Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 07:37 PM EST

PDB ID	:	1U1E
Title	:	Structure of e. coli uridine phosphorylase complexed to 5(phenylseleno)acycl ouridine (PSAU)
Authors	:	Bu, W.; Settembre, E.C.; Ealick, S.E.
Deposited on	:	2004-07-15
Resolution	:	2.00 Å(reported)

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

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

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

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

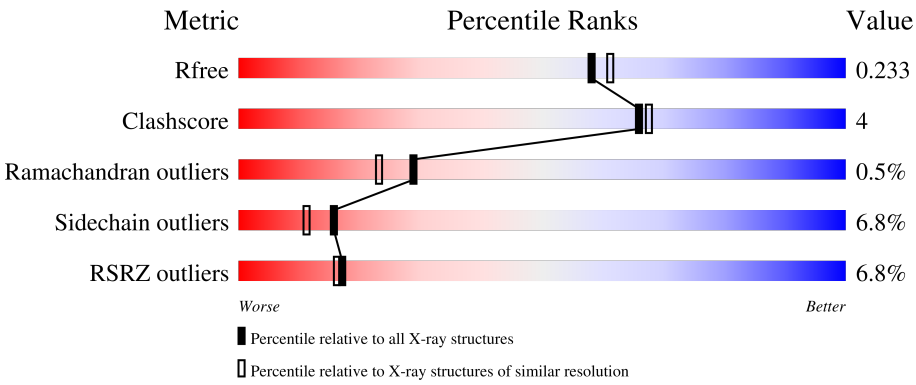
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	256	2%, 82%, 15%
1	B	256	4%, 81%, 16%
1	C	256	16%, 84%, 12%
1	D	256	9%, 82%, 14%
1	E	256	5%, 86%, 11%

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Mol	Chain	Length	Quality of chain
1	F	256	3% 83% 13%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11953 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	253	1895	1186	330	367	12	0	0	0
1	B	251	1881	1178	328	364	11	0	0	0
1	C	250	1872	1172	326	363	11	0	0	0
1	D	250	1872	1172	326	363	11	0	0	0
1	E	251	1881	1178	328	364	11	0	0	0
1	F	250	1872	1172	326	363	11	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P12758
A	-1	SER	-	cloning artifact	UNP P12758
A	0	HIS	-	cloning artifact	UNP P12758
A	1	MET	-	cloning artifact	UNP P12758
B	-2	GLY	-	cloning artifact	UNP P12758
B	-1	SER	-	cloning artifact	UNP P12758
B	0	HIS	-	cloning artifact	UNP P12758
B	1	MET	-	cloning artifact	UNP P12758
C	-2	GLY	-	cloning artifact	UNP P12758
C	-1	SER	-	cloning artifact	UNP P12758
C	0	HIS	-	cloning artifact	UNP P12758
C	1	MET	-	cloning artifact	UNP P12758
D	-2	GLY	-	cloning artifact	UNP P12758
D	-1	SER	-	cloning artifact	UNP P12758
D	0	HIS	-	cloning artifact	UNP P12758
D	1	MET	-	cloning artifact	UNP P12758
E	-2	GLY	-	cloning artifact	UNP P12758

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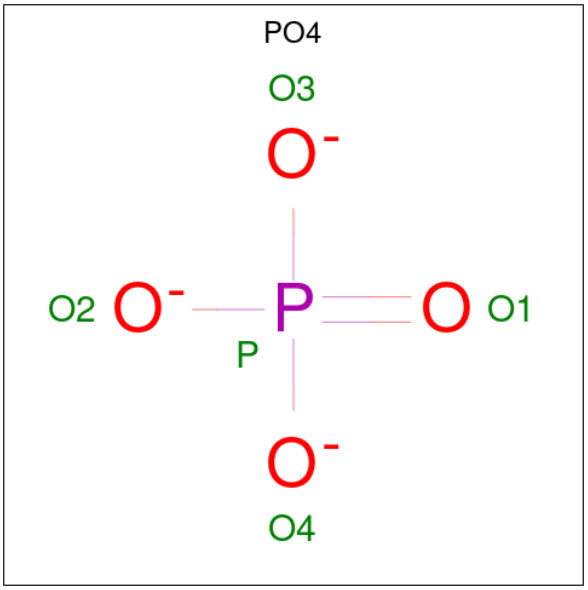
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	cloning artifact	UNP P12758
E	0	HIS	-	cloning artifact	UNP P12758
E	1	MET	-	cloning artifact	UNP P12758
F	-2	GLY	-	cloning artifact	UNP P12758
F	-1	SER	-	cloning artifact	UNP P12758
F	0	HIS	-	cloning artifact	UNP P12758
F	1	MET	-	cloning artifact	UNP P12758

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

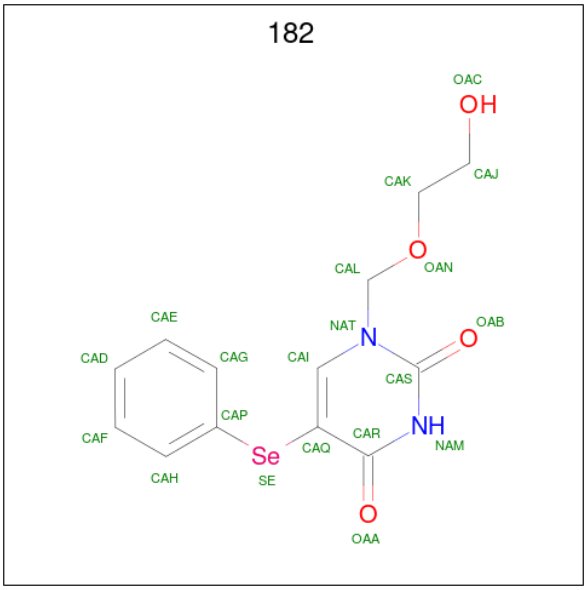


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
3	A	1	1	1	0	0
			Total	K		
3	C	1	1	1	0	0
			Total	K		
3	E	1	1	1	0	0

- Molecule 4 is 1-((2-HYDROXYETHOXY)METHYL)-5-(PHENYLSELANYL)PYRIMIDINE-2,4(1H,3H)-DIONE (three-letter code: 182) (formula: $C_{13}H_{14}N_2O_4Se$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	Se		
4	A	1	20	13	2	4	1	0	0
			Total	C	N	O	Se		
4	B	1	20	13	2	4	1	0	0
			Total	C	N	O	Se		
4	C	1	20	13	2	4	1	0	0
			Total	C	N	O	Se		
4	D	1	20	13	2	4	1	0	0
			Total	C	N	O	Se		
4	E	1	20	13	2	4	1	0	0
			Total	C	N	O	Se		
4	F	1	20	13	2	4	1	0	0

- Molecule 5 is water.

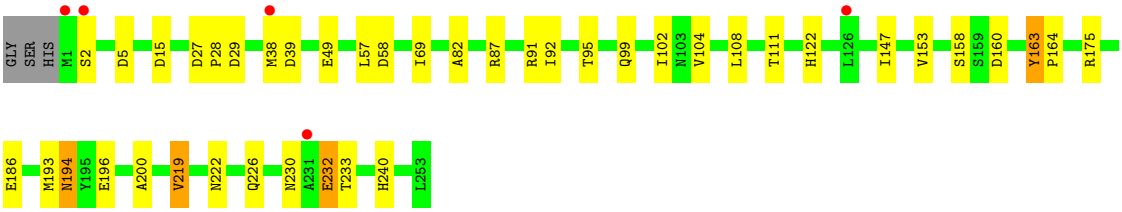
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	97	97	97	0	0
			Total	O		
5	B	110	110	110	0	0
			Total	O		
5	C	52	52	52	0	0
			Total	O		
5	D	64	64	64	0	0
			Total	O		
5	E	90	90	90	0	0
			Total	O		
5	F	114	114	114	0	0

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.

