Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 05:37 AM EDT

PDB ID	:	2QHX
Title	:	Structure of Pteridine Reductase from Leishmania major complexed with a ligand
Authors	:	Gibellini, F.; Mcluskey, K.; Tulloch, L.; Hunter, W.N.
Deposited on	:	2007-07-03
Resolution	:	2.61 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 following versions of software and data (see references (i)) were used in the production of this report:

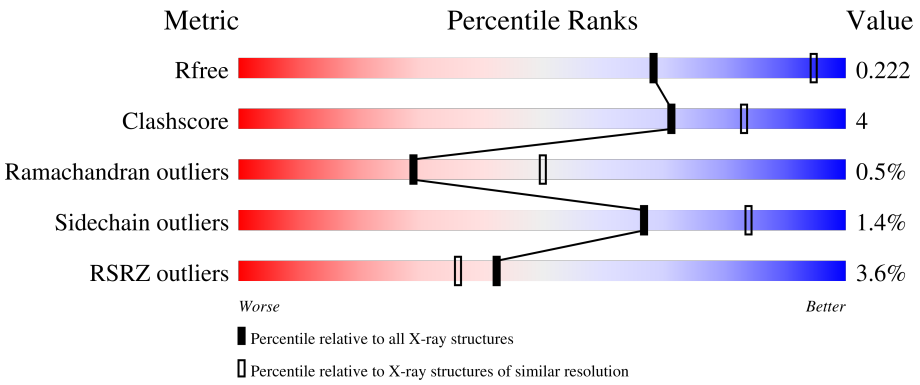
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	328	2% 74% 6% 20%
1	B	328	2% 75% 6% 19%
1	C	328	3% 72% 5% • 23%
1	D	328	4% 73% 6% 21%

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	IOD	A	1289	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8985 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 Pteridine reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	1979	1249	350	369	11	0	2	0
1	B	265	1987	1253	351	371	12	4	3	0
1	C	254	1897	1197	339	350	11	0	2	0
1	D	258	1926	1213	346	357	10	0	1	0

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-39	MET	-	expression tag	UNP Q01782
A	-38	GLY	-	expression tag	UNP Q01782
A	-37	SER	-	expression tag	UNP Q01782
A	-36	SER	-	expression tag	UNP Q01782
A	-35	HIS	-	expression tag	UNP Q01782
A	-34	HIS	-	expression tag	UNP Q01782
A	-33	HIS	-	expression tag	UNP Q01782
A	-32	HIS	-	expression tag	UNP Q01782
A	-31	HIS	-	expression tag	UNP Q01782
A	-30	HIS	-	expression tag	UNP Q01782
A	-29	SER	-	expression tag	UNP Q01782
A	-28	SER	-	expression tag	UNP Q01782
A	-27	GLY	-	expression tag	UNP Q01782
A	-26	LEU	-	expression tag	UNP Q01782
A	-25	VAL	-	expression tag	UNP Q01782
A	-24	PRO	-	expression tag	UNP Q01782
A	-23	ARG	-	expression tag	UNP Q01782
A	-22	GLY	-	expression tag	UNP Q01782
A	-21	SER	-	expression tag	UNP Q01782
A	-20	HIS	-	expression tag	UNP Q01782
A	-19	MET	-	expression tag	UNP Q01782

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP Q01782
A	-17	SER	-	expression tag	UNP Q01782
A	-16	SER	-	expression tag	UNP Q01782
A	-15	HIS	-	expression tag	UNP Q01782
A	-14	HIS	-	expression tag	UNP Q01782
A	-13	HIS	-	expression tag	UNP Q01782
A	-12	HIS	-	expression tag	UNP Q01782
A	-11	HIS	-	expression tag	UNP Q01782
A	-10	HIS	-	expression tag	UNP Q01782
A	-9	SER	-	expression tag	UNP Q01782
A	-8	SER	-	expression tag	UNP Q01782
A	-7	GLY	-	expression tag	UNP Q01782
A	-6	LEU	-	expression tag	UNP Q01782
A	-5	VAL	-	expression tag	UNP Q01782
A	-4	PRO	-	expression tag	UNP Q01782
A	-3	ARG	-	expression tag	UNP Q01782
A	-2	GLY	-	expression tag	UNP Q01782
A	-1	SER	-	expression tag	UNP Q01782
A	0	HIS	-	expression tag	UNP Q01782
A	162	VAL	PHE	SEE REMARK 999	UNP Q01782
B	-39	MET	-	expression tag	UNP Q01782
B	-38	GLY	-	expression tag	UNP Q01782
B	-37	SER	-	expression tag	UNP Q01782
B	-36	SER	-	expression tag	UNP Q01782
B	-35	HIS	-	expression tag	UNP Q01782
B	-34	HIS	-	expression tag	UNP Q01782
B	-33	HIS	-	expression tag	UNP Q01782
B	-32	HIS	-	expression tag	UNP Q01782
B	-31	HIS	-	expression tag	UNP Q01782
B	-30	HIS	-	expression tag	UNP Q01782
B	-29	SER	-	expression tag	UNP Q01782
B	-28	SER	-	expression tag	UNP Q01782
B	-27	GLY	-	expression tag	UNP Q01782
B	-26	LEU	-	expression tag	UNP Q01782
B	-25	VAL	-	expression tag	UNP Q01782
B	-24	PRO	-	expression tag	UNP Q01782
B	-23	ARG	-	expression tag	UNP Q01782
B	-22	GLY	-	expression tag	UNP Q01782
B	-21	SER	-	expression tag	UNP Q01782
B	-20	HIS	-	expression tag	UNP Q01782
B	-19	MET	-	expression tag	UNP Q01782
B	-18	GLY	-	expression tag	UNP Q01782

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP Q01782
B	-16	SER	-	expression tag	UNP Q01782
B	-15	HIS	-	expression tag	UNP Q01782
B	-14	HIS	-	expression tag	UNP Q01782
B	-13	HIS	-	expression tag	UNP Q01782
B	-12	HIS	-	expression tag	UNP Q01782
B	-11	HIS	-	expression tag	UNP Q01782
B	-10	HIS	-	expression tag	UNP Q01782
B	-9	SER	-	expression tag	UNP Q01782
B	-8	SER	-	expression tag	UNP Q01782
B	-7	GLY	-	expression tag	UNP Q01782
B	-6	LEU	-	expression tag	UNP Q01782
B	-5	VAL	-	expression tag	UNP Q01782
B	-4	PRO	-	expression tag	UNP Q01782
B	-3	ARG	-	expression tag	UNP Q01782
B	-2	GLY	-	expression tag	UNP Q01782
B	-1	SER	-	expression tag	UNP Q01782
B	0	HIS	-	expression tag	UNP Q01782
B	162	VAL	PHE	SEE REMARK 999	UNP Q01782
C	-39	MET	-	expression tag	UNP Q01782
C	-38	GLY	-	expression tag	UNP Q01782
C	-37	SER	-	expression tag	UNP Q01782
C	-36	SER	-	expression tag	UNP Q01782
C	-35	HIS	-	expression tag	UNP Q01782
C	-34	HIS	-	expression tag	UNP Q01782
C	-33	HIS	-	expression tag	UNP Q01782
C	-32	HIS	-	expression tag	UNP Q01782
C	-31	HIS	-	expression tag	UNP Q01782
C	-30	HIS	-	expression tag	UNP Q01782
C	-29	SER	-	expression tag	UNP Q01782
C	-28	SER	-	expression tag	UNP Q01782
C	-27	GLY	-	expression tag	UNP Q01782
C	-26	LEU	-	expression tag	UNP Q01782
C	-25	VAL	-	expression tag	UNP Q01782
C	-24	PRO	-	expression tag	UNP Q01782
C	-23	ARG	-	expression tag	UNP Q01782
C	-22	GLY	-	expression tag	UNP Q01782
C	-21	SER	-	expression tag	UNP Q01782
C	-20	HIS	-	expression tag	UNP Q01782
C	-19	MET	-	expression tag	UNP Q01782
C	-18	GLY	-	expression tag	UNP Q01782
C	-17	SER	-	expression tag	UNP Q01782

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	SER	-	expression tag	UNP Q01782
C	-15	HIS	-	expression tag	UNP Q01782
C	-14	HIS	-	expression tag	UNP Q01782
C	-13	HIS	-	expression tag	UNP Q01782
C	-12	HIS	-	expression tag	UNP Q01782
C	-11	HIS	-	expression tag	UNP Q01782
C	-10	HIS	-	expression tag	UNP Q01782
C	-9	SER	-	expression tag	UNP Q01782
C	-8	SER	-	expression tag	UNP Q01782
C	-7	GLY	-	expression tag	UNP Q01782
C	-6	LEU	-	expression tag	UNP Q01782
C	-5	VAL	-	expression tag	UNP Q01782
C	-4	PRO	-	expression tag	UNP Q01782
C	-3	ARG	-	expression tag	UNP Q01782
C	-2	GLY	-	expression tag	UNP Q01782
C	-1	SER	-	expression tag	UNP Q01782
C	0	HIS	-	expression tag	UNP Q01782
C	162	VAL	PHE	SEE REMARK 999	UNP Q01782
D	-39	MET	-	expression tag	UNP Q01782
D	-38	GLY	-	expression tag	UNP Q01782
D	-37	SER	-	expression tag	UNP Q01782
D	-36	SER	-	engineered mutation	UNP Q01782
D	-35	HIS	-	expression tag	UNP Q01782
D	-34	HIS	-	expression tag	UNP Q01782
D	-33	HIS	-	expression tag	UNP Q01782
D	-32	HIS	-	expression tag	UNP Q01782
D	-31	HIS	-	expression tag	UNP Q01782
D	-30	HIS	-	expression tag	UNP Q01782
D	-29	SER	-	expression tag	UNP Q01782
D	-28	SER	-	expression tag	UNP Q01782
D	-27	GLY	-	expression tag	UNP Q01782
D	-26	LEU	-	expression tag	UNP Q01782
D	-25	VAL	-	expression tag	UNP Q01782
D	-24	PRO	-	expression tag	UNP Q01782
D	-23	ARG	-	expression tag	UNP Q01782
D	-22	GLY	-	expression tag	UNP Q01782
D	-21	SER	-	expression tag	UNP Q01782
D	-20	HIS	-	expression tag	UNP Q01782
D	-19	MET	-	expression tag	UNP Q01782
D	-18	GLY	-	expression tag	UNP Q01782
D	-17	SER	-	expression tag	UNP Q01782
D	-16	SER	-	expression tag	UNP Q01782

Continued on next page...

