46	1.33
2	E	1230	PTY	O7-C8	4.43	1.46	1.34
2	A	1230	PTY	O4-C30	4.41	1.46	1.33
2	F	1230	PTY	O4-C30	4.26	1.45	1.33
2	D	1230	PTY	O4-C30	4.18	1.45	1.33
2	F	1230	PTY	O7-C8	4.16	1.46	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1230	PTY	O7-C8-C11	4.85	121.98	111.48
2	B	1230	PTY	O7-C8-C11	4.75	121.76	111.48
2	D	1230	PTY	O7-C8-C11	4.64	121.53	111.48
2	C	1230	PTY	O7-C8-C11	4.62	121.47	111.48
2	A	1230	PTY	O7-C8-C11	4.32	120.82	111.48
2	F	1230	PTY	O7-C8-C11	4.15	120.46	111.48
2	B	1230	PTY	O4-C30-C31	3.62	122.88	111.83
2	E	1230	PTY	O4-C30-C31	3.24	121.71	111.83
2	A	1230	PTY	O4-C30-C31	2.90	120.69	111.83
2	F	1230	PTY	O4-C30-C31	2.51	119.50	111.83
2	D	1230	PTY	O7-C8-O10	-2.42	118.04	123.70
2	D	1230	PTY	O4-C30-C31	2.36	119.03	111.83
2	C	1230	PTY	O4-C30-C31	2.31	118.88	111.83
2	B	1230	PTY	O4-C30-O30	-2.26	117.97	123.63
2	E	1230	PTY	O7-C8-O10	-2.20	118.55	123.70
2	C	1230	PTY	O7-C8-O10	-2.11	118.78	123.70
2	B	1230	PTY	O7-C8-O10	-2.03	118.96	123.70
2	A	1230	PTY	O4-C30-O30	-2.02	118.57	123.63
2	E	1230	PTY	O4-C30-O30	-2.00	118.62	123.63

There are no chirality outliers.

All (193) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1230	PTY	N1-C2-C3-O11
2	A	1230	PTY	C5-O14-P1-O11
2	A	1230	PTY	C5-O14-P1-O12
2	A	1230	PTY	C5-O14-P1-O13
2	B	1230	PTY	C6-C1-O4-C30
2	B	1230	PTY	C11-C8-O7-C6
2	C	1230	PTY	N1-C2-C3-O11