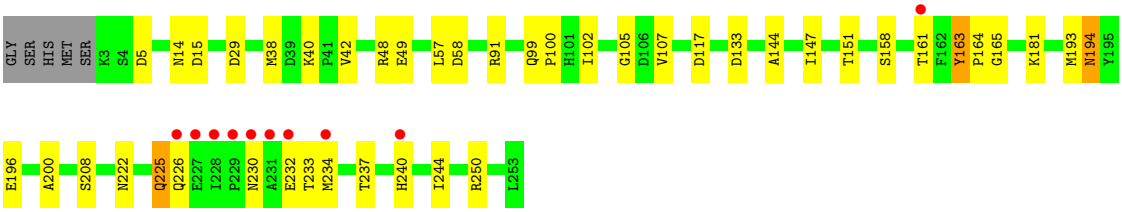
• Molecule 1: Uridine phosphorylase

Chain A:



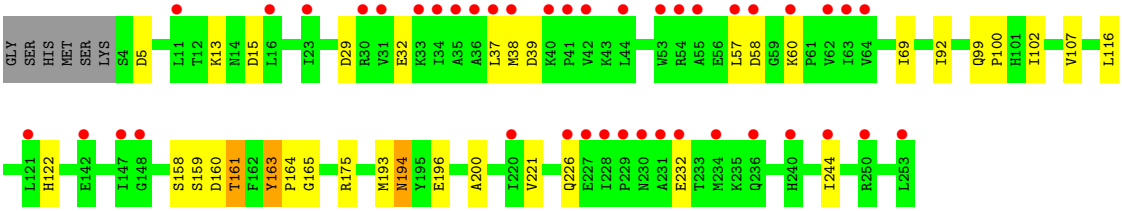
• Molecule 1: Uridine phosphorylase

Chain B:



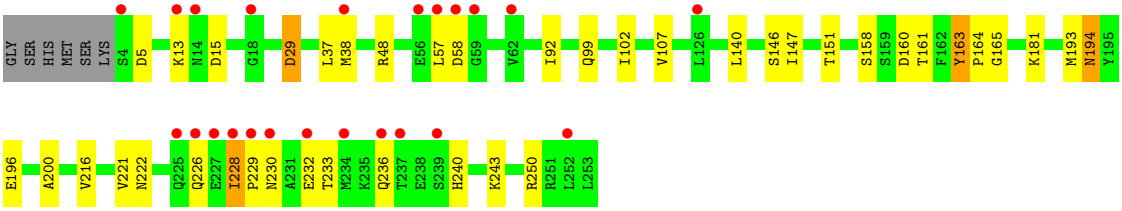
• Molecule 1: Uridine phosphorylase

Chain C:



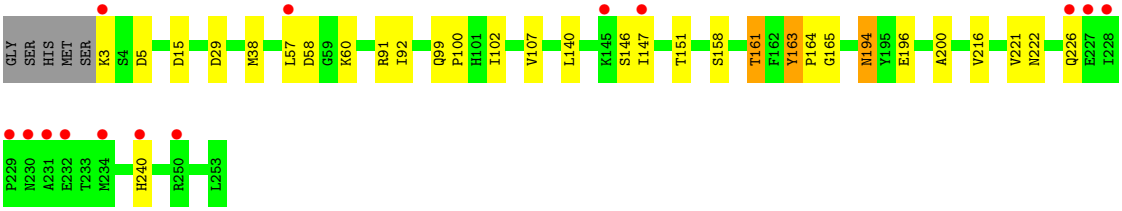
• Molecule 1: Uridine phosphorylase

Chain D:



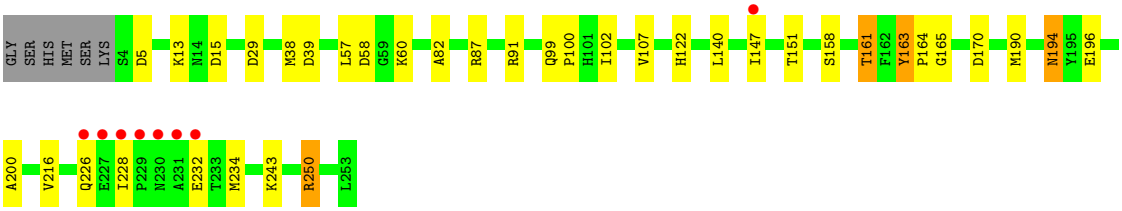
• Molecule 1: Uridine phosphorylase

Chain E:



• Molecule 1: Uridine phosphorylase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.08Å 125.69Å 140.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.00 48.56 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.80-2.00) 96.2 (48.56-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.76 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.24, CNS	Depositor
R, R_{free}	0.211 , 0.235 0.213 , 0.233	Depositor DCC
R_{free} test set	10934 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11953	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, K, 182

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	0.30	0/1927	0.66	5/2616 (0.2%)
1	B	0.30	0/1913	0.67	6/2598 (0.2%)
1	C	0.29	0/1904	0.65	5/2587 (0.2%)
1	D	0.29	0/1904	0.66	4/2587 (0.2%)
1	E	0.30	0/1913	0.66	4/2598 (0.2%)
1	F	0.30	0/1904	0.67	6/2587 (0.2%)
All	All	0.30	0/11465	0.66	30/15573 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	15	ASP	CB-CG-OD2	6.29	123.96	118.30
1	F	5	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	15	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	15	ASP	CB-CG-OD2	6.20	123.88	118.30
1	D	15	ASP	CB-CG-OD2	6.11	123.80	118.30
1	D	58	ASP	CB-CG-OD2	6.08	123.77	118.30
1	B	58	ASP	CB-CG-OD2	6.03	123.73	118.30
1	E	15	ASP	CB-CG-OD2	6.00	123.70	118.30
1	C	5	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	5	ASP	CB-CG-OD2	5.98	123.68	118.30
1	F	29	ASP	CB-CG-OD2	5.97	123.67	118.30
1	C	15	ASP	CB-CG-OD2	5.95	123.65	118.30
1	D	5	ASP	CB-CG-OD2	5.93	123.64	118.30
1	E	5	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	58	ASP	CB-CG-OD2	5.91	123.62	118.30
1	F	58	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	29	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	5	ASP	CB-CG-OD2	5.67	123.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	58	ASP	CB-CG-OD2	5.61	123.34	118.30
1	C	58	ASP	CB-CG-OD2	5.41	123.17	118.30
1	E	29	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	29	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	29	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	39	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	29	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	133	ASP	CB-CG-OD2	5.17	122.95	118.30
1	F	39	ASP	CB-CG-OD2	5.15	122.94	118.30
1	C	39	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	170	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	117	ASP	CB-CG-OD2	5.03	122.83	118.30