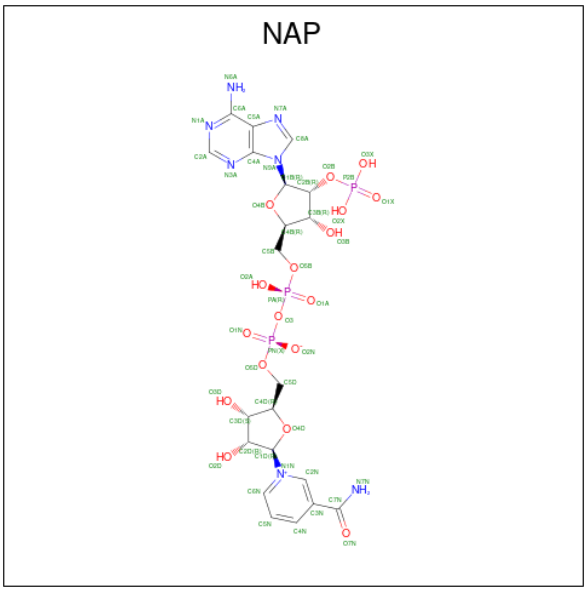
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	HIS	-	expression tag	UNP Q01782
D	-14	HIS	-	expression tag	UNP Q01782
D	-13	HIS	-	expression tag	UNP Q01782
D	-12	HIS	-	expression tag	UNP Q01782
D	-11	HIS	-	expression tag	UNP Q01782
D	-10	HIS	-	expression tag	UNP Q01782
D	-9	SER	-	expression tag	UNP Q01782
D	-8	SER	-	expression tag	UNP Q01782
D	-7	GLY	-	expression tag	UNP Q01782
D	-6	LEU	-	expression tag	UNP Q01782
D	-5	VAL	-	expression tag	UNP Q01782
D	-4	PRO	-	expression tag	UNP Q01782
D	-3	ARG	-	expression tag	UNP Q01782
D	-2	GLY	-	expression tag	UNP Q01782
D	-1	SER	-	expression tag	UNP Q01782
D	0	HIS	-	expression tag	UNP Q01782
D	162	VAL	PHE	SEE REMARK 999	UNP Q01782

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

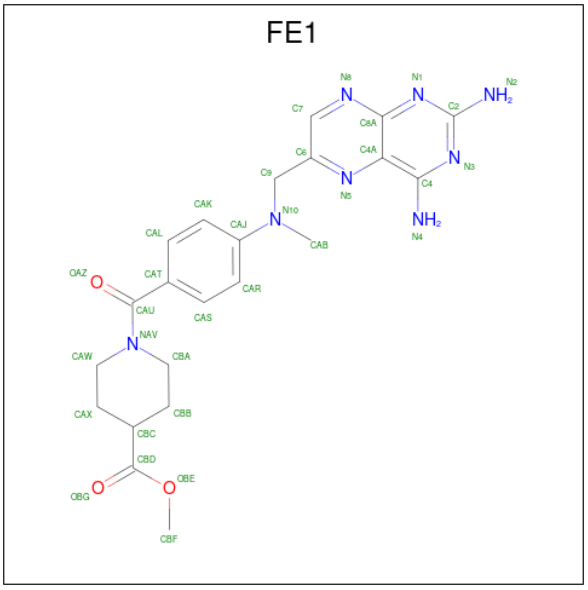
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
2	A	1	1	1	0	0
			Total	I		
2	B	1	1	1	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	B	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	C	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	D	1	48	21	7	17	3	0	0

- Molecule 4 is METHYL 1-(4-{[(2,4-DIAMINOPTERIDIN-6-YL)METHYL](METHYL)AMINO}BENZOYL)PIPERIDINE-4-CARBOXYLATE (three-letter code: FE1) (formula: $C_{22}H_{26}N_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	65	43	16	6	0	1
4	B	1	65	43	16	6	0	1
4	C	1	33	22	8	3	0	1
4	D	1	33	22	8	3	0	1

- Molecule 5 is water.

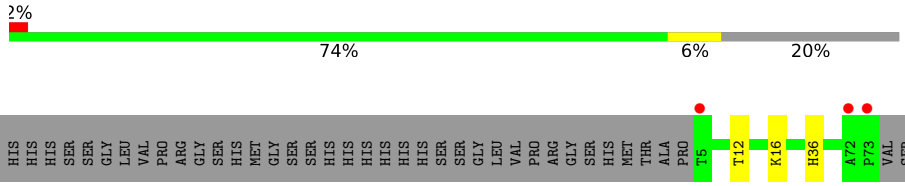
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	221	221	221	0	0
5	B	175	175	175	0	0
5	C	220	220	220	0	0
5	D	190	190	190	0	0

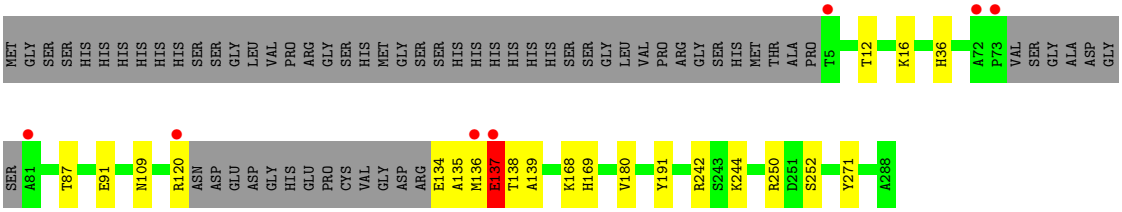
3 Residue-property plots (i)

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: Pteridine reductase 1

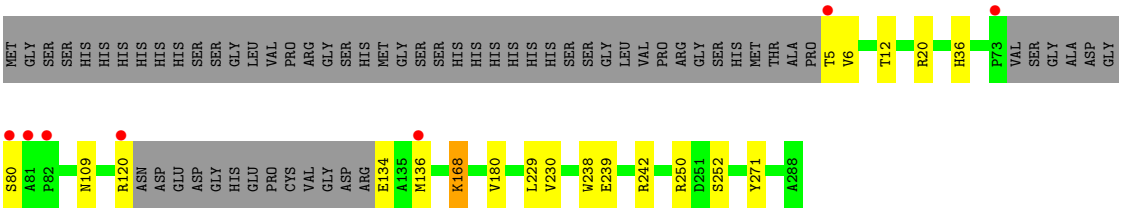
Chain A:





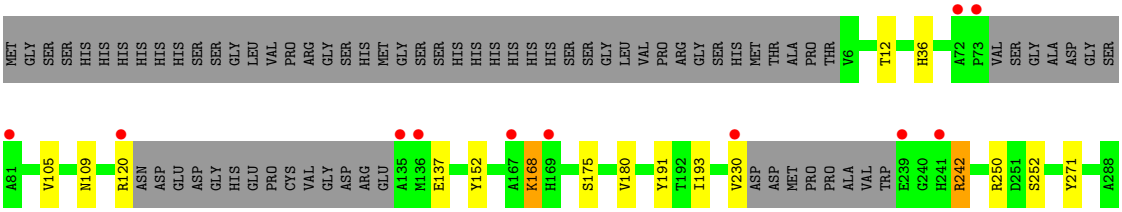
• Molecule 1: Pteridine reductase 1

Chain B:



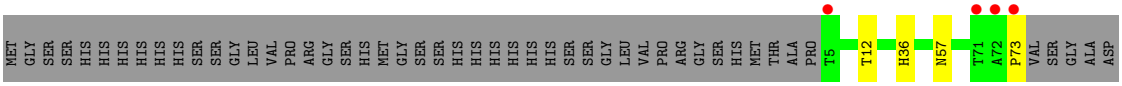
• Molecule 1: Pteridine reductase 1

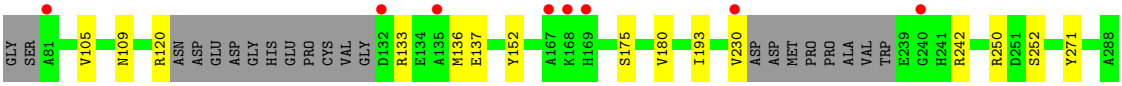
Chain C:



• Molecule 1: Pteridine reductase 1

Chain D:




GLY
SER
A81
V105
N109
R120
ASN
ASP
GLU
ASP
GLY
HIS
GLU
PRO
CYS
VAL
GLY
D132
R133
E134
A135
M136
E137
Y152
A167
K168
H169
S175
V180
I193
V230
ASP
ASP
MET
PRO
PRO
ALA
VAL
TRP
E239
G240
H241
R242
R250
D251
S252
Y271
A288

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.50Å 104.23Å 136.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.60 – 2.61 28.60 – 2.61	Depositor EDS
% Data completeness (in resolution range)	95.3 (28.60-2.61) 95.4 (28.60-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183 , 0.228 0.180 , 0.222	Depositor DCC
R_{free} test set	2030 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8985	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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 25.74 % 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 2.9968e-03. 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: FE1, IOD, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.40	0/2027	0.56	1/2762 (0.0%)
1	B	0.47	1/2039 (0.0%)	0.55	2/2778 (0.1%)
1	C	0.39	0/1939	0.51	0/2637
1	D	0.40	0/1965	0.52	0/2672
All	All	0.41	1/7970 (0.0%)	0.54	3/10849 (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	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	LYS	CB-CG	10.51	1.80	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	168	LYS	CB-CG-CD	5.98	127.14	111.60
1	B	168	LYS	CA-CB-CG	-5.42	101.47	113.40
1	A	137	GLU	N-CA-CB	5.34	120.21	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	ALA	Peptide
1	A	136	MET	Peptide
1	A	137	GLU	Peptide

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	1979	0	1982	14	1
1	B	1987	0	1988	11	0
1	C	1897	0	1916	14	0
1	D	1926	0	1939	13	1
2	A	1	0	0	2	0
2	B	1	0	0	1	0
3	A	48	0	25	0	0
3	B	48	0	25	0	0
3	C	48	0	25	0	0
3	D	48	0	25	0	0
4	A	65	0	52	6	0
4	B	65	0	52	4	0
4	C	33	0	26	2	0
4	D	33	0	26	1	0
5	A	221	0	0	4	0
5	B	175	0	0	6	0
5	C	220	0	0	3	0
5	D	190	0	0	5	0
All	All	8985	0	8081	57	1

