Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 01:16 PM EDT

PDB ID	:	5COB
Title	:	Crystal structure of iridoid synthase in complex with NADP+ and 8-oxogeranial at 2.65-angstrom resolution
Authors	:	Qin, L.; Zhu, Y.; Ding, Z.; Zhang, X.; Ye, S.; Zhang, R.
Deposited on	:	2015-07-20
Resolution	:	2.65 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:

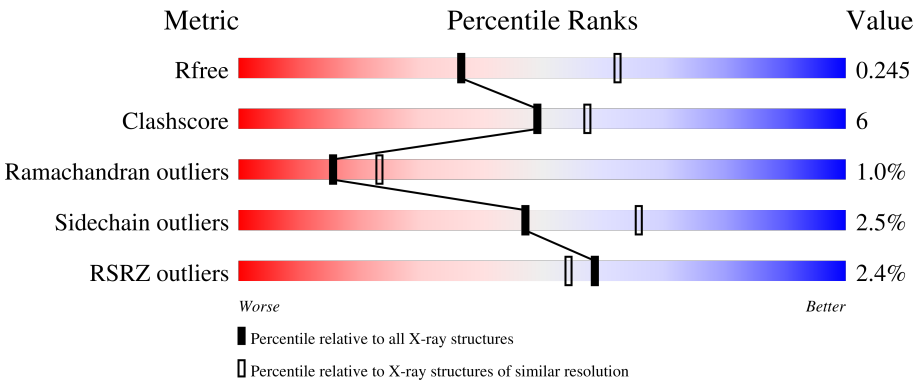
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	365	2% 86% 13% •
1	B	365	3% 82% 18% •
1	C	365	2% 85% 13% •
1	D	365	3% 83% 16% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12059 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 Iridoid synthase.

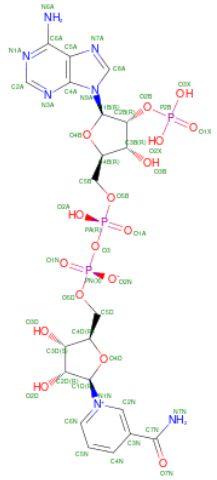
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	365	2895	1864	477	534	20	0	0	0
1	B	365	2895	1864	477	534	20	0	0	0
1	C	365	2895	1864	477	534	20	0	0	0
1	D	365	2895	1864	477	534	20	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	expression tag	UNP K7WDL7
A	25	ALA	-	expression tag	UNP K7WDL7
B	24	MET	-	expression tag	UNP K7WDL7
B	25	ALA	-	expression tag	UNP K7WDL7
C	24	MET	-	expression tag	UNP K7WDL7
C	25	ALA	-	expression tag	UNP K7WDL7
D	24	MET	-	expression tag	UNP K7WDL7
D	25	ALA	-	expression tag	UNP K7WDL7

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

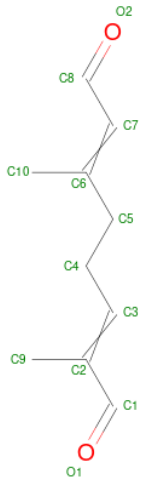
NAP



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

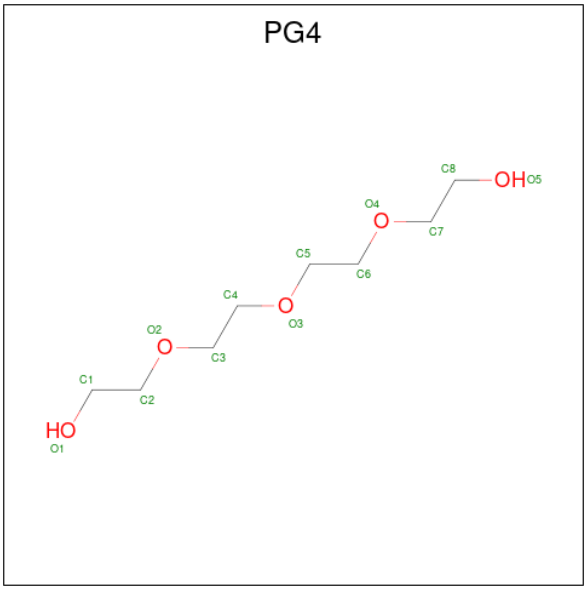
- Molecule 3 is (2E,6E)-2,6-dimethylocta-2,6-dienedial (three-letter code: XOG) (formula: $C_{10}H_{14}O_2$).

XOG



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	12	10	2	0	0
3	B	1	12	10	2	0	0
3	C	1	12	10	2	0	0
3	D	1	12	10	2	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	13	8	5	0	0
4	B	1	13	8	5	0	0
4	C	1	13	8	5	0	0
4	D	1	13	8	5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	48	48	48	0	0
5	B	52	52	52	0	0

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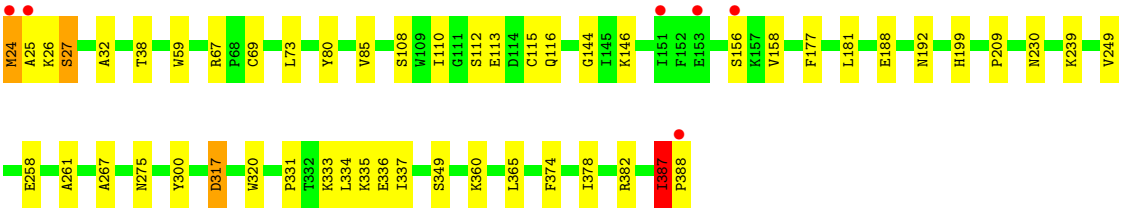
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	41	41	41	0	0
			Total	O		
5	D	46	46	46	0	0

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: Iridoid synthase

Chain A: 2% 86% 13%

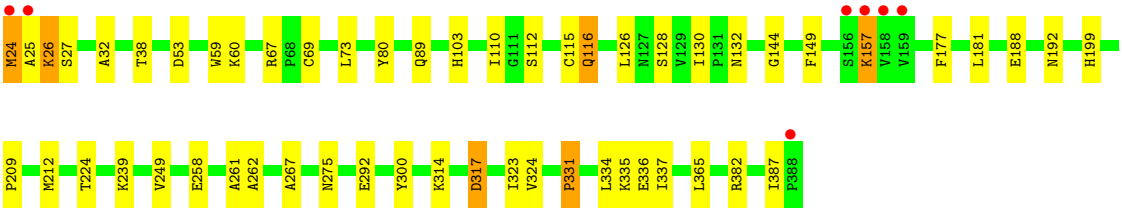


• Molecule 1: Iridoid synthase

Chain B: 3% 82% 18%

• Molecule 1: Iridoid synthase

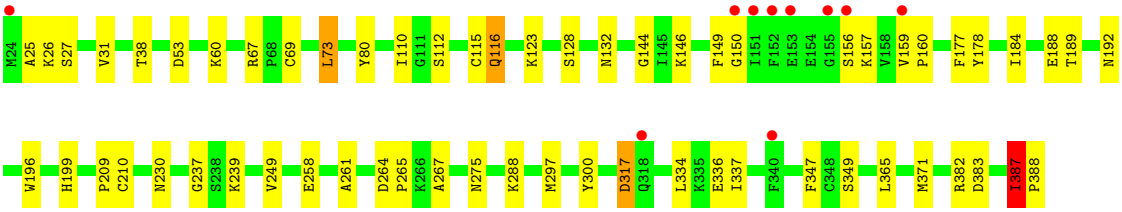
Chain C: 2% 85% 13%



• Molecule 1: Iridoid synthase

Chain D:

