Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 03:11 AM EDT

PDB ID	:	4HWK
Title	:	Crystal structure of human sepiapterin reductase in complex with sulfapyridine
Authors	:	Groenlund Pedersen, M.; Pojer, F.; Johnsson, K.
Deposited on	:	2012-11-08
Resolution	:	2.40 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:

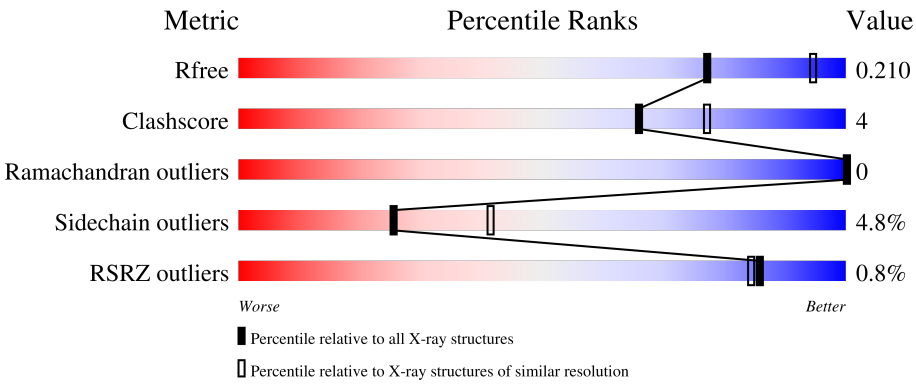
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	288	81% 7% • 11%
1	B	288	% 81% 7% • 11%
1	C	288	82% 6% • 11%
1	D	288	2% 78% 10% • 11%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8479 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 Sepiapterin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	257	1942	1223	344	365	10	0	1	0
1	B	257	1945	1225	345	366	9	0	1	0
1	C	257	1942	1223	344	365	10	0	1	0
1	D	257	1951	1228	346	367	10	0	2	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	expression tag	UNP P35270
A	-28	SER	-	expression tag	UNP P35270
A	-27	TYR	-	expression tag	UNP P35270
A	-26	TYR	-	expression tag	UNP P35270
A	-25	HIS	-	expression tag	UNP P35270
A	-24	HIS	-	expression tag	UNP P35270
A	-23	HIS	-	expression tag	UNP P35270
A	-22	HIS	-	expression tag	UNP P35270
A	-21	HIS	-	expression tag	UNP P35270
A	-20	HIS	-	expression tag	UNP P35270
A	-19	LEU	-	expression tag	UNP P35270
A	-18	GLU	-	expression tag	UNP P35270
A	-17	SER	-	expression tag	UNP P35270
A	-16	THR	-	expression tag	UNP P35270
A	-15	SER	-	expression tag	UNP P35270
A	-14	LEU	-	expression tag	UNP P35270
A	-13	TYR	-	expression tag	UNP P35270
A	-12	LYS	-	expression tag	UNP P35270
A	-11	LYS	-	expression tag	UNP P35270
A	-10	ALA	-	expression tag	UNP P35270
A	-9	GLY	-	expression tag	UNP P35270

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	LEU	-	expression tag	UNP P35270
A	-7	GLU	-	expression tag	UNP P35270
A	-6	GLY	-	expression tag	UNP P35270
A	-5	VAL	-	expression tag	UNP P35270
A	-4	ARG	-	expression tag	UNP P35270
A	-3	THR	-	expression tag	UNP P35270
B	-29	MET	-	expression tag	UNP P35270
B	-28	SER	-	expression tag	UNP P35270
B	-27	TYR	-	expression tag	UNP P35270
B	-26	TYR	-	expression tag	UNP P35270
B	-25	HIS	-	expression tag	UNP P35270
B	-24	HIS	-	expression tag	UNP P35270
B	-23	HIS	-	expression tag	UNP P35270
B	-22	HIS	-	expression tag	UNP P35270
B	-21	HIS	-	expression tag	UNP P35270
B	-20	HIS	-	expression tag	UNP P35270
B	-19	LEU	-	expression tag	UNP P35270
B	-18	GLU	-	expression tag	UNP P35270
B	-17	SER	-	expression tag	UNP P35270
B	-16	THR	-	expression tag	UNP P35270
B	-15	SER	-	expression tag	UNP P35270
B	-14	LEU	-	expression tag	UNP P35270
B	-13	TYR	-	expression tag	UNP P35270
B	-12	LYS	-	expression tag	UNP P35270
B	-11	LYS	-	expression tag	UNP P35270
B	-10	ALA	-	expression tag	UNP P35270
B	-9	GLY	-	expression tag	UNP P35270
B	-8	LEU	-	expression tag	UNP P35270
B	-7	GLU	-	expression tag	UNP P35270
B	-6	GLY	-	expression tag	UNP P35270
B	-5	VAL	-	expression tag	UNP P35270
B	-4	ARG	-	expression tag	UNP P35270
B	-3	THR	-	expression tag	UNP P35270
C	-29	MET	-	expression tag	UNP P35270
C	-28	SER	-	expression tag	UNP P35270
C	-27	TYR	-	expression tag	UNP P35270
C	-26	TYR	-	expression tag	UNP P35270
C	-25	HIS	-	expression tag	UNP P35270
C	-24	HIS	-	expression tag	UNP P35270
C	-23	HIS	-	expression tag	UNP P35270
C	-22	HIS	-	expression tag	UNP P35270
C	-21	HIS	-	expression tag	UNP P35270

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	expression tag	UNP P35270
C	-19	LEU	-	expression tag	UNP P35270
C	-18	GLU	-	expression tag	UNP P35270
C	-17	SER	-	expression tag	UNP P35270
C	-16	THR	-	expression tag	UNP P35270
C	-15	SER	-	expression tag	UNP P35270
C	-14	LEU	-	expression tag	UNP P35270
C	-13	TYR	-	expression tag	UNP P35270
C	-12	LYS	-	expression tag	UNP P35270
C	-11	LYS	-	expression tag	UNP P35270
C	-10	ALA	-	expression tag	UNP P35270
C	-9	GLY	-	expression tag	UNP P35270
C	-8	LEU	-	expression tag	UNP P35270
C	-7	GLU	-	expression tag	UNP P35270
C	-6	GLY	-	expression tag	UNP P35270
C	-5	VAL	-	expression tag	UNP P35270
C	-4	ARG	-	expression tag	UNP P35270
C	-3	THR	-	expression tag	UNP P35270
D	-29	MET	-	expression tag	UNP P35270
D	-28	SER	-	expression tag	UNP P35270
D	-27	TYR	-	expression tag	UNP P35270
D	-26	TYR	-	expression tag	UNP P35270
D	-25	HIS	-	expression tag	UNP P35270
D	-24	HIS	-	expression tag	UNP P35270
D	-23	HIS	-	expression tag	UNP P35270
D	-22	HIS	-	expression tag	UNP P35270
D	-21	HIS	-	expression tag	UNP P35270
D	-20	HIS	-	expression tag	UNP P35270
D	-19	LEU	-	expression tag	UNP P35270
D	-18	GLU	-	expression tag	UNP P35270
D	-17	SER	-	expression tag	UNP P35270
D	-16	THR	-	expression tag	UNP P35270
D	-15	SER	-	expression tag	UNP P35270
D	-14	LEU	-	expression tag	UNP P35270
D	-13	TYR	-	expression tag	UNP P35270
D	-12	LYS	-	expression tag	UNP P35270
D	-11	LYS	-	expression tag	UNP P35270
D	-10	ALA	-	expression tag	UNP P35270
D	-9	GLY	-	expression tag	UNP P35270
D	-8	LEU	-	expression tag	UNP P35270
D	-7	GLU	-	expression tag	UNP P35270
D	-6	GLY	-	expression tag	UNP P35270

