Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 08:36 pm GMT

PDB ID	:	4A0S
Title	:	STRUCTURE OF THE 2-OCTENOYL-COA CARBOXYLASE REDUCTASE CINF IN COMPLEX WITH NADP AND 2-OCTENOYL-COA
Authors	:	Quade, N.; Huo, L.; Rachid, S.; Heinz, D.W.; Muller, R.
Deposited on	:	2011-09-12
Resolution	:	1.90 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:

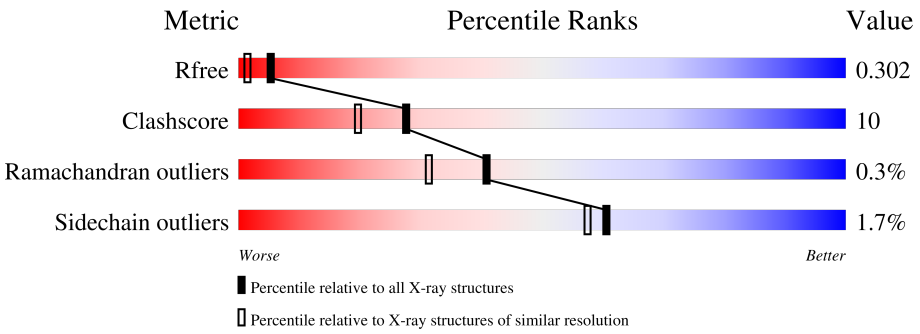
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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%

Mol	Chain	Length	Quality of chain
1	A	447	82% 17%
1	B	447	82% 17%
1	C	447	77% 21% ••
1	D	447	77% 21% ••

2 Entry composition (i)

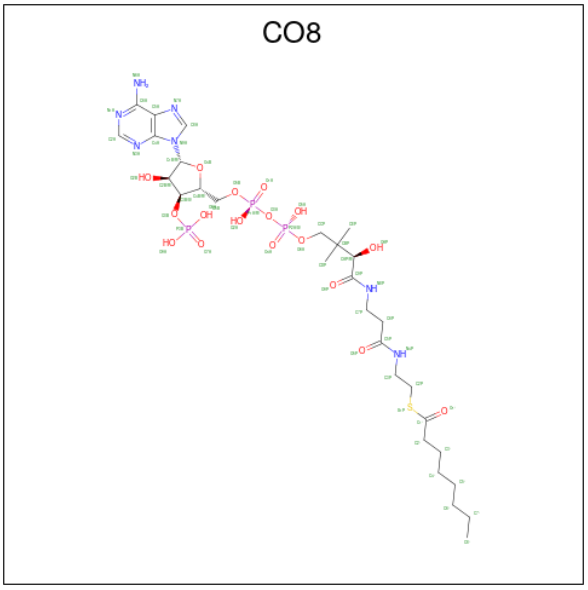
There are 4 unique types of molecules in this entry. The entry contains 15766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OCTENOYL-COA REDUCTASE/CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	445	3375	2115	613	631	16	0	3	0
1	B	445	3371	2112	615	628	16	0	2	0
1	C	444	3360	2106	609	629	16	0	2	0
1	D	444	3348	2098	608	626	16	0	0	0

- Molecule 2 is OCTANOYL-COENZYME A (three-letter code: CO8) (formula: $C_{29}H_{50}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	57	29	7	17	3	1	0	0
2	B	1	57	29	7	17	3	1	0	0

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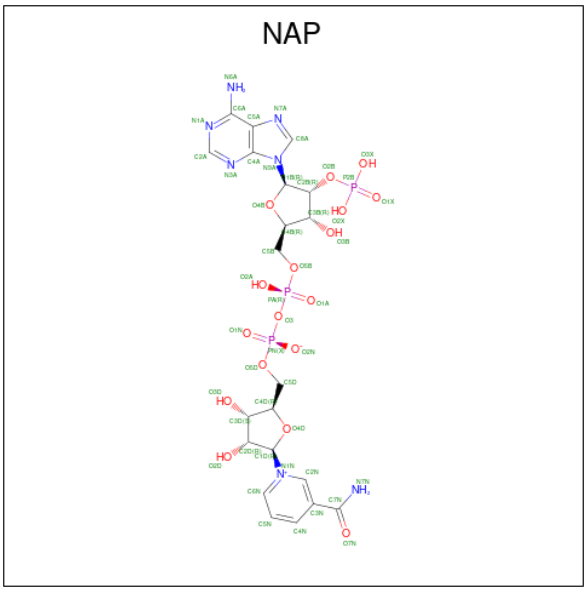
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	C	1	57	29	7	17	3	1	0	0
			Total	C	N	O	P	S		
2	D	1	57	29	7	17	3	1	0	0

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	522	522	522	0	0
			Total	O		
4	B	482	482	482	0	0
			Total	O		
4	C	457	457	457	0	0

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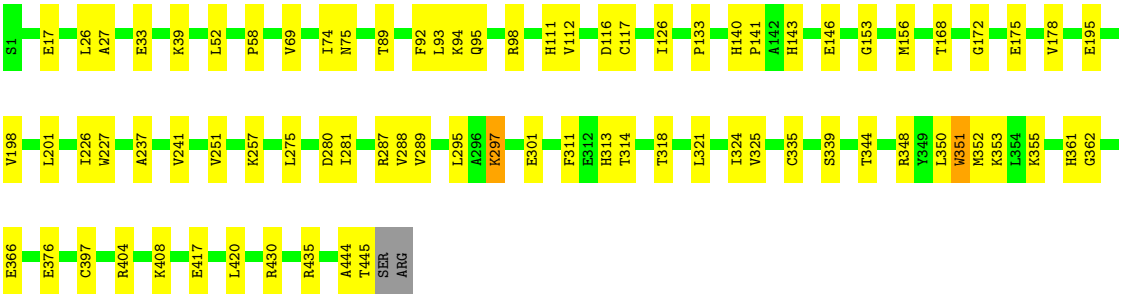
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	431	431	431	0	0

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. 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. 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.

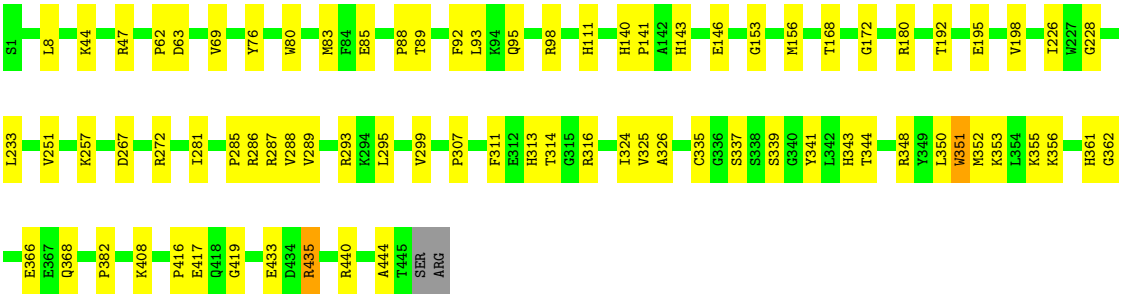
• Molecule 1: OCTENOYL-COA REDUCTASE/CARBOXYLASE

Chain A:



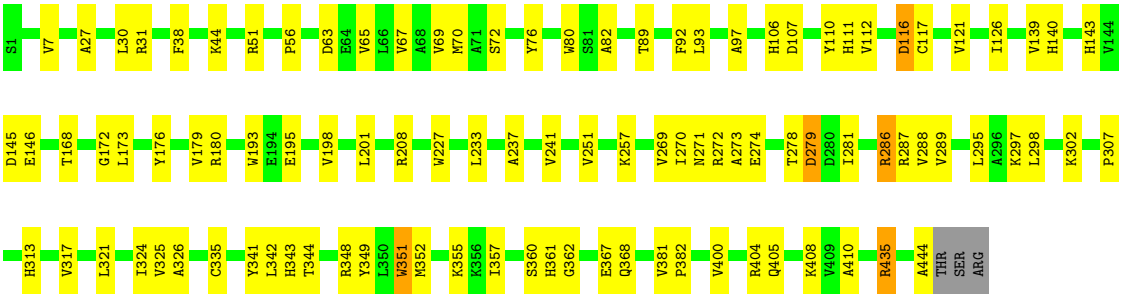
• Molecule 1: OCTENOYL-COA REDUCTASE/CARBOXYLASE

Chain B:



• Molecule 1: OCTENOYL-COA REDUCTASE/CARBOXYLASE

Chain C:



• Molecule 1: OCTENOYL-COA REDUCTASE/CARBOXYLASE

Chain D:

S1 F38 K39 K44 P56 P62 L66 V67 A68 V69 Y76 V79 W80 S81 A82 M83 T89 L93 Y110 H111 C117 R123 R130 W131 V137 I138 V139 H140 P141 A142 H143 E146 Q147 E148 M156 T159 F166 E167 T168 G172

Y176 K187 V198 L201 A216 I226 S230 K242 P248 V251 V252 Q256 K257 R272 L275 G276 I277 T278 D279 D280 I281 R287 V288 V289 E290 T291 K294 L295 A296 K297 L298 D308 I309 V310 F311 E312 H313 T314 G315 R316 V317 T318 I324 V325