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 (57) 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:137:GLU:HG2	5:C:1511:HOH:O	1.78	0.84
1:A:137:GLU:HA	5:A:1507:HOH:O	1.82	0.79
1:D:12:THR:HA	1:D:36:HIS:HB3	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:THR:HA	1:C:36:HIS:HB3	1.73	0.70
1:A:12:THR:HA	1:A:36:HIS:HB3	1.74	0.69
1:B:12:THR:HA	1:B:36:HIS:HB3	1.74	0.69
4:A:1301[B]:FE1:HAB1	5:D:1394:HOH:O	1.95	0.67
1:C:230:VAL:HG23	5:C:1514:HOH:O	1.93	0.67
4:A:1301[B]:FE1:CAB	5:D:1394:HOH:O	2.48	0.61
4:A:1301[A]:FE1:HAW2	4:A:1301[A]:FE1:CAL	2.32	0.60
1:C:191:TYR:OH	4:C:1305[A]:FE1:HBA1	2.01	0.60
2:A:1289:IOD:I	5:B:1443:HOH:O	2.87	0.59
1:B:136:MET:HB2	5:B:1350:HOH:O	2.02	0.59
1:A:168:LYS:HG3	1:A:169:HIS:ND1	2.18	0.59
1:B:6:VAL:HA	5:B:1463:HOH:O	2.03	0.57
1:C:230:VAL:HG21	5:C:1474:HOH:O	2.04	0.57
1:D:133:ARG:O	1:D:136:MET:HG2	2.04	0.57
4:A:1301[B]:FE1:HAW1	4:A:1301[B]:FE1:CAS	2.35	0.56
1:B:239:GLU:HG3	5:B:1437:HOH:O	2.07	0.53
2:A:1289:IOD:I	2:B:1288:IOD:I	3.68	0.51
4:C:1305[A]:FE1:HBA2	4:C:1305[A]:FE1:CAL	2.40	0.50
4:D:1307[A]:FE1:CAL	4:D:1307[A]:FE1:HBA2	2.43	0.49
1:A:271:TYR:CE2	1:C:252:SER:HB3	2.48	0.48
1:A:137:GLU:H	1:A:139:ALA:H	1.63	0.47
1:A:242:ARG:HB2	1:A:250:ARG:HA	1.95	0.47
1:C:193:ILE:HD11	1:D:152:TYR:CE2	2.49	0.47
1:D:242:ARG:HB2	1:D:250:ARG:HA	1.97	0.47
1:C:242:ARG:HB2	1:C:250:ARG:HA	1.96	0.47
1:B:229:LEU:HD12	4:B:1303[B]:FE1:HAB2	1.97	0.47
1:A:87:THR:O	1:A:91[A]:GLU:HG3	2.15	0.46
1:B:242:ARG:HB2	1:B:250:ARG:HA	1.97	0.46
1:D:230:VAL:HG23	5:D:1334:HOH:O	2.15	0.46
1:C:152:TYR:CE2	1:D:193:ILE:HD11	2.50	0.46
1:A:134:GLU:N	5:A:1459:HOH:O	2.49	0.45
1:A:12:THR:O	1:A:109:ASN:HB3	2.16	0.45
1:A:252:SER:HB3	1:C:271:TYR:CE2	2.51	0.45
1:A:244:LYS:NZ	5:A:1517:HOH:O	2.45	0.44
1:C:12:THR:O	1:C:109:ASN:HB3	2.17	0.44
1:D:12:THR:O	1:D:109:ASN:HB3	2.18	0.44
1:C:168:LYS:HD3	1:C:168:LYS:H	1.83	0.44
1:B:12:THR:O	1:B:109:ASN:HB3	2.18	0.44
1:D:73:PRO:HG3	5:D:1457:HOH:O	2.16	0.44
1:B:238:TRP:HZ2	5:B:1469:HOH:O	2.01	0.43
4:A:1301[A]:FE1:HAK	4:A:1301[A]:FE1:H92	1.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:SER:HB3	1:D:271:TYR:CE2	2.54	0.43
1:A:16:LYS:NZ	5:A:1444:HOH:O	2.51	0.43
1:B:20:ARG:HD2	5:B:1473:HOH:O	2.19	0.42
1:A:191:TYR:OH	4:A:1301[B]:FE1:HAW2	2.20	0.42
1:A:168:LYS:NZ	1:A:169:HIS:CE1	2.88	0.42
4:B:1303[B]:FE1:HAR	4:B:1303[B]:FE1:H91	1.74	0.42
1:B:271:TYR:CE2	1:D:252:SER:HB3	2.55	0.42
1:D:105:VAL:HA	1:D:175:SER:O	2.20	0.41
4:B:1303[A]:FE1:HAK	4:B:1303[A]:FE1:H92	1.82	0.41
4:B:1303[B]:FE1:CAB	4:B:1303[B]:FE1:N5	2.85	0.40
1:C:193:ILE:HD11	1:D:152:TYR:CD2	2.57	0.40
1:C:105:VAL:HA	1:C:175:SER:O	2.22	0.40
1:D:137:GLU:HG2	5:D:1493:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:O	1:D:57:ASN:OD1[2_564]	2.17	0.03

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	260/328 (79%)	244 (94%)	14 (5%)	2 (1%)	19	36
1	B	262/328 (80%)	248 (95%)	13 (5%)	1 (0%)	34	55
1	C	248/328 (76%)	236 (95%)	11 (4%)	1 (0%)	34	55
1	D	251/328 (76%)	240 (96%)	10 (4%)	1 (0%)	34	55
All	All	1021/1312 (78%)	968 (95%)	48 (5%)	5 (0%)	29	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	THR
1	B	180	VAL
1	D	180	VAL
1	A	180	VAL
1	C	180	VAL

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	207/257 (80%)	206 (100%)	1 (0%)	88	95
1	B	209/257 (81%)	203 (97%)	6 (3%)	42	67
1	C	198/257 (77%)	195 (98%)	3 (2%)	65	82
1	D	200/257 (78%)	199 (100%)	1 (0%)	88	95
All	All	814/1028 (79%)	803 (99%)	11 (1%)	67	84

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

Mol	Chain	Res	Type
1	A	120	ARG
1	B	5	THR
1	B	80	SER
1	B	120	ARG
1	B	134	GLU
1	B	168	LYS
1	B	230	VAL
1	C	120	ARG
1	C	168	LYS
1	C	242	ARG
1	D	120	ARG

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	169	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	216	GLN
1	A	249	GLN
1	B	216	GLN
1	C	216	GLN
1	D	216	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)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
3	NAP	A	1300	-	45,52,52	1.70	3 (6%)	56,80,80	1.10	1 (1%)
3	NAP	B	1302	-	45,52,52	1.66	4 (8%)	56,80,80	1.10	2 (3%)
4	FE1	A	1301[B]	-	36,36,36	1.14	2 (5%)	48,51,51	1.92	11 (22%)
4	FE1	B	1303[B]	-	36,36,36	1.16	2 (5%)	48,51,51	2.05	12 (25%)
3	NAP	C	1304	-	45,52,52	1.71	4 (8%)	56,80,80	1.06	1 (1%)
4	FE1	A	1301[A]	-	36,36,36	1.15	1 (2%)	48,51,51	1.96	12 (25%)
4	FE1	C	1305[A]	-	36,36,36	1.18	2 (5%)	48,51,51	1.95	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FE1	B	1303[A]	-	36,36,36	1.15	1 (2%)	48,51,51	2.26	16 (33%)
3	NAP	D	1306	-	45,52,52	1.72	3 (6%)	56,80,80	1.13	1 (1%)
4	FE1	D	1307[A]	-	36,36,36	1.19	2 (5%)	48,51,51	2.04	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	A	1300	-	-	0/31/67/67	0/5/5/5
3	NAP	B	1302	-	-	0/31/67/67	0/5/5/5
4	FE1	A	1301[B]	-	-	2/22/32/32	1/4/4/4
4	FE1	B	1303[B]	-	-	3/22/32/32	1/4/4/4
3	NAP	C	1304	-	-	0/31/67/67	0/5/5/5
4	FE1	A	1301[A]	-	-	3/22/32/32	0/4/4/4
4	FE1	C	1305[A]	-	-	2/22/32/32	1/4/4/4
4	FE1	B	1303[A]	-	-	3/22/32/32	1/4/4/4
3	NAP	D	1306	-	-	0/31/67/67	0/5/5/5
4	FE1	D	1307[A]	-	-	2/22/32/32	1/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1306	NAP	O7N-C7N	9.16	1.41	1.24
3	A	1300	NAP	O7N-C7N	9.00	1.41	1.24
3	C	1304	NAP	O7N-C7N	8.82	1.41	1.24
3	B	1302	NAP	O7N-C7N	8.62	1.40	1.24
4	C	1305[A]	FE1	OBE-CBD	5.57	1.46	1.33
4	B	1303[A]	FE1	OBE-CBD	5.56	1.46	1.33
4	D	1307[A]	FE1	OBE-CBD	5.55	1.46	1.33
4	B	1303[B]	FE1	OBE-CBD	5.51	1.46	1.33
4	A	1301[B]	FE1	OBE-CBD	5.42	1.46	1.33
4	A	1301[A]	FE1	OBE-CBD	5.42	1.46	1.33
3	C	1304	NAP	C2A-N3A	4.23	1.38	1.32
3	A	1300	NAP	C2A-N3A	3.92	1.38	1.32
3	D	1306	NAP	C2A-N3A	3.92	1.38	1.32
3	B	1302	NAP	C2A-N3A	3.62	1.37	1.32
3	A	1300	NAP	C2A-N1A	2.73	1.39	1.33
3	B	1302	NAP	C2A-N1A	2.72	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1304	NAP	C2A-N1A	2.59	1.38	1.33
3	D	1306	NAP	C2A-N1A	2.54	1.38	1.33
4	B	1303[B]	FE1	C7-N8	2.30	1.35	1.31
3	C	1304	NAP	C2N-N1N	2.25	1.37	1.35
3	B	1302	NAP	C2N-N1N	2.18	1.37	1.35
4	D	1307[A]	FE1	C6-N5	2.16	1.36	1.32
4	A	1301[B]	FE1	C7-N8	2.07	1.35	1.31
4	C	1305[A]	FE1	C6-N5	2.05	1.36	1.32