3%
83%
16%


M24 A25 K26 S27 V31 T38 D53 K60 R67 P68 C69 L73 Y80 I110 G111 S112 C115 Q116 K123 S128 N132 G144 I145 K146 F149 G150 I151 F152 E153 E154 G155 S156 K157 V158 V159 P160 F177 Y178 I184 E188 T189 N192
W196 H199 P209 C210 N230 G237 S238 K239 V249 E258 A261 D264 P265 K266 A267 N275 K288 M297 Y300 D317 Q318 L334 K335 E336 I337 F340 F347 C348 S349 L365 M371 R382 D383 I387 P388

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.99Å 171.91Å 66.03Å 90.00° 89.72° 90.00°	Depositor
Resolution (Å)	36.14 – 2.65 46.56 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.6 (36.14-2.65) 93.4 (46.56-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.09 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.194 , 0.245 0.194 , 0.245	Depositor DCC
R_{free} test set	2114 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.755	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.417 for -l,k,h 0.418 for h,-k,-l 0.477 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12059	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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: NAP, PG4, XOG

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	0.23	0/2970	0.40	0/4031
1	B	0.23	0/2970	0.40	0/4031
1	C	0.23	0/2970	0.40	0/4031
1	D	0.23	0/2970	0.41	0/4031
All	All	0.23	0/11880	0.40	0/16124

There are no bond length outliers.

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	2895	0	2866	34	0
1	B	2895	0	2866	44	0
1	C	2895	0	2866	35	0
1	D	2895	0	2866	33	0
2	A	48	0	23	4	0
2	B	48	0	23	2	0
2	C	48	0	23	3	0
2	D	48	0	23	1	0
3	A	12	0	14	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	14	2	0
3	C	12	0	14	3	0
3	D	12	0	14	5	0
4	A	13	0	18	2	0
4	B	13	0	18	1	0
4	C	13	0	18	0	0
4	D	13	0	18	1	0
5	A	48	0	0	2	0
5	B	52	0	0	2	0
5	C	41	0	0	2	0
5	D	46	0	0	1	0
All	All	12059	0	11684	140	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 6.