A326 R327 R328 G329 C335 G340 H343 R348 Y349 L350 W351 M352 K353 L354 K355 S360 H361 G362 Q368 E376 P382 T402 S403 R404 Q405 V406 G407 K408 V409 A410 D426 L431 G432 E433 D434 R435 L436 A444 THR SER ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.01Å 83.30Å 122.74Å 90.00° 110.96° 90.00°	Depositor
Resolution (Å)	47.21 – 1.90 47.21 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.21-1.90) 98.9 (47.21-1.90)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199 , 0.250 0.256 , 0.302	Depositor DCC
R_{free} test set	7037 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 15.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15766	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.55% 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: CO8, 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	0.53	0/3452	0.66	0/4687
1	B	0.54	0/3445	0.67	0/4677
1	C	0.52	0/3434	0.67	0/4663
1	D	0.51	0/3416	0.68	3/4639 (0.1%)
All	All	0.53	0/13747	0.67	3/18666 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	130	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	D	275	LEU	CA-CB-CG	5.06	126.93	115.30
1	D	130	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3375	0	3369	59	0
1	B	3371	0	3368	70	0
1	C	3360	0	3349	80	0
1	D	3348	0	3335	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	57	0	46	2	0
2	B	57	0	46	4	0
2	C	57	0	46	5	0
2	D	57	0	46	5	0
3	A	48	0	25	7	0
3	B	48	0	25	9	0
3	C	48	0	25	6	0
3	D	48	0	25	5	0
4	A	522	0	0	6	0
4	B	482	0	0	8	0
4	C	457	0	0	6	0
4	D	431	0	0	9	0
All	All	15766	0	13705	276	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (276) 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:D:79:VAL:HG12	1:D:83:MET:HE2	1.28	1.07
1:D:79:VAL:HG12	1:D:83:MET:CE	1.91	0.99
1:B:228:GLY:H	1:B:272[B]:ARG:HH22	1.11	0.97
1:C:362:GLY:H	3:C:1445:NAP:H72N	1.13	0.94
1:D:362:GLY:H	3:D:1445:NAP:H72N	1.06	0.94
1:A:362:GLY:H	3:A:1447:NAP:H72N	1.03	0.93
1:B:362:GLY:H	3:B:1446:NAP:H72N	0.89	0.88
1:B:362:GLY:N	3:B:1446:NAP:H72N	1.71	0.87
1:C:145:ASP:OD2	1:D:130:ARG:NH2	2.09	0.85
1:B:295:LEU:HD23	1:B:325:VAL:HG11	1.57	0.84
1:B:267:ASP:HB3	4:B:2307:HOH:O	1.77	0.84
1:C:233:LEU:HD21	1:C:335:CYS:SG	2.22	0.79
4:A:2380:HOH:O	2:D:1446:CO8:O4A	2.01	0.77
1:D:362:GLY:N	3:D:1445:NAP:H72N	1.83	0.76
1:D:281:ILE:HG13	1:D:287:ARG:HG2	1.66	0.76
1:C:297:LYS:HD3	4:C:2321:HOH:O	1.86	0.74
1:A:275:LEU:HD11	1:A:295:LEU:HD13	1.74	0.69
1:A:17:GLU:HG2	1:A:133:PRO:HG2	1.72	0.69
1:C:362:GLY:N	3:C:1445:NAP:H72N	1.89	0.67
1:C:63:ASP:OD2	4:C:2120:HOH:O	2.12	0.67
1:D:148:GLU:OE2	1:D:159:THR:HB	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LEU:HD23	1:C:325:VAL:HG11	1.75	0.67
1:D:376:GLU:OE1	4:D:2347:HOH:O	2.14	0.66
1:B:286:ARG:HH12	1:B:293[A]:ARG:NH2	1.94	0.65
1:A:362:GLY:N	3:A:1447:NAP:H72N	1.87	0.65
1:B:417:GLU:OE2	4:B:2438:HOH:O	2.14	0.65
1:A:376:GLU:OE2	4:A:2276:HOH:O	2.14	0.65
1:B:286:ARG:HH12	1:B:293[A]:ARG:HH22	1.46	0.63
2:B:1447:CO8:O7A	1:C:286:ARG:NH2	2.29	0.63
1:A:280:ASP:OD1	1:A:287[A]:ARG:NH2	2.32	0.63
1:C:278:THR:O	1:C:281:ILE:HG22	1.98	0.63
1:B:80:TRP:CE3	1:B:83:MET:CE	2.83	0.62
1:B:95:GLN:HG2	1:B:98:ARG:HH12	1.64	0.62
1:D:79:VAL:CG1	1:D:83:MET:CE	2.73	0.62
1:D:256:GLN:HG2	4:D:2262:HOH:O	1.98	0.62
1:D:278:THR:O	1:D:281:ILE:HG22	2.00	0.61
1:D:279:ASP:HA	1:D:317:VAL:HG12	1.82	0.61
1:A:289:VAL:HA	1:A:324:ILE:HD13	1.82	0.61
1:B:281:ILE:HG13	1:B:287:ARG:HG2	1.81	0.61
1:B:80:TRP:CE3	1:B:83:MET:HE3	2.36	0.61
1:C:289:VAL:HA	1:C:324:ILE:HD13	1.84	0.60
1:B:348:ARG:O	1:B:352:MET:HB2	2.01	0.60
1:B:80:TRP:HE3	1:B:83:MET:HE3	1.68	0.59
2:B:1447:CO8:P3B	1:C:286:ARG:HH22	2.26	0.59
1:D:317:VAL:HG23	1:D:318:THR:HG23	1.84	0.58
1:B:63:ASP:OD2	4:B:2102:HOH:O	2.16	0.58
1:B:295:LEU:CD2	1:B:325:VAL:HG11	2.30	0.57
1:B:435:ARG:NH1	4:B:2467:HOH:O	2.37	0.57
1:B:335:CYS:O	3:B:1446:NAP:H2N	2.04	0.57
1:B:228:GLY:H	1:B:272[B]:ARG:NH2	1.93	0.57
1:A:95:GLN:HG2	1:A:98:ARG:NH1	2.20	0.56
1:A:335:CYS:O	3:A:1447:NAP:H2N	2.06	0.56
3:B:1446:NAP:C7N	2:B:1447:CO8:H2'1	2.36	0.55
1:D:335:CYS:O	3:D:1445:NAP:H2N	2.07	0.55
1:D:295:LEU:HG	1:D:325:VAL:HG11	1.89	0.55
1:C:335:CYS:O	3:C:1445:NAP:H2N	2.07	0.55
1:A:417:GLU:HG2	1:A:420:LEU:HD11	1.90	0.54
3:B:1446:NAP:H8A	3:B:1446:NAP:H3B	1.89	0.54
1:C:404:ARG:NH2	4:C:2092:HOH:O	2.40	0.54
1:C:198:VAL:O	1:C:408:LYS:HE2	2.07	0.54
1:D:348:ARG:O	1:D:352:MET:HB2	2.08	0.54
1:D:297:LYS:NZ	4:D:2297:HOH:O	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:LEU:HD11	2:D:1446:CO8:H4'1	1.89	0.54
1:A:95:GLN:HG2	1:A:98:ARG:HH12	1.74	0.53
1:C:56:PRO:HD2	1:C:110:TYR:CZ	2.43	0.53
1:C:307:PRO:HD2	1:C:325:VAL:O	2.08	0.53
1:D:81:SER:HB2	1:D:89:THR:HG21	1.90	0.53
1:A:146[B]:GLU:HB2	1:B:146:GLU:HB3	1.91	0.53
1:C:348:ARG:O	1:C:352:MET:HB2	2.08	0.53
1:D:198:VAL:O	1:D:408:LYS:HE2	2.09	0.53
1:A:348:ARG:O	1:A:352:MET:HB2	2.09	0.52
1:C:227:TRP:CZ3	1:C:251:VAL:HG11	2.44	0.52
1:D:433:GLU:HG2	4:D:2398:HOH:O	2.10	0.52
1:B:140:HIS:CG	1:B:368:GLN:HG3	2.45	0.52
1:C:279:ASP:HA	1:C:317:VAL:HG22	1.90	0.52
1:D:166:PHE:CE2	2:D:1446:CO8:H32	2.45	0.52
1:D:308:ASP:HA	1:D:327:ARG:HG2	1.92	0.51
1:B:433:GLU:HG2	1:B:440:ARG:HH22	1.75	0.51
1:B:287:ARG:HD2	4:B:2329:HOH:O	2.10	0.51
1:C:198:VAL:CG1	1:C:410:ALA:HB2	2.40	0.51
1:C:341:TYR:CD1	1:C:342:LEU:HD12	2.46	0.51
1:B:228:GLY:N	1:B:272[B]:ARG:HH22	1.93	0.51
1:C:69:VAL:HG13	1:C:117:CYS:HB2	1.93	0.51
1:A:227:TRP:CZ3	1:A:251:VAL:HG11	2.45	0.51
1:C:295:LEU:CD2	1:C:325:VAL:HG11	2.41	0.51
1:B:95:GLN:HG2	1:B:98:ARG:NH1	2.27	0.50
1:B:289:VAL:HA	1:B:324:ILE:HD13	1.93	0.50
1:C:271:ASN:O	1:C:274:GLU:HB2	2.11	0.50
1:C:69:VAL:HG11	1:C:172:GLY:O	2.11	0.50
1:A:351:TRP:O	1:D:361:HIS:HB2	2.11	0.50
1:C:271:ASN:O	1:C:274:GLU:CB	2.60	0.50
1:B:433:GLU:HG2	1:B:440:ARG:NH2	2.27	0.50
1:D:66:LEU:HB3	1:D:123:ARG:HB2	1.94	0.50
1:D:289:VAL:HA	1:D:324:ILE:HD13	1.92	0.50
1:C:146:GLU:HB3	1:D:146:GLU:HB3	1.92	0.50
1:A:93:LEU:HD11	1:A:111:HIS:CG	2.47	0.49
1:A:201:LEU:HD11	2:A:1446:CO8:H4'1	1.93	0.49
1:C:76:TYR:CE1	1:C:80:TRP:NE1	2.80	0.49
1:D:56:PRO:HD2	1:D:110:TYR:CZ	2.46	0.49
1:A:297:LYS:O	1:A:301:GLU:HG3	2.12	0.49
1:D:295:LEU:CG	1:D:325:VAL:HG11	2.42	0.49
1:B:180:ARG:HD3	4:B:2102:HOH:O	2.12	0.49
1:D:38:PHE:HB3	1:D:44:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ALA:CB	1:C:107:ASP:HB2	2.42	0.49
1:D:426:ASP:HB2	4:D:2388:HOH:O	2.12	0.49
1:D:81:SER:HB2	1:D:89:THR:CG2	2.41	0.49
1:A:140:HIS:HB2	1:A:141:PRO:HD2	1.94	0.48
1:C:38:PHE:HB3	1:C:44:LYS:HG2	1.95	0.48
1:A:143:HIS:CG	1:A:168:THR:HG21	2.48	0.48
1:B:251:VAL:HG12	1:B:272[A]:ARG:HG3	1.94	0.48
1:A:146[A]:GLU:HB3	1:B:146:GLU:HG2	1.96	0.48
1:D:431:LEU:HD23	1:D:436:LEU:HD21	1.95	0.48
1:B:140:HIS:HB2	1:B:141:PRO:HD2	1.94	0.48
1:C:31:ARG:HG2	1:C:51:ARG:HD2	1.96	0.48
1:C:281:ILE:HG13	1:C:287:ARG:HG2	1.94	0.48
1:C:251:VAL:HG12	1:C:272:ARG:HG2	1.95	0.48
1:C:65:VAL:HG13	1:C:121:VAL:HG13	1.95	0.48
1:C:195:GLU:HB3	1:C:382:PRO:HG2	1.96	0.48
1:A:344:THR:HA	1:D:343:HIS:O	2.14	0.47
1:D:69:VAL:HG11	1:D:172:GLY:O	2.13	0.47
1:B:289:VAL:O	1:B:293[A]:ARG:HG3	2.13	0.47
1:A:69:VAL:HG13	1:A:117:CYS:HB2	1.96	0.47