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	1895	0	1893	16	0
1	B	1881	0	1875	19	0
1	C	1872	0	1862	15	0
1	D	1872	0	1863	16	0
1	E	1881	0	1875	15	0
1	F	1872	0	1862	16	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	20	0	14	0	0
4	B	20	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	20	0	14	0	0
4	D	20	0	14	0	0
4	E	20	0	14	0	0
4	F	20	0	14	0	0
5	A	97	0	0	0	0
5	B	110	0	0	0	0
5	C	52	0	0	0	0
5	D	64	0	0	0	0
5	E	90	0	0	0	0
5	F	114	0	0	1	0
All	All	11953	0	11314	90	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (90) 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:105:GLY:HA2	1:B:237:THR:HG22	1.65	0.77
1:A:122:HIS:ND1	1:B:161:THR:HG22	2.10	0.66
1:F:161:THR:CG2	1:F:165:GLY:H	2.09	0.66
1:E:161:THR:CG2	1:E:165:GLY:H	2.09	0.65
1:F:161:THR:HG21	1:F:164:PRO:HG2	1.79	0.64
1:C:158:SER:HB3	1:C:200:ALA:HB2	1.79	0.64
1:E:161:THR:HG21	1:E:164:PRO:HG2	1.79	0.64
1:B:230:ASN:HD22	1:B:233:THR:H	1.48	0.61
1:F:158:SER:HB3	1:F:200:ALA:HB2	1.80	0.61
1:B:161:THR:CG2	1:B:165:GLY:H	2.14	0.60
1:F:38:MET:HG2	1:F:57:LEU:HD13	1.86	0.57
1:E:38:MET:HG2	1:E:57:LEU:HD13	1.86	0.57
1:E:158:SER:HB3	1:E:200:ALA:HB2	1.87	0.56
1:E:102:ILE:O	1:E:222:ASN:ND2	2.39	0.56
1:F:161:THR:HG22	1:F:165:GLY:H	1.71	0.56
1:E:161:THR:HG21	1:E:165:GLY:H	1.71	0.55
1:D:161:THR:HG21	1:D:164:PRO:HG2	1.87	0.55
1:D:158:SER:HB3	1:D:200:ALA:HB2	1.90	0.54
1:D:163:TYR:HB2	1:D:164:PRO:CD	2.37	0.54
1:B:158:SER:HB3	1:B:200:ALA:HB2	1.90	0.54
1:C:161:THR:CG2	1:C:165:GLY:H	2.21	0.53
1:B:163:TYR:HB2	1:B:164:PRO:HD3	1.91	0.52
1:A:38:MET:HG2	1:A:57:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:MET:HB2	1:C:194:ASN:HD22	1.74	0.51
1:A:158:SER:HB3	1:A:200:ALA:HB2	1.93	0.51
1:C:116:LEU:HB2	1:C:159:SER:HA	1.93	0.51
1:E:163:TYR:HB2	1:E:164:PRO:CD	2.40	0.51
1:A:82:ALA:O	1:A:87:ARG:NH2	2.44	0.51
1:B:38:MET:HG2	1:B:57:LEU:HD13	1.93	0.50
1:D:99:GLN:HB2	1:D:102:ILE:HD12	1.93	0.50
1:D:161:THR:CG2	1:D:165:GLY:H	2.25	0.50
1:D:193:MET:HB2	1:D:194:ASN:HD22	1.76	0.50
1:B:163:TYR:HB2	1:B:164:PRO:CD	2.43	0.49
1:D:163:TYR:HB2	1:D:164:PRO:HD3	1.95	0.49
1:F:82:ALA:O	1:F:87:ARG:NH2	2.45	0.48
1:E:194:ASN:N	1:E:194:ASN:HD22	2.12	0.48
1:E:161:THR:HG22	1:E:165:GLY:H	1.77	0.48
1:C:163:TYR:HB2	1:C:164:PRO:CD	2.44	0.48
1:F:163:TYR:HB2	1:F:164:PRO:CD	2.44	0.47
1:C:161:THR:HG21	1:C:164:PRO:HG2	1.95	0.47
1:A:193:MET:HB2	1:A:194:ASN:HD22	1.79	0.47
1:B:107:VAL:HG13	1:B:151:THR:HG23	1.95	0.47
1:C:69:ILE:HD11	1:D:48:ARG:HD3	1.95	0.47
1:A:104:VAL:HA	1:A:219:VAL:HG22	1.96	0.47
1:D:140:LEU:HD22	1:D:216:VAL:HB	1.97	0.47
1:E:161:THR:HB	1:F:122:HIS:ND1	2.31	0.46
1:F:107:VAL:HG13	1:F:151:THR:HG23	1.96	0.46
1:D:38:MET:HG2	1:D:57:LEU:HD13	1.96	0.46
1:A:99:GLN:HB2	1:A:102:ILE:HD12	1.98	0.45
1:B:161:THR:HG21	1:B:164:PRO:HG2	1.98	0.45
1:B:193:MET:HB2	1:B:194:ASN:HD22	1.81	0.45
1:C:161:THR:HG22	1:C:165:GLY:H	1.81	0.45
1:D:230:ASN:HD22	1:D:233:THR:H	1.64	0.45
1:D:228:ILE:HA	1:D:229:PRO:HD3	1.82	0.44
1:C:107:VAL:HG21	1:C:244:ILE:HD13	1.98	0.44
1:B:102:ILE:O	1:B:222:ASN:ND2	2.46	0.44
1:C:99:GLN:HB2	1:C:102:ILE:HD12	2.00	0.44
1:F:161:THR:HG21	1:F:165:GLY:H	1.81	0.44
1:C:99:GLN:HA	1:C:100:PRO:HD3	1.90	0.43
1:D:102:ILE:O	1:D:222:ASN:ND2	2.49	0.43
1:E:99:GLN:HB2	1:E:102:ILE:HD12	2.00	0.43
1:A:163:TYR:HB2	1:A:164:PRO:HD3	1.99	0.43
1:C:38:MET:HG2	1:C:57:LEU:HD13	2.01	0.43
1:E:140:LEU:HD22	1:E:216:VAL:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLU:HB3	1:B:49:GLU:HB3	2.00	0.43
1:D:163:TYR:CB	1:D:164:PRO:CD	2.96	0.43
1:B:161:THR:HG23	1:B:165:GLY:H	1.81	0.43
1:C:163:TYR:HB2	1:C:164:PRO:HD3	2.01	0.42
1:A:230:ASN:HD22	1:A:233:THR:H	1.68	0.42
1:F:57:LEU:HG	1:F:250:ARG:HG3	2.00	0.42
1:A:102:ILE:O	1:A:222:ASN:ND2	2.53	0.41
1:A:111:THR:HG23	1:A:153:VAL:HG12	2.02	0.41
1:F:140:LEU:HD22	1:F:216:VAL:HB	2.02	0.41
1:A:27:ASP:HA	1:A:28:PRO:HD2	1.91	0.41
1:D:107:VAL:HG13	1:D:151:THR:HG23	2.03	0.41
1:E:99:GLN:HA	1:E:100:PRO:HD3	1.92	0.41
1:E:107:VAL:HG13	1:E:151:THR:HG23	2.01	0.41
1:F:99:GLN:HB2	1:F:102:ILE:HD12	2.02	0.41
1:A:69:ILE:HD11	1:B:48:ARG:HD3	2.01	0.41
1:E:163:TYR:CB	1:E:164:PRO:CD	2.97	0.41
1:C:163:TYR:CB	1:C:164:PRO:CD	2.99	0.41
1:F:99:GLN:HA	1:F:100:PRO:HD3	1.94	0.41
1:A:95:THR:HG21	1:A:108:LEU:HD12	2.02	0.40
1:A:175:ARG:HD2	5:F:8450:HOH:O	2.21	0.40
1:F:194:ASN:HD22	1:F:194:ASN:N	2.19	0.40
1:B:144:ALA:HA	1:B:244:ILE:HG12	2.02	0.40
1:C:122:HIS:ND1	1:D:161:THR:HG22	2.36	0.40
1:B:99:GLN:HA	1:B:100:PRO:HD3	1.90	0.40
1:B:208:SER:HB2	1:F:190:MET:HG2	2.04	0.40
1:B:222:ASN:HB3	1:B:225:GLN:HG2	2.04	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	251/256 (98%)	246 (98%)	3 (1%)	2 (1%)	19	13
1	B	249/256 (97%)	245 (98%)	3 (1%)	1 (0%)	34	30
1	C	248/256 (97%)	238 (96%)	9 (4%)	1 (0%)	34	30
1	D	248/256 (97%)	241 (97%)	6 (2%)	1 (0%)	34	30
1	E	249/256 (97%)	246 (99%)	2 (1%)	1 (0%)	34	30
1	F	248/256 (97%)	244 (98%)	3 (1%)	1 (0%)	34	30
All	All	1493/1536 (97%)	1460 (98%)	26 (2%)	7 (0%)	29	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	TYR
1	D	163	TYR
1	E	163	TYR
1	F	163	TYR
1	A	232	GLU
1	C	163	TYR
1	A	163	TYR