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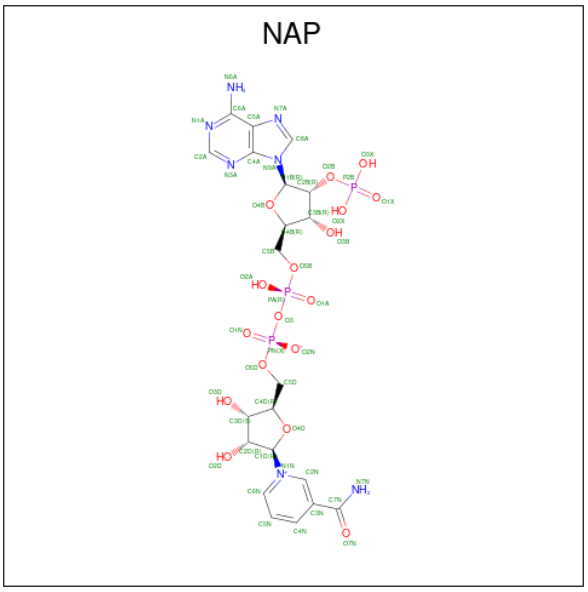
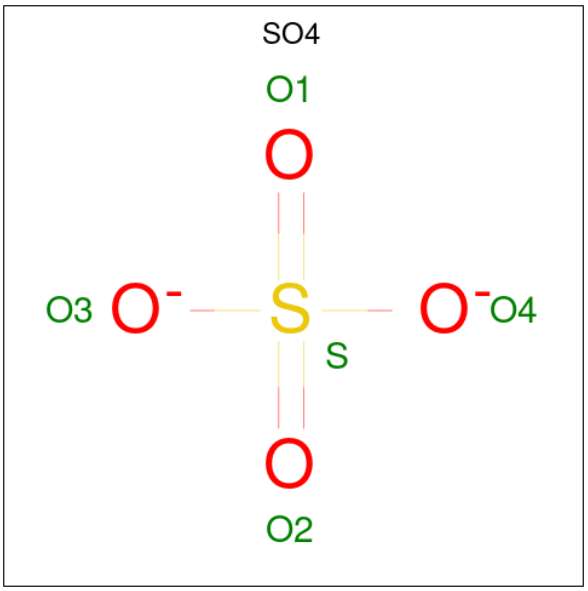
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	VAL	-	expression tag	UNP P35270
D	-4	ARG	-	expression tag	UNP P35270
D	-3	THR	-	expression tag	UNP P35270

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



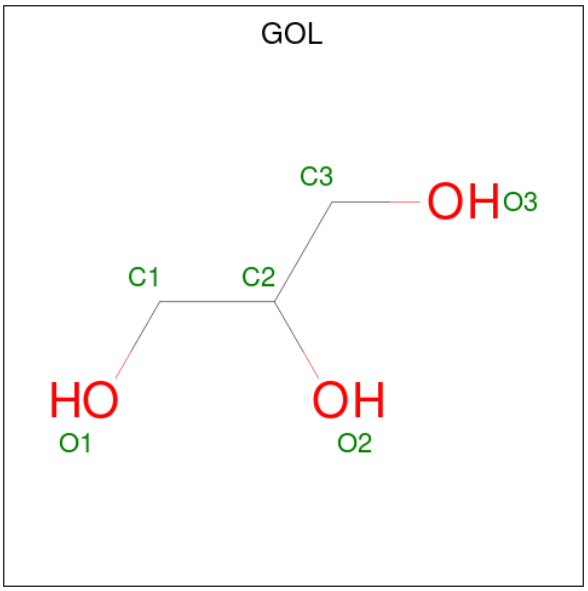
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	B	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	C	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	D	1	48	21	7	17	3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



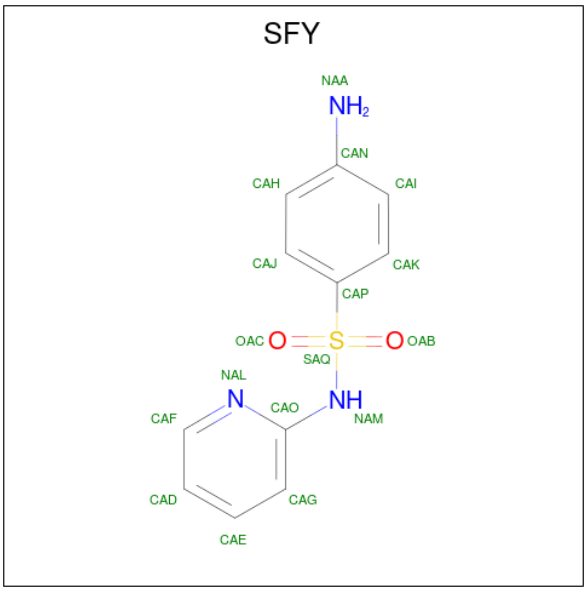
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	D	1	5	4	1		0	0
			Total	O	S			
3	D	1	5	4	1		0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



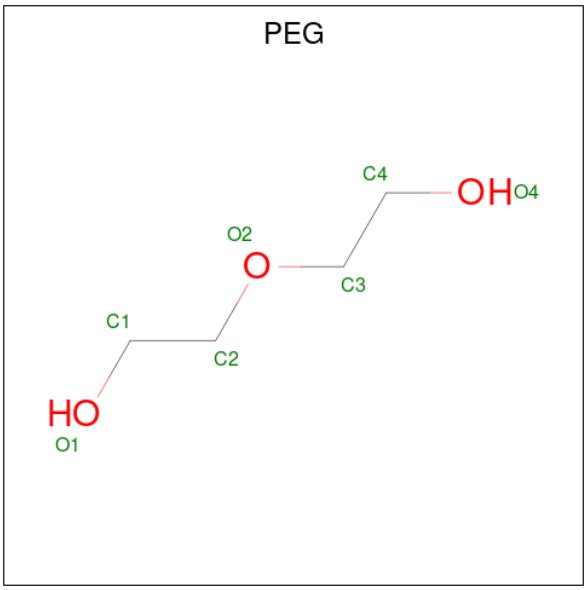
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	C	1	6	3	3	0	0

- Molecule 5 is 4-amino-N-(pyridin-2-yl)benzenesulfonamide (three-letter code: SFY) (formula: $C_{11}H_{11}N_3O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	17	11	3	2	1	0	0
			Total	C	N	O	S		
5	B	1	17	11	3	2	1	0	0
			Total	C	N	O	S		
5	C	1	17	11	3	2	1	0	0
			Total	C	N	O	S		
5	D	1	17	11	3	2	1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	7	4	3	0	0
			Total	C	O		
6	C	1	7	4	3	0	0

- Molecule 7 is water.

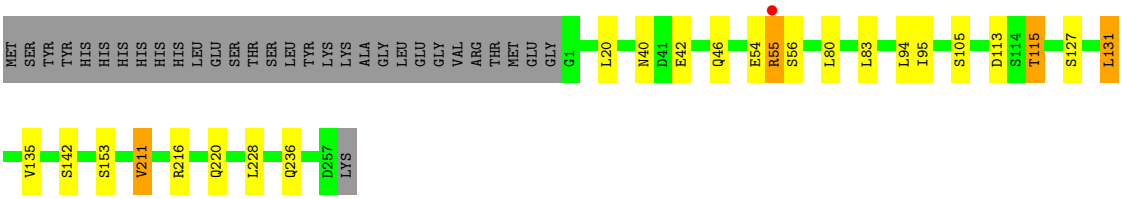
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	104	104	104	0	0
			Total	O		
7	B	101	101	101	0	0
			Total	O		
7	C	85	85	85	0	0
			Total	O		
7	D	48	48	48	0	0

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: Sepiapterin reductase

Chain A:

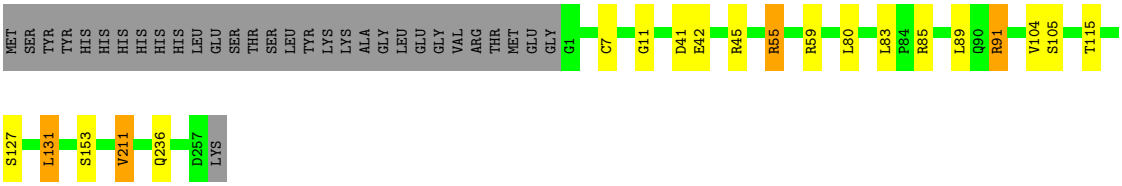


• Molecule 1: Sepiapterin reductase

Chain B:

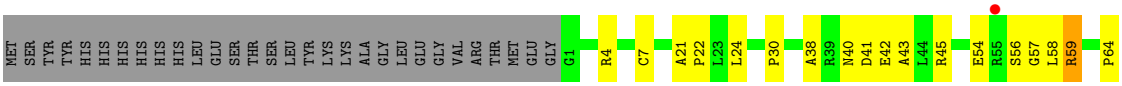
• Molecule 1: Sepiapterin reductase

Chain C:



• Molecule 1: Sepiapterin reductase

Chain D:



L80
R81
E82
L83
T115
Q116
S127
L131
S142
S153
W164
A173
R216
K217
Q220
A224
K225
G226
K227
D257
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	148.45Å 148.45Å 179.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.91 – 2.40 46.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.91-2.40) 99.7 (46.91-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.194 , 0.211 0.194 , 0.210	Depositor DCC
R_{free} test set	4377 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8479	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: SO4, PEG, SFY, NAP, GOL

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	0.39	0/1969	0.53	0/2664
1	B	0.39	1/1972 (0.1%)	0.54	0/2668
1	C	0.39	0/1969	0.55	0/2664
1	D	0.40	1/1978 (0.1%)	0.55	0/2676
All	All	0.39	2/7888 (0.0%)	0.54	0/10672

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	164	TRP	CD2-CE2	5.14	1.47	1.41
1	B	121	TRP	CD2-CE2	5.13	1.47	1.41

There are no bond angle outliers.

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	1942	0	2007	19	0
1	B	1945	0	2010	17	0
1	C	1942	0	2007	10	0
1	D	1951	0	2014	24	0
2	A	48	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	25	1	0
2	C	48	0	25	2	0
2	D	48	0	25	1	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	A	24	0	32	1	0
4	B	12	0	16	1	0
4	C	6	0	8	0	0
5	A	17	0	11	0	0
5	B	17	0	11	1	0
5	C	17	0	11	0	0
5	D	17	0	11	0	0
6	A	7	0	10	0	0
6	C	7	0	10	0	0
7	A	104	0	0	2	0
7	B	101	0	0	1	0
7	C	85	0	0	1	0
7	D	48	0	0	0	0
All	All	8479	0	8258	66	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 (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ARG:O	1:A:220:GLN:HG3	1.66	0.94
1:D:216:ARG:O	1:D:220:GLN:HG3	1.76	0.85
1:C:91:ARG:HG2	1:C:91:ARG:HH11	1.44	0.82
1:D:30:PRO:HA	1:D:57:GLY:HA3	1.66	0.76
1:A:46:GLN:HE21	1:B:59:ARG:HH11	1.35	0.74
1:D:81:ARG:HG3	1:D:81:ARG:NH1	2.03	0.73
1:D:40:ASN:ND2	1:D:43:ALA:CB	2.54	0.70
1:D:81:ARG:HG3	1:D:81:ARG:HH11	1.57	0.69
1:B:220:GLN:NE2	7:B:973:HOH:O	2.25	0.68
1:A:115:THR:HG22	7:A:966:HOH:O	1.93	0.68
1:A:54:GLU:HG3	1:B:55:ARG:O	1.94	0.67
5:B:806:SFY:H4	4:B:807:GOL:H12	1.60	0.65
1:D:40:ASN:ND2	1:D:43:ALA:HB2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:HH11	1:C:91:ARG:CG	2.10	0.63
1:A:228:LEU:HB2	4:A:806:GOL:H11	1.82	0.61
1:C:105:SER:O	1:C:211:VAL:HG13	2.03	0.58
1:A:153:SER:O	2:A:801:NAP:H6N	2.03	0.58
1:C:153:SER:O	2:C:801:NAP:H6N	2.04	0.58
1:D:7[B]:CYS:SG	1:D:24:LEU:HD21	2.45	0.56
1:D:153:SER:O	2:D:801:NAP:H6N	2.06	0.55
1:A:46:GLN:HE21	1:B:59:ARG:NH1	2.03	0.55
1:B:153:SER:O	2:B:801:NAP:H6N	2.07	0.55
1:B:21:ALA:HB3	1:B:22:PRO:HD3	1.88	0.55
1:D:40:ASN:HD21	1:D:43:ALA:HB2	1.72	0.54
1:B:105:SER:O	1:B:211:VAL:HG13	2.08	0.53
1:A:46:GLN:NE2	1:B:59:ARG:HH11	2.05	0.52
1:D:40:ASN:ND2	1:D:43:ALA:HB3	2.24	0.52
1:D:81:ARG:HH11	1:D:81:ARG:CG	2.18	0.50
1:D:40:ASN:HD22	1:D:43:ALA:HB3	1.78	0.48
1:D:56:SER:O	1:D:58:LEU:N	2.44	0.48
1:A:55:ARG:HG2	1:A:56:SER:N	2.28	0.48
1:D:21:ALA:HB3	1:D:22:PRO:HD3	1.94	0.48
1:C:91:ARG:CG	1:C:91:ARG:NH1	2.75	0.48
1:A:113:ASP:OD1	1:A:115:THR:HG23	2.14	0.47
1:A:105:SER:O	1:A:211:VAL:HG13	2.14	0.47
1:A:127:SER:O	1:A:131:LEU:HB2	2.14	0.47
1:D:40:ASN:HD22	1:D:43:ALA:CB	2.27	0.47
1:A:40:ASN:OD1	1:A:42:GLU:HB3	2.15	0.47
1:B:50:GLU:O	1:B:50:GLU:CG	2.62	0.46
1:D:30:PRO:CA	1:D:57:GLY:HA3	2.40	0.46
1:D:30:PRO:HA	1:D:57:GLY:CA	2.40	0.46
1:D:40:ASN:OD1	1:D:42:GLU:HB3	2.15	0.46
1:D:41:ASP:O	1:D:45:ARG:HG3	2.16	0.45
1:C:127:SER:O	1:C:131:LEU:HB2	2.17	0.45
1:A:220:GLN:NE2	7:A:970:HOH:O	2.30	0.45
1:D:40:ASN:ND2	1:D:43:ALA:H	2.14	0.45
1:B:38:ALA:O	1:B:64:PRO:HA	2.18	0.44
1:D:38:ALA:O	1:D:64:PRO:HA	2.18	0.44
1:A:94:LEU:HD11	1:A:131:LEU:HD13	2.00	0.43
1:A:80:LEU:HD21	1:A:135:VAL:HG22	2.00	0.43
1:C:55:ARG:HD3	7:C:960:HOH:O	2.19	0.43
1:D:59:ARG:HE	1:D:59:ARG:HB2	1.45	0.43
1:C:41:ASP:O	1:C:45:ARG:HG3	2.19	0.43
1:B:127:SER:O	1:B:131:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LEU:O	1:B:80:LEU:HB2	2.19	0.42
1:D:127:SER:O	1:D:131:LEU:HB2	2.19	0.42
1:B:51:LEU:HD12	1:B:51:LEU:HA	1.91	0.42
1:B:50:GLU:O	1:B:50:GLU:HG2	2.19	0.42
1:C:104:VAL:O	1:C:211:VAL:HG22	2.19	0.42
1:B:18:ARG:HH22	1:B:46:GLN:HG3	1.86	0.41
1:A:20:LEU:HD21	1:A:95:ILE:HD13	2.02	0.41
1:A:216:ARG:O	1:A:220:GLN:CG	2.54	0.41
1:B:173:ALA:HB2	1:D:173:ALA:HB2	2.03	0.41
1:C:11:GLY:HA2	2:C:801:NAP:H1B	2.02	0.40
1:B:18:ARG:HH22	1:B:46:GLN:CG	2.34	0.40
1:A:55:ARG:HH11	1:A:55:ARG:HD3	1.77	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	256/288 (89%)	252 (98%)	4 (2%)	0	100	100
1	B	256/288 (89%)	252 (98%)	4 (2%)	0	100	100
1	C	256/288 (89%)	251 (98%)	5 (2%)	0	100	100
1	D	257/288 (89%)	253 (98%)	4 (2%)	0	100	100
All	All	1025/1152 (89%)	1008 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	210/236 (89%)	203 (97%)	7 (3%)	38	57
1	B	210/236 (89%)	200 (95%)	10 (5%)	25	41
1	C	210/236 (89%)	196 (93%)	14 (7%)	16	26
1	D	211/236 (89%)	200 (95%)	11 (5%)	23	38
All	All	841/944 (89%)	799 (95%)	42 (5%)	25	40