1:C:287:ARG:HG3	4:C:2317:HOH:O	2.13	0.47
1:D:251:VAL:HG12	1:D:272:ARG:CG	2.44	0.47
1:D:143:HIS:CG	1:D:168:THR:HG21	2.49	0.47
1:A:33:GLU:HG2	4:A:2047:HOH:O	2.15	0.47
1:D:79:VAL:CG1	1:D:83:MET:HE1	2.45	0.47
1:A:74:ILE:HG21	1:A:397:CYS:HA	1.95	0.47
1:A:350:LEU:HD12	1:A:355:LYS:HB2	1.95	0.47
1:B:339:SER:HB3	3:B:1446:NAP:H2A	1.96	0.47
1:D:350:LEU:HD12	1:D:355:LYS:HB2	1.96	0.47
1:B:337:SER:HB3	1:B:341:TYR:HA	1.97	0.46
1:C:288:VAL:HG12	1:C:324:ILE:HD12	1.97	0.46
1:D:329:GLY:HA2	1:D:354:LEU:O	2.14	0.46
3:A:1447:NAP:H8A	3:A:1447:NAP:H3B	1.98	0.46
1:B:288:VAL:HG12	1:B:324:ILE:CD1	2.46	0.46
1:A:404:ARG:NH1	1:A:445:THR:HG21	2.30	0.46
1:B:69:VAL:HG11	1:B:172:GLY:O	2.15	0.46
1:C:198:VAL:HB	1:C:408:LYS:CB	2.46	0.46
1:A:94:LYS:HE2	4:A:2059:HOH:O	2.15	0.46
1:B:156:MET:HE2	1:B:361:HIS:O	2.15	0.46
1:C:321:LEU:O	1:C:325:VAL:HG13	2.16	0.46
1:A:75:ASN:OD1	1:A:201:LEU:HD22	2.15	0.46
1:B:8:LEU:HD22	1:B:416:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:VAL:O	1:B:408:LYS:HE2	2.15	0.46
1:B:353:LYS:NZ	2:C:1446:CO8:H121	2.31	0.46
3:C:1445:NAP:H52A	3:C:1445:NAP:H52N	1.97	0.46
1:A:288:VAL:HG12	1:A:324:ILE:HD12	1.97	0.45
1:A:295:LEU:HG	1:A:325:VAL:HG21	1.97	0.45
1:B:285:PRO:CG	1:C:342:LEU:HD21	2.46	0.45
1:D:156:MET:HE2	1:D:361:HIS:O	2.16	0.45
1:C:30:LEU:HD21	1:C:82:ALA:HA	1.98	0.45
1:D:201:LEU:C	1:D:201:LEU:HD23	2.36	0.45
1:D:376:GLU:OE2	4:D:2207:HOH:O	2.21	0.45
1:B:295:LEU:HD23	1:B:325:VAL:CG1	2.39	0.45
1:D:140:HIS:HB2	1:D:141:PRO:HD2	1.98	0.45
1:A:26:LEU:HD11	1:A:52:LEU:HG	1.98	0.45
1:B:299:VAL:HG11	1:B:307:PRO:HD3	1.98	0.45
1:C:27:ALA:HB1	1:C:112:VAL:HG13	1.99	0.45
1:A:27:ALA:HB1	1:A:112:VAL:HG13	1.99	0.45
1:C:400:VAL:HA	1:C:405:GLN:OE1	2.17	0.45
1:D:198:VAL:CG1	1:D:410:ALA:HB2	2.47	0.45
1:D:353:LYS:HD2	4:D:2315:HOH:O	2.17	0.45
1:B:343:HIS:O	1:C:344:THR:HA	2.17	0.45
1:C:72:SER:HB3	1:C:173:LEU:HD23	1.99	0.45
1:D:79:VAL:O	1:D:83:MET:HG3	2.17	0.45
1:A:201:LEU:HD23	1:A:201:LEU:C	2.38	0.45
1:B:344:THR:HA	1:C:343:HIS:O	2.17	0.45
1:C:140:HIS:CG	1:C:368:GLN:HG3	2.52	0.45
1:A:195:GLU:O	1:A:198:VAL:HG22	2.17	0.44
2:A:1446:CO8:H2'1	3:A:1447:NAP:C7N	2.47	0.44
1:B:93:LEU:HD11	1:B:111:HIS:CG	2.52	0.44
1:C:273:ALA:O	1:C:274:GLU:C	2.55	0.44
1:D:257:LYS:HE3	1:D:444:ALA:HB1	1.97	0.44
1:C:361:HIS:CE1	2:C:1446:CO8:H5'1	2.53	0.44
1:B:47:ARG:HD2	4:B:2069:HOH:O	2.17	0.44
1:B:326:ALA:HB3	1:B:355:LYS:HD3	1.98	0.44
1:C:106:HIS:CE1	1:C:168:THR:HB	2.52	0.44
1:D:226:ILE:HA	1:D:311:PHE:HB3	1.98	0.44
1:A:146[A]:GLU:HG2	1:B:146:GLU:HB3	1.98	0.44
1:B:89:THR:HA	1:B:92:PHE:CD2	2.53	0.44
1:C:208:ARG:HG3	1:C:367:GLU:OE2	2.17	0.44
1:C:143:HIS:CG	1:C:168:THR:HG21	2.52	0.44
1:D:382:PRO:HB2	4:D:2354:HOH:O	2.18	0.44
1:D:198:VAL:HB	1:D:408:LYS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:LEU:HD11	1:C:111:HIS:CG	2.52	0.44
1:D:316:ARG:HB3	1:D:340:GLY:O	2.18	0.44
3:C:1445:NAP:C7N	2:C:1446:CO8:H2'1	2.48	0.43
1:A:126:ILE:HG13	1:B:62:PRO:HG3	1.99	0.43
1:A:153:GLY:HA3	1:B:366:GLU:OE1	2.17	0.43
1:D:146:GLU:CD	1:D:146:GLU:H	2.22	0.43
1:D:402:THR:OG1	1:D:404:ARG:HD2	2.17	0.43
1:B:195:GLU:HB3	1:B:382:PRO:HG2	2.00	0.43
1:B:257:LYS:HE3	1:B:444:ALA:HB1	1.99	0.43
1:C:67:VAL:O	1:C:176:TYR:HA	2.18	0.43
1:C:201:LEU:C	1:C:201:LEU:HD23	2.39	0.43
1:C:351:TRP:CD1	1:C:351:TRP:C	2.91	0.43
1:A:89:THR:HA	1:A:92:PHE:CD2	2.54	0.43
1:B:146:GLU:OE1	1:B:146:GLU:N	2.50	0.43
1:A:297:LYS:HG2	4:A:2381:HOH:O	2.17	0.43
1:B:361:HIS:CE1	2:B:1447:CO8:H5'1	2.54	0.43
1:B:44:LYS:HD2	1:B:85:GLU:OE2	2.19	0.43
1:C:116:ASP:O	1:C:117:CYS:HB3	2.18	0.43
1:C:335:CYS:HA	1:C:360:SER:O	2.18	0.43
1:D:287:ARG:HD2	4:D:2279:HOH:O	2.19	0.43
1:A:156:MET:HE2	1:A:361:HIS:O	2.19	0.43
1:B:198:VAL:HB	1:B:408:LYS:CB	2.49	0.43
1:B:356:LYS:HE2	4:B:2364:HOH:O	2.19	0.43
1:A:198:VAL:O	1:A:408:LYS:HE2	2.19	0.43
1:B:192:THR:HG21	1:B:419:GLY:HA2	2.00	0.43
3:C:1445:NAP:C4N	2:C:1446:CO8:H3'2	2.49	0.43
1:D:67:VAL:O	1:D:176:TYR:HA	2.19	0.43
1:A:69:VAL:HG11	1:A:172:GLY:O	2.19	0.43
1:C:70:MET:HG3	1:C:193:TRP:CE2	2.54	0.43
1:D:140:HIS:CG	1:D:368:GLN:HG3	2.54	0.43
1:A:237:ALA:O	1:A:241:VAL:HG23	2.19	0.42
1:C:257:LYS:HE3	1:C:444:ALA:HB1	2.01	0.42
1:C:269:VAL:O	1:C:302:LYS:HE3	2.18	0.42
1:D:242:LYS:HG2	1:D:248:PRO:HG3	2.00	0.42
1:A:281:ILE:HG13	1:A:287[A]:ARG:HG2	1.99	0.42
1:D:251:VAL:HG12	1:D:272:ARG:HG3	2.00	0.42
3:B:1446:NAP:H8A	3:B:1446:NAP:C3B	2.49	0.42
1:D:230:SER:HB2	1:D:406:VAL:HG22	2.00	0.42
1:B:350:LEU:HD21	1:C:357:ILE:HG22	2.02	0.42
1:D:288:VAL:HG12	1:D:324:ILE:HD12	2.02	0.42
1:B:285:PRO:HG3	1:C:342:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:VAL:HB	1:C:408:LYS:HB3	2.01	0.42
1:B:226:ILE:HA	1:B:311:PHE:HB3	2.02	0.42
1:D:69:VAL:HG13	1:D:117:CYS:HB2	2.01	0.42
1:C:126:ILE:HG13	1:D:62:PRO:HG3	2.02	0.42
1:A:318:THR:HA	1:A:321:LEU:HD12	2.02	0.41
1:A:353:LYS:NZ	2:D:1446:CO8:H121	2.35	0.41
1:B:337:SER:CB	1:B:341:TYR:HA	2.50	0.41
1:B:351:TRP:CD1	1:B:351:TRP:C	2.94	0.41
3:B:1446:NAP:H52A	3:B:1446:NAP:H52N	2.01	0.41
1:C:381:VAL:HG11	1:C:435:ARG:HD3	2.01	0.41
1:A:430:ARG:NH1	4:A:2504:HOH:O	2.53	0.41
1:C:139:VAL:HG21	1:C:179:VAL:HG11	2.02	0.41
1:C:286:ARG:NE	4:C:2313:HOH:O	2.54	0.41
1:C:180:ARG:HD3	4:C:2120:HOH:O	2.20	0.41
1:C:349:TYR:O	1:C:355:LYS:HE3	2.21	0.41
1:D:297:LYS:HA	1:D:297:LYS:HD3	1.53	0.41
3:D:1445:NAP:C7N	2:D:1446:CO8:H2'1	2.50	0.41
1:A:257:LYS:NZ	3:A:1447:NAP:O3X	2.41	0.41
1:A:257:LYS:HE3	1:A:444:ALA:HB1	2.02	0.41
1:C:237:ALA:O	1:C:241:VAL:HG23	2.20	0.41
1:C:326:ALA:HB3	1:C:355:LYS:HD3	2.03	0.41
1:D:216:ALA:HB1	1:D:309:ILE:HG12	2.01	0.41
1:C:7:VAL:CG1	1:C:70:MET:HE3	2.51	0.41
1:C:30:LEU:O	1:C:110:TYR:HA	2.21	0.41
1:D:131:TRP:CZ3	1:D:137:VAL:HG12	2.56	0.41
1:D:252:VAL:HA	3:D:1445:NAP:O1X	2.20	0.41
1:A:351:TRP:CD1	1:A:351:TRP:C	2.94	0.41
1:B:361:HIS:HB2	1:C:351:TRP:O	2.21	0.41
1:A:58:PRO:HG2	1:A:178:VAL:HG21	2.02	0.41
1:D:93:LEU:HD11	1:D:111:HIS:CG	2.55	0.41
1:D:295:LEU:HD23	1:D:325:VAL:HG11	2.03	0.41
1:A:366:GLU:OE1	1:B:153:GLY:HA3	2.21	0.41
1:B:143:HIS:CG	1:B:168:THR:HG21	2.56	0.41
1:D:251:VAL:CG1	1:D:272:ARG:HG2	2.51	0.41
1:D:291:THR:HA	1:D:294:LYS:HE3	2.03	0.41
1:B:352:MET:HG3	2:C:1446:CO8:CEP	2.51	0.40
1:A:26:LEU:HB3	1:A:175:GLU:HG3	2.02	0.40
1:C:89:THR:HA	1:C:92:PHE:CD2	2.56	0.40
1:C:381:VAL:HG11	1:C:435:ARG:CD	2.51	0.40
1:A:226:ILE:HA	1:A:311:PHE:HB3	2.03	0.40
1:A:361:HIS:HB2	1:D:351:TRP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:CYS:HA	1:D:360:SER:O	2.22	0.40
1:A:116:ASP:O	1:A:117:CYS:HB3	2.21	0.40
1:B:233:LEU:HD12	3:B:1446:NAP:H51N	2.03	0.40
1:C:251:VAL:HG12	1:C:272:ARG:CG	2.52	0.40
1:C:251:VAL:CG1	1:C:272:ARG:HG2	2.52	0.40
1:D:138:ILE:HG23	1:D:187:LYS:HA	2.03	0.40
1:A:339:SER:HB3	3:A:1447:NAP:H2A	2.03	0.40
1:C:270:ILE:HG23	1:C:298:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/447 (100%)	433 (97%)	12 (3%)	1 (0%)	47	38
1	B	445/447 (100%)	433 (97%)	11 (2%)	1 (0%)	47	38
1	C	444/447 (99%)	429 (97%)	14 (3%)	1 (0%)	47	38
1	D	442/447 (99%)	427 (97%)	13 (3%)	2 (0%)	29	18
All	All	1777/1788 (99%)	1722 (97%)	50 (3%)	5 (0%)	41	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	C	313	HIS
1	D	313	HIS
1	B	313	HIS
1	D	277	ILE