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Mol	Chain	Res	Type	Atoms
2	C	1230	PTY	C11-C8-O7-C6
2	D	1230	PTY	C6-C5-O14-P1
2	D	1230	PTY	C11-C8-O7-C6
2	D	1230	PTY	C3-O11-P1-O12
2	E	1230	PTY	N1-C2-C3-O11
2	E	1230	PTY	C6-C5-O14-P1
2	E	1230	PTY	C11-C8-O7-C6
2	F	1230	PTY	C3-O11-P1-O12
2	F	1230	PTY	C3-O11-P1-O13
2	F	1230	PTY	C3-O11-P1-O14
2	F	1230	PTY	C5-O14-P1-O11
2	F	1230	PTY	C5-O14-P1-O12
2	F	1230	PTY	C5-O14-P1-O13
2	A	1230	PTY	O30-C30-O4-C1
2	E	1230	PTY	C6-C1-O4-C30
2	A	1230	PTY	C31-C30-O4-C1
2	B	1230	PTY	O30-C30-O4-C1
2	D	1230	PTY	O30-C30-O4-C1
2	B	1230	PTY	O10-C8-O7-C6
2	C	1230	PTY	O10-C8-O7-C6
2	E	1230	PTY	O10-C8-O7-C6
2	B	1230	PTY	C31-C30-O4-C1
2	D	1230	PTY	C31-C30-O4-C1
2	E	1230	PTY	O30-C30-O4-C1
2	D	1230	PTY	O10-C8-O7-C6
2	C	1230	PTY	C31-C30-O4-C1
2	E	1230	PTY	C31-C30-O4-C1
2	F	1230	PTY	C31-C30-O4-C1
2	C	1230	PTY	C35-C36-C37-C38
2	C	1230	PTY	O30-C30-O4-C1
2	F	1230	PTY	O30-C30-O4-C1
2	F	1230	PTY	O4-C1-C6-O7
2	C	1230	PTY	C6-C1-O4-C30
2	F	1230	PTY	C30-C31-C32-C33
2	A	1230	PTY	C36-C37-C38-C39
2	B	1230	PTY	C22-C23-C24-C25
2	E	1230	PTY	C25-C26-C27-C28
2	B	1230	PTY	C33-C34-C35-C36
2	E	1230	PTY	C11-C12-C13-C14
2	E	1230	PTY	C15-C16-C17-C18
2	A	1230	PTY	C39-C40-C41-C42
2	D	1230	PTY	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
2	F	1230	PTY	C36-C37-C38-C39
2	A	1230	PTY	C17-C18-C19-C20
2	B	1230	PTY	C15-C16-C17-C18
2	B	1230	PTY	C16-C17-C18-C19
2	A	1230	PTY	C18-C19-C20-C21
2	A	1230	PTY	C34-C35-C36-C37
2	D	1230	PTY	C34-C35-C36-C37
2	F	1230	PTY	C37-C38-C39-C40
2	A	1230	PTY	C11-C8-O7-C6
2	A	1230	PTY	C20-C21-C22-C23
2	A	1230	PTY	C37-C38-C39-C40
2	B	1230	PTY	C31-C32-C33-C34
2	D	1230	PTY	C21-C22-C23-C24
2	E	1230	PTY	C17-C18-C19-C20
2	E	1230	PTY	C36-C37-C38-C39
2	C	1230	PTY	C36-C37-C38-C39
2	E	1230	PTY	C34-C35-C36-C37
2	E	1230	PTY	C35-C36-C37-C38
2	F	1230	PTY	C32-C33-C34-C35
2	B	1230	PTY	C36-C37-C38-C39
2	B	1230	PTY	C40-C41-C42-C43
2	A	1230	PTY	C12-C13-C14-C15
2	B	1230	PTY	C18-C19-C20-C21
2	D	1230	PTY	C37-C38-C39-C40
2	D	1230	PTY	C6-C1-O4-C30
2	D	1230	PTY	C36-C37-C38-C39
2	E	1230	PTY	C24-C25-C26-C27
2	B	1230	PTY	C19-C20-C21-C22
2	D	1230	PTY	C19-C20-C21-C22
2	C	1230	PTY	C18-C19-C20-C21
2	F	1230	PTY	C8-C11-C12-C13
2	A	1230	PTY	O10-C8-O7-C6
2	B	1230	PTY	C34-C35-C36-C37
2	C	1230	PTY	C39-C40-C41-C42
2	F	1230	PTY	C20-C21-C22-C23
2	A	1230	PTY	C21-C22-C23-C24
2	B	1230	PTY	C21-C22-C23-C24
2	B	1230	PTY	C20-C21-C22-C23
2	F	1230	PTY	C19-C20-C21-C22
2	D	1230	PTY	C16-C17-C18-C19
2	B	1230	PTY	C17-C18-C19-C20
2	D	1230	PTY	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
2	E	1230	PTY	C39-C40-C41-C42
2	C	1230	PTY	C38-C39-C40-C41
2	B	1230	PTY	C39-C40-C41-C42
2	F	1230	PTY	C13-C14-C15-C16
2	C	1230	PTY	C11-C12-C13-C14
2	B	1230	PTY	C23-C24-C25-C26
2	F	1230	PTY	C22-C23-C24-C25
2	E	1230	PTY	C23-C24-C25-C26