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1305[A]	FE1	OBE-CBD-CBC	6.27	121.36	111.76
4	B	1303[A]	FE1	CAT-CAU-NAV	6.23	126.63	118.72
4	D	1307[A]	FE1	OBE-CBD-CBC	6.15	121.17	111.76
4	B	1303[A]	FE1	OBE-CBD-CBC	6.02	120.97	111.76
3	D	1306	NAP	N3A-C2A-N1A	-5.87	119.51	128.68
4	B	1303[B]	FE1	OBE-CBD-CBC	5.46	120.12	111.76
3	C	1304	NAP	N3A-C2A-N1A	-5.41	120.23	128.68
3	B	1302	NAP	N3A-C2A-N1A	-5.40	120.23	128.68
3	A	1300	NAP	N3A-C2A-N1A	-5.35	120.31	128.68
4	B	1303[B]	FE1	N8-C8A-N1	5.26	121.82	115.82
4	A	1301[A]	FE1	OBE-CBD-CBC	5.04	119.48	111.76
4	D	1307[A]	FE1	N1-C2-N3	-5.01	120.53	127.22
4	D	1307[A]	FE1	C2-N1-C8A	4.92	120.98	115.36
4	B	1303[B]	FE1	N1-C2-N3	-4.91	120.67	127.22
4	A	1301[B]	FE1	N8-C8A-N1	4.85	121.36	115.82
4	A	1301[B]	FE1	N1-C2-N3	-4.83	120.77	127.22
4	A	1301[B]	FE1	OBE-CBD-CBC	4.73	119.00	111.76
4	C	1305[A]	FE1	N1-C2-N3	-4.60	121.08	127.22
4	A	1301[A]	FE1	N8-C8A-N1	4.54	121.00	115.82
4	A	1301[A]	FE1	N1-C2-N3	-4.53	121.18	127.22
4	A	1301[B]	FE1	C2-N1-C8A	4.51	120.51	115.36
4	A	1301[A]	FE1	C2-N1-C8A	4.47	120.46	115.36
4	B	1303[A]	FE1	C2-N1-C8A	4.45	120.44	115.36
4	B	1303[B]	FE1	C2-N1-C8A	4.32	120.30	115.36
4	B	1303[A]	FE1	N1-C2-N3	-4.24	121.57	127.22
4	B	1303[B]	FE1	C7-N8-C8A	4.10	120.81	116.69
4	C	1305[A]	FE1	C2-N1-C8A	4.09	120.03	115.36
4	D	1307[A]	FE1	N8-C8A-N1	4.01	120.40	115.82
4	C	1305[A]	FE1	N8-C8A-N1	3.92	120.30	115.82
4	B	1303[A]	FE1	N8-C8A-N1	3.90	120.27	115.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1303[A]	FE1	C6-C7-N8	-3.66	119.54	123.13
4	A	1301[A]	FE1	C7-N8-C8A	3.64	120.35	116.69
4	A	1301[B]	FE1	C7-N8-C8A	3.63	120.34	116.69
4	A	1301[A]	FE1	C6-C7-N8	-3.54	119.66	123.13
4	B	1303[A]	FE1	C7-N8-C8A	3.54	120.25	116.69
4	C	1305[A]	FE1	C7-N8-C8A	3.52	120.23	116.69
4	D	1307[A]	FE1	C7-N8-C8A	3.35	120.06	116.69
4	B	1303[A]	FE1	CBB-CBA-NAV	-3.32	105.77	110.82
4	A	1301[B]	FE1	C6-C7-N8	-3.27	119.92	123.13
4	B	1303[B]	FE1	C6-C7-N8	-3.14	120.05	123.13
4	D	1307[A]	FE1	C6-C7-N8	-3.13	120.06	123.13
4	C	1305[A]	FE1	C6-C7-N8	-3.11	120.08	123.13
4	B	1303[B]	FE1	C7-C6-N5	-2.97	118.91	120.85
4	C	1305[A]	FE1	OBE-CBD-OBG	-2.93	118.10	123.84
4	B	1303[B]	FE1	OBE-CBD-OBG	-2.93	118.11	123.84
4	B	1303[A]	FE1	OAZ-CAU-NAV	-2.76	117.77	122.34
4	A	1301[A]	FE1	OBE-CBD-OBG	-2.76	118.45	123.84
4	D	1307[A]	FE1	OBE-CBD-OBG	-2.73	118.49	123.84
4	A	1301[A]	FE1	C4A-C4-N3	-2.71	119.23	121.01
4	C	1305[A]	FE1	CBB-CBA-NAV	-2.66	106.78	110.82
4	B	1303[A]	FE1	C8A-C4A-N5	-2.61	119.26	122.41
4	A	1301[A]	FE1	CAX-CAW-NAV	-2.61	106.86	110.82
4	C	1305[A]	FE1	CBF-OBE-CBD	2.61	121.83	115.94
4	B	1303[A]	FE1	OBE-CBD-OBG	-2.59	118.78	123.84
4	A	1301[B]	FE1	C4A-C4-N3	-2.57	119.32	121.01
4	B	1303[A]	FE1	C4A-C4-N3	-2.57	119.33	121.01
4	B	1303[B]	FE1	C4A-C4-N3	-2.51	119.36	121.01
4	A	1301[B]	FE1	CAT-CAU-NAV	2.50	121.90	118.72
4	D	1307[A]	FE1	CBA-NAV-CAW	2.44	117.32	112.62
4	B	1303[A]	FE1	OAZ-CAU-CAT	-2.39	115.58	120.23
4	B	1303[B]	FE1	CBF-OBE-CBD	2.38	121.32	115.94
4	D	1307[A]	FE1	CBF-OBE-CBD	2.38	121.31	115.94
4	C	1305[A]	FE1	CAW-CAX-CBC	2.37	114.35	110.41
4	A	1301[B]	FE1	OBE-CBD-OBG	-2.37	119.21	123.84
4	A	1301[A]	FE1	CAT-CAU-NAV	2.36	121.72	118.72
4	B	1303[A]	FE1	CBF-OBE-CBD	2.33	121.20	115.94
4	A	1301[B]	FE1	CBF-OBE-CBD	2.32	121.18	115.94
4	B	1303[A]	FE1	CAW-CAX-CBC	2.30	114.24	110.41
4	C	1305[A]	FE1	C9-C6-N5	2.27	120.60	116.96
4	D	1307[A]	FE1	C4A-C4-N3	-2.26	119.53	121.01
4	B	1303[B]	FE1	CBB-CBA-NAV	-2.26	107.39	110.82
4	C	1305[A]	FE1	C4A-C4-N3	-2.26	119.53	121.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1302	NAP	C3D-C2D-C1D	2.25	104.37	100.98
4	A	1301[A]	FE1	C8A-C4A-N5	-2.24	119.70	122.41
4	A	1301[B]	FE1	CAR-CAJ-N10	-2.22	118.43	121.62
4	D	1307[A]	FE1	C8A-C4A-N5	-2.17	119.79	122.41
4	A	1301[A]	FE1	CBF-OBE-CBD	2.16	120.82	115.94
4	B	1303[A]	FE1	CBA-NAV-CAW	2.14	116.74	112.62
4	B	1303[B]	FE1	C8A-C4A-N5	-2.03	119.95	122.41

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301[A]	FE1	CBC-CBD-OBE-CBF
4	B	1303[B]	FE1	CBC-CBD-OBE-CBF
4	B	1303[B]	FE1	C6-C9-N10-CAJ
4	C	1305[A]	FE1	CBC-CBD-OBE-CBF
4	A	1301[A]	FE1	OBG-CBD-OBE-CBF
4	A	1301[B]	FE1	OBG-CBD-OBE-CBF
4	A	1301[B]	FE1	CBC-CBD-OBE-CBF
4	B	1303[A]	FE1	CBC-CBD-OBE-CBF
4	D	1307[A]	FE1	CBC-CBD-OBE-CBF
4	B	1303[A]	FE1	OBG-CBD-OBE-CBF
4	B	1303[B]	FE1	OBG-CBD-OBE-CBF
4	C	1305[A]	FE1	OBG-CBD-OBE-CBF
4	D	1307[A]	FE1	OBG-CBD-OBE-CBF
4	A	1301[A]	FE1	C6-C9-N10-CAJ
4	B	1303[A]	FE1	CBB-CBC-CBD-OBE

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1303[A]	FE1	CAW-CAX-CBA-CBB-CBC-NAV
4	C	1305[A]	FE1	CAW-CAX-CBA-CBB-CBC-NAV
4	B	1303[B]	FE1	CAW-CAX-CBA-CBB-CBC-NAV
4	D	1307[A]	FE1	CAW-CAX-CBA-CBB-CBC-NAV
4	A	1301[B]	FE1	CAW-CAX-CBA-CBB-CBC-NAV

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301[B]	FE1	4	0

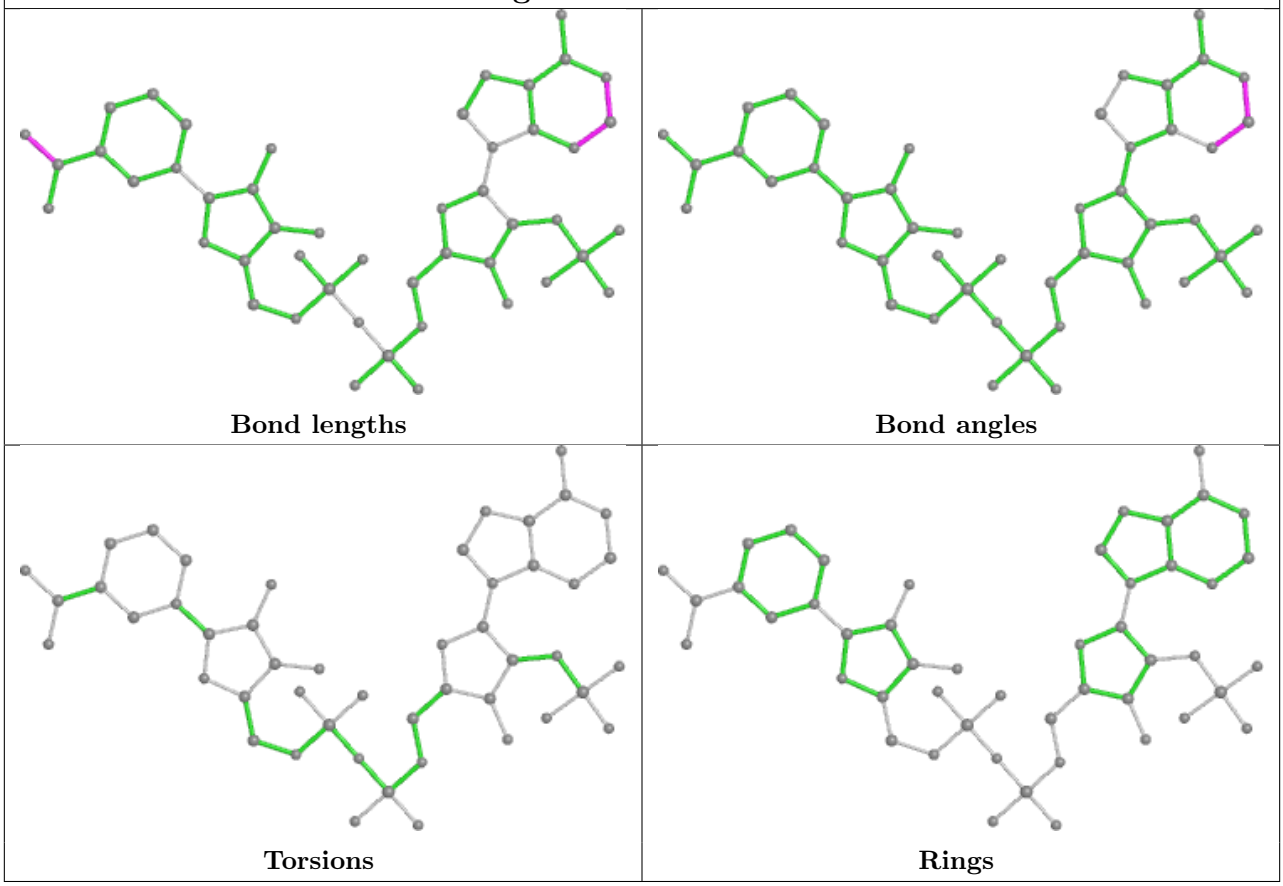
Continued on next page...

Continued from previous page...