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	351/350 (100%)	346 (99%)	5 (1%)	67	65
1	B	350/350 (100%)	344 (98%)	6 (2%)	60	57
1	C	349/350 (100%)	344 (99%)	5 (1%)	67	65
1	D	347/350 (99%)	340 (98%)	7 (2%)	55	51
All	All	1397/1400 (100%)	1374 (98%)	23 (2%)	60	60

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	297	LYS
1	A	314	THR
1	A	351	TRP
1	A	435	ARG
1	B	76	TYR
1	B	88	PRO
1	B	314	THR
1	B	316	ARG
1	B	351	TRP
1	B	435	ARG
1	C	116	ASP
1	C	279	ASP
1	C	286	ARG
1	C	351	TRP
1	C	435	ARG
1	D	39	LYS
1	D	76	TYR
1	D	279	ASP
1	D	298	LEU
1	D	314	THR
1	D	351	TRP
1	D	435	ARG

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	95	GLN
1	B	217	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	NAP	B	1446	-	45,52,52	1.60	7 (15%)	56,80,80	1.38	6 (10%)
3	NAP	C	1445	-	45,52,52	1.63	8 (17%)	56,80,80	2.30	10 (17%)
2	CO8	D	1446	-	51,59,59	2.09	6 (11%)	62,85,85	1.45	9 (14%)
3	NAP	A	1447	-	45,52,52	1.67	5 (11%)	56,80,80	1.75	12 (21%)
2	CO8	A	1446	-	51,59,59	2.34	10 (19%)	62,85,85	1.64	10 (16%)
2	CO8	C	1446	-	51,59,59	2.18	9 (17%)	62,85,85	1.36	6 (9%)
3	NAP	D	1445	-	45,52,52	1.75	8 (17%)	56,80,80	2.45	17 (30%)
2	CO8	B	1447	-	51,59,59	2.09	6 (11%)	62,85,85	1.29	5 (8%)

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	B	1446	-	-	4/31/67/67	0/5/5/5
3	NAP	C	1445	-	-	6/31/67/67	0/5/5/5
2	CO8	D	1446	-	-	12/54/74/74	0/3/3/3
3	NAP	A	1447	-	-	4/31/67/67	0/5/5/5
2	CO8	A	1446	-	-	13/54/74/74	0/3/3/3
2	CO8	C	1446	-	-	13/54/74/74	0/3/3/3
3	NAP	D	1445	-	-	3/31/67/67	0/5/5/5
2	CO8	B	1447	-	-	9/54/74/74	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1446	CO8	C2'-C1'	-12.38	1.38	1.50
2	B	1447	CO8	C2'-C1'	-11.27	1.39	1.50
2	C	1446	CO8	C2'-C1'	-11.03	1.39	1.50
2	D	1446	CO8	C2'-C1'	-10.99	1.39	1.50
3	A	1447	NAP	O4B-C1B	6.58	1.50	1.41
3	C	1445	NAP	P2B-O2B	5.59	1.69	1.59
3	D	1445	NAP	P2B-O1X	5.45	1.68	1.50
2	C	1446	CO8	O4B-C1B	5.33	1.48	1.41
3	B	1446	NAP	O4B-C1B	5.11	1.48	1.41
3	D	1445	NAP	P2B-O2B	5.07	1.68	1.59
3	C	1445	NAP	P2B-O1X	4.85	1.66	1.50
2	B	1447	CO8	O4B-C1B	4.62	1.47	1.41
2	D	1446	CO8	O4B-C1B	4.44	1.47	1.41
3	D	1445	NAP	O4B-C1B	4.44	1.47	1.41
2	A	1446	CO8	P1A-O1A	4.31	1.66	1.50
2	A	1446	CO8	O4B-C1B	4.10	1.46	1.41
3	A	1447	NAP	P2B-O1X	3.98	1.63	1.50
2	A	1446	CO8	P3B-O7A	3.97	1.63	1.50
2	A	1446	CO8	C3'-C2'	-3.84	1.38	1.52
2	C	1446	CO8	P3B-O7A	3.79	1.62	1.50
2	D	1446	CO8	P3B-O7A	3.77	1.62	1.50
2	B	1447	CO8	C3'-C2'	-3.74	1.38	1.52
3	B	1446	NAP	C2N-N1N	3.68	1.39	1.35
3	A	1447	NAP	O4D-C1D	3.58	1.46	1.41
2	D	1446	CO8	P1A-O1A	3.56	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1447	CO8	P2A-O4A	3.56	1.63	1.50
2	C	1446	CO8	C3'-C2'	-3.47	1.39	1.52
3	D	1445	NAP	P2B-O2X	3.44	1.68	1.54
2	D	1446	CO8	C3'-C2'	-3.43	1.39	1.52
3	C	1445	NAP	P2B-O2X	3.43	1.68	1.54
2	C	1446	CO8	P2A-O4A	3.37	1.62	1.50
3	B	1446	NAP	P2B-O2B	3.25	1.65	1.59
3	D	1445	NAP	PN-O1N	3.24	1.62	1.50
2	C	1446	CO8	P1A-O1A	3.22	1.62	1.50
3	A	1447	NAP	C6N-N1N	3.16	1.43	1.35
3	B	1446	NAP	C6N-N1N	3.01	1.42	1.35
2	D	1446	CO8	P2A-O4A	2.99	1.61	1.50
3	B	1446	NAP	P2B-O1X	2.84	1.59	1.50
3	C	1445	NAP	C2N-N1N	2.80	1.38	1.35
3	A	1447	NAP	C2N-N1N	2.73	1.38	1.35
3	D	1445	NAP	C6N-N1N	2.69	1.42	1.35
2	A	1446	CO8	P3B-O8A	2.66	1.65	1.54
2	B	1447	CO8	P3B-O9A	2.65	1.65	1.54
3	C	1445	NAP	C2D-C1D	-2.62	1.49	1.53
2	A	1446	CO8	P2A-O4A	2.60	1.60	1.50
3	B	1446	NAP	O4D-C4D	2.53	1.50	1.45
3	C	1445	NAP	C6N-N1N	2.51	1.41	1.35
2	A	1446	CO8	OAP-CAP	2.48	1.46	1.42
3	D	1445	NAP	O4D-C1D	2.47	1.44	1.41
3	C	1445	NAP	O4B-C1B	2.43	1.44	1.41
2	A	1446	CO8	O1'-C1'	2.39	1.24	1.21
2	C	1446	CO8	C4'-C3'	-2.20	1.39	1.51
3	C	1445	NAP	PN-O1N	2.17	1.58	1.50
2	B	1447	CO8	OAP-CAP	2.16	1.46	1.42
3	B	1446	NAP	PA-O1A	2.14	1.58	1.50
2	C	1446	CO8	P3B-O3B	2.14	1.63	1.59
2	C	1446	CO8	C6P-C5P	2.10	1.55	1.51
3	D	1445	NAP	C2N-N1N	2.08	1.37	1.35
2	A	1446	CO8	C6P-C5P	2.03	1.55	1.51