All (140) 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:67:ARG:NH2	2:C:1001:NAP:O2X	2.22	0.72
1:D:249:VAL:HB	1:D:275:ASN:HA	1.70	0.72
1:A:249:VAL:HB	1:A:275:ASN:HA	1.74	0.70
1:D:67:ARG:NH1	1:D:336:GLU:OE2	2.25	0.70
1:D:67:ARG:NH2	2:D:1001:NAP:O2X	2.24	0.69
1:C:67:ARG:NH1	1:C:336:GLU:OE2	2.24	0.69
1:B:236:PRO:HG3	1:B:309:LEU:HD13	1.76	0.68
1:B:24:MET:N	1:B:28:TYR:O	2.27	0.67
1:B:249:VAL:HB	1:B:275:ASN:HA	1.77	0.65
1:C:249:VAL:HB	1:C:275:ASN:HA	1.79	0.64
1:C:365:LEU:HD13	1:D:365:LEU:HD13	1.80	0.63
1:B:72:TRP:O	1:C:116:GLN:NE2	2.32	0.63
1:A:113:GLU:OE2	1:A:146:LYS:NZ	2.31	0.63
1:A:67:ARG:NH1	1:A:336:GLU:OE2	2.32	0.63
1:B:67:ARG:NH1	1:B:336:GLU:OE2	2.33	0.62
1:C:188:GLU:O	1:C:192:ASN:ND2	2.31	0.62
1:B:67:ARG:NH2	2:B:1001:NAP:O2X	2.26	0.62
1:A:317:ASP:OD1	1:A:317:ASP:N	2.33	0.61
1:D:188:GLU:O	1:D:192:ASN:ND2	2.31	0.61
1:B:76:LYS:HD3	1:C:116:GLN:HE21	1.65	0.60
1:D:110:ILE:HG23	1:D:112:SER:H	1.67	0.58
1:A:144:GLY:HA3	3:A:1002:XOG:H2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:LEU:HD12	1:B:312:LEU:HD11	1.87	0.57
1:B:115:CYS:HA	1:B:177:PHE:HB3	1.86	0.57
1:A:67:ARG:NH2	2:A:1001:NAP:O2X	2.29	0.56
1:C:317:ASP:OD1	1:C:317:ASP:N	2.31	0.56
1:B:110:ILE:HG23	1:B:112:SER:H	1.70	0.56
1:B:333:LYS:HG2	1:B:335:LYS:HD3	1.88	0.56
1:B:188:GLU:O	1:B:192:ASN:ND2	2.35	0.56
1:D:382:ARG:HA	1:D:388:PRO:HD3	1.88	0.55
1:A:110:ILE:HG23	1:A:112:SER:H	1.70	0.55
1:C:25:ALA:O	1:C:27:SER:N	2.41	0.54
1:A:382:ARG:HA	1:A:388:PRO:HD3	1.90	0.54
1:D:239:LYS:HB2	1:D:300:TYR:CZ	2.43	0.53
1:B:288:LYS:NZ	5:B:1105:HOH:O	2.42	0.53
1:D:144:GLY:HA3	3:D:1002:XOG:H2	1.90	0.53
1:C:110:ILE:HG23	1:C:112:SER:H	1.73	0.52
1:B:75:LYS:HB3	1:C:115:CYS:HB2	1.89	0.52
1:B:144:GLY:HA3	3:B:1002:XOG:H2	1.91	0.52
1:D:146:LYS:HB2	3:D:1002:XOG:O2	2.09	0.52
1:C:144:GLY:HA3	3:C:1002:XOG:H2	1.92	0.52
1:B:157:LYS:NZ	5:B:1106:HOH:O	2.42	0.51
1:D:31:VAL:HG22	1:D:60:LYS:HB3	1.93	0.51
1:C:199:HIS:CE1	1:C:258:GLU:HA	2.45	0.51
1:C:128:SER:O	1:C:132:ASN:ND2	2.44	0.51
1:D:199:HIS:CE1	1:D:258:GLU:HA	2.46	0.50
1:A:25:ALA:O	1:A:27:SER:N	2.45	0.49
1:C:224:THR:HG22	1:C:323:ILE:HD13	1.93	0.49
1:C:103:HIS:CD2	1:C:262:ALA:HB1	2.48	0.49
1:D:25:ALA:O	1:D:27:SER:N	2.45	0.49
1:B:50:LYS:HG3	1:B:77:PRO:HG2	1.94	0.48
1:A:349:SER:OG	3:A:1002:XOG:O1	2.23	0.48
1:B:31:VAL:HG22	1:B:60:LYS:HB3	1.95	0.48
1:D:115:CYS:HA	1:D:177:PHE:HB3	1.96	0.48
1:B:24:MET:HE3	1:B:135:ASN:HD22	1.79	0.47
1:C:103:HIS:HD2	1:C:262:ALA:HB1	1.80	0.47
1:B:128:SER:O	1:B:132:ASN:ND2	2.45	0.47
1:A:387:ILE:H	1:A:388:PRO:CD	2.28	0.47
1:A:188:GLU:O	1:A:192:ASN:ND2	2.41	0.47
1:A:115:CYS:HA	1:A:177:PHE:HB3	1.95	0.47
1:A:69:CYS:HB2	1:A:80:TYR:CD2	2.50	0.46
1:A:146:LYS:HB2	3:A:1002:XOG:O2	2.14	0.46
1:A:209:PRO:HA	1:A:337:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LYS:NZ	5:C:1111:HOH:O	2.48	0.46
1:A:108:SER:HB2	2:A:1001:NAP:O4B	2.15	0.46
1:A:317:ASP:OD2	5:A:1101:HOH:O	2.21	0.46
1:B:149:PHE:HZ	3:B:1002:XOG:H14	1.79	0.46
1:B:384:TYR:CE1	1:C:116:GLN:HB2	2.51	0.46
1:C:149:PHE:HZ	3:C:1002:XOG:H14	1.81	0.46
1:B:239:LYS:HB2	1:B:300:TYR:CZ	2.51	0.45
1:A:199:HIS:CE1	1:A:258:GLU:HA	2.52	0.45
3:A:1002:XOG:H8	4:A:1003:PG4:H82	1.98	0.45
1:B:24:MET:HE2	1:B:100:ASP:HA	1.97	0.45
1:B:28:TYR:HA	1:B:58:PRO:HG2	1.99	0.45
1:B:138:HIS:ND1	1:B:195:THR:OG1	2.38	0.45
1:C:69:CYS:HB2	1:C:80:TYR:CD2	2.52	0.45
1:D:116:GLN:H	1:D:116:GLN:HG2	1.48	0.45
1:A:38:THR:HG22	1:A:73:LEU:HD12	1.99	0.45
1:C:382:ARG:HA	1:C:387:ILE:O	2.17	0.45
1:A:24:MET:HB3	1:A:25:ALA:H	1.59	0.45
1:A:67:ARG:HD2	2:A:1001:NAP:O2X	2.17	0.44
1:A:333:LYS:HG2	1:A:335:LYS:HD3	1.99	0.44
1:B:25:ALA:O	1:B:27:SER:N	2.50	0.44
1:C:209:PRO:HA	1:C:337:ILE:HG13	1.98	0.44
1:D:387:ILE:H	1:D:388:PRO:CD	2.30	0.44
1:A:261:ALA:HA	1:A:267:ALA:HB3	1.99	0.44
1:D:288:LYS:HG3	1:D:371:MET:SD	2.58	0.44
1:D:189:THR:HG21	1:D:196:TRP:HB3	1.99	0.44
1:B:103:HIS:CD2	1:B:138:HIS:HB3	2.53	0.44
1:C:292:GLU:O	1:C:382:ARG:NH2	2.35	0.44
1:C:126:LEU:HD22	1:C:130:ILE:HD11	2.00	0.44
1:C:38:THR:HG21	1:C:67:ARG:HD3	1.99	0.44
1:B:199:HIS:CE1	1:B:258:GLU:HA	2.53	0.43
1:B:103:HIS:CD2	1:B:262:ALA:HB1	2.53	0.43
1:D:349:SER:OG	3:D:1002:XOG:O1	2.26	0.43
1:A:334:LEU:HB3	5:A:1101:HOH:O	2.18	0.43
1:B:67:ARG:HD2	2:B:1001:NAP:O2X	2.19	0.43
1:D:150:GLY:HA3	4:D:1003:PG4:H12	2.00	0.43
1:B:24:MET:HE1	1:B:135:ASN:HB2	2.01	0.43
1:B:221:VAL:HG22	1:B:320:TRP:CH2	2.54	0.43
1:B:69:CYS:HB2	1:B:80:TYR:CD2	2.54	0.42
1:C:334:LEU:HB3	5:C:1106:HOH:O	2.19	0.42
1:A:177:PHE:O	1:A:181:LEU:HG	2.19	0.42
1:A:374:PHE:O	1:A:378:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:LYS:HG3	1:D:184:ILE:HD13	2.02	0.42
1:D:69:CYS:HB2	1:D:80:TYR:CD2	2.54	0.42
1:C:239:LYS:HB2	1:C:300:TYR:CZ	2.55	0.42
1:A:365:LEU:HD13	1:B:365:LEU:HD13	2.00	0.42
1:C:177:PHE:O	1:C:181:LEU:HG	2.19	0.42
1:D:149:PHE:HZ	3:D:1002:XOG:H14	1.83	0.42
1:A:239:LYS:HB2	1:A:300:TYR:CZ	2.54	0.42
1:B:32:ALA:HB2	1:B:59:TRP:CZ3	2.54	0.42
1:B:123:LYS:HG3	1:B:184:ILE:HD13	2.01	0.42
2:C:1001:NAP:C2N	3:C:1002:XOG:H7	2.50	0.42
1:D:178:TYR:OH	3:D:1002:XOG:O2	2.31	0.42
1:A:85:VAL:HG23	2:A:1001:NAP:H2A	2.01	0.42
1:C:32:ALA:HB2	1:C:59:TRP:CE3	2.55	0.42
1:B:372:LYS:O	1:C:89:GLN:NE2	2.52	0.42
1:C:24:MET:HB3	1:C:25:ALA:H	1.61	0.42
1:D:38:THR:HG22	1:D:73:LEU:HD12	2.02	0.42
1:D:317:ASP:OD1	1:D:317:ASP:N	2.34	0.42
1:B:261:ALA:HA	1:B:267:ALA:HB3	2.01	0.41
1:B:288:LYS:HG3	1:B:371:MET:SD	2.59	0.41
1:D:261:ALA:HA	1:D:267:ALA:HB3	2.01	0.41
1:D:264:ASP:HA	1:D:265:PRO:HD3	1.86	0.41
1:D:159:VAL:HA	1:D:160:PRO:HD2	1.95	0.41
1:A:32:ALA:HB2	1:A:59:TRP:CZ3	2.56	0.41
1:C:261:ALA:HA	1:C:267:ALA:HB3	2.03	0.41
1:A:360:LYS:HB3	1:B:367:PHE:CZ	2.56	0.41
1:B:335:LYS:HE2	1:B:335:LYS:HB2	1.89	0.41
1:D:334:LEU:HB3	5:D:1108:HOH:O	2.21	0.41
1:B:176:ASN:OD1	4:B:1003:PG4:H32	2.21	0.41
1:C:324:VAL:HG11	1:C:331:PRO:HA	2.03	0.41
1:B:65:ALA:HB3	1:B:80:TYR:OH	2.21	0.40
1:C:67:ARG:HD2	2:C:1001:NAP:O2X	2.20	0.40
1:D:128:SER:O	1:D:132:ASN:ND2	2.49	0.40
1:D:237:GLY:HA3	1:D:347:PHE:HB3	2.04	0.40
1:A:320:TRP:HH2	1:A:387:ILE:HD12	1.86	0.40
1:D:209:PRO:HA	1:D:337:ILE:HG13	2.03	0.40
1:A:146:LYS:HD2	4:A:1003:PG4:H42	2.02	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	363/365 (100%)	339 (93%)	19 (5%)	5 (1%)	11	16
1	B	363/365 (100%)	345 (95%)	16 (4%)	2 (1%)	25	37
1	C	363/365 (100%)	343 (94%)	17 (5%)	3 (1%)	19	29
1	D	363/365 (100%)	344 (95%)	15 (4%)	4 (1%)	14	21
All	All	1452/1460 (100%)	1371 (94%)	67 (5%)	14 (1%)	15	23