2	A	1230	PTY	C31-C32-C33-C34
2	C	1230	PTY	O4-C1-C6-C5
2	E	1230	PTY	O4-C1-C6-C5
2	A	1230	PTY	C33-C34-C35-C36
2	B	1230	PTY	C14-C15-C16-C17
2	C	1230	PTY	C23-C24-C25-C26
2	D	1230	PTY	C13-C14-C15-C16
2	D	1230	PTY	C20-C21-C22-C23
2	B	1230	PTY	C37-C38-C39-C40
2	E	1230	PTY	C14-C15-C16-C17
2	F	1230	PTY	C23-C24-C25-C26
2	D	1230	PTY	C18-C19-C20-C21
2	C	1230	PTY	C16-C17-C18-C19
2	C	1230	PTY	C21-C22-C23-C24
2	E	1230	PTY	C41-C42-C43-C44
2	F	1230	PTY	C26-C27-C28-C29
2	D	1230	PTY	C41-C42-C43-C44
2	E	1230	PTY	C26-C27-C28-C29
2	B	1230	PTY	C24-C25-C26-C27
2	A	1230	PTY	C6-C5-O14-P1
2	B	1230	PTY	C26-C27-C28-C29
2	C	1230	PTY	O14-C5-C6-C1
2	D	1230	PTY	O14-C5-C6-C1
2	E	1230	PTY	O14-C5-C6-C1
2	F	1230	PTY	C31-C32-C33-C34
2	E	1230	PTY	C32-C33-C34-C35
2	F	1230	PTY	C24-C25-C26-C27
2	C	1230	PTY	C24-C25-C26-C27
2	B	1230	PTY	O4-C1-C6-C5
2	F	1230	PTY	O4-C1-C6-C5
2	D	1230	PTY	C31-C32-C33-C34
2	E	1230	PTY	O14-C5-C6-O7
2	B	1230	PTY	C6-C5-O14-P1
2	D	1230	PTY	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
2	F	1230	PTY	C25-C26-C27-C28
2	E	1230	PTY	C20-C21-C22-C23
2	E	1230	PTY	C18-C19-C20-C21
2	A	1230	PTY	C41-C42-C43-C44
2	D	1230	PTY	C32-C33-C34-C35
2	D	1230	PTY	C26-C27-C28-C29
2	C	1230	PTY	C26-C27-C28-C29
2	A	1230	PTY	O14-C5-C6-C1
2	D	1230	PTY	C12-C13-C14-C15
2	B	1230	PTY	C5-C6-O7-C8
2	D	1230	PTY	C22-C23-C24-C25
2	A	1230	PTY	C14-C15-C16-C17
2	F	1230	PTY	C41-C42-C43-C44
2	B	1230	PTY	C13-C14-C15-C16
2	F	1230	PTY	C39-C40-C41-C42
2	C	1230	PTY	C20-C21-C22-C23
2	A	1230	PTY	C35-C36-C37-C38
2	B	1230	PTY	C35-C36-C37-C38
2	C	1230	PTY	C34-C35-C36-C37
2	A	1230	PTY	C3-O11-P1-O12
2	A	1230	PTY	C3-O11-P1-O13
2	A	1230	PTY	C3-O11-P1-O14
2	B	1230	PTY	C3-O11-P1-O13
2	D	1230	PTY	C3-O11-P1-O13
2	D	1230	PTY	C3-O11-P1-O14
2	C	1230	PTY	C6-C5-O14-P1
2	E	1230	PTY	C40-C41-C42-C43
2	C	1230	PTY	C1-C6-O7-C8
2	D	1230	PTY	C5-C6-O7-C8
2	C	1230	PTY	C14-C15-C16-C17
2	A	1230	PTY	O14-C5-C6-O7
2	F	1230	PTY	C14-C15-C16-C17
2	B	1230	PTY	C25-C26-C27-C28
2	F	1230	PTY	C33-C34-C35-C36
2	A	1230	PTY	C40-C41-C42-C43
2	E	1230	PTY	C22-C23-C24-C25
2	C	1230	PTY	O4-C1-C6-O7
2	C	1230	PTY	C12-C13-C14-C15
2	E	1230	PTY	C21-C22-C23-C24
2	E	1230	PTY	C1-C6-O7-C8
2	A	1230	PTY	C19-C20-C21-C22
2	E	1230	PTY	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
2	D	1230	PTY	O4-C1-C6-C5
2	F	1230	PTY	C12-C13-C14-C15
2	C	1230	PTY	C32-C33-C34-C35
2	A	1230	PTY	C25-C26-C27-C28
2	C	1230	PTY	C22-C23-C24-C25
2	B	1230	PTY	O4-C30-C31-C32
2	F	1230	PTY	C11-C12-C13-C14
2	E	1230	PTY	C16-C17-C18-C19
2	D	1230	PTY	C15-C16-C17-C18
2	B	1230	PTY	O4-C1-C6-O7
2	D	1230	PTY	C23-C24-C25-C26
2	C	1230	PTY	C13-C14-C15-C16
2	C	1230	PTY	C31-C32-C33-C34
2	B	1230	PTY	C12-C11-C8-O7
2	A	1230	PTY	O4-C30-C31-C32
2	E	1230	PTY	O4-C30-C31-C32
2	B	1230	PTY	C38-C39-C40-C41
2	B	1230	PTY	C12-C11-C8-O10