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1445	NAP	O3X-P2B-O1X	-9.67	72.81	110.68
3	D	1445	NAP	O3X-P2B-O2X	-9.64	70.78	107.64
3	C	1445	NAP	O3X-P2B-O2X	-7.22	80.03	107.64
3	D	1445	NAP	O3X-P2B-O1X	-6.25	86.19	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1445	NAP	N3A-C2A-N1A	-6.00	119.31	128.68
2	A	1446	CO8	C2P-C3P-N4P	-5.35	101.17	112.42
3	B	1446	NAP	N3A-C2A-N1A	-5.19	120.57	128.68
3	D	1445	NAP	O3X-P2B-O2B	-5.06	83.31	105.99
2	A	1446	CO8	C3'-C2'-C1'	4.90	123.20	112.33
3	C	1445	NAP	N3A-C2A-N1A	-4.89	121.04	128.68
2	A	1446	CO8	N3A-C2A-N1A	-4.77	121.22	128.68
2	C	1446	CO8	N3A-C2A-N1A	-4.69	121.35	128.68
2	B	1447	CO8	N3A-C2A-N1A	-4.68	121.36	128.68
3	A	1447	NAP	C3N-C2N-N1N	-4.64	115.90	120.43
2	D	1446	CO8	N3A-C2A-N1A	-4.57	121.53	128.68
3	C	1445	NAP	O3X-P2B-O2B	-4.52	85.75	105.99
3	A	1447	NAP	C3N-C7N-N7N	-4.39	112.48	117.75
2	B	1447	CO8	C3'-C2'-C1'	4.37	122.02	112.33
2	C	1446	CO8	C2'-C1'-S1P	4.37	118.54	113.46
3	D	1445	NAP	C3N-C7N-N7N	-4.36	112.52	117.75
2	D	1446	CO8	C3'-C2'-C1'	4.32	121.92	112.33
3	A	1447	NAP	N3A-C2A-N1A	-4.15	122.19	128.68
2	A	1446	CO8	C3P-N4P-C5P	4.11	130.47	122.84
3	C	1445	NAP	C3N-C7N-N7N	-3.98	112.97	117.75
3	A	1447	NAP	C2N-C3N-C4N	3.92	122.71	118.26
3	D	1445	NAP	O2X-P2B-O2B	3.73	122.69	105.99
3	D	1445	NAP	C2N-C3N-C4N	3.72	122.48	118.26
2	D	1446	CO8	C2'-C1'-S1P	3.56	117.61	113.46
3	A	1447	NAP	O2B-P2B-O1X	-3.44	96.11	109.39
3	B	1446	NAP	PN-O3-PA	-3.20	121.83	132.83
2	C	1446	CO8	C4'-C3'-C2'	3.12	124.40	113.19
3	D	1445	NAP	C5B-C4B-C3B	-3.08	103.64	115.18
3	C	1445	NAP	O2B-P2B-O1X	3.07	121.23	109.39
3	D	1445	NAP	O2X-P2B-O1X	2.95	122.23	110.68
2	C	1446	CO8	C3'-C2'-C1'	2.83	118.61	112.33
3	A	1447	NAP	O4D-C1D-C2D	-2.81	102.82	106.93
2	D	1446	CO8	O1'-C1'-S1P	-2.78	119.00	122.61
3	A	1447	NAP	O3D-C3D-C4D	-2.74	103.14	111.05
3	A	1447	NAP	PN-O3-PA	-2.72	123.48	132.83
2	D	1446	CO8	C4'-C3'-C2'	2.72	122.98	113.19
3	D	1445	NAP	O4B-C4B-C5B	-2.72	100.43	109.37
3	B	1446	NAP	N6A-C6A-N1A	2.70	124.17	118.57
2	A	1446	CO8	C6P-C5P-N4P	2.65	120.88	116.42
3	A	1447	NAP	O3X-P2B-O2X	2.62	117.67	107.64
2	B	1447	CO8	CEP-CBP-CAP	2.62	113.36	108.82
3	D	1445	NAP	O7N-C7N-N7N	2.54	126.18	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1445	NAP	O2N-PN-O5D	2.52	119.44	107.75
3	B	1446	NAP	C2A-N1A-C6A	2.51	123.05	118.75
3	D	1445	NAP	C3N-C2N-N1N	-2.51	117.97	120.43
2	C	1446	CO8	O1'-C1'-S1P	-2.49	119.38	122.61
3	D	1445	NAP	C2A-N1A-C6A	2.45	122.94	118.75
2	B	1447	CO8	C6'-C5'-C4'	-2.38	102.36	114.42
3	C	1445	NAP	O7N-C7N-C3N	2.36	122.46	119.63
2	D	1446	CO8	P2A-O3A-P1A	-2.36	124.74	132.83
3	B	1446	NAP	C3N-C7N-N7N	-2.28	115.02	117.75
2	D	1446	CO8	C2P-S1P-C1'	-2.27	94.81	101.87
2	B	1447	CO8	C4'-C3'-C2'	2.27	121.33	113.19
2	D	1446	CO8	C7P-C6P-C5P	-2.26	108.59	112.36
3	C	1445	NAP	C3D-C2D-C1D	-2.26	97.58	100.98
3	D	1445	NAP	O5D-PN-O1N	2.24	117.81	109.07
2	A	1446	CO8	O8A-P3B-O7A	-2.23	101.94	110.68
2	A	1446	CO8	O5P-C5P-N4P	-2.20	118.86	123.01
2	A	1446	CO8	C7P-C6P-C5P	-2.18	108.72	112.36
2	D	1446	CO8	C2P-C3P-N4P	-2.16	107.88	112.42
3	D	1445	NAP	O2N-PN-O1N	2.15	122.89	112.24
3	B	1446	NAP	O4D-C1D-C2D	-2.12	103.83	106.93
3	C	1445	NAP	C1B-N9A-C4A	-2.12	122.92	126.64
3	D	1445	NAP	C1B-N9A-C4A	-2.09	122.97	126.64
2	A	1446	CO8	CDP-CBP-CAP	2.08	112.43	108.82
2	A	1446	CO8	C1B-N9A-C4A	-2.07	123.00	126.64
2	C	1446	CO8	O6A-CCP-CBP	2.06	113.86	110.55
3	A	1447	NAP	O7N-C7N-N7N	2.06	125.51	122.58
3	D	1445	NAP	O2N-PN-O5D	2.05	117.28	107.75
3	A	1447	NAP	C6N-C5N-C4N	-2.03	116.49	119.44
3	A	1447	NAP	C1B-N9A-C4A	-2.01	123.11	126.64

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1446	CO8	C4B-C5B-O5B-P1A
2	A	1446	CO8	CCP-O6A-P2A-O3A
2	A	1446	CO8	CCP-O6A-P2A-O5A
2	A	1446	CO8	C5P-C6P-C7P-N8P
2	A	1446	CO8	S1P-C2P-C3P-N4P
2	B	1447	CO8	C4B-C5B-O5B-P1A
2	B	1447	CO8	CCP-O6A-P2A-O3A
2	B	1447	CO8	CCP-O6A-P2A-O5A

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Mol	Chain	Res	Type	Atoms
2	C	1446	CO8	CAP-CBP-CCP-O6A
2	C	1446	CO8	C5P-C6P-C7P-N8P
2	C	1446	CO8	S1P-C2P-C3P-N4P
2	C	1446	CO8	O1'-C1'-S1P-C2P
2	C	1446	CO8	C2'-C1'-S1P-C2P
2	D	1446	CO8	CCP-O6A-P2A-O3A
2	D	1446	CO8	CCP-O6A-P2A-O5A
2	D	1446	CO8	O1'-C1'-S1P-C2P
2	D	1446	CO8	C2'-C1'-S1P-C2P
3	A	1447	NAP	O4D-C1D-N1N-C6N
3	B	1446	NAP	O4D-C1D-N1N-C6N
3	C	1445	NAP	C2B-O2B-P2B-O1X
3	C	1445	NAP	C5D-O5D-PN-O1N
3	C	1445	NAP	O4D-C1D-N1N-C6N
3	D	1445	NAP	C5D-O5D-PN-O1N
3	D	1445	NAP	O4D-C1D-N1N-C6N
2	A	1446	CO8	C6P-C5P-N4P-C3P
2	C	1446	CO8	C6P-C5P-N4P-C3P
2	D	1446	CO8	C6P-C5P-N4P-C3P
2	C	1446	CO8	C2'-C3'-C4'-C5'
2	D	1446	CO8	C2'-C3'-C4'-C5'
2	A	1446	CO8	C2'-C3'-C4'-C5'
2	A	1446	CO8	O5P-C5P-N4P-C3P
2	C	1446	CO8	O5P-C5P-N4P-C3P
2	D	1446	CO8	O5P-C5P-N4P-C3P
2	B	1447	CO8	C2'-C3'-C4'-C5'
2	C	1446	CO8	CEP-CBP-CCP-O6A
2	D	1446	CO8	C4B-C5B-O5B-P1A
2	C	1446	CO8	CDP-CBP-CCP-O6A
2	A	1446	CO8	P1A-O3A-P2A-O4A
2	B	1447	CO8	P1A-O3A-P2A-O4A
2	C	1446	CO8	C4B-C5B-O5B-P1A
2	A	1446	CO8	O1'-C1'-S1P-C2P
2	B	1447	CO8	O1'-C1'-S1P-C2P
2	A	1446	CO8	P1A-O3A-P2A-O6A
2	B	1447	CO8	P1A-O3A-P2A-O6A
2	D	1446	CO8	P1A-O3A-P2A-O6A
2	A	1446	CO8	C2'-C1'-S1P-C2P
2	B	1447	CO8	C2'-C1'-S1P-C2P
3	A	1447	NAP	C2B-O2B-P2B-O2X
3	C	1445	NAP	C2B-O2B-P2B-O3X
3	C	1445	NAP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	C	1446	CO8	CBP-CCP-O6A-P2A
2	A	1446	CO8	CCP-O6A-P2A-O4A
2	B	1447	CO8	CCP-O6A-P2A-O4A
2	D	1446	CO8	CCP-O6A-P2A-O4A
2	D	1446	CO8	C5P-C6P-C7P-N8P
2	C	1446	CO8	C3P-C2P-S1P-C1'
2	D	1446	CO8	C3P-C2P-S1P-C1'
3	C	1445	NAP	O4B-C4B-C5B-O5B
3	A	1447	NAP	O4B-C4B-C5B-O5B
3	A	1447	NAP	C2D-C1D-N1N-C2N
3	B	1446	NAP	C2D-C1D-N1N-C2N
3	B	1446	NAP	C2D-C1D-N1N-C6N
3	B	1446	NAP	O4B-C4B-C5B-O5B
3	D	1445	NAP	O4B-C4B-C5B-O5B

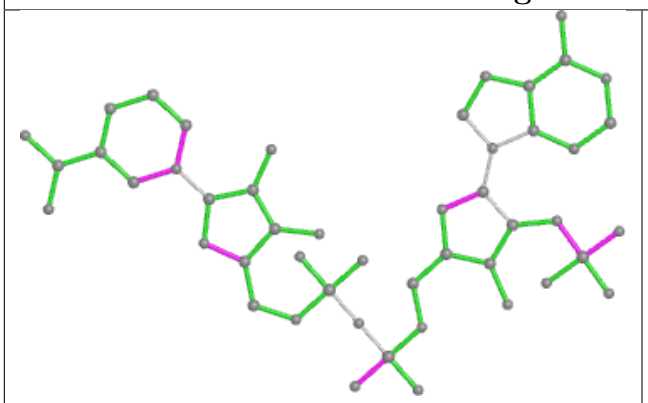
There are no ring outliers.

8 monomers are involved in 38 short contacts:

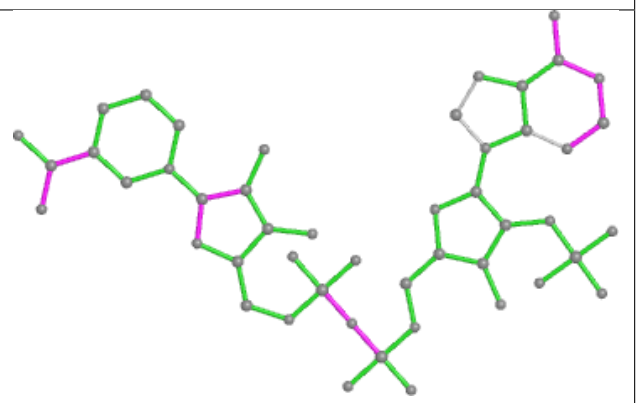
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1446	NAP	9	0
3	C	1445	NAP	6	0
2	D	1446	CO8	5	0
3	A	1447	NAP	7	0
2	A	1446	CO8	2	0
2	C	1446	CO8	5	0
3	D	1445	NAP	5	0
2	B	1447	CO8	4	0

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.