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	387	ILE
1	D	156	SER
1	A	26	LYS
1	B	26	LYS
1	C	26	LYS
1	D	26	LYS
1	D	387	ILE
1	A	156	SER
1	A	158	VAL
1	B	158	VAL
1	D	157	LYS
1	C	157	LYS
1	A	331	PRO
1	C	331	PRO

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	323/323 (100%)	317 (98%)	6 (2%)	57	74
1	B	323/323 (100%)	316 (98%)	7 (2%)	52	70
1	C	323/323 (100%)	313 (97%)	10 (3%)	40	57
1	D	323/323 (100%)	314 (97%)	9 (3%)	43	61
All	All	1292/1292 (100%)	1260 (98%)	32 (2%)	47	66

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	27	SER
1	A	116	GLN
1	A	230	ASN
1	A	317	ASP
1	A	387	ILE
1	B	116	GLN
1	B	154	GLU
1	B	157	LYS
1	B	297	MET
1	B	317	ASP
1	B	335	LYS
1	B	387	ILE
1	C	24	MET
1	C	26	LYS
1	C	53	ASP
1	C	73	LEU
1	C	116	GLN
1	C	157	LYS
1	C	212	MET
1	C	314	LYS
1	C	317	ASP
1	C	335	LYS
1	D	53	ASP
1	D	73	LEU
1	D	116	GLN
1	D	210	CYS
1	D	230	ASN
1	D	297	MET
1	D	317	ASP
1	D	383	ASP
1	D	387	ILE

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

Mol	Chain	Res	Type
1	B	135	ASN
1	C	116	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)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	D	1001	-	45,52,52	1.37	3 (6%)	56,80,80	1.19	4 (7%)
4	PG4	B	1003	-	12,12,12	0.45	0	11,11,11	0.31	0
4	PG4	C	1003	-	12,12,12	0.45	0	11,11,11	0.30	0
4	PG4	D	1003	-	12,12,12	0.45	0	11,11,11	0.30	0
3	XOG	A	1002	-	11,11,11	3.74	4 (36%)	10,12,12	6.52	4 (40%)
2	NAP	C	1001	-	45,52,52	1.38	3 (6%)	56,80,80	1.18	4 (7%)
4	PG4	A	1003	-	12,12,12	0.46	0	11,11,11	0.29	0
2	NAP	B	1001	-	45,52,52	1.37	3 (6%)	56,80,80	1.17	4 (7%)
3	XOG	C	1002	-	11,11,11	3.73	4 (36%)	10,12,12	6.63	4 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	XOG	D	1002	-	11,11,11	3.77	4 (36%)	10,12,12	6.44	4 (40%)
3	XOG	B	1002	-	11,11,11	3.77	4 (36%)	10,12,12	6.50	4 (40%)
2	NAP	A	1001	-	45,52,52	1.37	3 (6%)	56,80,80	1.16	4 (7%)

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	D	1001	-	-	15/31/67/67	0/5/5/5
4	PG4	B	1003	-	-	0/10/10/10	-
4	PG4	C	1003	-	-	0/10/10/10	-
4	PG4	D	1003	-	-	0/10/10/10	-
3	XOG	A	1002	-	-	3/11/11/11	-
2	NAP	C	1001	-	-	11/31/67/67	0/5/5/5
4	PG4	A	1003	-	-	0/10/10/10	-
2	NAP	B	1001	-	-	10/31/67/67	0/5/5/5
3	XOG	C	1002	-	-	3/11/11/11	-
3	XOG	D	1002	-	-	3/11/11/11	-
3	XOG	B	1002	-	-	3/11/11/11	-
2	NAP	A	1001	-	-	12/31/67/67	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	XOG	O1-C1	9.32	1.43	1.22
3	C	1002	XOG	O1-C1	9.30	1.43	1.22
3	D	1002	XOG	O1-C1	9.28	1.43	1.22
3	A	1002	XOG	O1-C1	9.24	1.43	1.22
3	D	1002	XOG	O2-C8	6.70	1.43	1.22
3	A	1002	XOG	O2-C8	6.70	1.43	1.22
3	B	1002	XOG	O2-C8	6.67	1.43	1.22
3	C	1002	XOG	O2-C8	6.63	1.43	1.22
2	C	1001	NAP	C7N-N7N	-5.56	1.22	1.33
2	B	1001	NAP	C7N-N7N	-5.56	1.22	1.33
2	A	1001	NAP	C7N-N7N	-5.53	1.22	1.33
2	D	1001	NAP	C7N-N7N	-5.50	1.22	1.33
2	D	1001	NAP	O7N-C7N	5.03	1.33	1.24
2	B	1001	NAP	O7N-C7N	5.03	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	NAP	O7N-C7N	5.00	1.33	1.24
2	C	1001	NAP	O7N-C7N	4.99	1.33	1.24
3	B	1002	XOG	C1-C2	4.00	1.51	1.46
3	D	1002	XOG	C1-C2	3.95	1.51	1.46
3	A	1002	XOG	C1-C2	3.87	1.50	1.46
3	C	1002	XOG	C1-C2	3.75	1.50	1.46
3	D	1002	XOG	C7-C8	2.98	1.51	1.44
3	A	1002	XOG	C7-C8	2.90	1.51	1.44
3	B	1002	XOG	C7-C8	2.87	1.51	1.44
3	C	1002	XOG	C7-C8	2.83	1.51	1.44
2	C	1001	NAP	C5A-C4A	2.51	1.47	1.40
2	D	1001	NAP	C5A-C4A	2.50	1.47	1.40
2	A	1001	NAP	C5A-C4A	2.48	1.47	1.40
2	B	1001	NAP	C5A-C4A	2.45	1.47	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1002	XOG	O1-C1-C2	-18.01	106.85	125.16
3	A	1002	XOG	O1-C1-C2	-17.30	107.57	125.16
3	B	1002	XOG	O1-C1-C2	-17.29	107.58	125.16
3	D	1002	XOG	O1-C1-C2	-17.18	107.69	125.16
3	A	1002	XOG	O2-C8-C7	-10.30	111.13	123.66
3	B	1002	XOG	O2-C8-C7	-10.12	111.34	123.66
3	D	1002	XOG	O2-C8-C7	-9.94	111.56	123.66
3	C	1002	XOG	O2-C8-C7	-9.63	111.94	123.66
2	B	1001	NAP	N3A-C2A-N1A	-3.30	123.51	128.68
2	A	1001	NAP	N3A-C2A-N1A	-3.29	123.54	128.68
2	C	1001	NAP	N3A-C2A-N1A	-3.23	123.63	128.68
2	D	1001	NAP	N3A-C2A-N1A	-3.17	123.72	128.68
2	D	1001	NAP	PN-O3-PA	-3.16	121.98	132.83
2	C	1001	NAP	PN-O3-PA	-3.08	122.27	132.83
2	B	1001	NAP	PN-O3-PA	-2.96	122.68	132.83
2	A	1001	NAP	PN-O3-PA	-2.93	122.77	132.83
2	C	1001	NAP	C4A-C5A-N7A	-2.77	106.51	109.40
3	B	1002	XOG	C8-C7-C6	-2.72	119.79	125.60
2	A	1001	NAP	C4A-C5A-N7A	-2.71	106.57	109.40
2	B	1001	NAP	C4A-C5A-N7A	-2.71	106.57	109.40
3	C	1002	XOG	C10-C6-C5	2.70	119.81	115.27
2	D	1001	NAP	C4A-C5A-N7A	-2.69	106.59	109.40
3	C	1002	XOG	C8-C7-C6	-2.59	120.06	125.60
3	B	1002	XOG	C10-C6-C5	2.57	119.59	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1002	XOG	C8-C7-C6	-2.55	120.15	125.60
3	A	1002	XOG	C10-C6-C5	2.52	119.51	115.27
3	A	1002	XOG	C8-C7-C6	-2.46	120.33	125.60
3	D	1002	XOG	C10-C6-C5	2.36	119.25	115.27
2	A	1001	NAP	O3X-P2B-O2X	2.31	116.45	107.64
2	B	1001	NAP	O3X-P2B-O2X	2.19	116.02	107.64
2	D	1001	NAP	O3X-P2B-O2X	2.19	116.02	107.64
2	C	1001	NAP	O3X-P2B-O2X	2.16	115.90	107.64