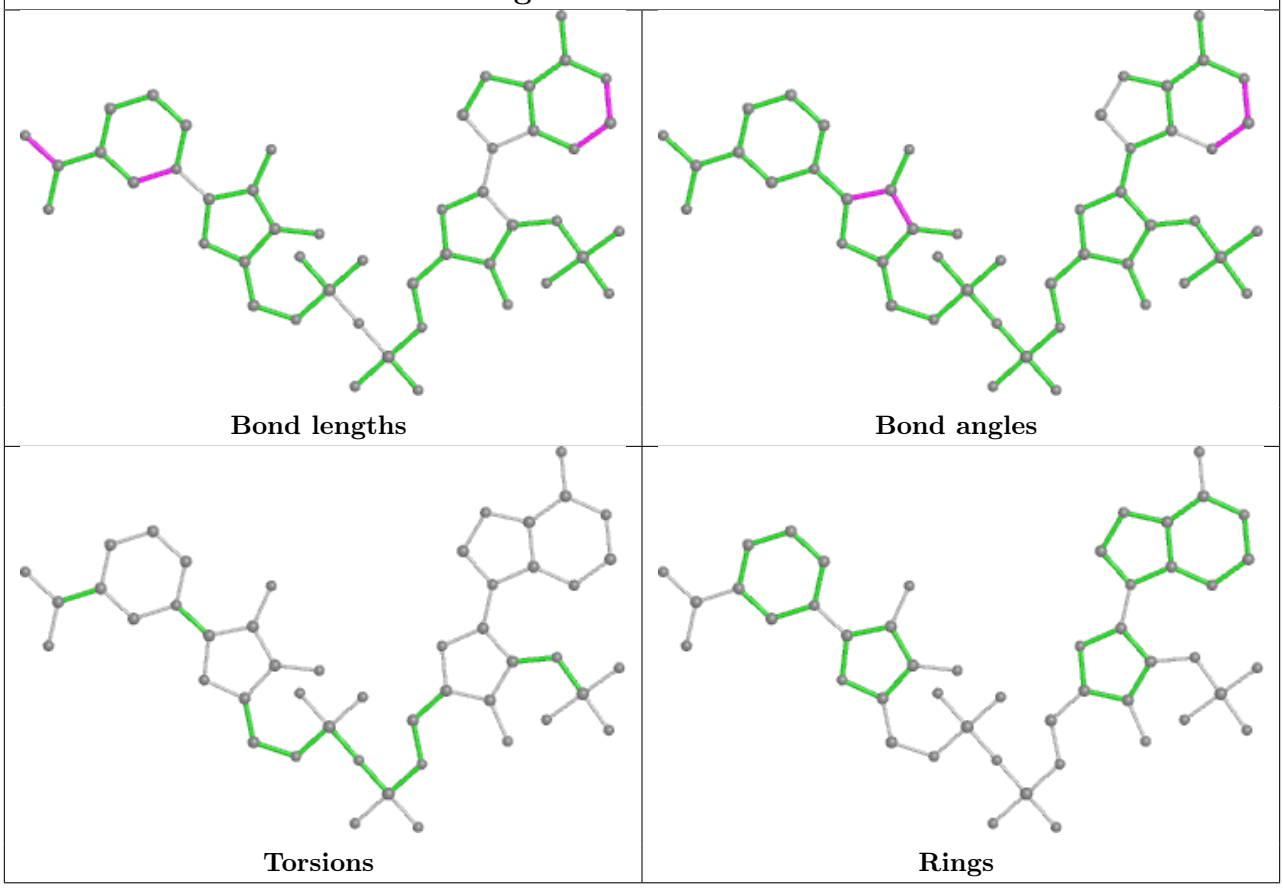
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1303[B]	FE1	3	0
4	A	1301[A]	FE1	2	0
4	C	1305[A]	FE1	2	0
4	B	1303[A]	FE1	1	0
4	D	1307[A]	FE1	1	0

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.

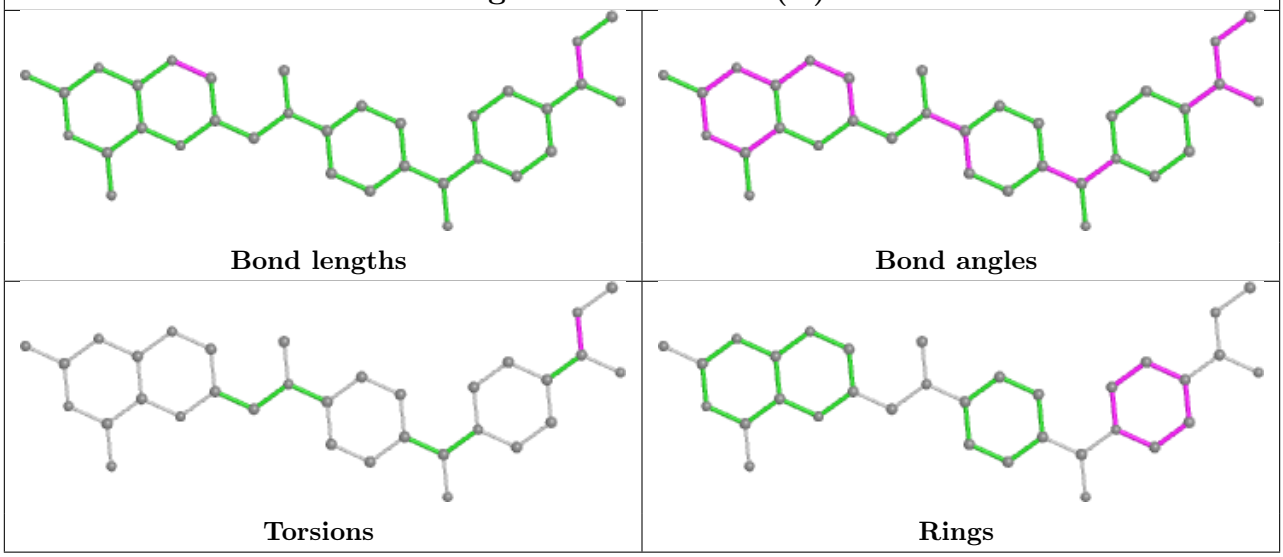
Ligand NAP A 1300



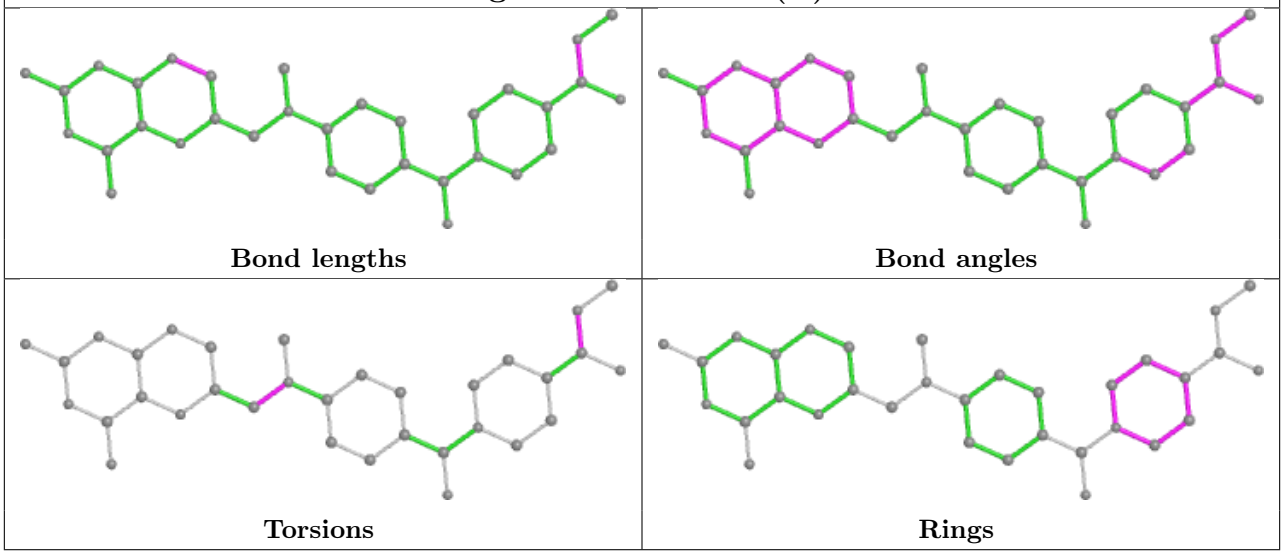
Ligand NAP B 1302



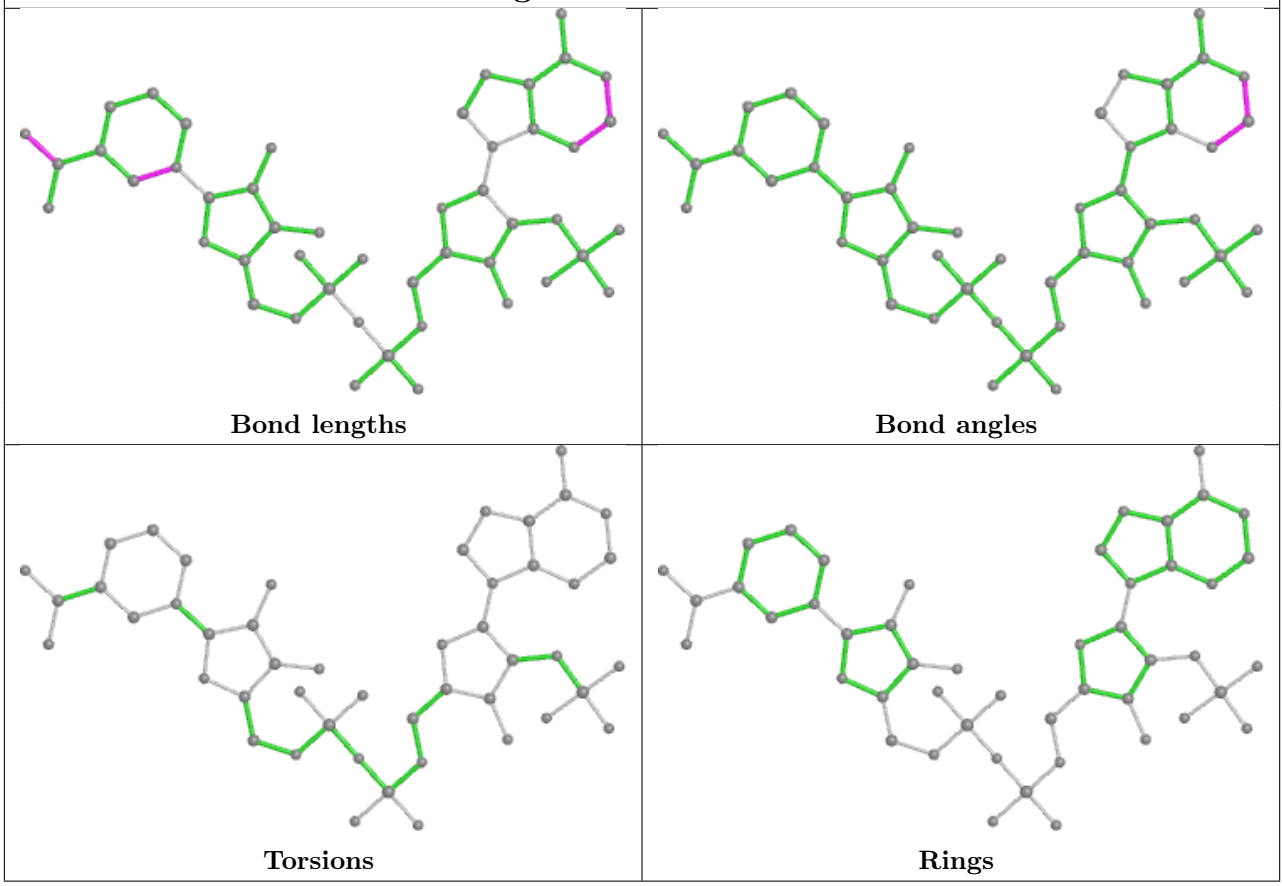
Ligand FE1 A 1301 (B)