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	202/206 (98%)	190 (94%)	12 (6%)	19	15
1	B	200/206 (97%)	186 (93%)	14 (7%)	15	10
1	C	199/206 (97%)	186 (94%)	13 (6%)	17	12
1	D	199/206 (97%)	181 (91%)	18 (9%)	9	6
1	E	200/206 (97%)	188 (94%)	12 (6%)	19	14
1	F	199/206 (97%)	186 (94%)	13 (6%)	17	12
All	All	1199/1236 (97%)	1117 (93%)	82 (7%)	16	11

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	91	ARG
1	A	92	ILE
1	A	147	ILE
1	A	160	ASP
1	A	186	GLU
1	A	194	ASN
1	A	196	GLU
1	A	219	VAL
1	A	226	GLN
1	A	232	GLU
1	A	240	HIS
1	B	14	ASN
1	B	40	LYS
1	B	42	VAL
1	B	91	ARG
1	B	147	ILE
1	B	181	LYS
1	B	194	ASN
1	B	196	GLU
1	B	225	GLN
1	B	226	GLN
1	B	232	GLU
1	B	234	MET
1	B	240	HIS
1	B	250	ARG
1	C	13	LYS
1	C	32	GLU
1	C	37	LEU
1	C	60	LYS
1	C	92	ILE
1	C	160	ASP
1	C	161	THR
1	C	175	ARG
1	C	194	ASN
1	C	196	GLU
1	C	221	VAL
1	C	226	GLN
1	C	232	GLU
1	D	13	LYS
1	D	29	ASP
1	D	37	LEU
1	D	92	ILE

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Mol	Chain	Res	Type
1	D	146	SER
1	D	147	ILE
1	D	160	ASP
1	D	181	LYS
1	D	194	ASN
1	D	196	GLU
1	D	221	VAL
1	D	226	GLN
1	D	228	ILE
1	D	232	GLU
1	D	236	GLN
1	D	240	HIS
1	D	243	LYS
1	D	250	ARG
1	E	3	LYS
1	E	60	LYS
1	E	91	ARG
1	E	92	ILE
1	E	146	SER
1	E	147	ILE
1	E	161	THR
1	E	194	ASN
1	E	196	GLU
1	E	221	VAL
1	E	226	GLN
1	E	240	HIS
1	F	13	LYS
1	F	60	LYS
1	F	91	ARG
1	F	147	ILE
1	F	161	THR
1	F	194	ASN
1	F	196	GLU
1	F	226	GLN
1	F	228	ILE
1	F	232	GLU
1	F	234	MET
1	F	243	LYS
1	F	250	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	47	HIS
1	A	194	ASN
1	A	230	ASN
1	B	194	ASN
1	B	230	ASN
1	C	152	HIS
1	C	194	ASN
1	D	194	ASN
1	D	230	ASN
1	E	194	ASN
1	F	17	GLN
1	F	47	HIS
1	F	194	ASN
1	F	230	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	A	3401	-	4,4,4	0.89	0	6,6,6	0.44	0
2	PO4	B	4401	-	4,4,4	0.88	0	6,6,6	0.45	0
2	PO4	D	6401	-	4,4,4	0.93	0	6,6,6	0.41	0
4	182	B	4400	-	16,21,21	5.23	4 (25%)	17,27,27	1.97	2 (11%)
2	PO4	E	7401	-	4,4,4	0.91	0	6,6,6	0.41	0
4	182	C	5400	-	16,21,21	5.24	5 (31%)	17,27,27	1.95	2 (11%)
4	182	A	3400	-	16,21,21	5.25	4 (25%)	17,27,27	1.94	2 (11%)
4	182	D	6400	-	16,21,21	5.21	4 (25%)	17,27,27	1.95	2 (11%)
4	182	E	7400	-	16,21,21	5.14	5 (31%)	17,27,27	1.90	2 (11%)
2	PO4	F	8401	-	4,4,4	0.89	0	6,6,6	0.44	0
4	182	F	8400	-	16,21,21	5.13	5 (31%)	17,27,27	1.85	2 (11%)
2	PO4	C	5401	-	4,4,4	0.91	0	6,6,6	0.41	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
4	182	B	4400	-	-	1/8/9/9	0/2/2/2
4	182	E	7400	-	-	1/8/9/9	0/2/2/2
4	182	C	5400	-	-	1/8/9/9	0/2/2/2
4	182	A	3400	-	-	1/8/9/9	0/2/2/2
4	182	D	6400	-	-	1/8/9/9	0/2/2/2
4	182	F	8400	-	-	1/8/9/9	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3400	182	SE-CAP	-14.74	1.75	1.92
4	C	5400	182	SE-CAP	-14.39	1.75	1.92
4	B	4400	182	SE-CAP	-14.37	1.75	1.92
4	D	6400	182	SE-CAP	-14.02	1.75	1.92
4	F	8400	182	SE-CAP	-14.00	1.76	1.92
4	E	7400	182	SE-CAP	-13.97	1.76	1.92
4	D	6400	182	SE-CAQ	-13.53	1.76	1.92
4	C	5400	182	SE-CAQ	-13.27	1.76	1.92
4	B	4400	182	SE-CAQ	-13.23	1.76	1.92
4	E	7400	182	SE-CAQ	-13.09	1.76	1.92
4	F	8400	182	SE-CAQ	-13.06	1.76	1.92
4	A	3400	182	SE-CAQ	-12.98	1.77	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	7400	182	CAR-NAM	5.06	1.41	1.33
4	B	4400	182	CAR-NAM	5.05	1.41	1.33
4	D	6400	182	CAR-NAM	5.05	1.41	1.33
4	C	5400	182	CAR-NAM	5.01	1.41	1.33
4	A	3400	182	CAR-NAM	4.99	1.41	1.33
4	F	8400	182	CAR-NAM	4.92	1.41	1.33
4	A	3400	182	CAI-NAT	2.49	1.42	1.36
4	B	4400	182	CAI-NAT	2.48	1.42	1.36
4	C	5400	182	CAI-NAT	2.46	1.42	1.36
4	F	8400	182	CAI-NAT	2.45	1.42	1.36
4	E	7400	182	CAI-NAT	2.33	1.41	1.36
4	D	6400	182	CAI-NAT	2.32	1.41	1.36
4	E	7400	182	CAE-CAG	2.06	1.43	1.38
4	F	8400	182	CAE-CAG	2.04	1.43	1.38
4	C	5400	182	CAE-CAG	2.01	1.43	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3400	182	CAS-NAM-CAR	5.73	119.98	115.14
4	C	5400	182	CAS-NAM-CAR	5.68	119.94	115.14
4	E	7400	182	CAS-NAM-CAR	5.63	119.90	115.14
4	B	4400	182	CAS-NAM-CAR	5.59	119.86	115.14
4	D	6400	182	CAS-NAM-CAR	5.49	119.78	115.14
4	F	8400	182	CAS-NAM-CAR	5.47	119.76	115.14
4	D	6400	182	CAQ-SE-CAP	4.81	105.95	99.40
4	B	4400	182	CAQ-SE-CAP	4.73	105.85	99.40
4	C	5400	182	CAQ-SE-CAP	4.50	105.53	99.40
4	A	3400	182	CAQ-SE-CAP	4.49	105.52	99.40
4	F	8400	182	CAQ-SE-CAP	4.15	105.05	99.40
4	E	7400	182	CAQ-SE-CAP	4.14	105.05	99.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