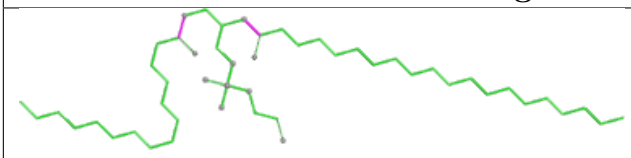
There are no ring outliers.

6 monomers are involved in 24 short contacts:

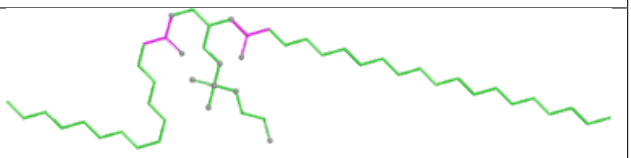
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1230	PTY	1	0
2	C	1230	PTY	8	0
2	A	1230	PTY	5	0
2	E	1230	PTY	3	0
2	F	1230	PTY	6	0
2	D	1230	PTY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

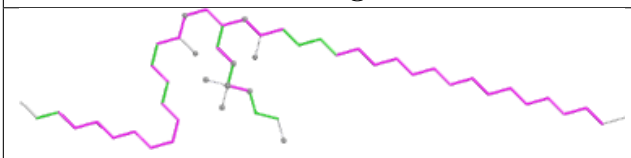
Ligand PTY B 1230



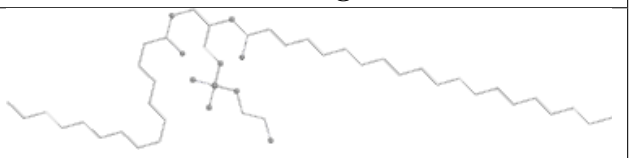
Bond lengths



Bond angles

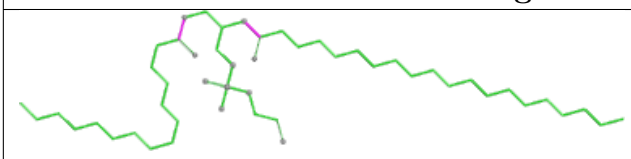


Torsions

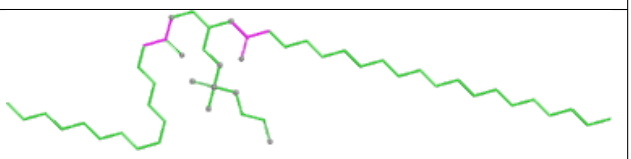


Rings

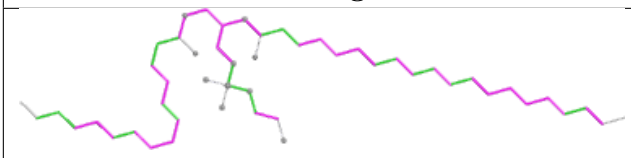
Ligand PTY C 1230



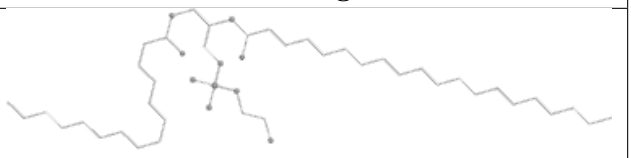
Bond lengths



Bond angles

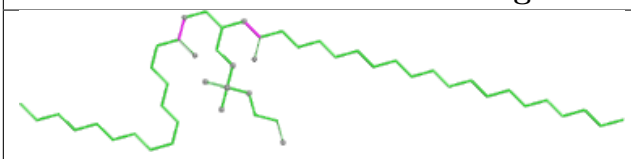


Torsions

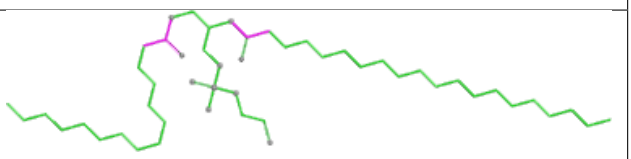


Rings

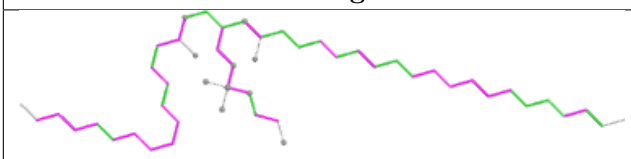
Ligand PTY A 1230



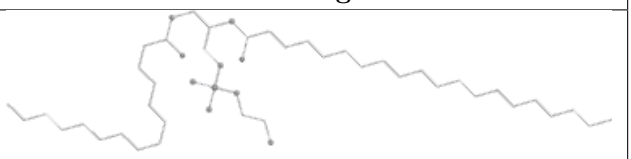
Bond lengths



Bond angles

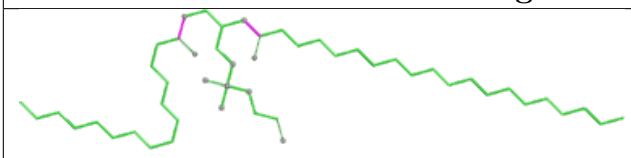


Torsions

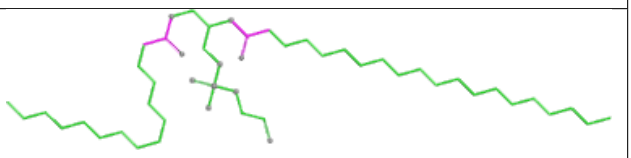


Rings

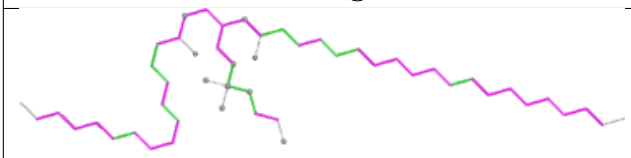
Ligand PTY E 1230



Bond lengths

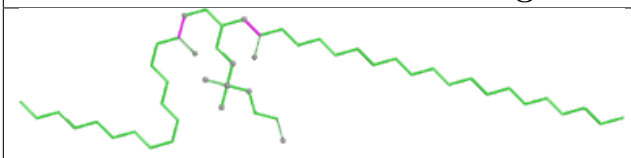
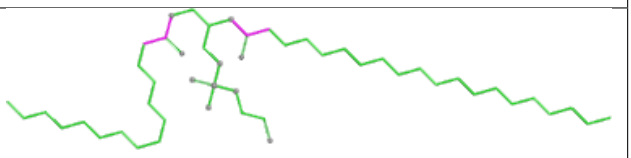
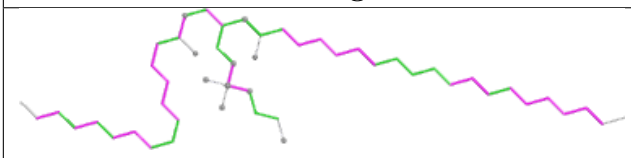
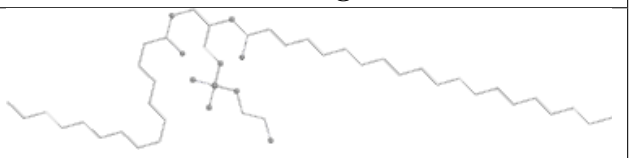