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	A	83	LEU
1	A	115	THR
1	A	131	LEU
1	A	142	SER
1	A	211	VAL
1	A	236	GLN
1	B	46	GLN
1	B	51	LEU
1	B	82	GLU
1	B	83	LEU
1	B	115	THR
1	B	131	LEU
1	B	205	LEU
1	B	211	VAL
1	B	217	LYS
1	B	220	GLN
1	C	7[A]	CYS
1	C	7[B]	CYS
1	C	42	GLU
1	C	55	ARG
1	C	59	ARG
1	C	80	LEU
1	C	83	LEU
1	C	85	ARG
1	C	89	LEU
1	C	91	ARG
1	C	115	THR

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Mol	Chain	Res	Type
1	C	131	LEU
1	C	211	VAL
1	C	236	GLN
1	D	4	ARG
1	D	54	GLU
1	D	59	ARG
1	D	80	LEU
1	D	81	ARG
1	D	83	LEU
1	D	115	THR
1	D	116[A]	GLN
1	D	116[B]	GLN
1	D	131	LEU
1	D	142	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	D	40	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)

26 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	808	-	4,4,4	0.34	0	6,6,6	0.06	0
5	SFY	A	807	-	18,18,18	2.93	4 (22%)	25,25,25	2.17	4 (16%)
3	SO4	D	802	-	4,4,4	0.33	0	6,6,6	0.07	0
4	GOL	A	803	-	5,5,5	0.35	0	5,5,5	0.28	0
4	GOL	B	807	-	5,5,5	0.37	0	5,5,5	0.20	0
4	GOL	A	809	-	5,5,5	0.40	0	5,5,5	0.23	0
2	NAP	D	801	-	45,52,52	1.58	5 (11%)	56,80,80	1.10	4 (7%)
6	PEG	C	805	-	6,6,6	0.46	0	5,5,5	0.27	0
3	SO4	A	805	-	4,4,4	0.33	0	6,6,6	0.06	0
3	SO4	A	802	-	4,4,4	0.29	0	6,6,6	0.08	0
3	SO4	C	802	-	4,4,4	0.33	0	6,6,6	0.07	0
5	SFY	C	804	-	18,18,18	2.96	4 (22%)	25,25,25	2.15	4 (16%)
2	NAP	C	801	-	45,52,52	1.57	6 (13%)	56,80,80	1.14	4 (7%)
5	SFY	B	806	-	18,18,18	2.96	4 (22%)	25,25,25	2.21	5 (20%)
2	NAP	B	801	-	45,52,52	1.56	5 (11%)	56,80,80	1.11	3 (5%)
3	SO4	B	805	-	4,4,4	0.33	0	6,6,6	0.07	0
4	GOL	B	803	-	5,5,5	0.40	0	5,5,5	0.37	0
4	GOL	C	803	-	5,5,5	0.36	0	5,5,5	0.23	0
3	SO4	D	804	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	B	804	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	A	804	-	5,5,5	0.36	0	5,5,5	0.27	0
2	NAP	A	801	-	45,52,52	1.53	5 (11%)	56,80,80	1.11	3 (5%)
5	SFY	D	803	-	18,18,18	2.93	4 (22%)	25,25,25	2.28	5 (20%)
3	SO4	B	802	-	4,4,4	0.30	0	6,6,6	0.10	0
4	GOL	A	806	-	5,5,5	0.40	0	5,5,5	0.54	0
6	PEG	A	810	-	6,6,6	0.43	0	5,5,5	0.35	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
2	NAP	B	801	-	-	2/31/67/67	0/5/5/5
4	GOL	A	809	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SFY	D	803	-	-	4/11/11/11	0/2/2/2
5	SFY	B	806	-	-	4/11/11/11	0/2/2/2
4	GOL	B	803	-	-	2/4/4/4	-
4	GOL	C	803	-	-	2/4/4/4	-
5	SFY	A	807	-	-	4/11/11/11	0/2/2/2
6	PEG	A	810	-	-	3/4/4/4	-
4	GOL	A	803	-	-	3/4/4/4	-
4	GOL	A	804	-	-	0/4/4/4	-
4	GOL	B	807	-	-	4/4/4/4	-
5	SFY	C	804	-	-	4/11/11/11	0/2/2/2
4	GOL	A	806	-	-	3/4/4/4	-
2	NAP	C	801	-	-	5/31/67/67	0/5/5/5
2	NAP	D	801	-	-	7/31/67/67	0/5/5/5
2	NAP	A	801	-	-	5/31/67/67	0/5/5/5
6	PEG	C	805	-	-	3/4/4/4	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	804	SFY	CAP-SAQ	-10.07	1.60	1.76
5	B	806	SFY	CAP-SAQ	-10.06	1.60	1.76
5	D	803	SFY	CAP-SAQ	-9.96	1.61	1.76
5	A	807	SFY	CAP-SAQ	-9.92	1.61	1.76
2	D	801	NAP	O7N-C7N	6.09	1.35	1.24
2	B	801	NAP	O7N-C7N	6.07	1.35	1.24
2	A	801	NAP	O7N-C7N	6.05	1.35	1.24
2	C	801	NAP	O7N-C7N	6.02	1.35	1.24
2	D	801	NAP	C2N-N1N	5.36	1.41	1.35
2	B	801	NAP	C2N-N1N	5.01	1.41	1.35
2	A	801	NAP	C2N-N1N	4.98	1.41	1.35
2	C	801	NAP	C2N-N1N	4.86	1.40	1.35
5	C	804	SFY	OAB-SAQ	4.49	1.48	1.43
5	D	803	SFY	OAC-SAQ	4.46	1.48	1.43
5	B	806	SFY	OAB-SAQ	4.44	1.48	1.43
5	A	807	SFY	OAB-SAQ	4.40	1.48	1.43
5	A	807	SFY	OAC-SAQ	4.37	1.48	1.43
5	B	806	SFY	OAC-SAQ	4.31	1.48	1.43
5	D	803	SFY	OAB-SAQ	4.19	1.48	1.43
5	C	804	SFY	OAC-SAQ	4.16	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	NAP	O4D-C1D	3.45	1.45	1.41
2	C	801	NAP	O4D-C1D	3.43	1.45	1.41
5	A	807	SFY	CAN-NAA	3.19	1.49	1.38
5	C	804	SFY	CAN-NAA	3.17	1.49	1.38
5	B	806	SFY	CAN-NAA	3.15	1.49	1.38
5	D	803	SFY	CAN-NAA	3.12	1.49	1.38
2	D	801	NAP	O4D-C1D	2.71	1.44	1.41
2	C	801	NAP	O4B-C1B	2.62	1.44	1.41
2	A	801	NAP	O4D-C1D	2.57	1.44	1.41
2	A	801	NAP	O4B-C1B	2.49	1.44	1.41
2	B	801	NAP	O4B-C1B	2.26	1.44	1.41
2	D	801	NAP	C3N-C7N	2.24	1.53	1.50
2	C	801	NAP	C6N-N1N	2.23	1.40	1.35
2	D	801	NAP	C6N-N1N	2.11	1.40	1.35
2	A	801	NAP	C6N-N1N	2.08	1.40	1.35
2	C	801	NAP	C3N-C7N	2.07	1.53	1.50
2	B	801	NAP	C6N-N1N	2.06	1.40	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	803	SFY	OAC-SAQ-OAB	-8.61	108.96	119.55
5	A	807	SFY	OAC-SAQ-OAB	-8.41	109.20	119.55
5	B	806	SFY	OAC-SAQ-OAB	-8.34	109.30	119.55
5	C	804	SFY	OAC-SAQ-OAB	-7.93	109.80	119.55
2	C	801	NAP	N3A-C2A-N1A	-4.73	121.28	128.68
2	D	801	NAP	N3A-C2A-N1A	-4.54	121.59	128.68
2	A	801	NAP	N3A-C2A-N1A	-4.50	121.64	128.68
2	B	801	NAP	N3A-C2A-N1A	-4.41	121.78	128.68
5	C	804	SFY	NAM-CAO-NAL	3.77	118.37	114.12
5	B	806	SFY	NAM-CAO-NAL	3.76	118.36	114.12
5	D	803	SFY	NAM-CAO-NAL	3.72	118.31	114.12
5	A	807	SFY	NAM-CAO-NAL	3.68	118.27	114.12
5	D	803	SFY	CAF-NAL-CAO	3.40	122.04	117.22
5	D	803	SFY	CAP-SAQ-NAM	3.28	110.96	106.83
5	B	806	SFY	CAF-NAL-CAO	3.14	121.67	117.22
5	C	804	SFY	CAF-NAL-CAO	3.13	121.66	117.22
5	C	804	SFY	CAP-SAQ-NAM	3.03	110.64	106.83
2	B	801	NAP	PN-O3-PA	-2.99	122.56	132.83
5	A	807	SFY	CAF-NAL-CAO	2.98	121.44	117.22
2	D	801	NAP	PN-O3-PA	-2.74	123.43	132.83
5	B	806	SFY	CAP-SAQ-NAM	2.70	110.23	106.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	NAP	PN-O3-PA	-2.69	123.58	132.83
2	B	801	NAP	C6N-N1N-C2N	-2.40	119.78	121.97
2	C	801	NAP	C6N-N1N-C2N	-2.36	119.82	121.97
2	C	801	NAP	O4D-C1D-C2D	-2.22	103.68	106.93
2	A	801	NAP	PN-O3-PA	-2.19	125.30	132.83
2	D	801	NAP	C6N-N1N-C2N	-2.18	119.99	121.97
5	D	803	SFY	CAG-CAO-NAL	-2.08	119.32	122.57
5	A	807	SFY	CAP-SAQ-NAM	2.07	109.44	106.83
2	A	801	NAP	O4D-C1D-C2D	-2.06	103.91	106.93
5	B	806	SFY	OAB-SAQ-CAP	2.04	110.48	107.97
2	D	801	NAP	O4D-C1D-C2D	-2.01	103.98	106.93