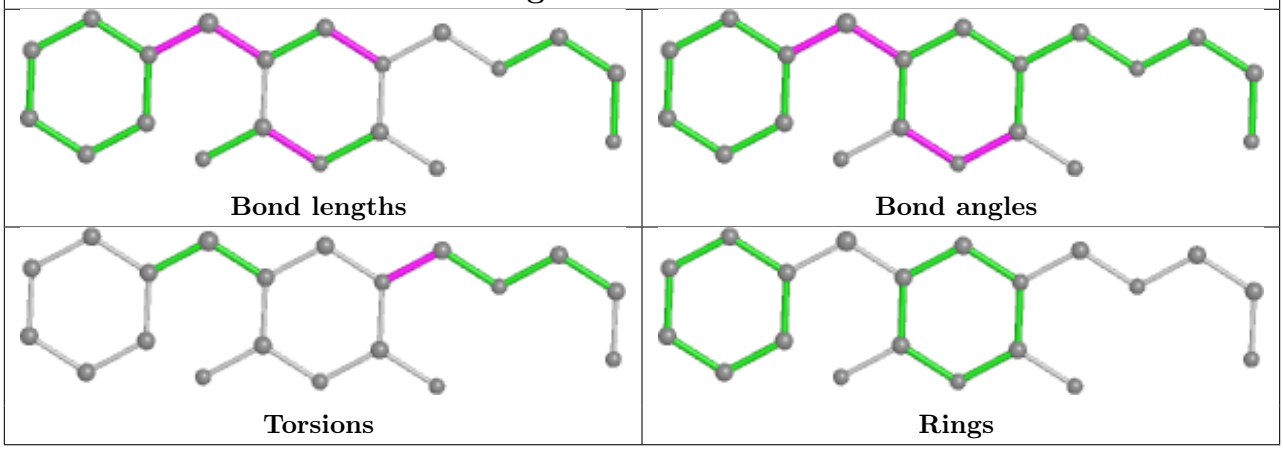
Mol	Chain	Res	Type	Atoms
4	A	3400	182	OAN-CAL-NAT-CAI
4	B	4400	182	OAN-CAL-NAT-CAI
4	C	5400	182	OAN-CAL-NAT-CAI
4	D	6400	182	OAN-CAL-NAT-CAI
4	E	7400	182	OAN-CAL-NAT-CAI
4	F	8400	182	OAN-CAL-NAT-CAI

There are no ring outliers.

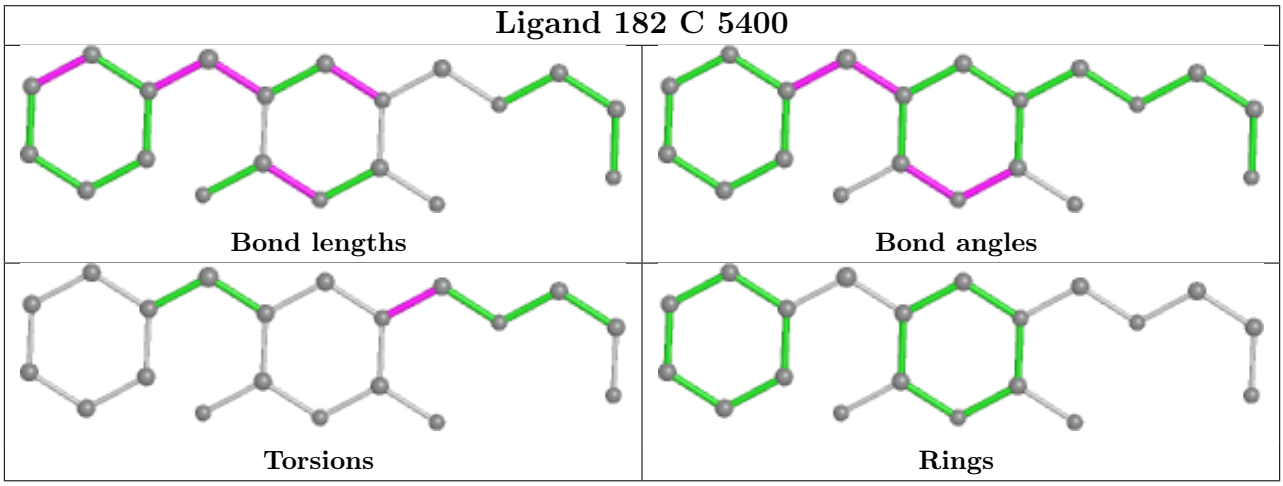
No monomer is involved in short contacts.

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.

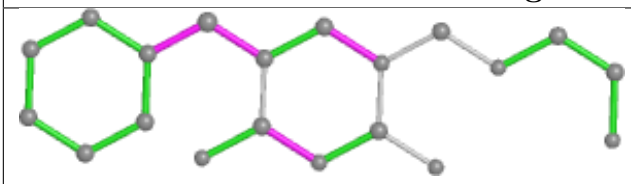
Ligand 182 B 4400



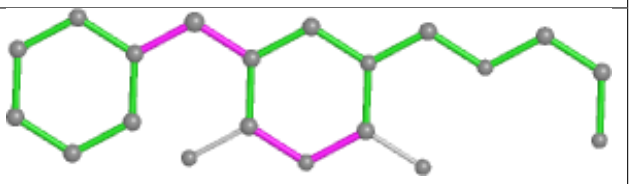
Ligand 182 C 5400



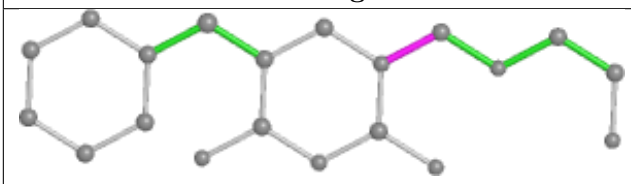
Ligand 182 A 3400



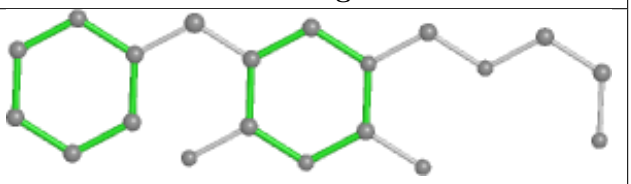
Bond lengths



Bond angles

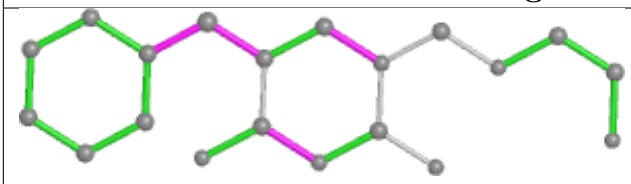


Torsions

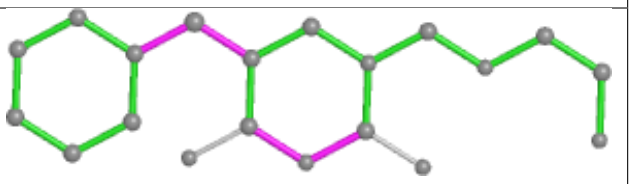


Rings

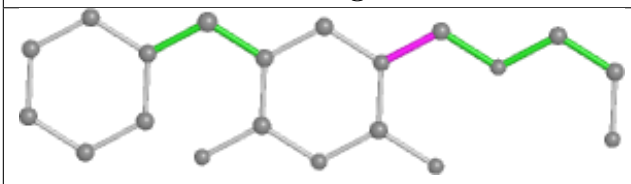
Ligand 182 D 6400



Bond lengths



Bond angles



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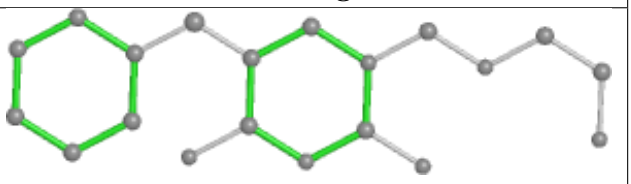
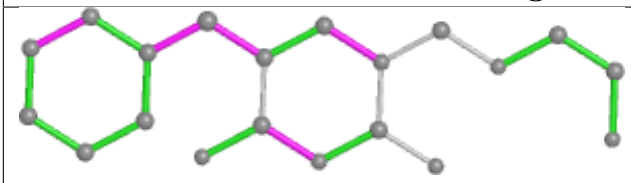
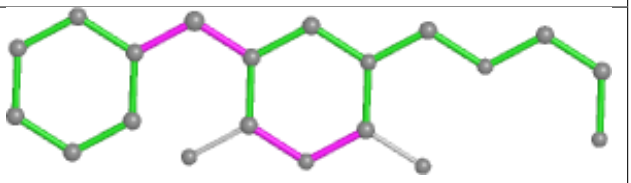