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	NAP	C5D-O5D-PN-O1N
2	A	1001	NAP	C5D-O5D-PN-O2N
2	A	1001	NAP	O4D-C1D-N1N-C2N
2	A	1001	NAP	O4D-C1D-N1N-C6N
2	A	1001	NAP	C2D-C1D-N1N-C2N
2	A	1001	NAP	C2D-C1D-N1N-C6N
2	B	1001	NAP	C5D-O5D-PN-O1N
2	B	1001	NAP	C5D-O5D-PN-O2N
2	B	1001	NAP	O4D-C1D-N1N-C2N
2	B	1001	NAP	O4D-C1D-N1N-C6N
2	B	1001	NAP	C2D-C1D-N1N-C2N
2	B	1001	NAP	C2D-C1D-N1N-C6N
2	C	1001	NAP	C5D-O5D-PN-O1N
2	C	1001	NAP	C5D-O5D-PN-O2N
2	C	1001	NAP	O4D-C1D-N1N-C2N
2	C	1001	NAP	O4D-C1D-N1N-C6N
2	C	1001	NAP	C2D-C1D-N1N-C2N
2	C	1001	NAP	C2D-C1D-N1N-C6N
2	D	1001	NAP	C5B-O5B-PA-O3
2	D	1001	NAP	C5D-O5D-PN-O1N
2	D	1001	NAP	C5D-O5D-PN-O2N
2	D	1001	NAP	O4D-C1D-N1N-C2N
2	D	1001	NAP	O4D-C1D-N1N-C6N
2	D	1001	NAP	C2D-C1D-N1N-C2N
2	D	1001	NAP	C2D-C1D-N1N-C6N
3	A	1002	XOG	C6-C7-C8-O2
3	B	1002	XOG	C6-C7-C8-O2
3	C	1002	XOG	C6-C7-C8-O2
3	D	1002	XOG	C6-C7-C8-O2

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Mol	Chain	Res	Type	Atoms
3	B	1002	XOG	C4-C5-C6-C10
3	D	1002	XOG	C4-C5-C6-C10
3	B	1002	XOG	C4-C5-C6-C7
3	D	1002	XOG	C4-C5-C6-C7
3	A	1002	XOG	C4-C5-C6-C10
3	A	1002	XOG	C4-C5-C6-C7
2	A	1001	NAP	C5B-O5B-PA-O3
2	B	1001	NAP	C5B-O5B-PA-O3
2	D	1001	NAP	C2B-O2B-P2B-O3X
2	D	1001	NAP	C5D-O5D-PN-O3
2	C	1001	NAP	PN-O3-PA-O1A
2	D	1001	NAP	C5B-O5B-PA-O1A
2	D	1001	NAP	C5B-O5B-PA-O2A
2	A	1001	NAP	O4D-C4D-C5D-O5D
2	D	1001	NAP	O4B-C4B-C5B-O5B
3	C	1002	XOG	C4-C5-C6-C7
3	C	1002	XOG	C4-C5-C6-C10
2	A	1001	NAP	C3D-C4D-C5D-O5D
2	D	1001	NAP	PN-O3-PA-O1A
2	C	1001	NAP	O4B-C4B-C5B-O5B
2	D	1001	NAP	C3D-C4D-C5D-O5D
2	D	1001	NAP	O4D-C4D-C5D-O5D
2	A	1001	NAP	O4B-C4B-C5B-O5B
2	A	1001	NAP	C5D-O5D-PN-O3
2	B	1001	NAP	C2B-O2B-P2B-O3X
2	B	1001	NAP	C5D-O5D-PN-O3
2	C	1001	NAP	C5B-O5B-PA-O3
2	C	1001	NAP	C2B-O2B-P2B-O3X
2	C	1001	NAP	C5D-O5D-PN-O3
2	B	1001	NAP	O4B-C4B-C5B-O5B
2	A	1001	NAP	C5B-O5B-PA-O1A

There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	NAP	1	0
4	B	1003	PG4	1	0
4	D	1003	PG4	1	0
3	A	1002	XOG	4	0
2	C	1001	NAP	3	0
4	A	1003	PG4	2	0