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAP	C5D-O5D-PN-O1N
2	A	801	NAP	C5D-O5D-PN-O2N
2	A	801	NAP	O4D-C1D-N1N-C2N
2	B	801	NAP	O4D-C1D-N1N-C2N
2	C	801	NAP	C5D-O5D-PN-O2N
2	C	801	NAP	O4D-C1D-N1N-C2N
2	D	801	NAP	C2B-O2B-P2B-O1X
2	D	801	NAP	C2B-O2B-P2B-O2X
2	D	801	NAP	C5D-O5D-PN-O3
2	D	801	NAP	O4D-C1D-N1N-C2N
4	A	803	GOL	O1-C1-C2-C3
4	A	809	GOL	O1-C1-C2-C3
4	B	803	GOL	O1-C1-C2-C3
4	B	807	GOL	O1-C1-C2-C3
6	A	810	PEG	O2-C3-C4-O4
6	A	810	PEG	O1-C1-C2-O2
6	C	805	PEG	O1-C1-C2-O2
4	A	803	GOL	C1-C2-C3-O3
4	A	806	GOL	O1-C1-C2-C3
4	A	806	GOL	C1-C2-C3-O3
4	A	809	GOL	C1-C2-C3-O3
4	B	807	GOL	C1-C2-C3-O3
4	C	803	GOL	O1-C1-C2-C3
5	D	803	SFY	CAJ-CAP-SAQ-OAC
5	A	807	SFY	CAK-CAP-SAQ-OAC
5	B	806	SFY	CAK-CAP-SAQ-OAC

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Mol	Chain	Res	Type	Atoms
5	D	803	SFY	CAK-CAP-SAQ-OAC
5	B	806	SFY	CAJ-CAP-SAQ-OAC
5	A	807	SFY	CAJ-CAP-SAQ-OAC
5	C	804	SFY	CAJ-CAP-SAQ-OAC
4	A	803	GOL	O1-C1-C2-O2
4	A	806	GOL	O1-C1-C2-O2
4	A	809	GOL	O1-C1-C2-O2
4	B	803	GOL	O1-C1-C2-O2
4	B	807	GOL	O1-C1-C2-O2
5	C	804	SFY	CAK-CAP-SAQ-OAC
5	D	803	SFY	CAJ-CAP-SAQ-NAM
5	B	806	SFY	CAJ-CAP-SAQ-NAM
5	D	803	SFY	CAK-CAP-SAQ-NAM
5	B	806	SFY	CAK-CAP-SAQ-NAM
5	A	807	SFY	CAJ-CAP-SAQ-NAM
6	A	810	PEG	C1-C2-O2-C3
6	C	805	PEG	C1-C2-O2-C3
5	A	807	SFY	CAK-CAP-SAQ-NAM
2	C	801	NAP	C5D-O5D-PN-O3
4	B	807	GOL	O2-C2-C3-O3
6	C	805	PEG	O2-C3-C4-O4
2	C	801	NAP	C5D-O5D-PN-O1N
2	D	801	NAP	C5D-O5D-PN-O1N
5	C	804	SFY	CAJ-CAP-SAQ-NAM
2	D	801	NAP	PA-O3-PN-O2N
5	C	804	SFY	CAK-CAP-SAQ-NAM
2	C	801	NAP	O4B-C4B-C5B-O5B
2	D	801	NAP	O4B-C4B-C5B-O5B
4	C	803	GOL	O1-C1-C2-O2
2	A	801	NAP	O4B-C4B-C5B-O5B
2	A	801	NAP	C5D-O5D-PN-O3
4	A	809	GOL	O2-C2-C3-O3
2	B	801	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	807	GOL	1	0
2	D	801	NAP	1	0
2	C	801	NAP	2	0
5	B	806	SFY	1	0