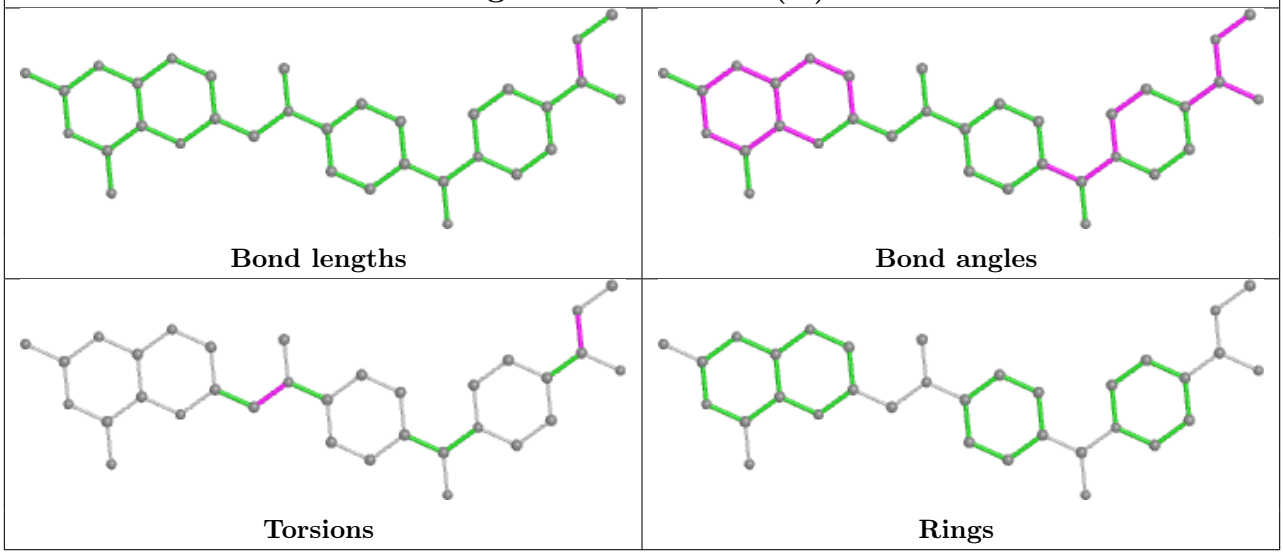
Ligand FE1 B 1303 (B)



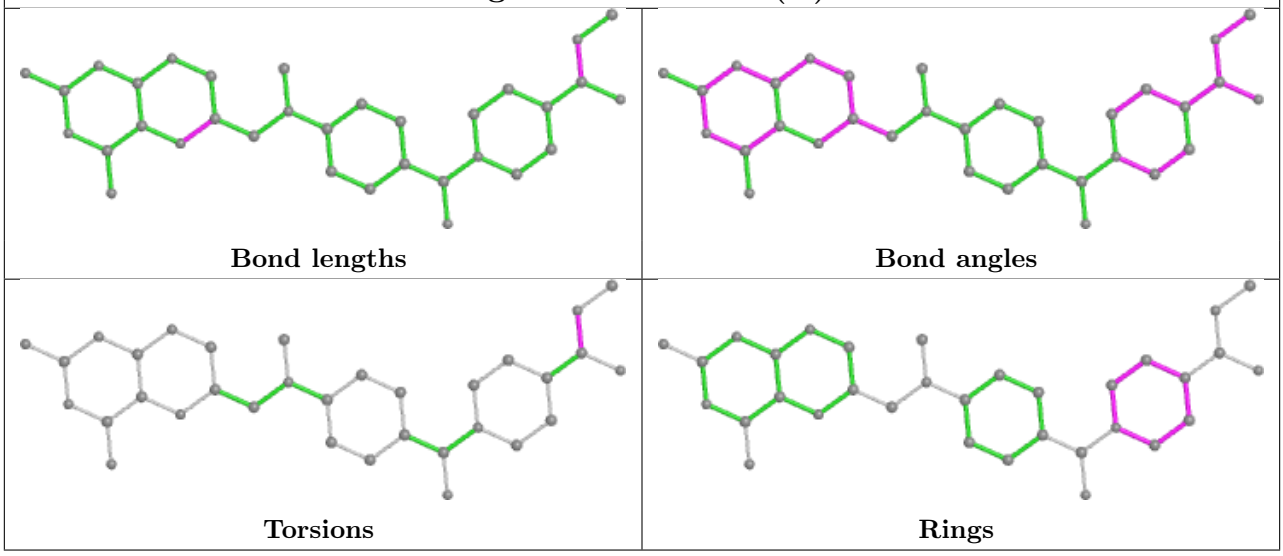
Ligand NAP C 1304



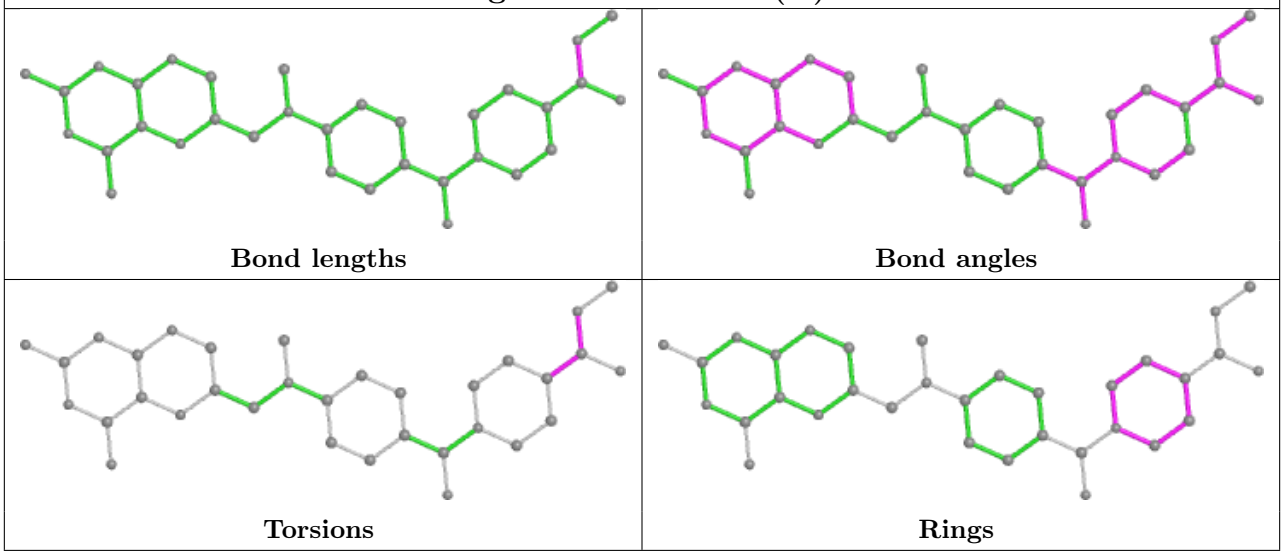
Ligand FE1 A 1301 (A)



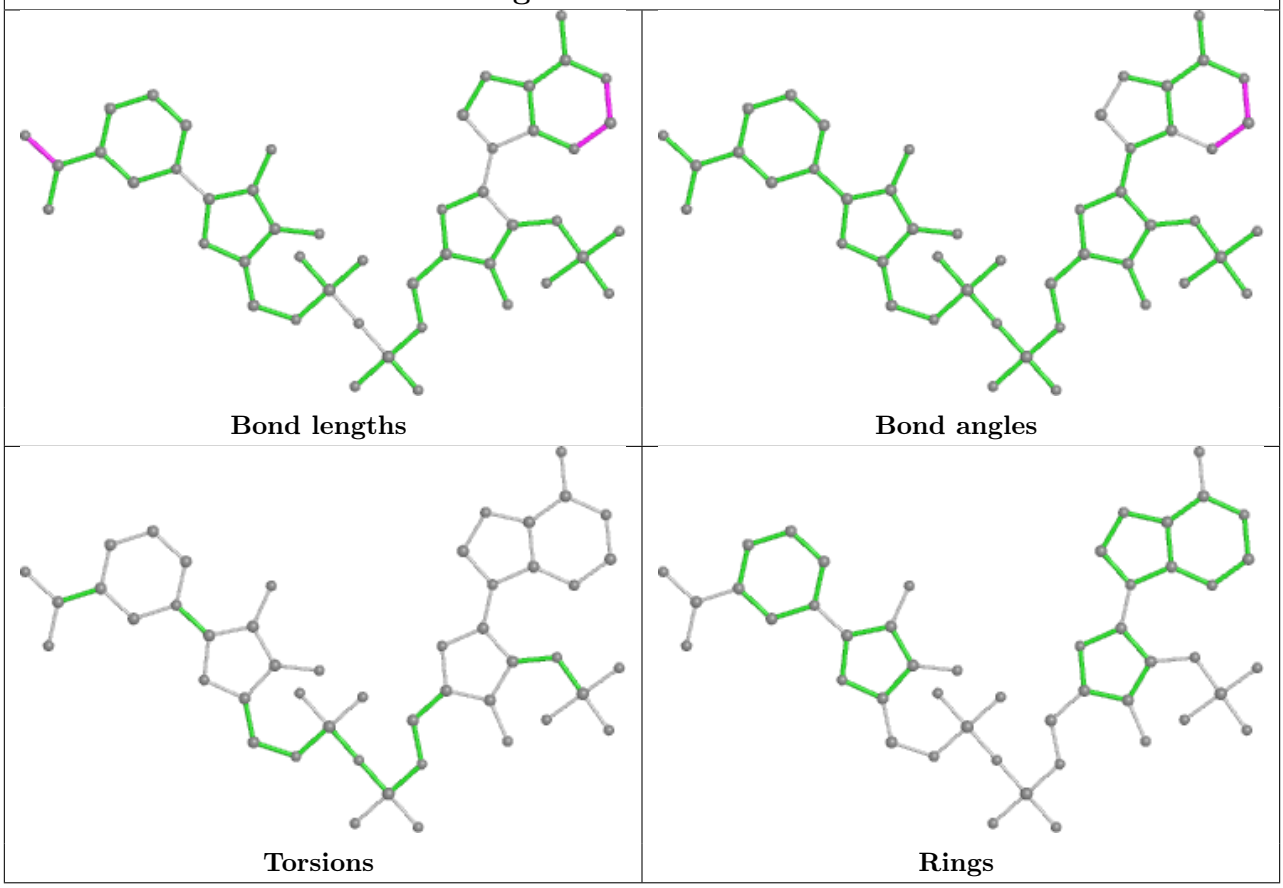
Ligand FE1 C 1305 (A)



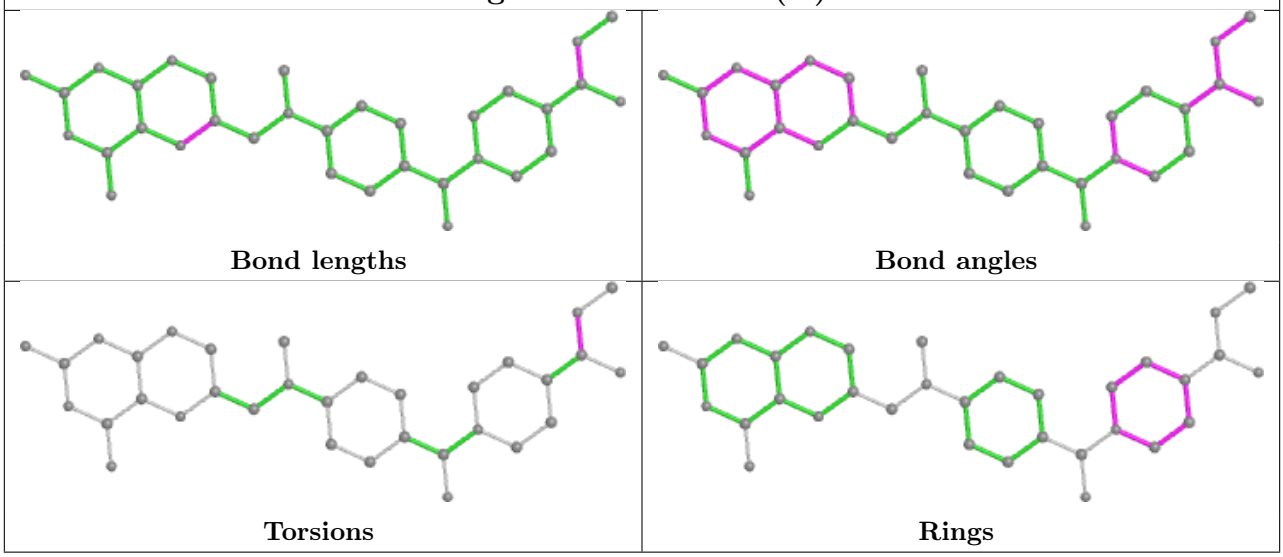
Ligand FE1 B 1303 (A)