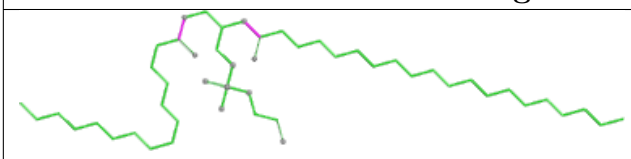
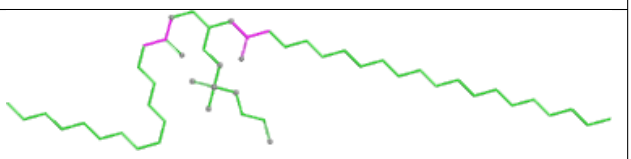
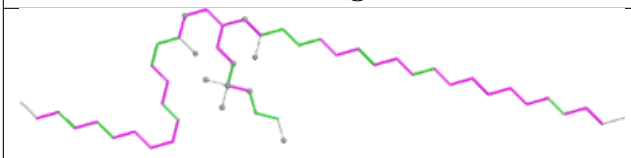
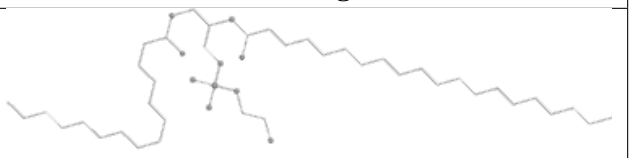
Bond angles



Torsions

Rings

Ligand PTY F 1230	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PTY D 1230	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 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	97/101 (96%)	0.01	4 (4%)	37	40	4, 15, 42, 56	0
1	B	97/101 (96%)	-0.03	3 (3%)	49	52	3, 13, 45, 60	0
1	C	97/101 (96%)	-0.03	5 (5%)	27	29	4, 12, 44, 61	0
1	D	97/101 (96%)	0.00	3 (3%)	49	52	3, 14, 43, 60	0
1	E	97/101 (96%)	0.13	4 (4%)	37	40	6, 18, 56, 72	0
1	F	97/101 (96%)	0.16	4 (4%)	37	40	5, 15, 49, 63	0
All	All	582/606 (96%)	0.04	23 (3%)	38	41	3, 15, 46, 72	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	ASN	4.8
1	D	142	LYS	4.4
1	C	130	ASN	4.2
1	F	130	ASN	3.9
1	E	139	ILE	3.9
1	D	131	LYS	3.8
1	E	130	ASN	3.8
1	F	131	LYS	3.5
1	D	130	ASN	3.4
1	F	142	LYS	3.2
1	B	131	LYS	2.9
1	F	229	ASN	2.8
1	E	131	LYS	2.8
1	A	131	LYS	2.7
1	C	133	ASN	2.5
1	B	226	GLN	2.3
1	A	130	ASN	2.3
1	C	203	TYR	2.3
1	C	131	LYS	2.2

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Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	133	ASN	2.2
1	C	132	ILE	2.2
1	A	140	GLU	2.2
1	E	133	ASN	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)