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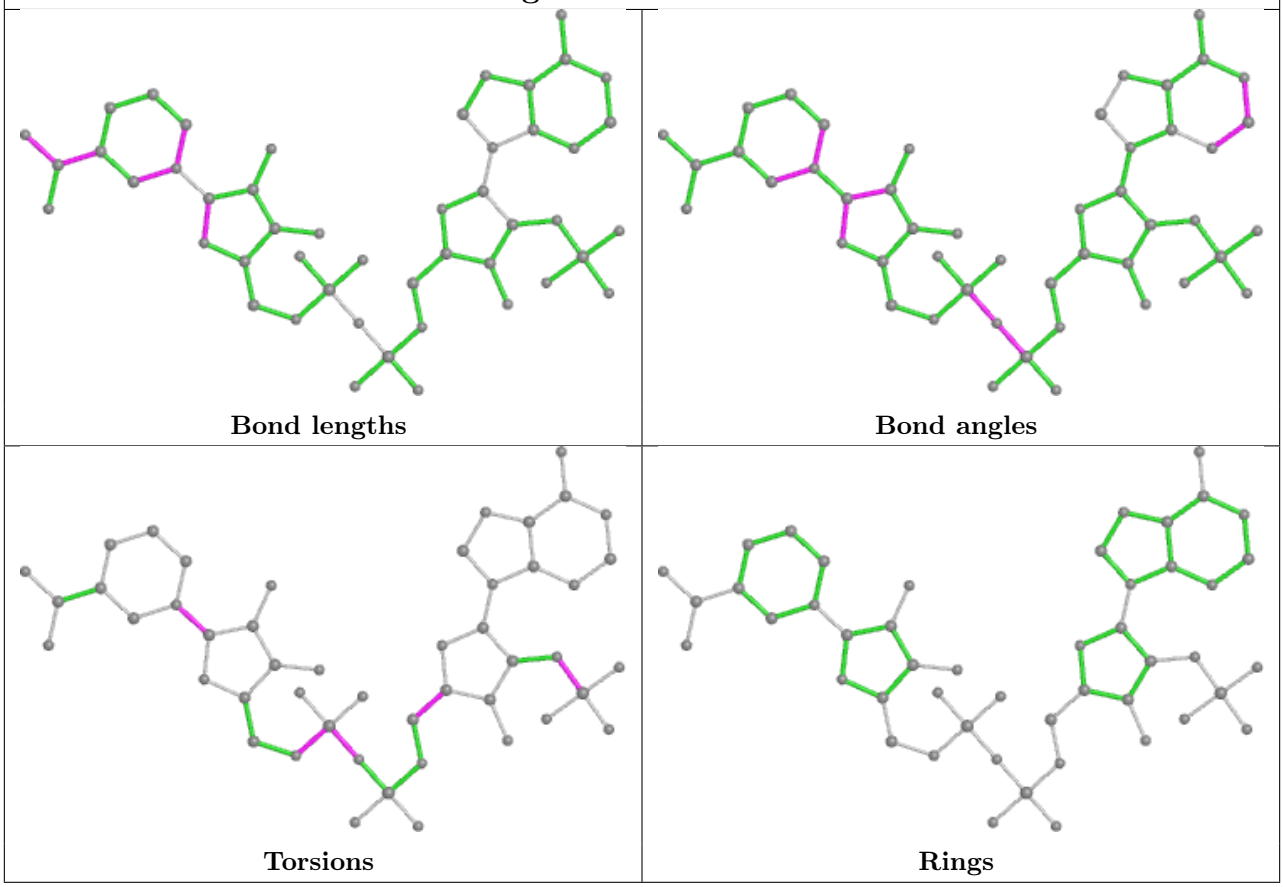
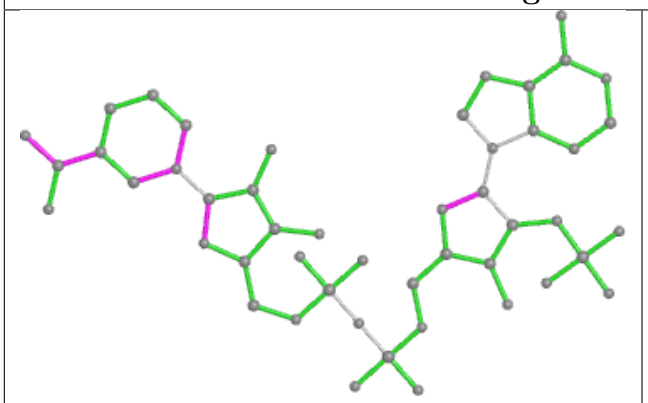
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	NAP	1	0
2	A	801	NAP	1	0
4	A	806	GOL	1	0

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.