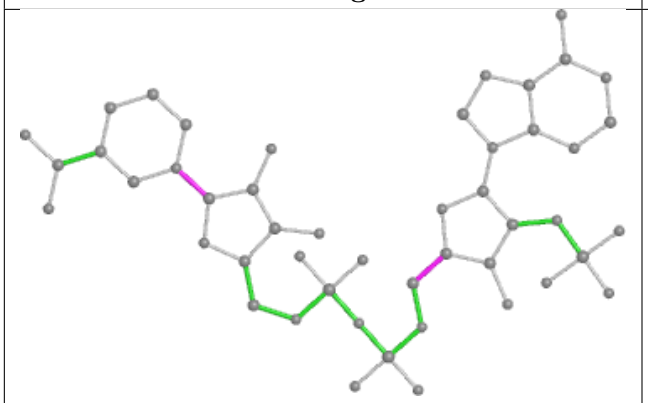
Ligand NAP B 1446



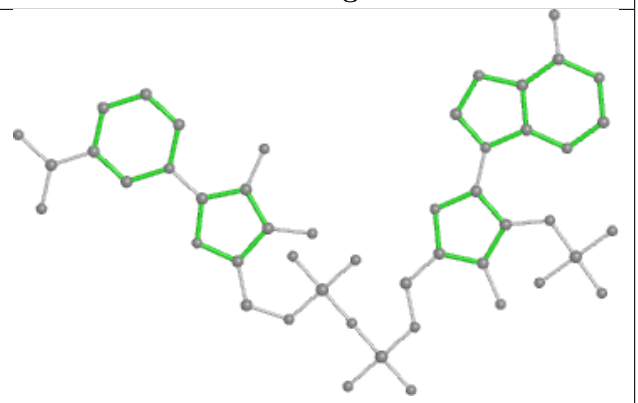
Bond lengths



Bond angles

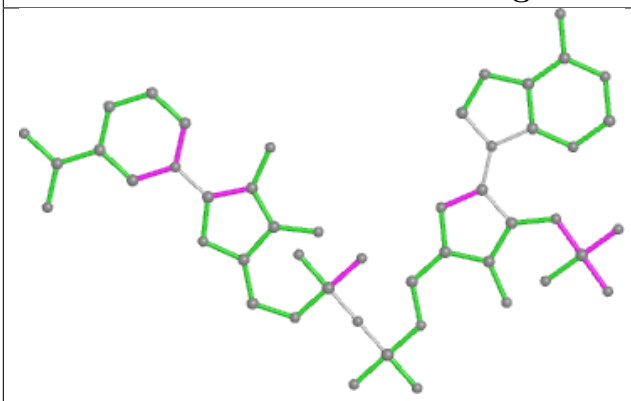


Torsions

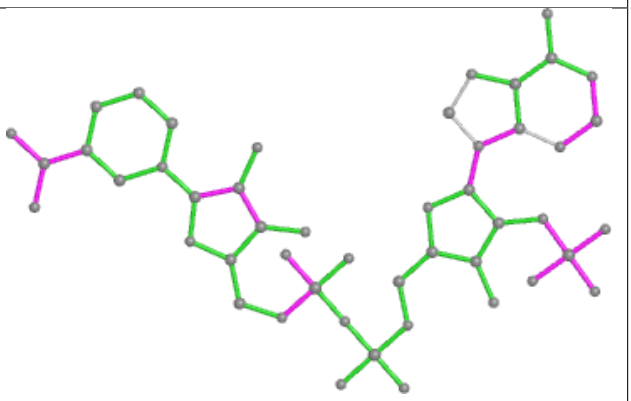


Rings

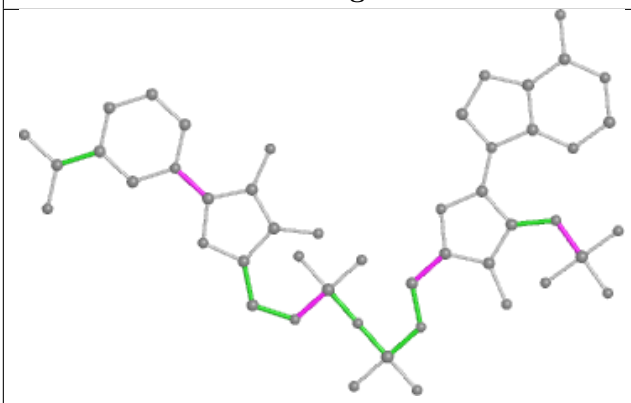
Ligand NAP C 1445



Bond lengths



Bond angles



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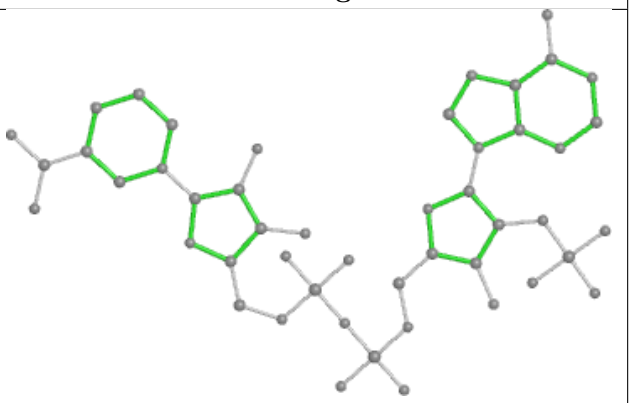
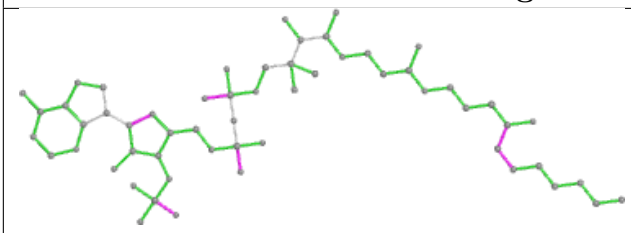
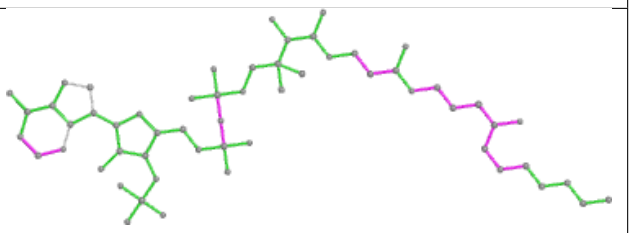