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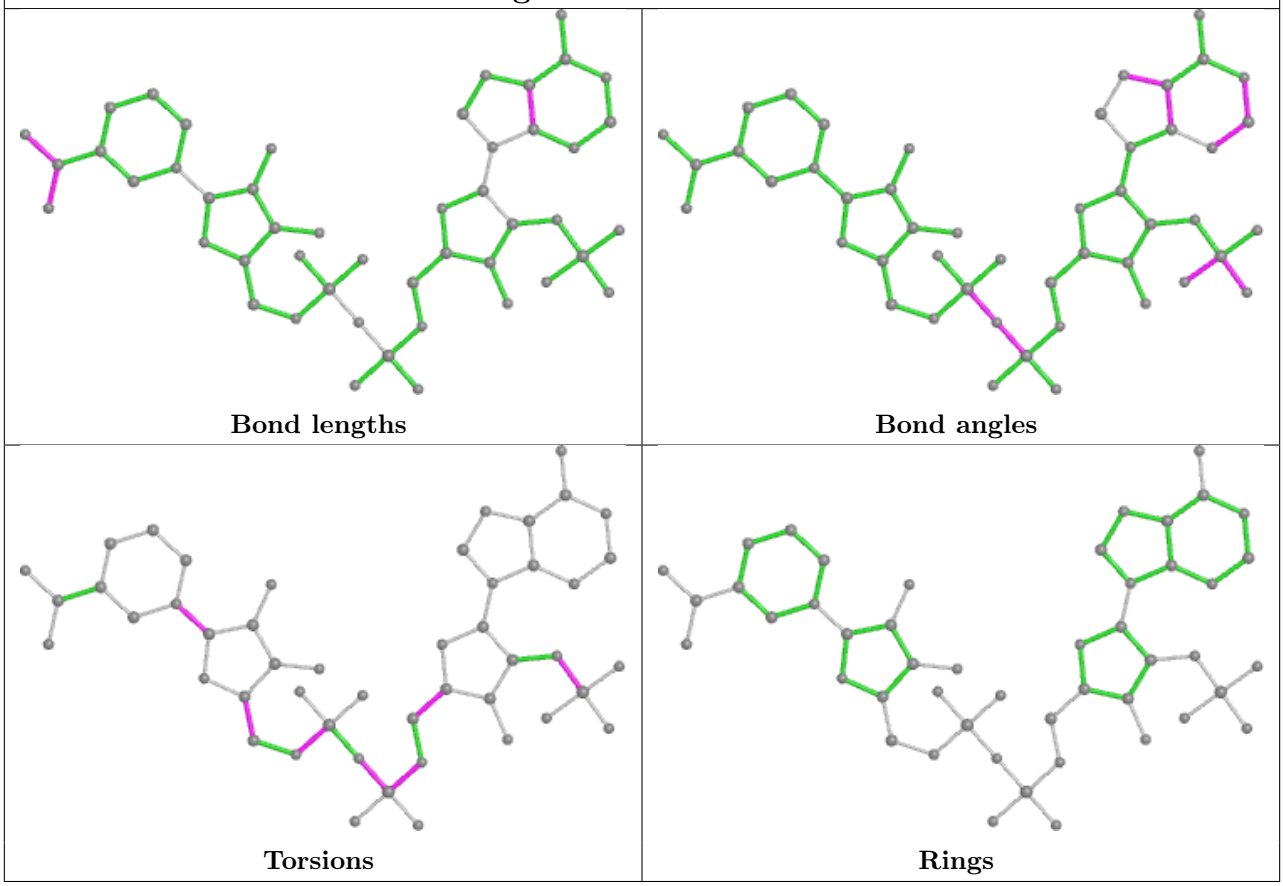
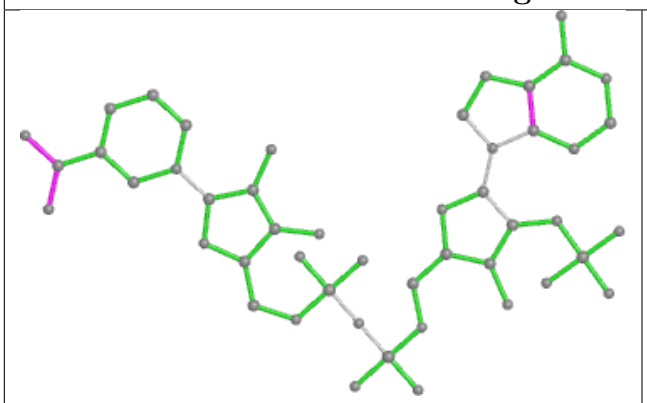
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	NAP	2	0
3	C	1002	XOG	3	0
3	D	1002	XOG	5	0
3	B	1002	XOG	2	0
2	A	1001	NAP	4	0

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.