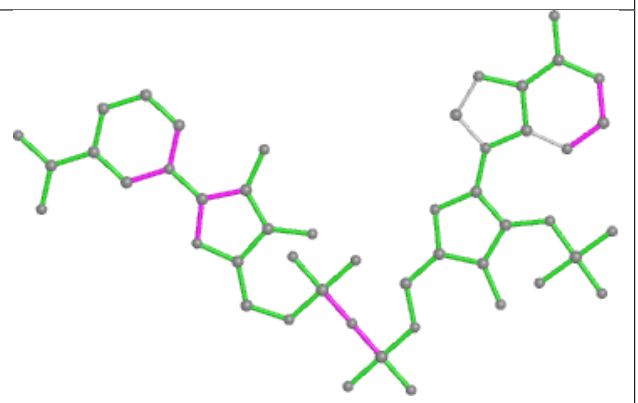
Ligand NAP D 801



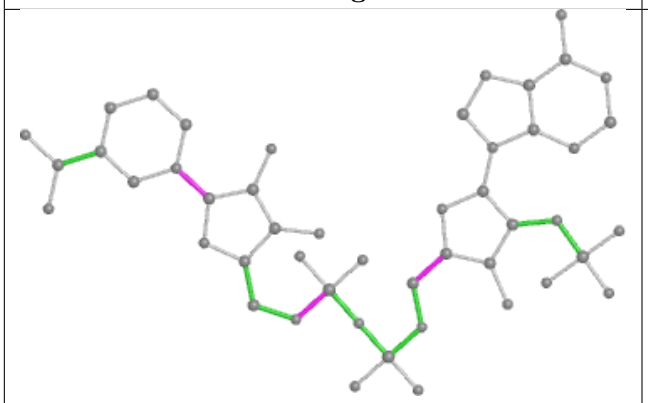
Ligand NAP C 801



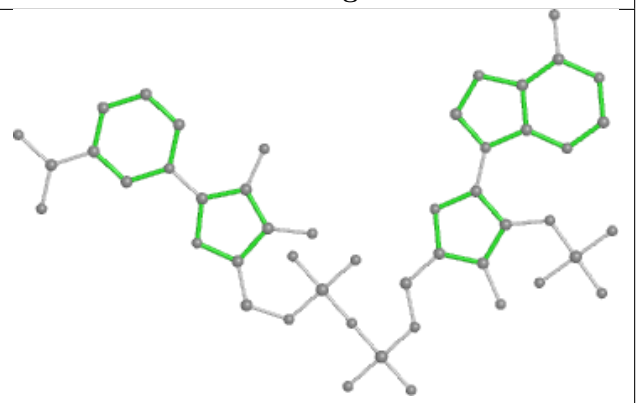
Bond lengths



Bond angles

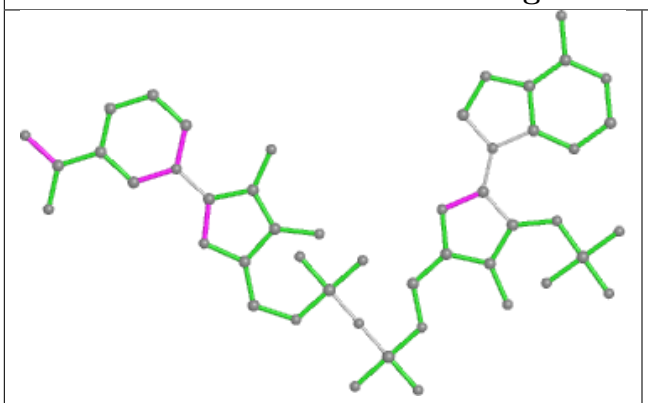


Torsions

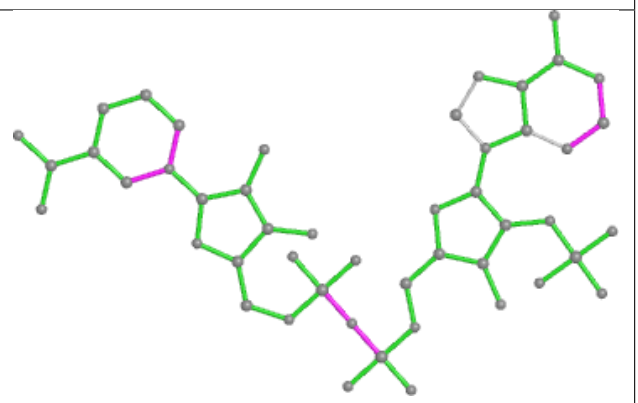


Rings

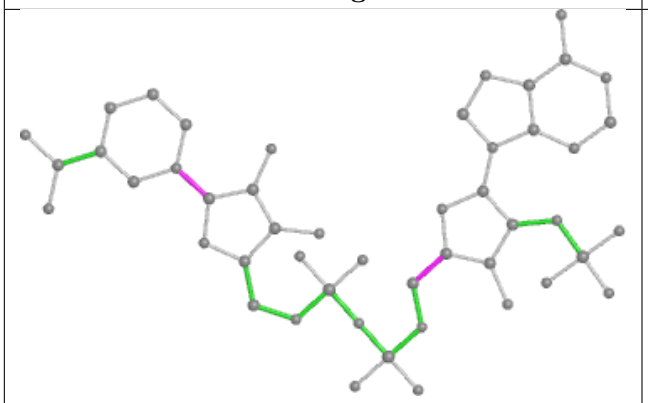
Ligand NAP B 801



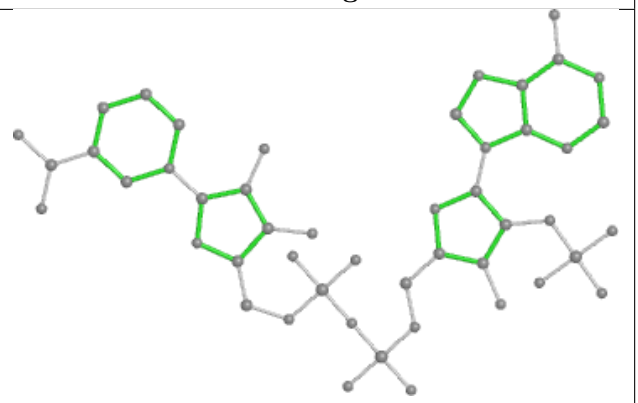
Bond lengths



Bond angles

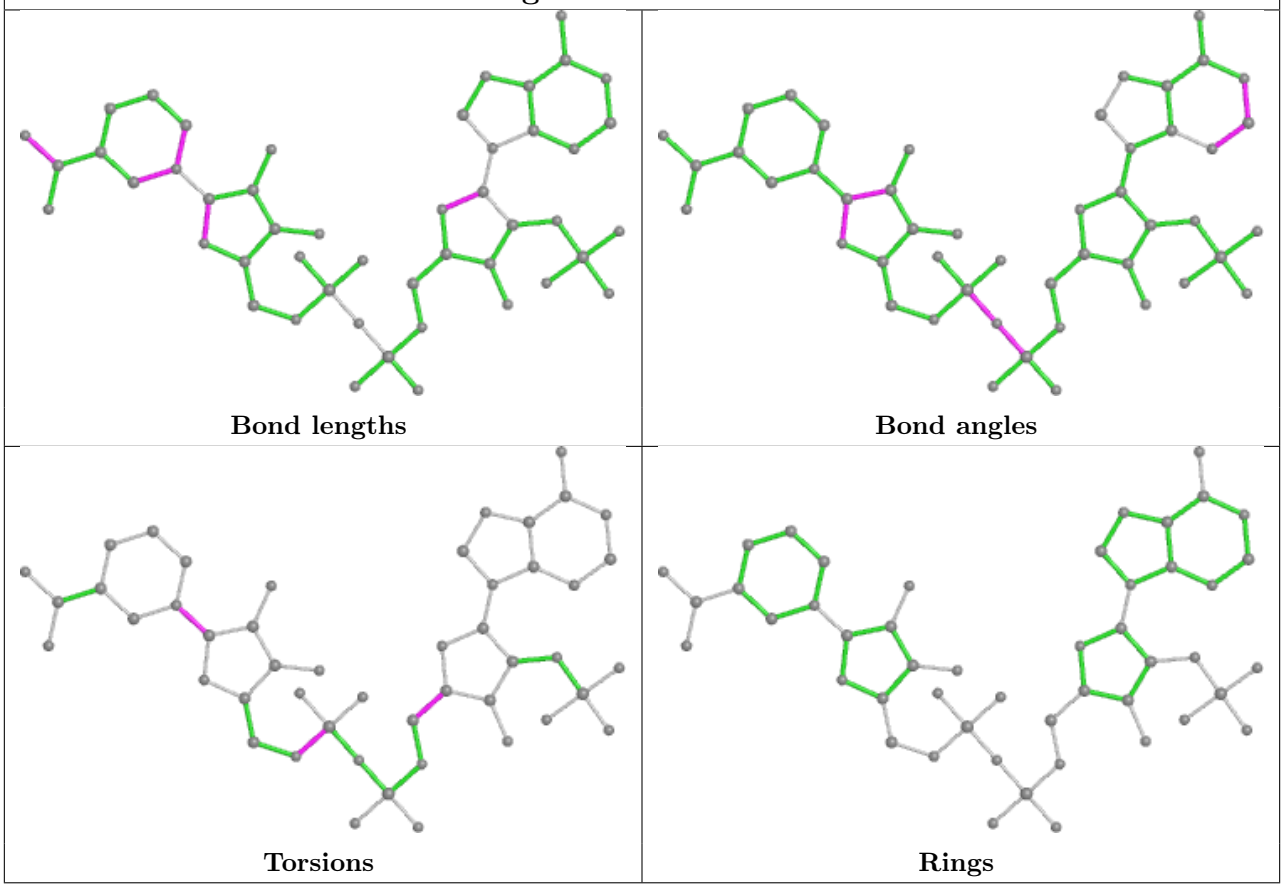


Torsions



Rings

Ligand NAP A 801



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	257/288 (89%)	-0.59	1 (0%)	92	91	18, 30, 46, 68	0
1	B	257/288 (89%)	-0.56	2 (0%)	86	84	21, 32, 51, 86	0
1	C	257/288 (89%)	-0.51	0	100	100	19, 33, 52, 66	0
1	D	257/288 (89%)	-0.22	5 (1%)	66	64	23, 40, 68, 92	0
All	All	1028/1152 (89%)	-0.47	8 (0%)	86	84	18, 33, 56, 92	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	224	ALA	4.8
1	D	227	LYS	3.0
1	B	54	GLU	2.9
1	D	55	ARG	2.8
1	D	217	LYS	2.6
1	B	55	ARG	2.4
1	D	225	LYS	2.2
1	A	55	ARG	2.1

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)

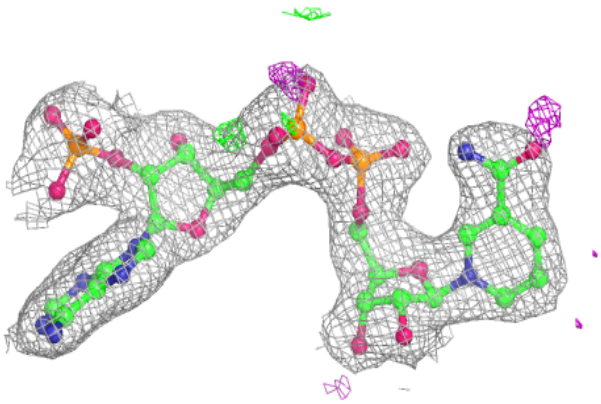
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