Rings

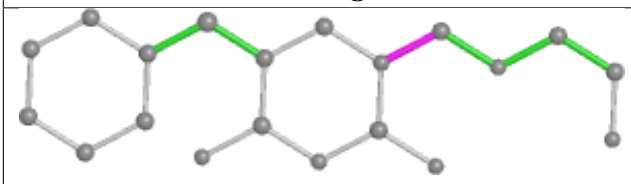
Ligand 182 E 7400



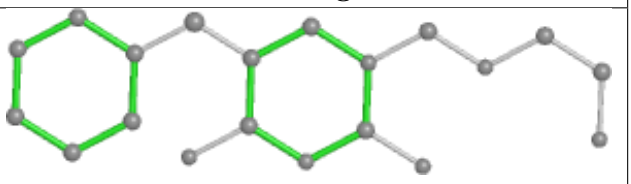
Bond lengths



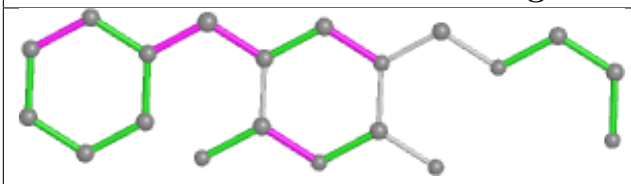
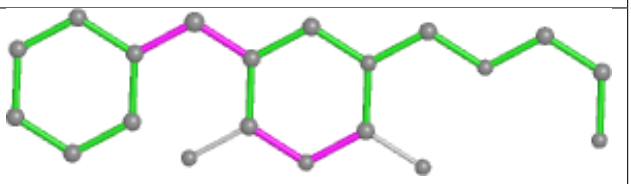
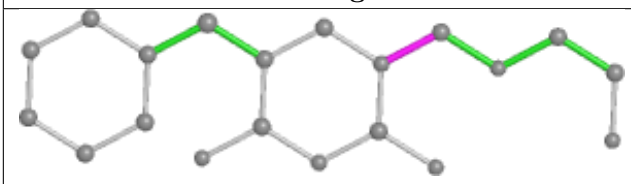
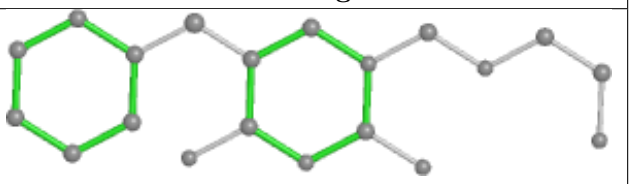
Bond angles



Torsions



Rings

Ligand 182 F 8400	
 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	253/256 (98%)	0.28	5 (1%)	65	63	8, 11, 14, 18	0
1	B	251/256 (98%)	0.24	10 (3%)	38	37	9, 11, 17, 22	0
1	C	250/256 (97%)	0.99	42 (16%)	1	1	10, 12, 14, 16	0
1	D	250/256 (97%)	0.66	23 (9%)	9	8	9, 11, 14, 18	0
1	E	251/256 (98%)	0.36	14 (5%)	24	23	8, 11, 16, 21	0
1	F	250/256 (97%)	0.17	8 (3%)	47	46	8, 11, 17, 20	0
All	All	1505/1536 (97%)	0.45	102 (6%)	17	16	8, 11, 15, 22	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	228	ILE	12.9
1	D	228	ILE	10.0
1	A	2	SER	9.5
1	C	228	ILE	9.2
1	C	229	PRO	8.5
1	F	228	ILE	7.6
1	B	228	ILE	7.5
1	C	34	ILE	6.9
1	C	37	LEU	6.8
1	B	227	GLU	6.7
1	C	41	PRO	6.5
1	C	227	GLU	6.4
1	D	229	PRO	6.4
1	F	226	GLN	6.4
1	E	226	GLN	6.2
1	D	227	GLU	6.2
1	E	227	GLU	5.9
1	D	226	GLN	5.4
1	B	226	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	226	GLN	5.3
1	E	229	PRO	5.3
1	F	231	ALA	5.3
1	D	232	GLU	5.2
1	C	231	ALA	5.1
1	C	253	LEU	5.0
1	D	57	LEU	5.0
1	E	234	MET	4.9
1	C	57	LEU	4.8
1	A	1	MET	4.8
1	B	229	PRO	4.8
1	C	36	ALA	4.8
1	C	53	TRP	4.6
1	B	231	ALA	4.4
1	C	38	MET	4.3
1	B	230	ASN	4.3
1	C	234	MET	4.3
1	F	232	GLU	4.2
1	D	230	ASN	4.1
1	C	31	VAL	4.0
1	A	231	ALA	3.6
1	E	231	ALA	3.6
1	E	230	ASN	3.5
1	C	58	ASP	3.4
1	E	3	LYS	3.4
1	E	147	ILE	3.4
1	C	236	GLN	3.4
1	F	227	GLU	3.4
1	D	62	VAL	3.3
1	C	23	ILE	3.2
1	C	250	ARG	3.1
1	C	230	ASN	3.1
1	D	236	GLN	3.1
1	D	252	LEU	3.1
1	C	60	LYS	3.0
1	C	220	ILE	3.0
1	B	240	HIS	3.0
1	C	40	LYS	3.0
1	D	234	MET	2.9
1	F	229	PRO	2.9
1	C	42	VAL	2.9
1	C	232	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	64	VAL	2.8
1	D	38	MET	2.8
1	E	240	HIS	2.8
1	C	244	ILE	2.7
1	F	147	ILE	2.7
1	D	14	ASN	2.7
1	B	232	GLU	2.7
1	B	234	MET	2.7
1	D	237	THR	2.7
1	C	148	GLY	2.6
1	C	62	VAL	2.6
1	C	16	LEU	2.6
1	E	57	LEU	2.6
1	E	232	GLU	2.5
1	B	161	THR	2.5
1	D	18	GLY	2.4
1	C	54	ARG	2.4
1	C	147	ILE	2.4
1	A	38	MET	2.4
1	D	4	SER	2.4
1	C	30	ARG	2.3
1	D	56	GLU	2.3
1	C	44	LEU	2.2
1	C	121	LEU	2.2
1	C	63	ILE	2.2
1	A	126	LEU	2.2
1	C	142	GLU	2.2
1	D	239	SER	2.2
1	F	230	ASN	2.2
1	C	33	LYS	2.1
1	D	225	GLN	2.1
1	D	13	LYS	2.1
1	D	59	GLY	2.1
1	D	126	LEU	2.1
1	C	55	ALA	2.1
1	C	240	HIS	2.1
1	E	145	LYS	2.1
1	D	58	ASP	2.0
1	C	11	LEU	2.0
1	C	35	ALA	2.0
1	E	250	ARG	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)