Rings

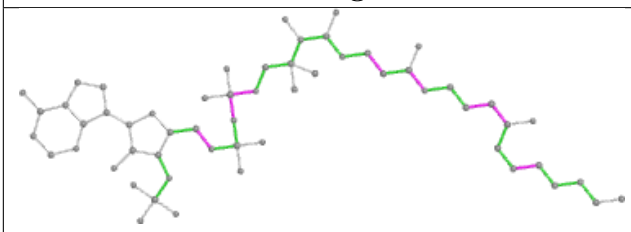
Ligand CO8 D 1446



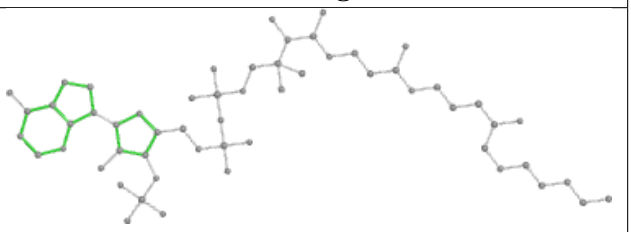
Bond lengths



Bond angles

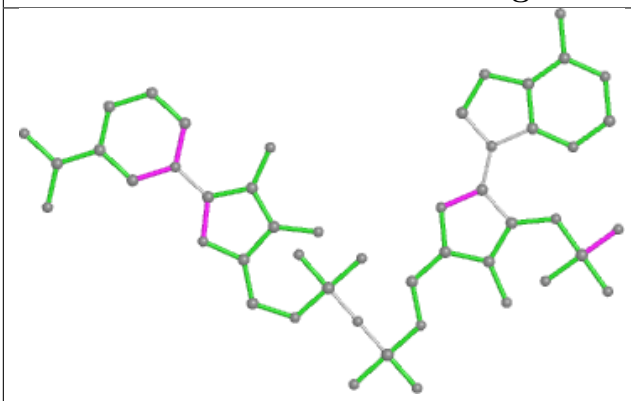


Torsions

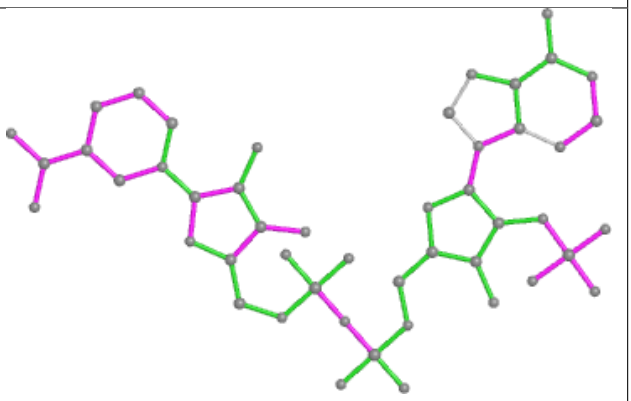


Rings

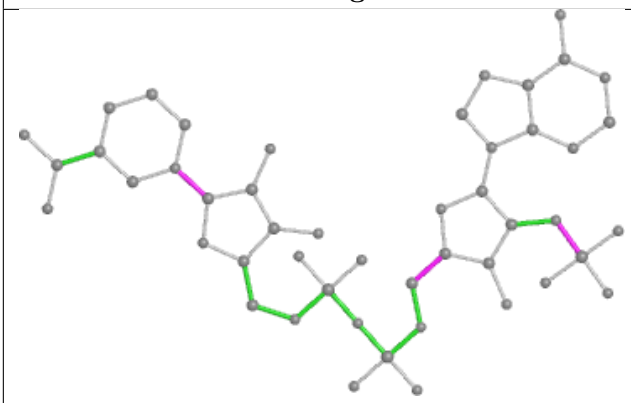
Ligand NAP A 1447



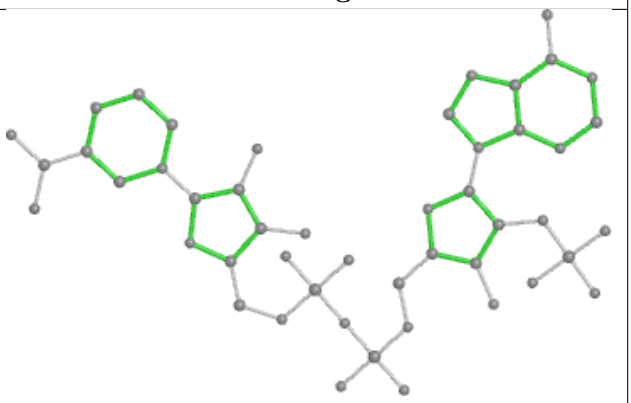
Bond lengths



Bond angles

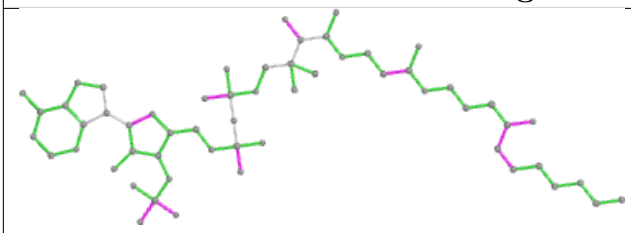


Torsions

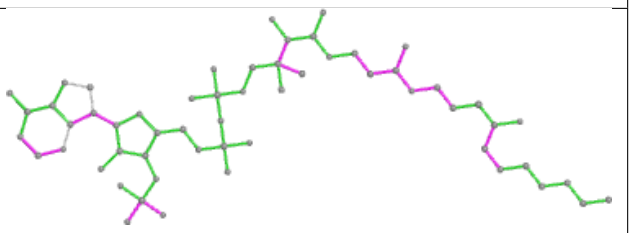


Rings

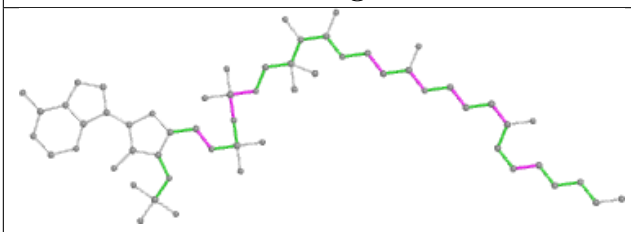
Ligand CO8 A 1446



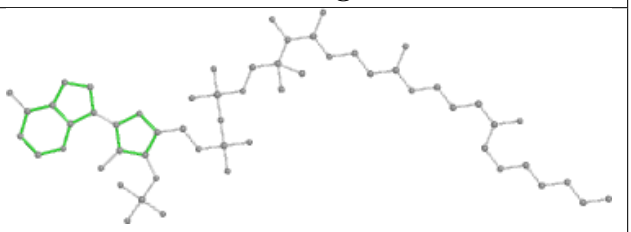
Bond lengths



Bond angles

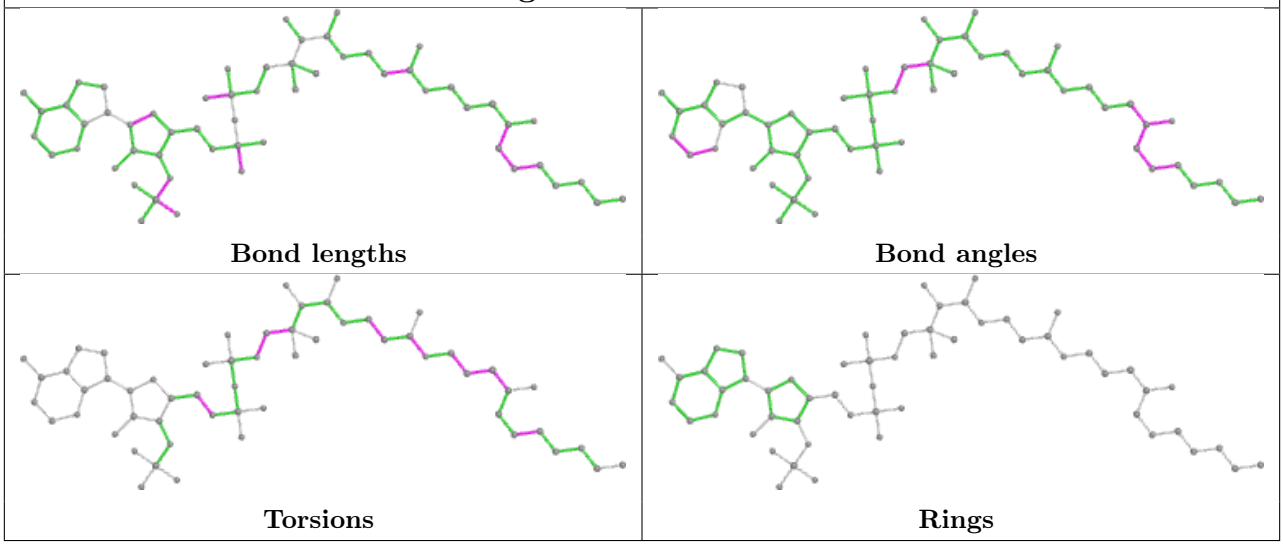


Torsions

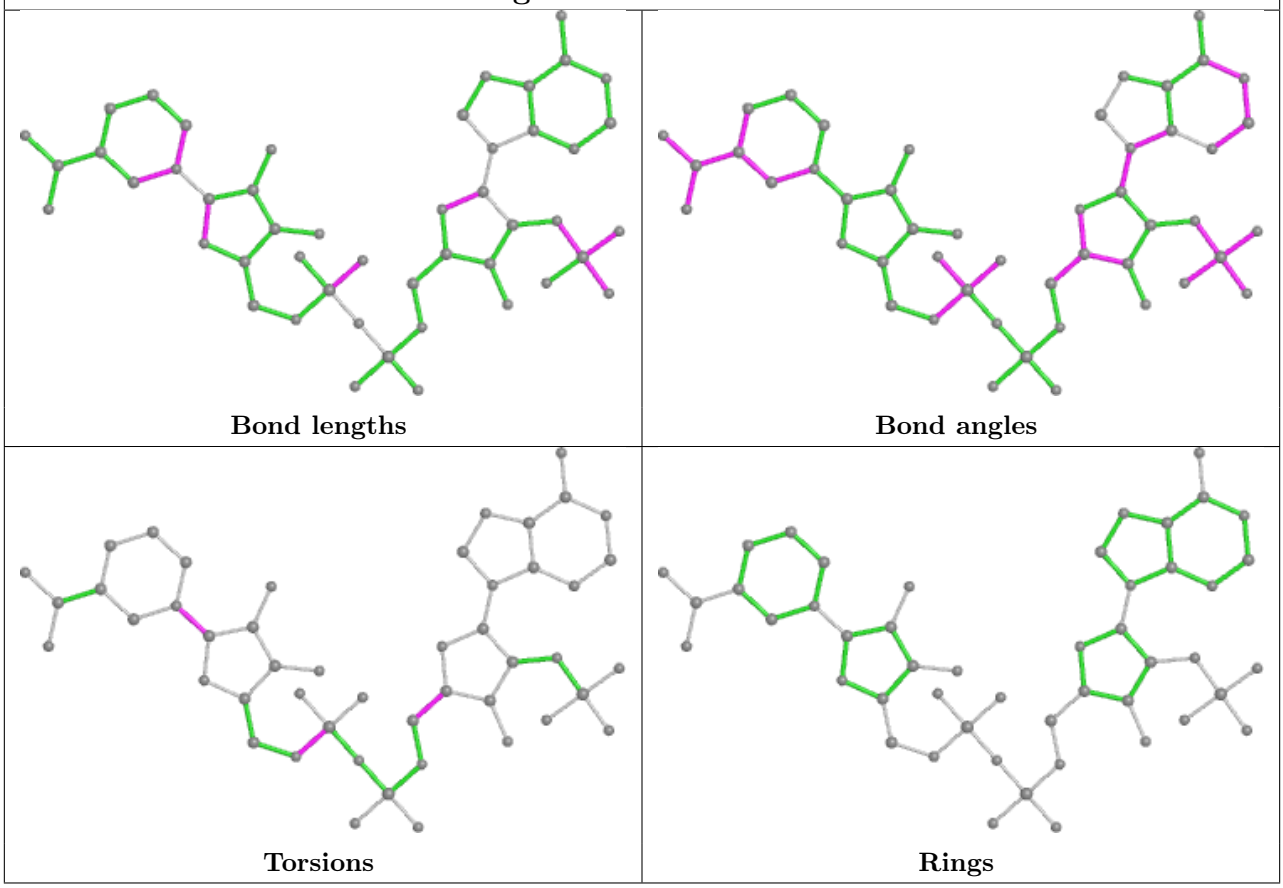


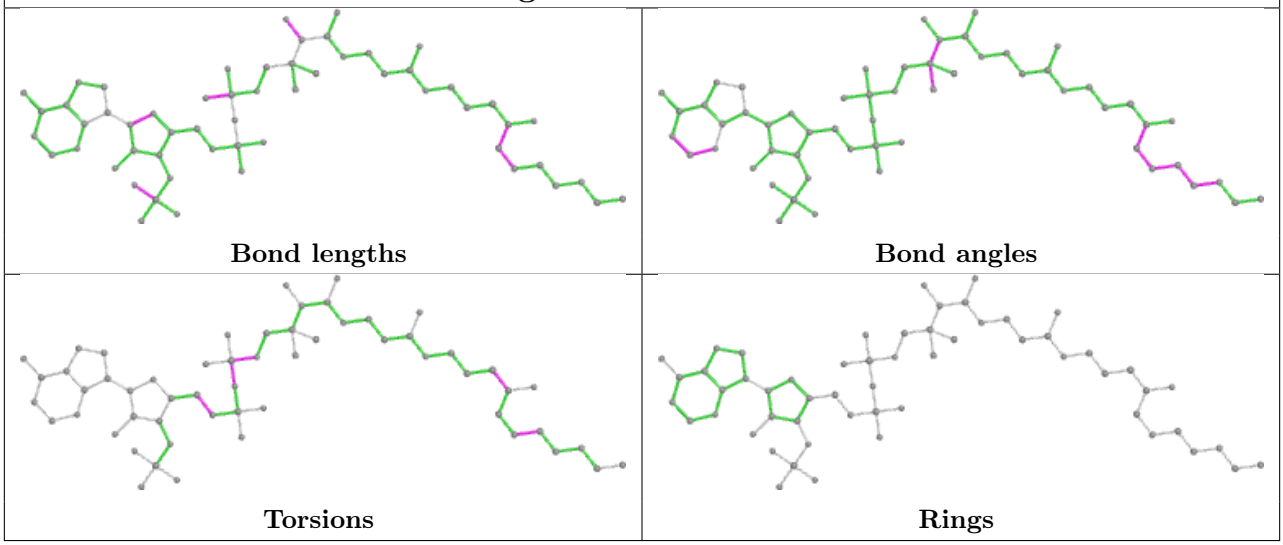
Rings

Ligand CO8 C 1446



Ligand NAP D 1445



Ligand CO8 B 1447	
	
Bond lengths	Bond angles
Torsions	Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