Ligand NAP D 1306



Ligand FE1 D 1307 (A)



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	264/328 (80%)	-0.52	7 (2%)	54	49	10, 17, 35, 55	4 (1%)
1	B	265/328 (80%)	-0.40	7 (2%)	56	50	10, 17, 37, 54	2 (0%)
1	C	254/328 (77%)	-0.43	11 (4%)	35	29	10, 17, 35, 54	1 (0%)
1	D	258/328 (78%)	-0.39	12 (4%)	31	25	10, 17, 36, 74	4 (1%)
All	All	1041/1312 (79%)	-0.44	37 (3%)	42	36	10, 17, 36, 74	11 (1%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	80	SER	5.7
1	D	73	PRO	5.5
1	B	81	ALA	4.9
1	A	136	MET	4.8
1	C	230	VAL	4.7
1	D	72	ALA	4.6
1	B	136	MET	4.1
1	D	81	ALA	4.1
1	C	136	MET	4.1
1	A	81	ALA	4.0
1	A	72	ALA	3.9
1	A	73	PRO	3.7
1	B	5	THR	3.3
1	B	120	ARG	3.1
1	D	230	VAL	3.1
1	C	120	ARG	3.1
1	D	135	ALA	2.9
1	C	72	ALA	2.9
1	D	167	ALA	2.8
1	C	73	PRO	2.8
1	D	5	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	168	LYS	2.7
1	D	169	HIS	2.7
1	A	137	GLU	2.7
1	C	81	ALA	2.7
1	C	135	ALA	2.6
1	D	240	GLY	2.6
1	C	169	HIS	2.6
1	C	239	GLU	2.6
1	A	120	ARG	2.5
1	C	241	HIS	2.4
1	B	82	PRO	2.3
1	C	167	ALA	2.2
1	D	132	ASP	2.2
1	A	5	THR	2.2
1	B	73	PRO	2.1
1	D	71	THR	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
4	FE1	A	1301[A]	33/33	0.83	0.37	34,47,63,63	32
4	FE1	A	1301[B]	33/33	0.83	0.37	32,43,56,57	32
4	FE1	C	1305[A]	33/33	0.83	0.29	27,50,80,82	0
4	FE1	D	1307[A]	33/33	0.84	0.27	28,45,74,78	0
4	FE1	B	1303[A]	33/33	0.85	0.35	35,43,55,55	32
4	FE1	B	1303[B]	33/33	0.85	0.35	35,45,53,57	32
3	NAP	A	1300	48/48	0.98	0.11	11,14,17,19	0

Continued on next page...

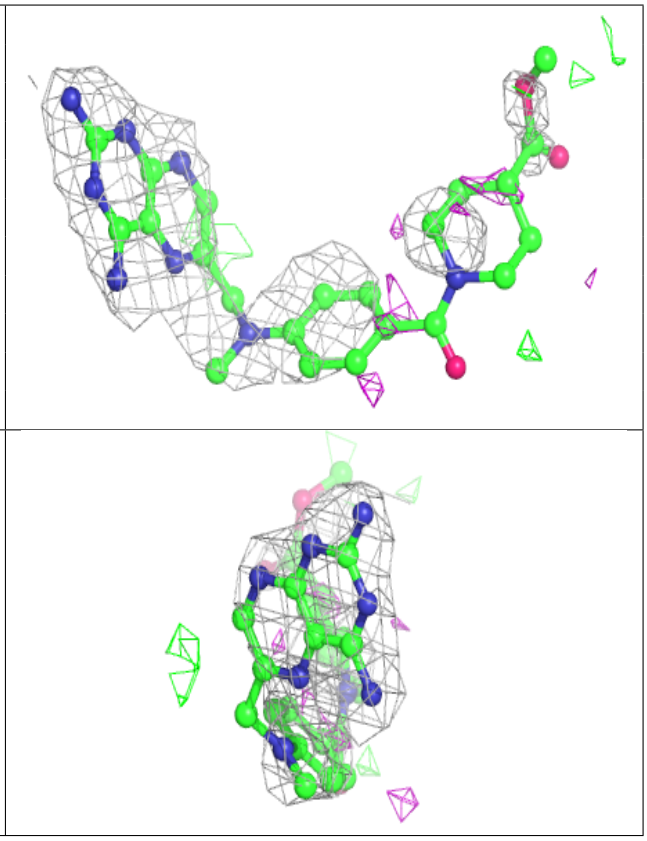
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAP	B	1302	48/48	0.98	0.09	11,14,18,19	0
3	NAP	C	1304	48/48	0.98	0.10	11,14,17,19	0
3	NAP	D	1306	48/48	0.98	0.08	11,14,18,19	0
2	IOD	B	1288	1/1	0.98	0.06	44,44,44,44	1
2	IOD	A	1289	1/1	0.99	0.05	30,30,30,30	1

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.

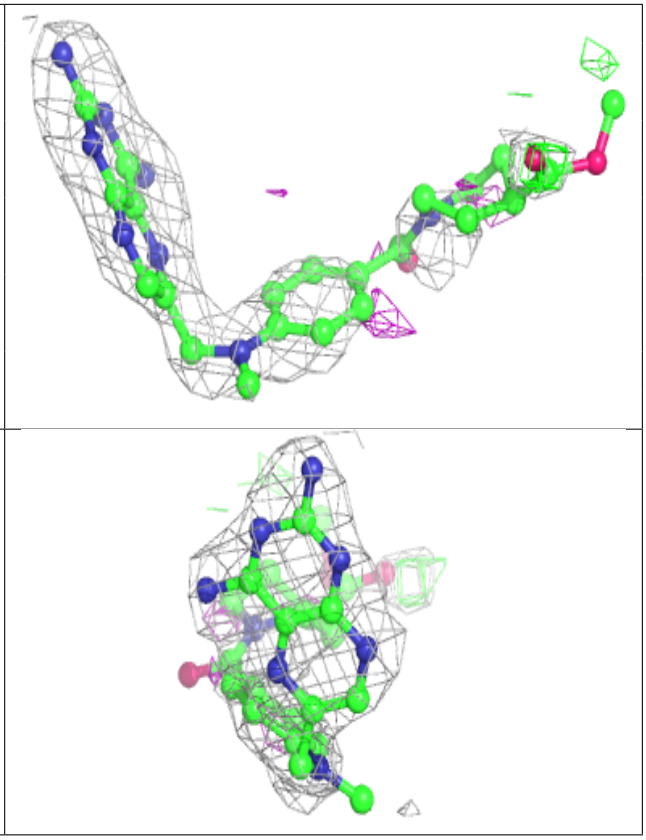
Electron density around FE1 A 1301 (A):

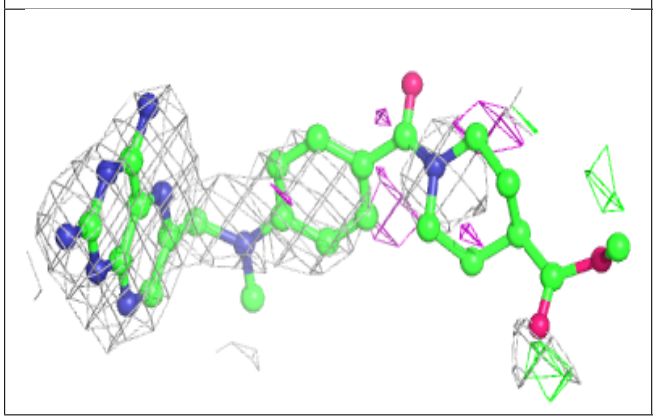
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE1 A 1301 (B):

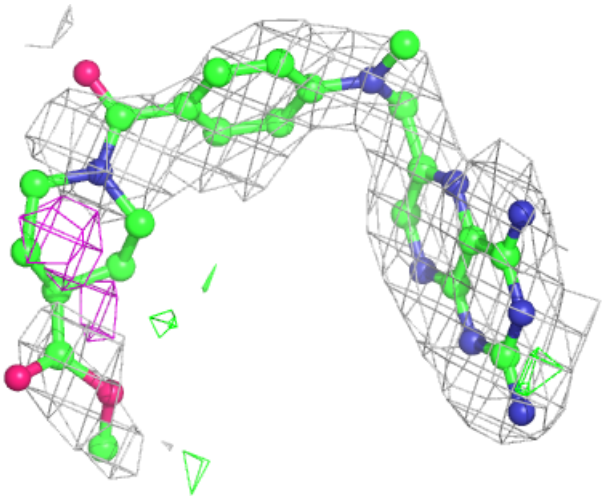
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

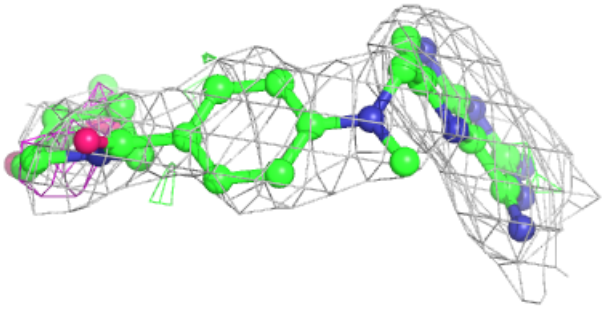


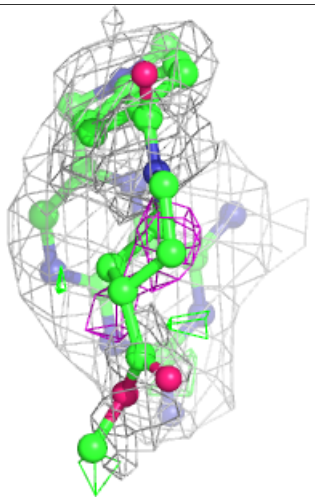


Electron density around FE1 C 1305 (A):

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

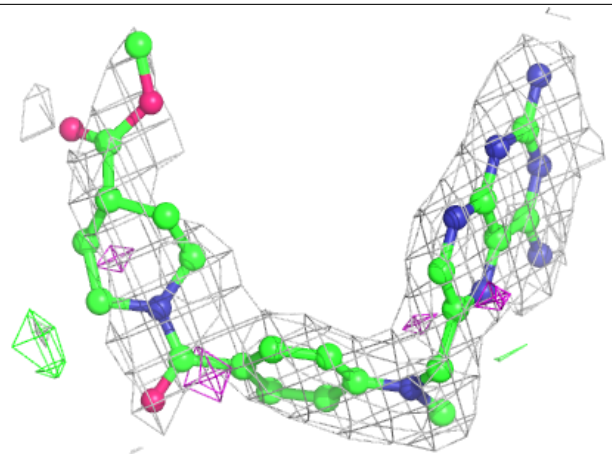


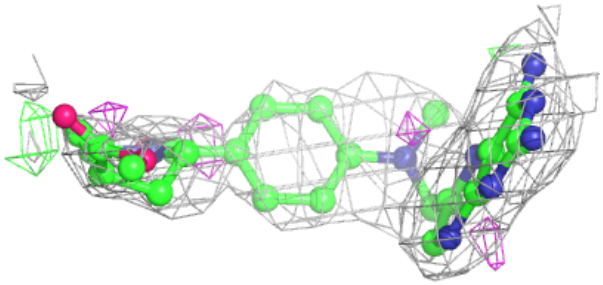


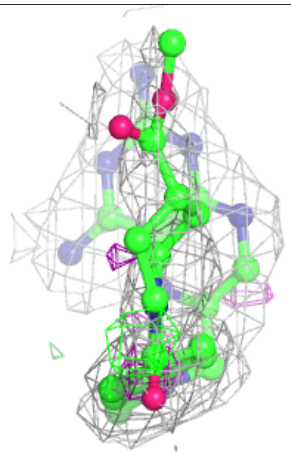


Electron density around FE1 D 1307 (A):