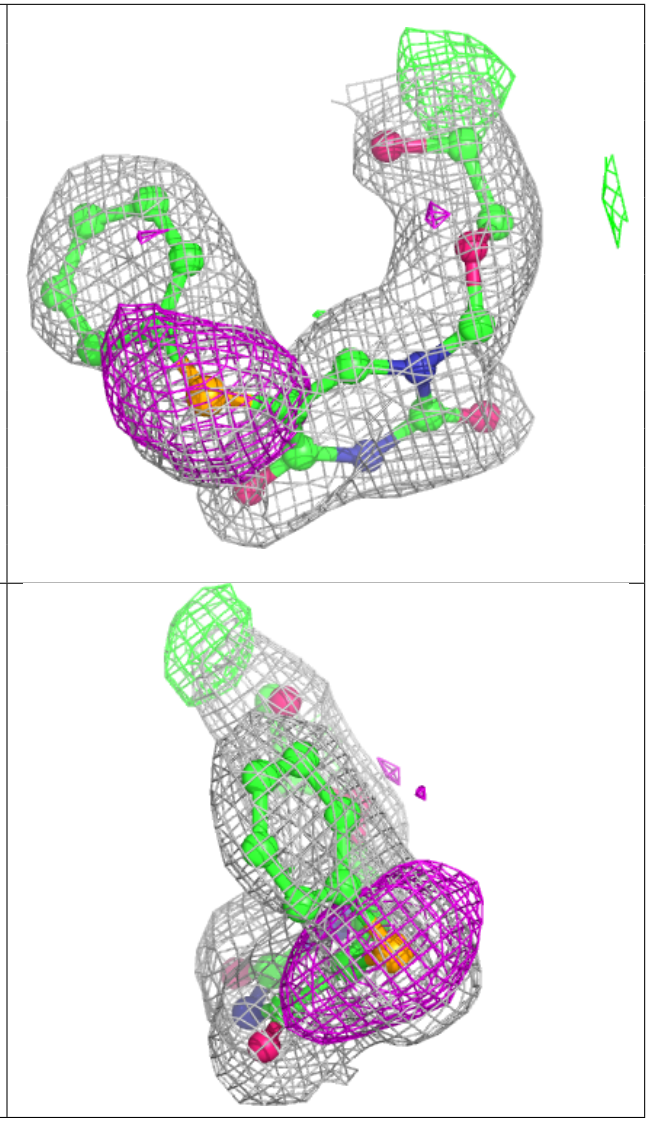
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K	C	1003	1/1	0.78	0.33	69,69,69,69	0
3	K	A	1002	1/1	0.79	0.15	63,63,63,63	0
4	182	C	5400	20/20	0.86	0.22	40,41,42,43	0
4	182	A	3400	20/20	0.88	0.17	29,32,35,35	0
4	182	B	4400	20/20	0.92	0.13	29,31,32,33	0
4	182	D	6400	20/20	0.92	0.15	36,37,40,41	0
4	182	F	8400	20/20	0.92	0.15	26,29,32,32	0
4	182	E	7400	20/20	0.93	0.14	25,27,29,29	0
2	PO4	E	7401	5/5	0.94	0.12	39,40,40,40	0
3	K	E	1001	1/1	0.94	0.28	53,53,53,53	0
2	PO4	F	8401	5/5	0.95	0.10	37,37,37,37	0
2	PO4	A	3401	5/5	0.95	0.12	39,39,39,39	0
2	PO4	D	6401	5/5	0.96	0.10	46,46,46,46	0
2	PO4	C	5401	5/5	0.96	0.19	47,47,47,47	0
2	PO4	B	4401	5/5	0.97	0.09	42,42,42,42	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.

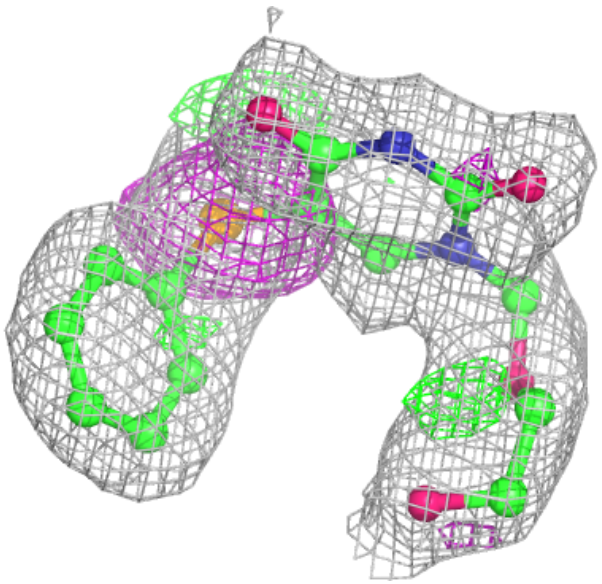
Electron density around 182 C 5400:

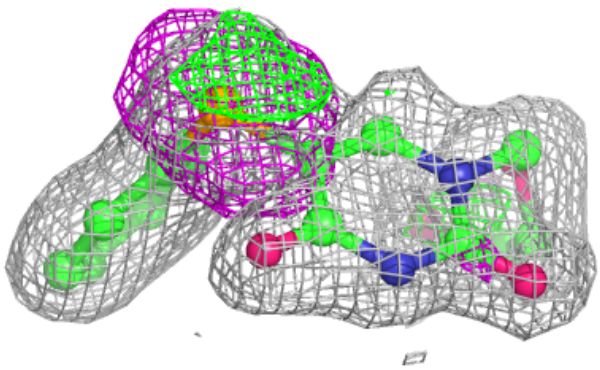
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

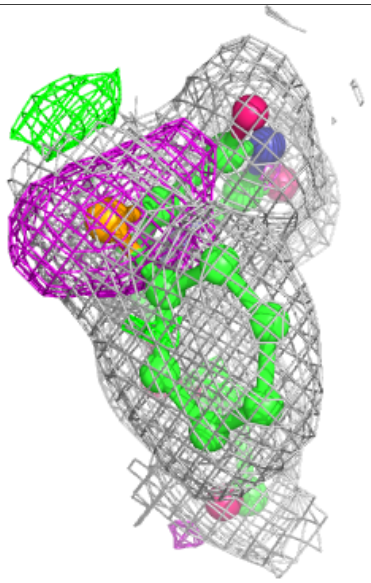


Electron density around 182 A 3400:

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

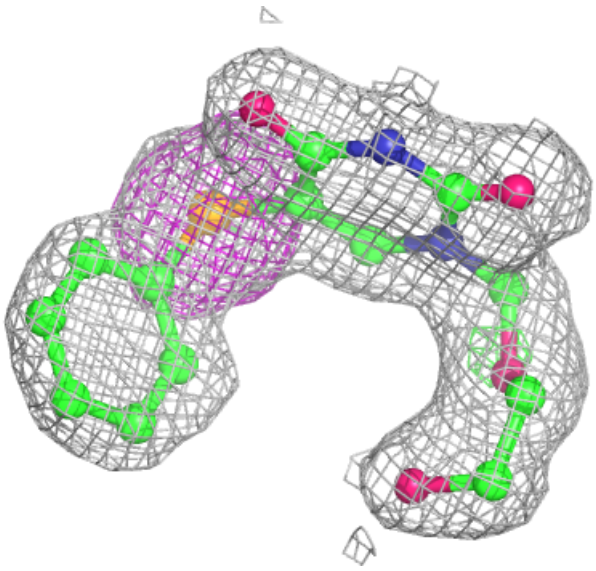


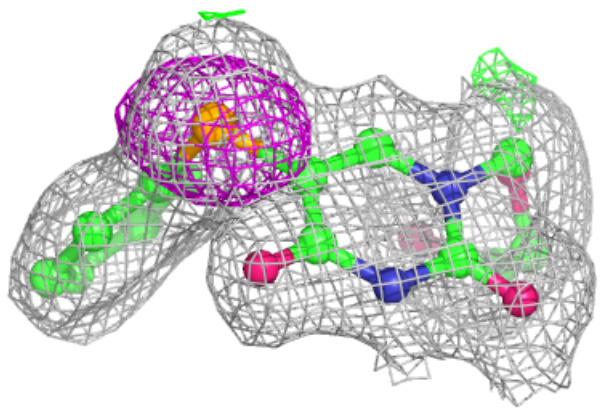


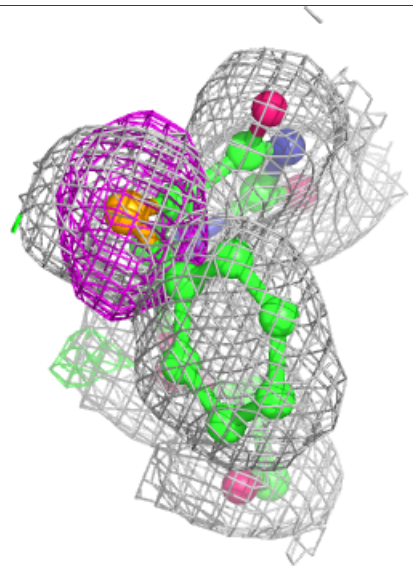


Electron density around 182 B 4400:

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

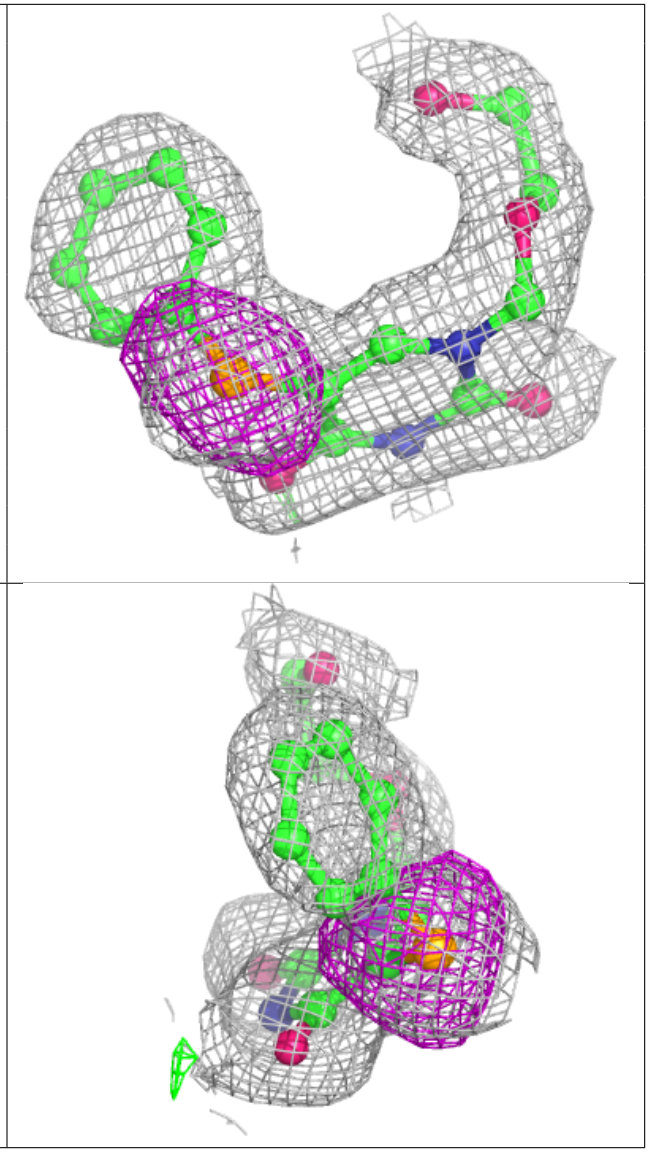






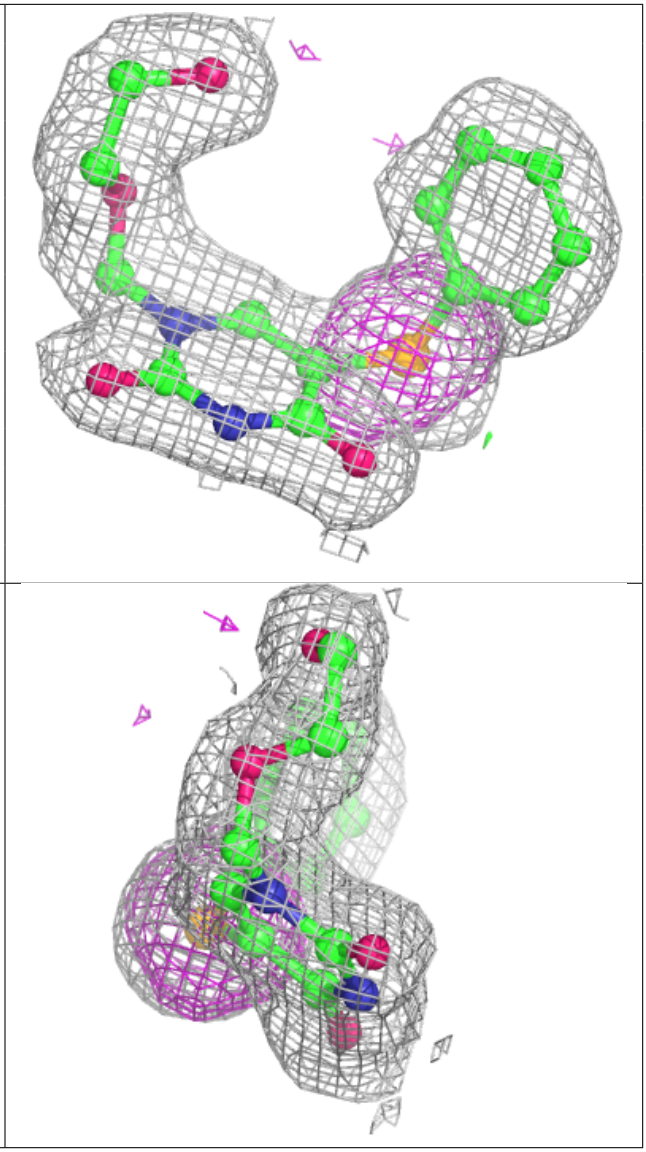
Electron density around 182 D 6400:

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



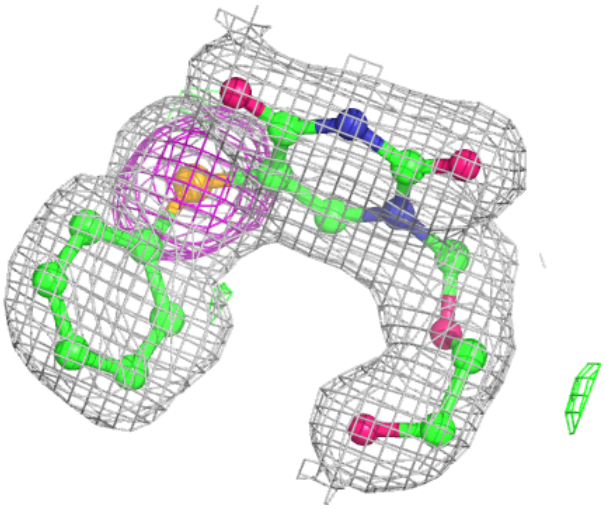
Electron density around 182 F 8400:

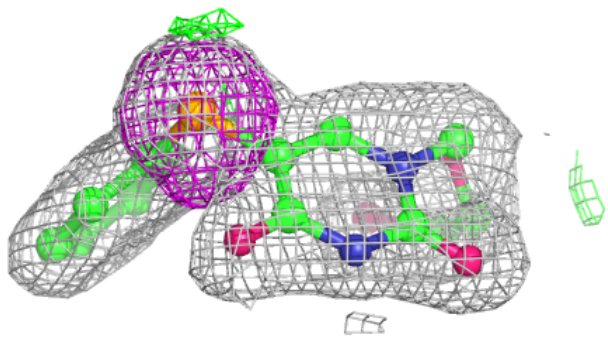
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

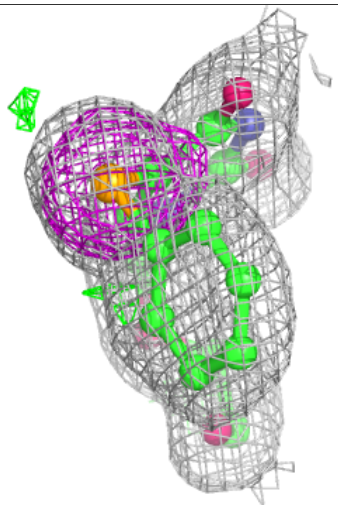


Electron density around 182 E 7400:

$2mF_o$-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.