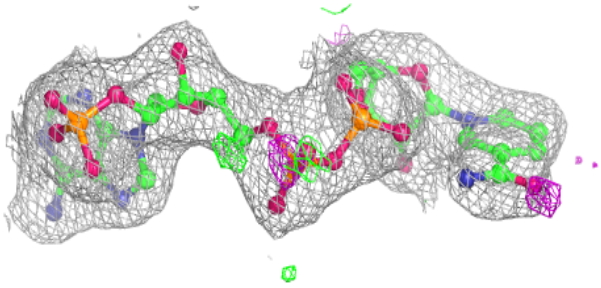
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	807	6/6	0.56	0.35	58,62,62,63	0
6	PEG	C	805	7/7	0.63	0.29	71,73,75,75	0
4	GOL	A	806	6/6	0.67	0.34	51,53,54,55	0
6	PEG	A	810	7/7	0.76	0.22	61,62,64,64	0
3	SO4	A	805	5/5	0.77	0.23	97,98,99,99	0
4	GOL	A	809	6/6	0.80	0.22	50,51,52,53	0
3	SO4	A	808	5/5	0.80	0.34	117,118,119,120	0
3	SO4	D	804	5/5	0.82	0.25	105,105,107,108	0
4	GOL	A	803	6/6	0.85	0.17	54,55,56,56	0
3	SO4	B	805	5/5	0.88	0.20	95,95,97,99	0
3	SO4	B	804	5/5	0.89	0.24	73,74,75,76	0
4	GOL	C	803	6/6	0.91	0.13	55,57,58,58	0
4	GOL	B	803	6/6	0.91	0.20	47,49,50,53	0
4	GOL	A	804	6/6	0.91	0.15	51,54,54,55	0
3	SO4	D	802	5/5	0.95	0.18	73,73,73,74	0
3	SO4	B	802	5/5	0.96	0.14	58,58,60,60	0
2	NAP	D	801	48/48	0.97	0.12	34,37,41,42	0
5	SFY	D	803	17/17	0.97	0.15	38,39,45,45	0
5	SFY	B	806	17/17	0.98	0.12	19,22,25,26	0
5	SFY	C	804	17/17	0.98	0.10	26,28,32,33	0
3	SO4	A	802	5/5	0.98	0.12	53,54,55,55	0
2	NAP	C	801	48/48	0.98	0.11	23,26,28,29	0
3	SO4	C	802	5/5	0.98	0.08	56,57,57,58	0
5	SFY	A	807	17/17	0.99	0.09	20,22,25,25	0
2	NAP	A	801	48/48	0.99	0.10	19,21,23,23	0
2	NAP	B	801	48/48	0.99	0.10	18,23,27,27	0

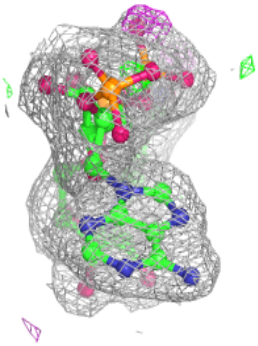
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP D 801:

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

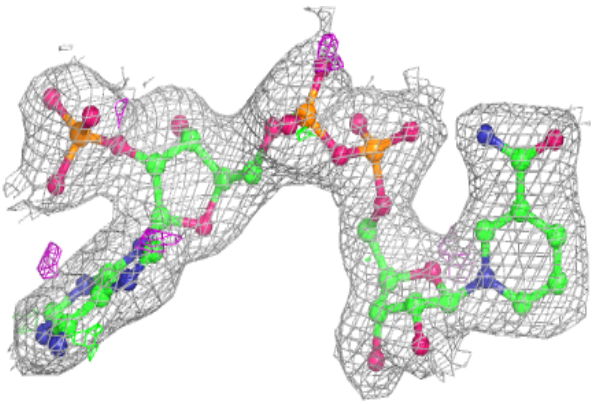


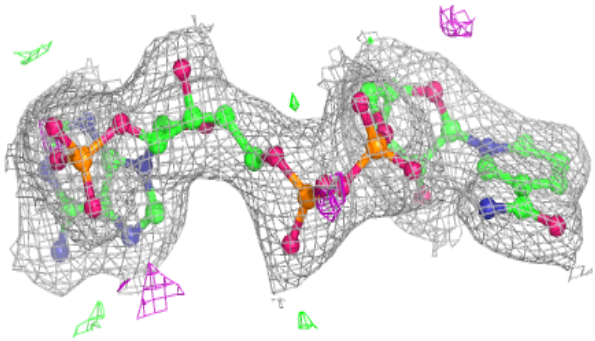


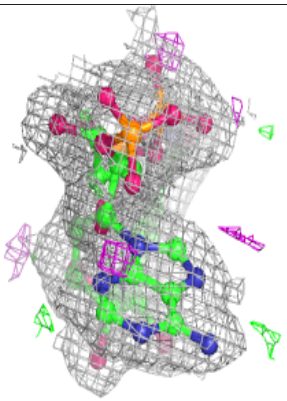


Electron density around NAP C 801:

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

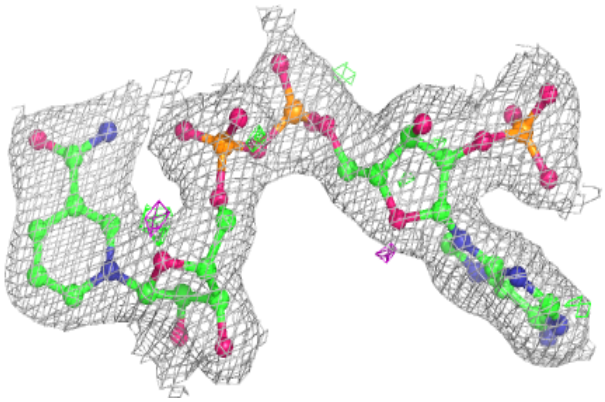


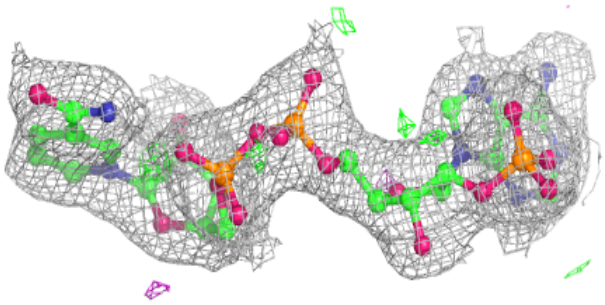


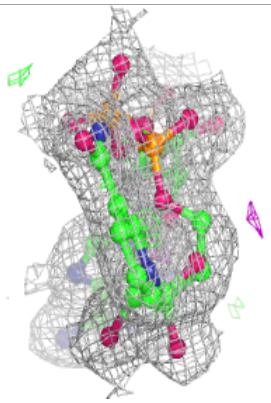


Electron density around NAP A 801:

$2mF_o$-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 801:

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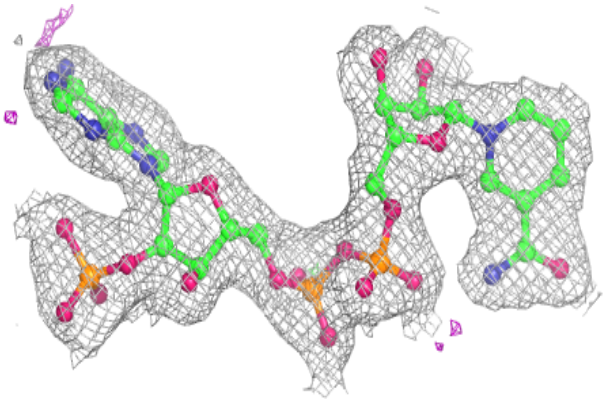
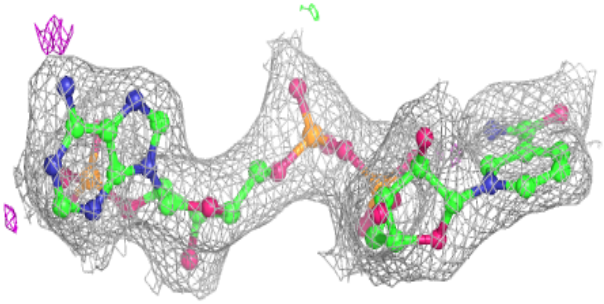
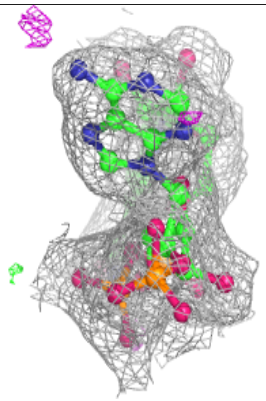
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.