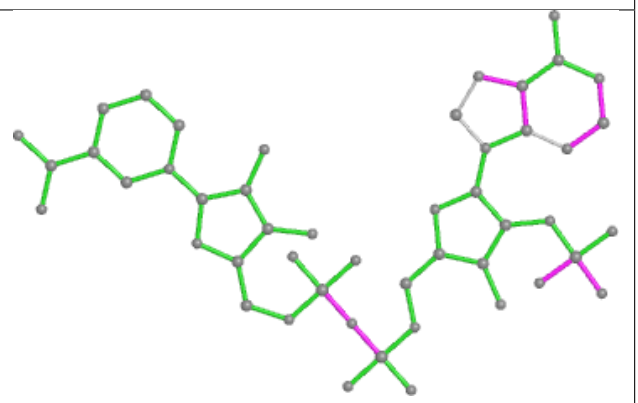
Ligand NAP D 1001



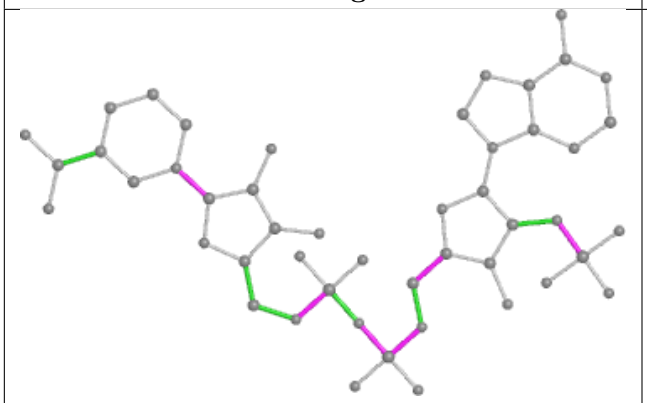
Ligand NAP C 1001



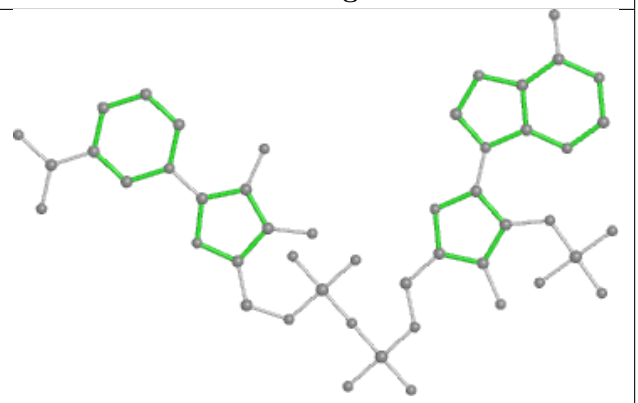
Bond lengths



Bond angles

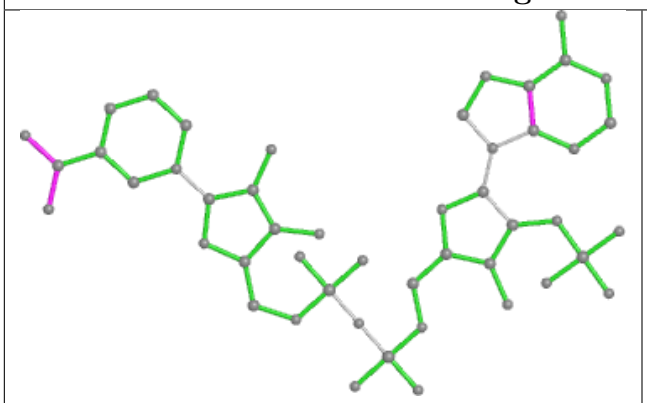


Torsions

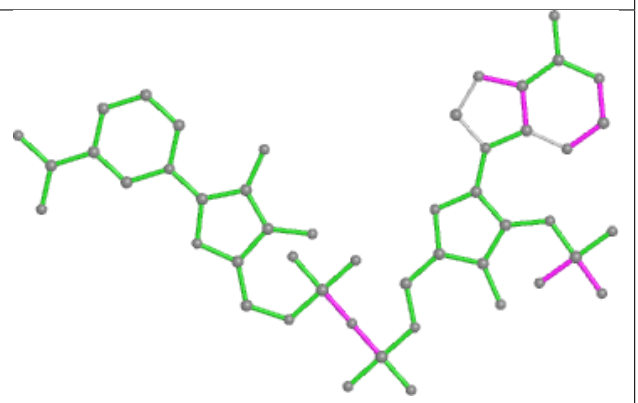


Rings

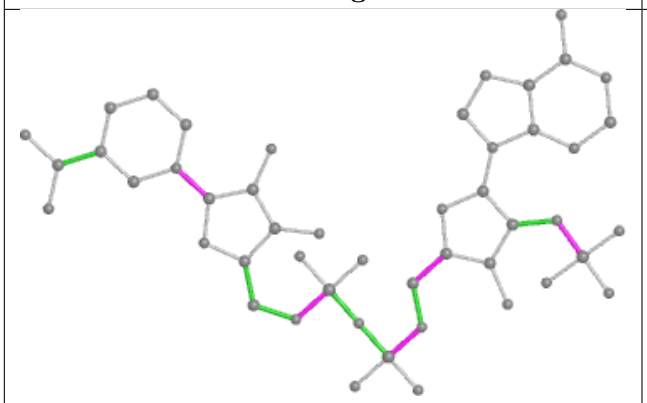
Ligand NAP B 1001



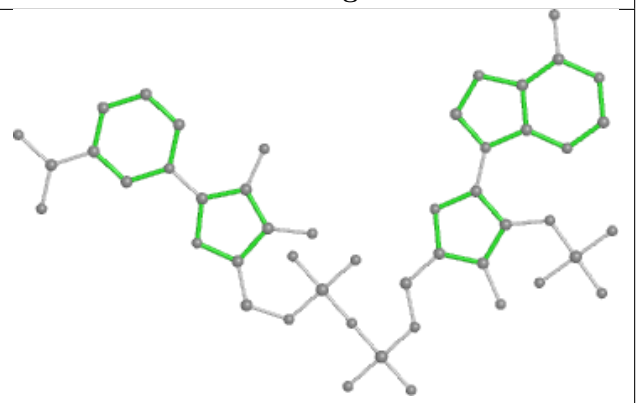
Bond lengths



Bond angles

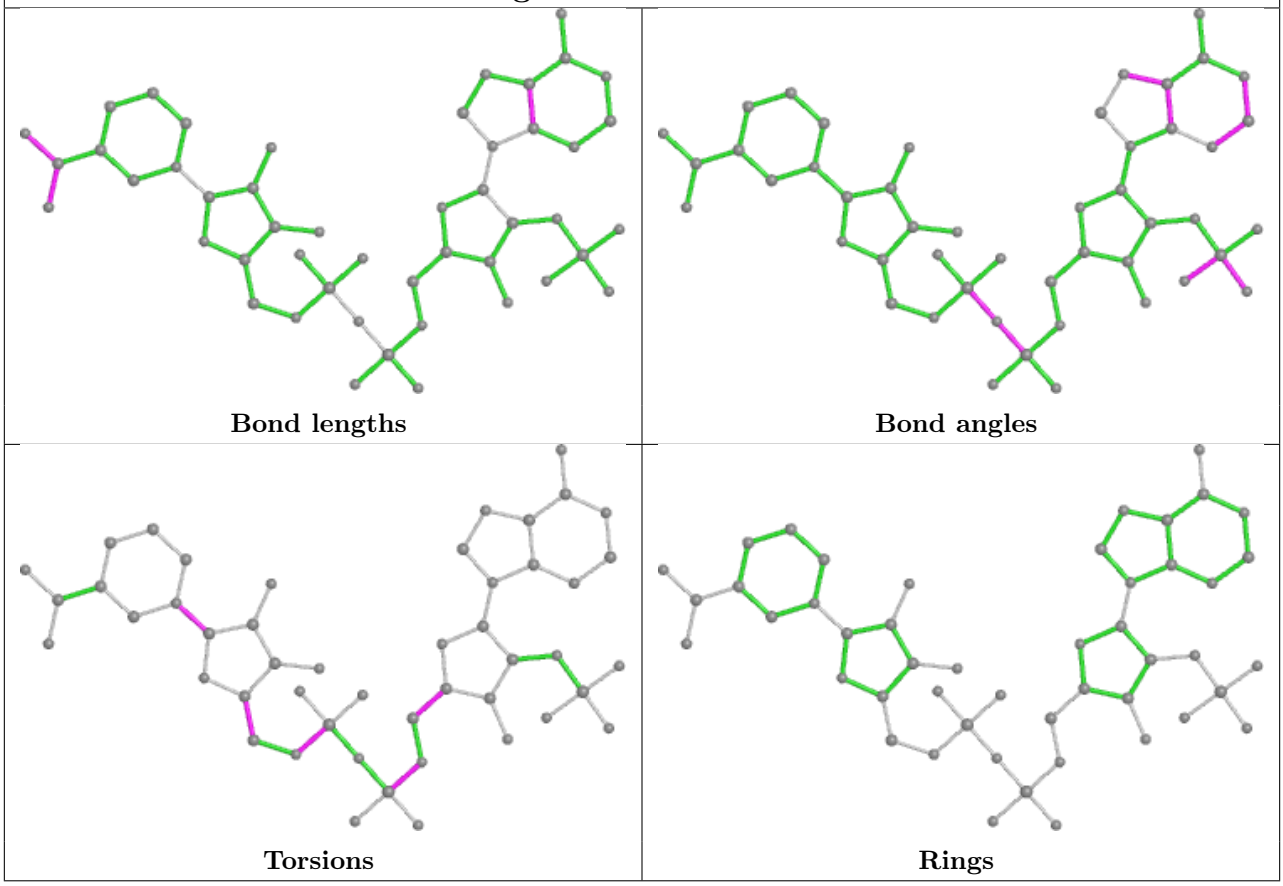


Torsions



Rings

Ligand NAP A 1001



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	365/365 (100%)	-0.04	6 (1%)	72	69	35, 57, 94, 170	0
1	B	365/365 (100%)	0.03	12 (3%)	46	43	36, 57, 96, 176	0
1	C	365/365 (100%)	-0.03	7 (1%)	66	63	38, 58, 96, 154	0
1	D	365/365 (100%)	-0.02	10 (2%)	54	50	34, 58, 100, 177	0
All	All	1460/1460 (100%)	-0.01	35 (2%)	59	54	34, 58, 98, 177	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	PRO	7.2
1	A	156	SER	6.5
1	C	156	SER	6.0
1	D	155	GLY	5.6
1	D	156	SER	5.3
1	B	150	GLY	5.0
1	B	153	GLU	4.6
1	B	158	VAL	4.6
1	B	159	VAL	4.3
1	B	157	LYS	3.9
1	D	151	ILE	3.8
1	A	151	ILE	3.5
1	A	24	MET	3.4
1	C	158	VAL	3.2
1	D	150	GLY	3.2
1	B	156	SER	3.1
1	B	303	GLY	3.1
1	B	151	ILE	3.0
1	D	24	MET	3.0
1	D	159	VAL	2.9
1	C	24	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	388	PRO	2.8
1	A	25	ALA	2.7
1	D	153	GLU	2.7
1	B	25	ALA	2.6
1	C	388	PRO	2.6
1	D	318	GLN	2.5
1	A	153	GLU	2.4
1	B	152	PHE	2.3
1	B	24	MET	2.3
1	D	340	PHE	2.3
1	C	159	VAL	2.3
1	C	157	LYS	2.2
1	D	152	PHE	2.1
1	C	25	ALA	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	XOG	C	1002	12/12	0.80	0.37	71,78,84,84	0
3	XOG	B	1002	12/12	0.81	0.40	75,77,79,81	0
4	PG4	B	1003	13/13	0.82	0.25	76,78,86,88	0
3	XOG	D	1002	12/12	0.84	0.49	78,80,89,90	0
3	XOG	A	1002	12/12	0.85	0.38	72,76,81,81	0
4	PG4	C	1003	13/13	0.85	0.27	68,74,81,83	0
4	PG4	D	1003	13/13	0.86	0.29	75,80,85,87	0
4	PG4	A	1003	13/13	0.88	0.33	77,80,83,83	0
2	NAP	A	1001	48/48	0.96	0.14	27,54,61,83	0