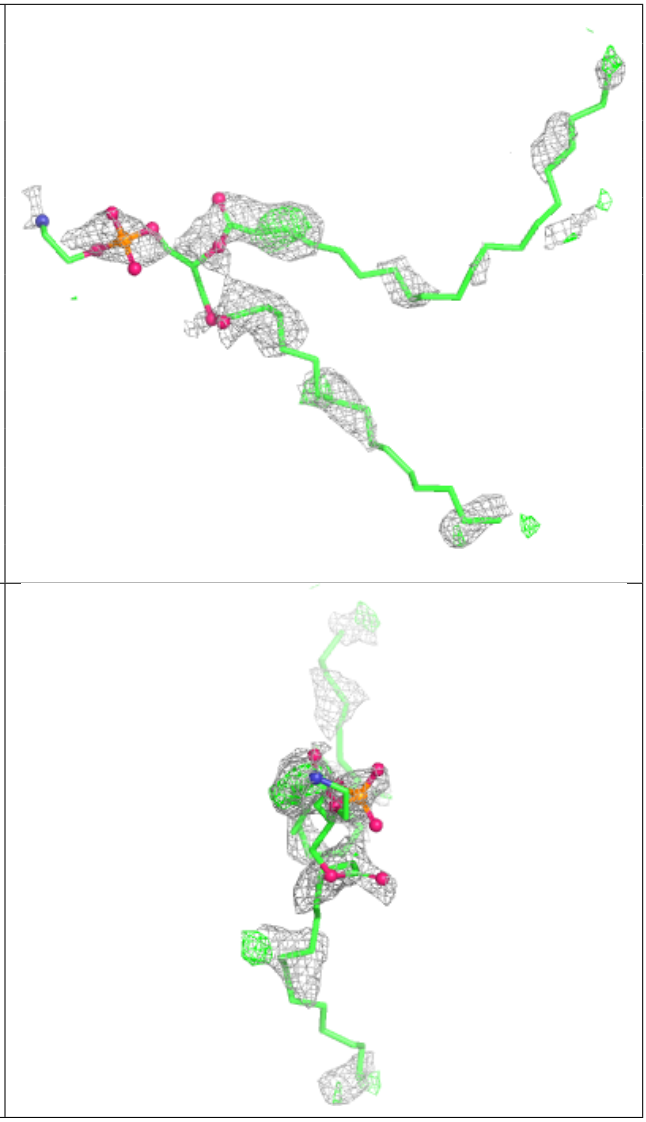
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PTY	B	1230	50/50	0.48	0.46	35,50,54,54	50
2	PTY	E	1230	50/50	0.48	0.49	45,55,65,65	50
2	PTY	A	1230	50/50	0.50	0.47	47,54,60,60	50
2	PTY	D	1230	50/50	0.53	0.43	31,36,40,41	50
2	PTY	C	1230	50/50	0.65	0.36	17,43,47,48	50
2	PTY	F	1230	50/50	0.71	0.30	16,30,33,34	50

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.

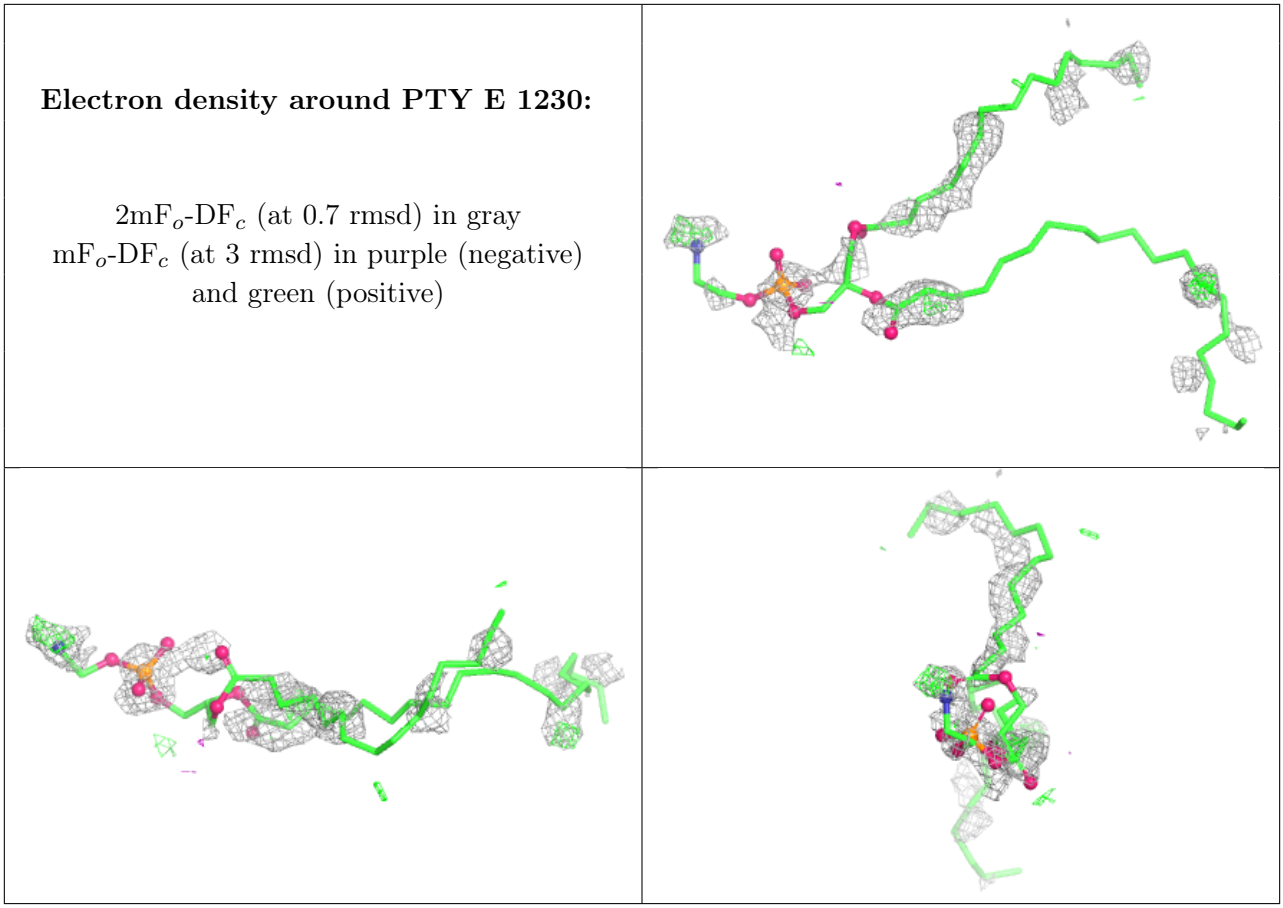
Electron density around PTY B 1230:

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



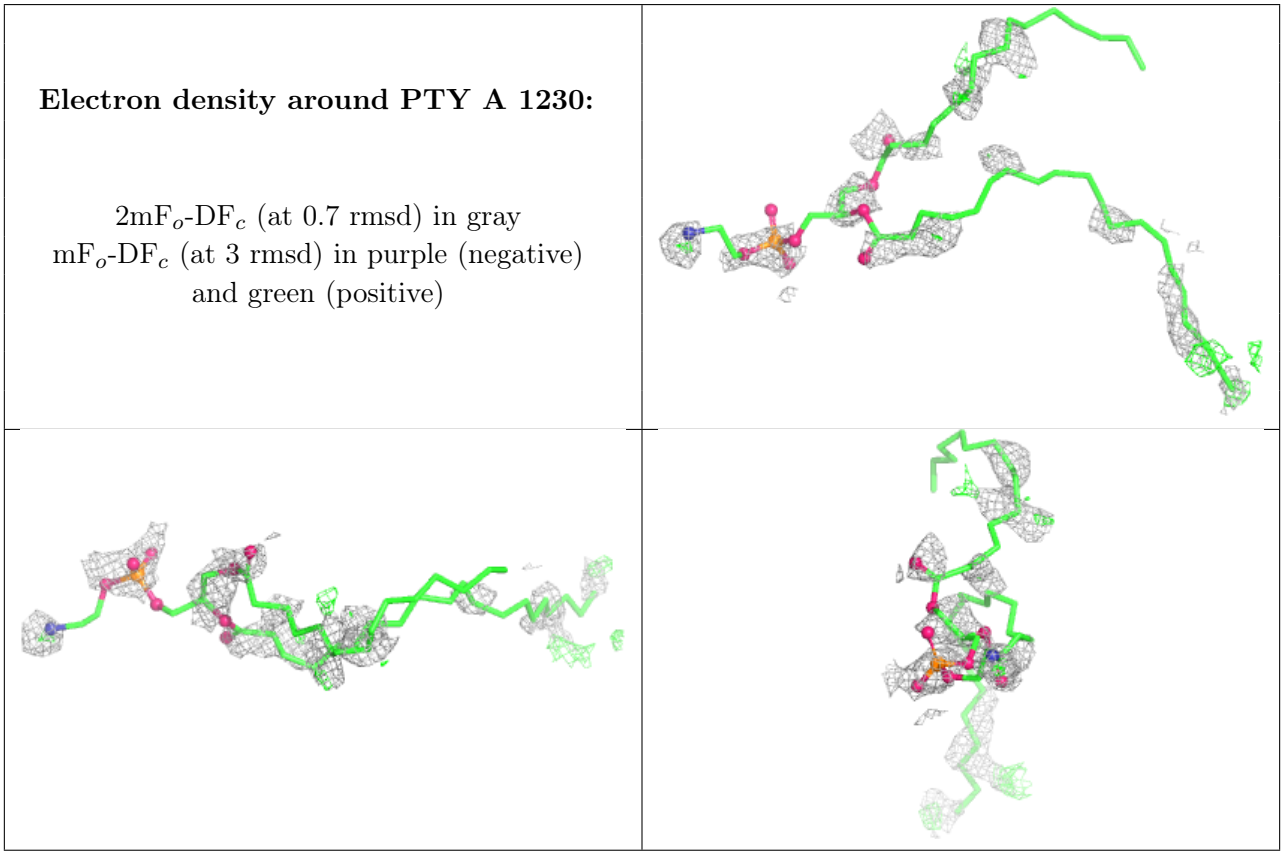
Electron density around PTY E 1230:

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



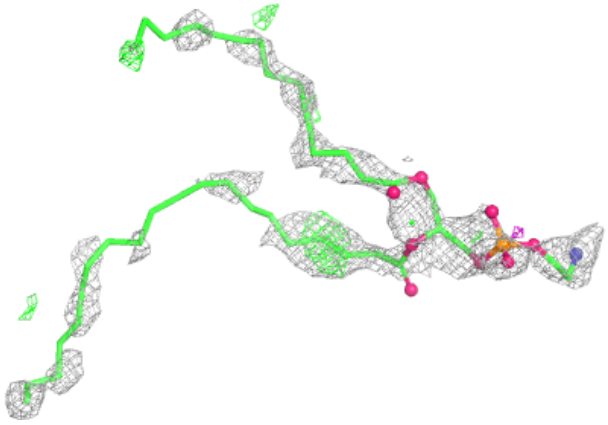
Electron density around PTY A 1230:

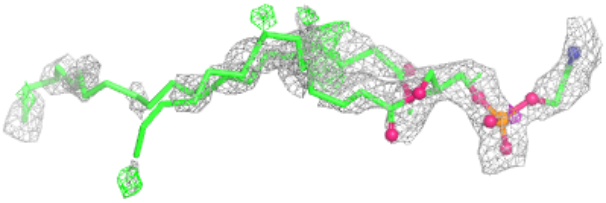
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PTY D 1230:

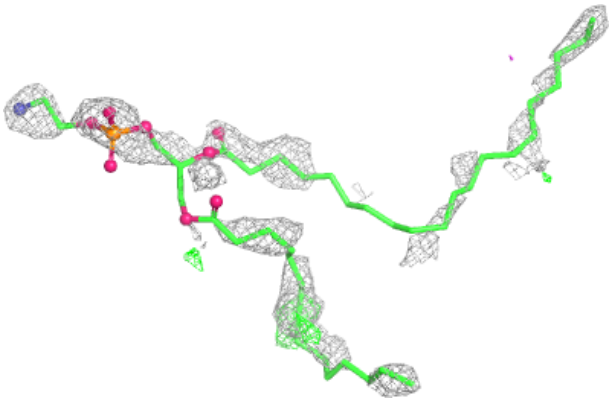
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

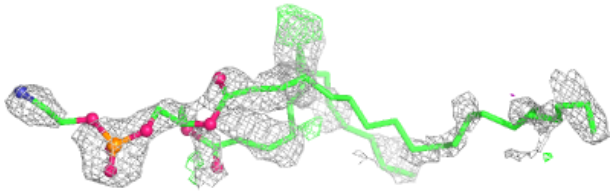


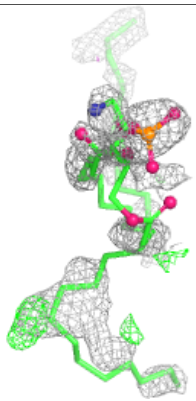


Electron density around PTY C 1230:

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

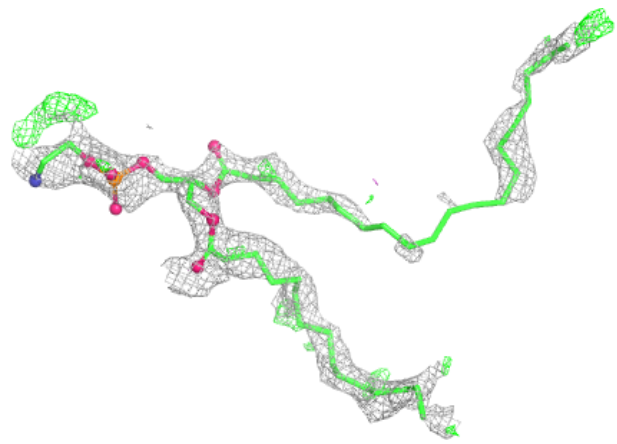


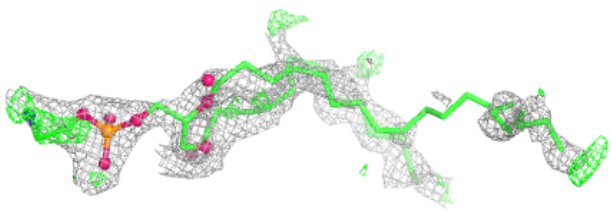




Electron density around PTY F 1230:

$2mF_o$-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.