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

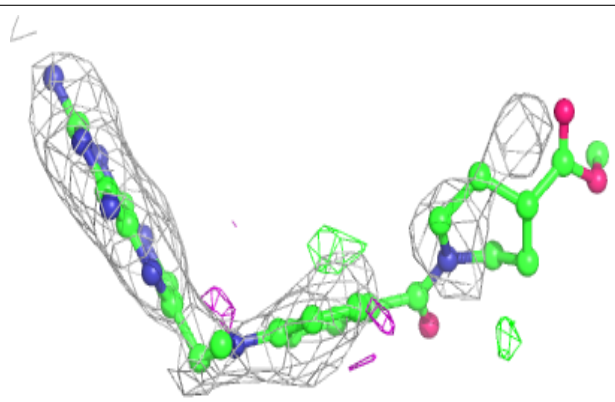


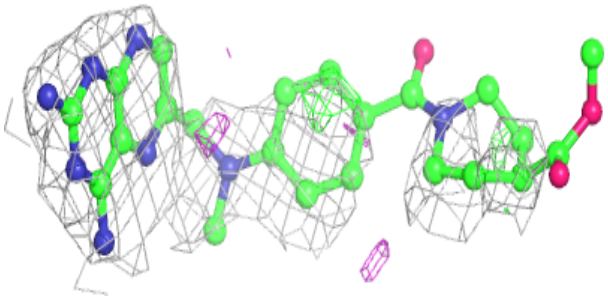


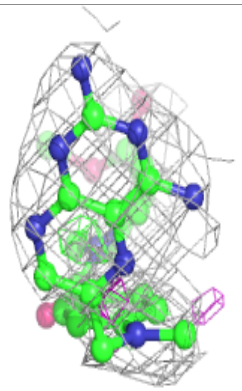


Electron density around FE1 B 1303 (A):

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

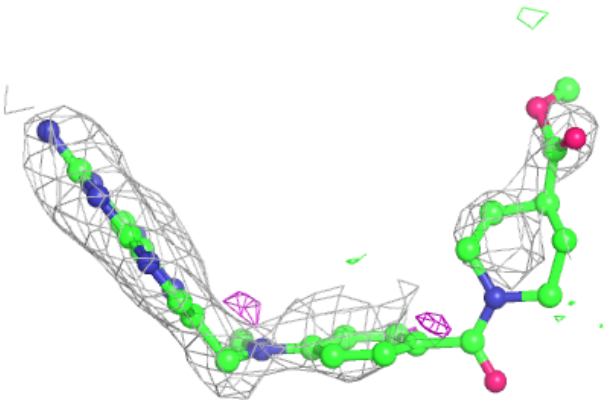


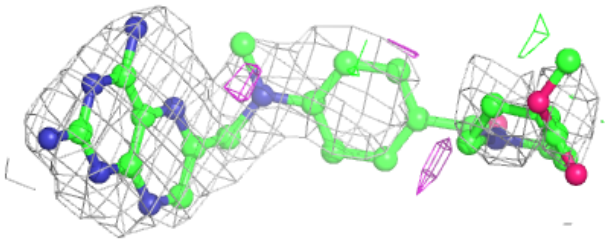


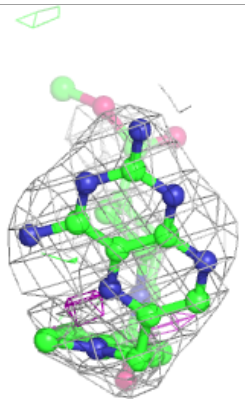


Electron density around FE1 B 1303 (B):

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

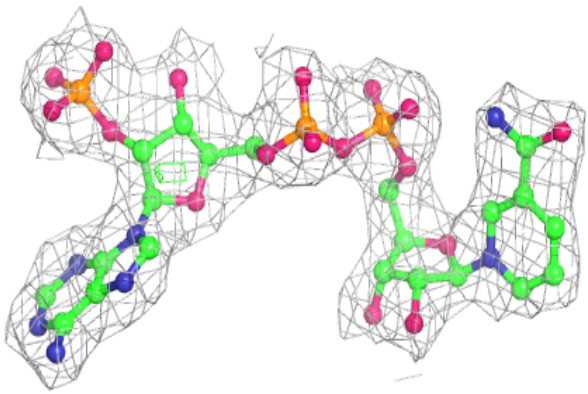


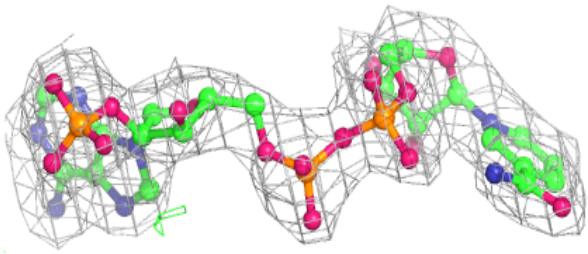


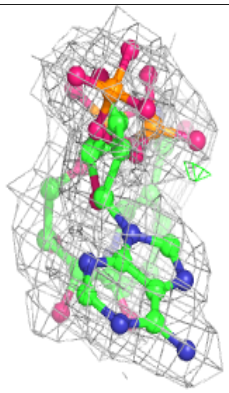


Electron density around NAP A 1300:

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

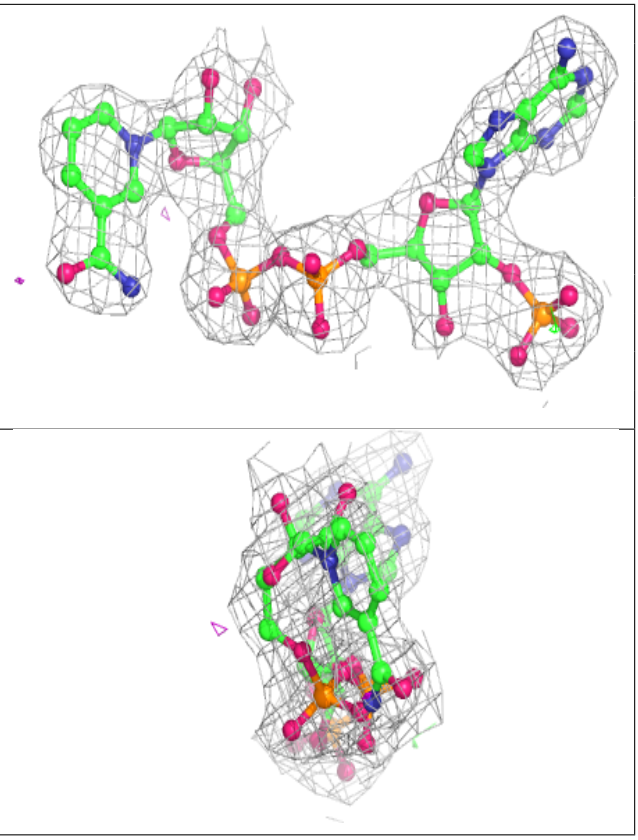






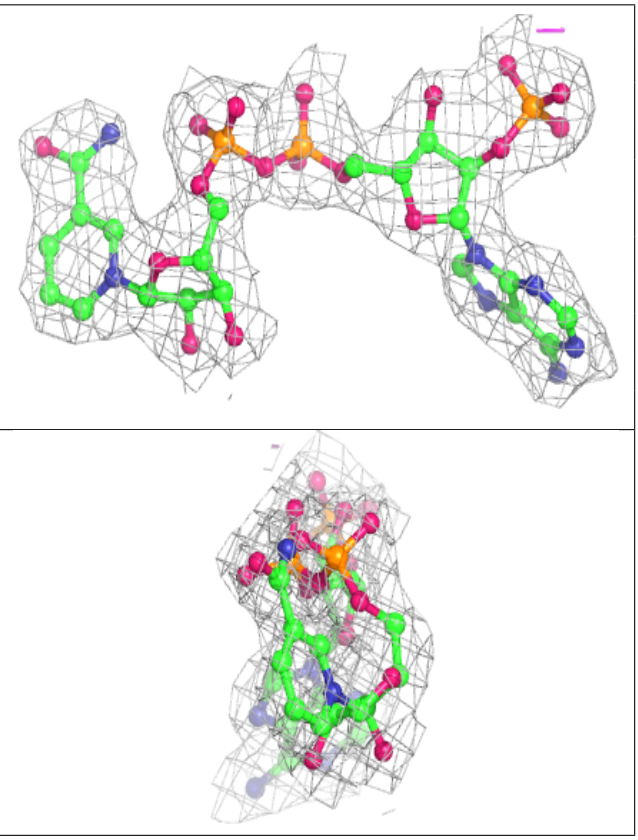
Electron density around NAP B 1302:

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



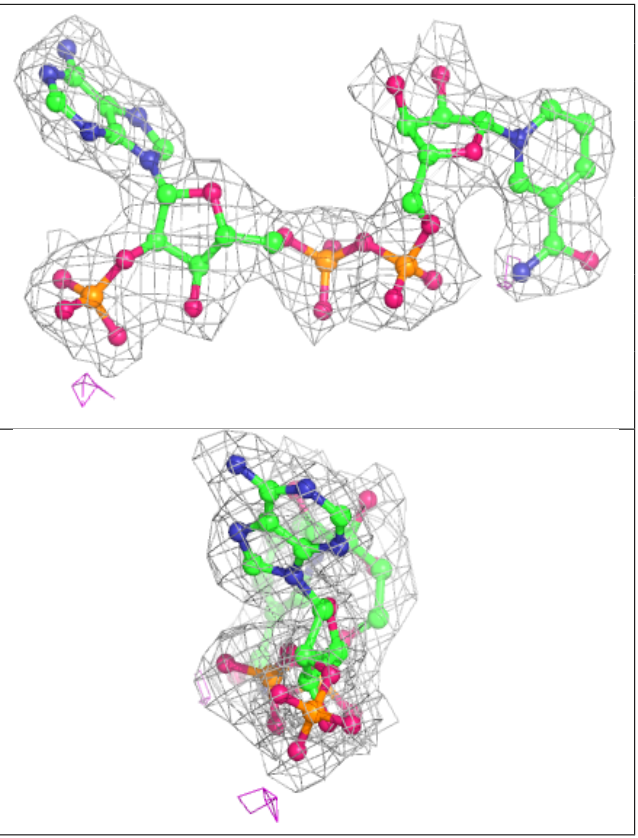
Electron density around NAP C 1304:

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



Electron density around NAP D 1306:

$2mF_o$-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.