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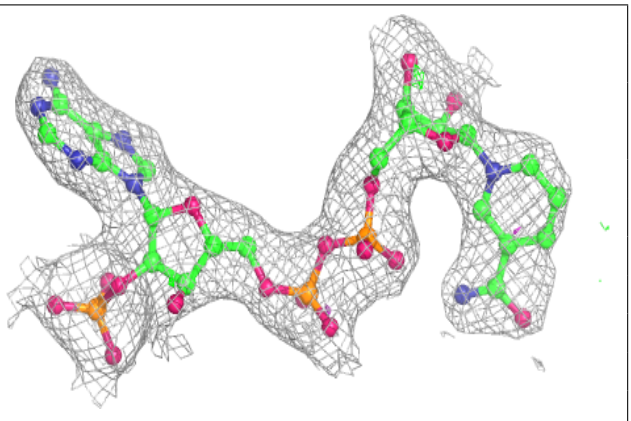
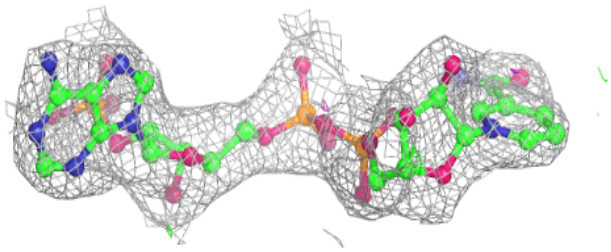
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	D	1001	48/48	0.97	0.13	31,54,67,93	0
2	NAP	B	1001	48/48	0.97	0.14	31,55,65,105	0
2	NAP	C	1001	48/48	0.97	0.14	32,57,62,84	0

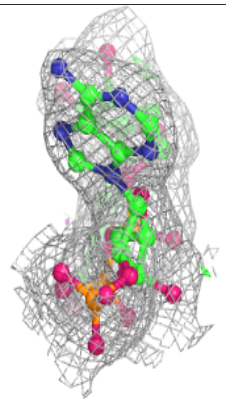
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP A 1001:

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

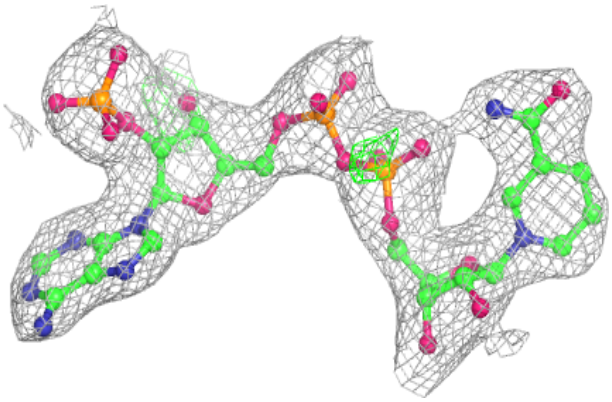


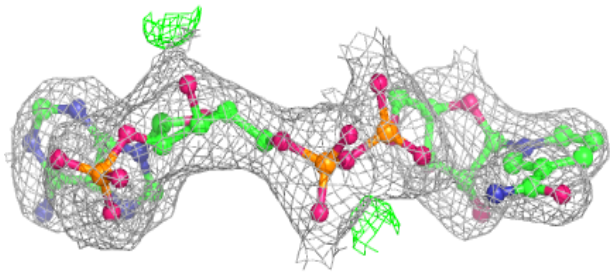


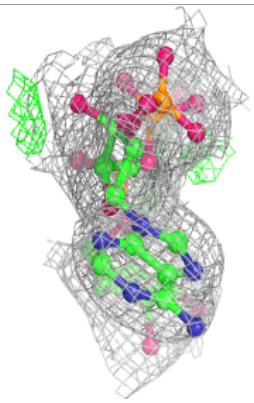


Electron density around NAP D 1001:

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

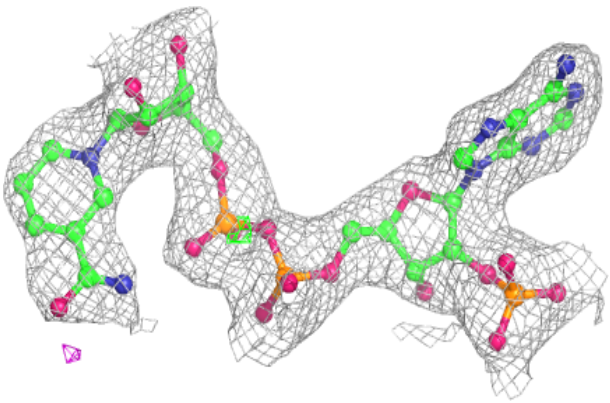


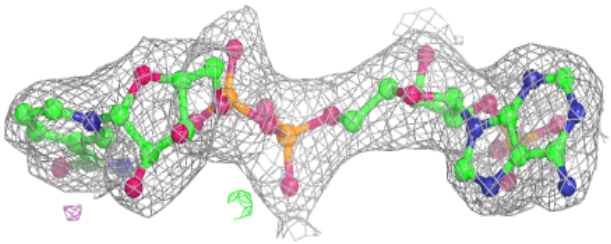


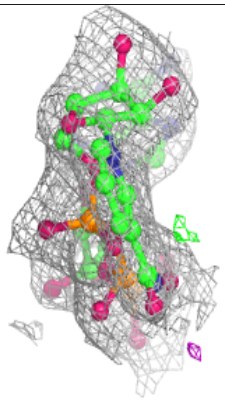


Electron density around NAP B 1001:

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

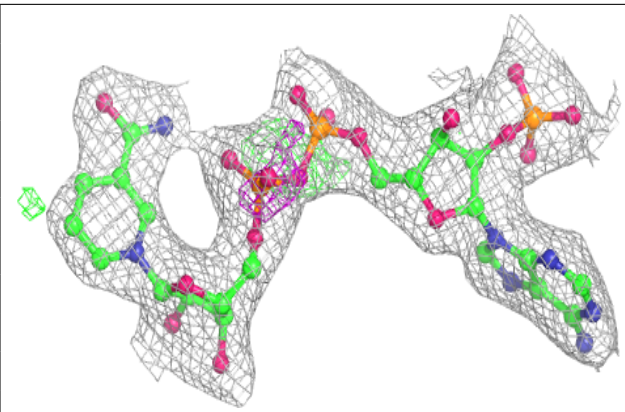


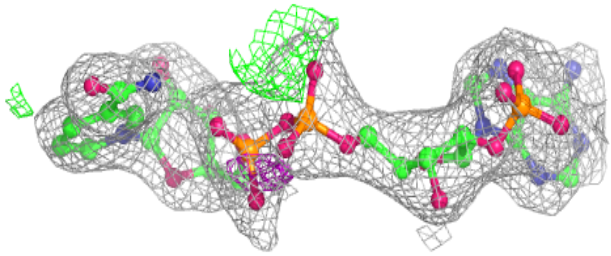


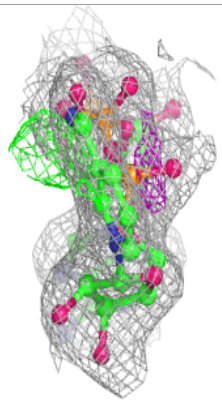


Electron density around NAP C 1001:

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.