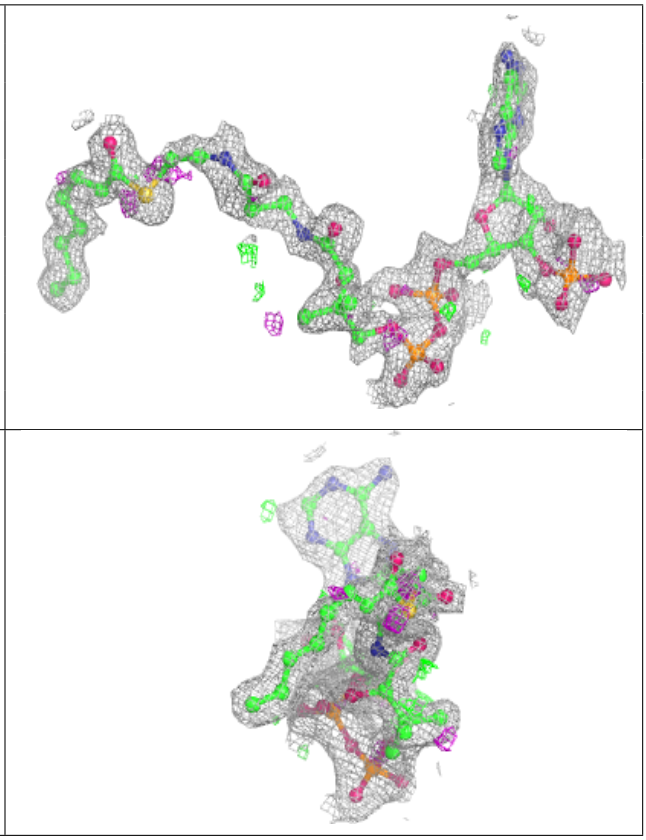
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

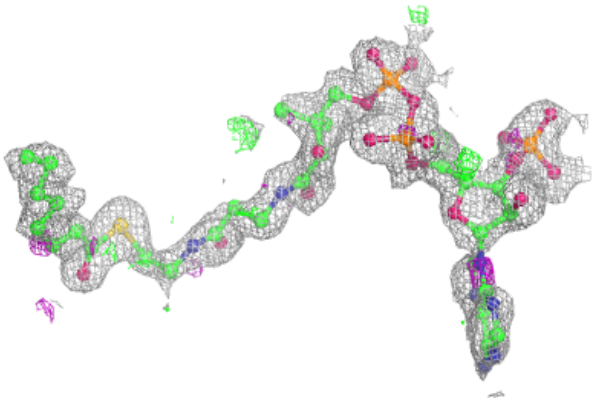
Electron density around CO8 A 1446:

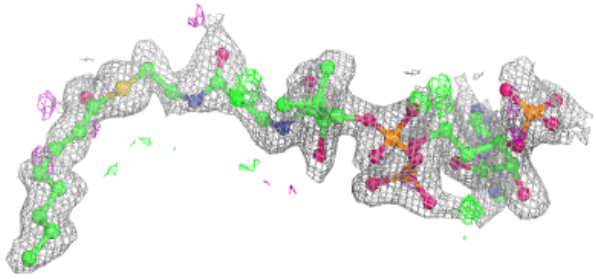
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CO8 B 1447:

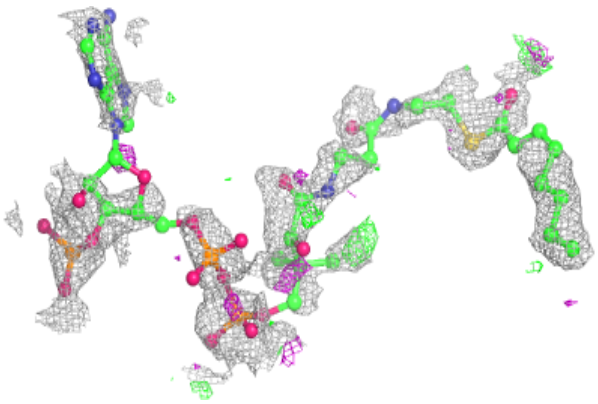
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

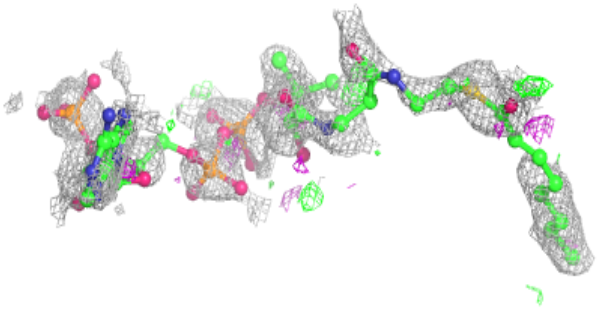




Electron density around CO8 C 1446:

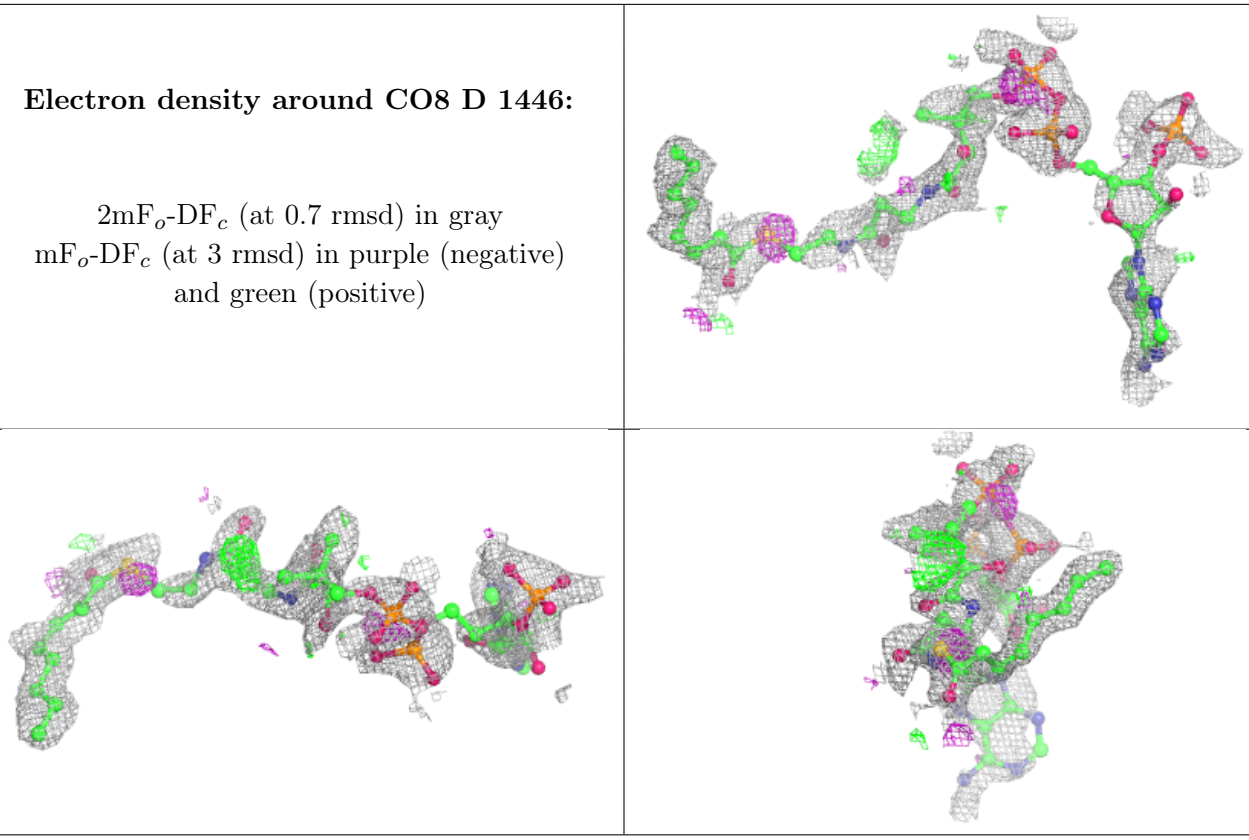
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





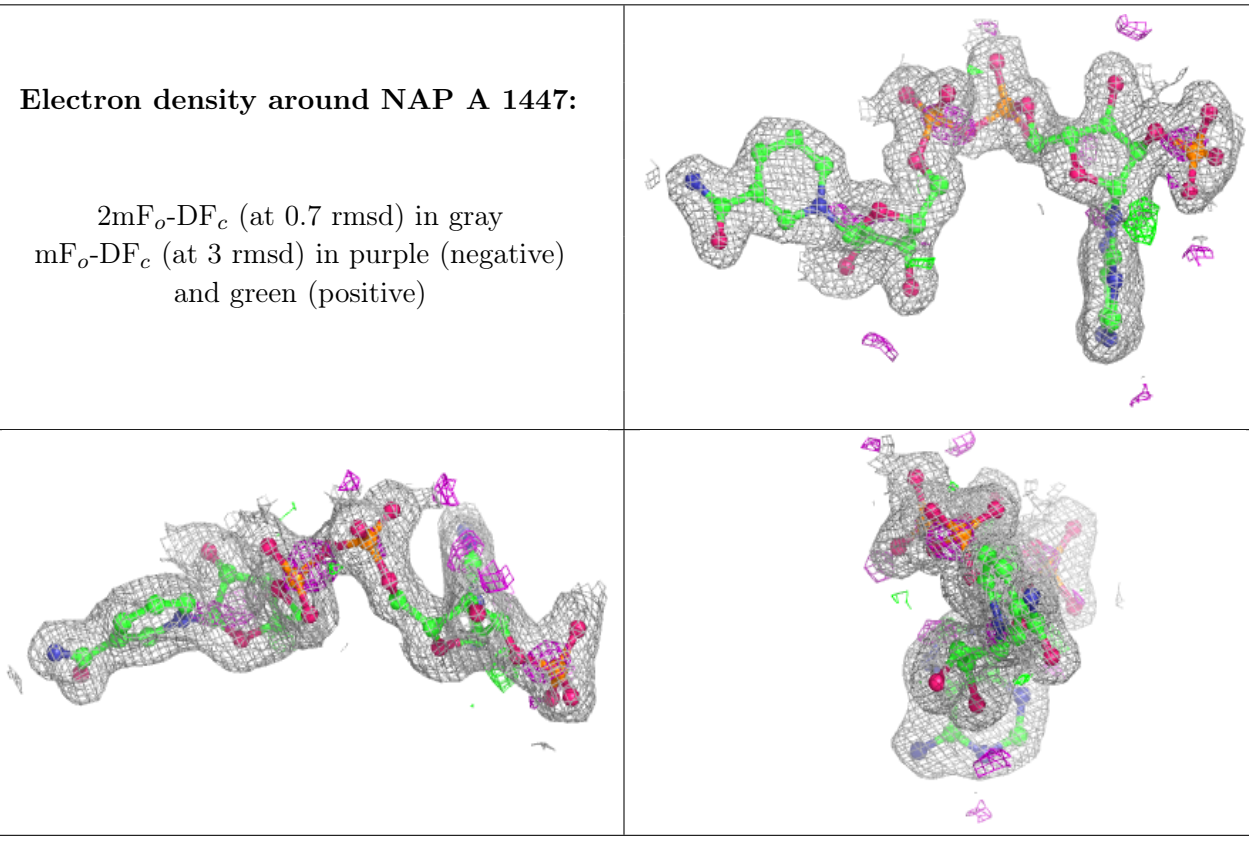
Electron density around CO8 D 1446:

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



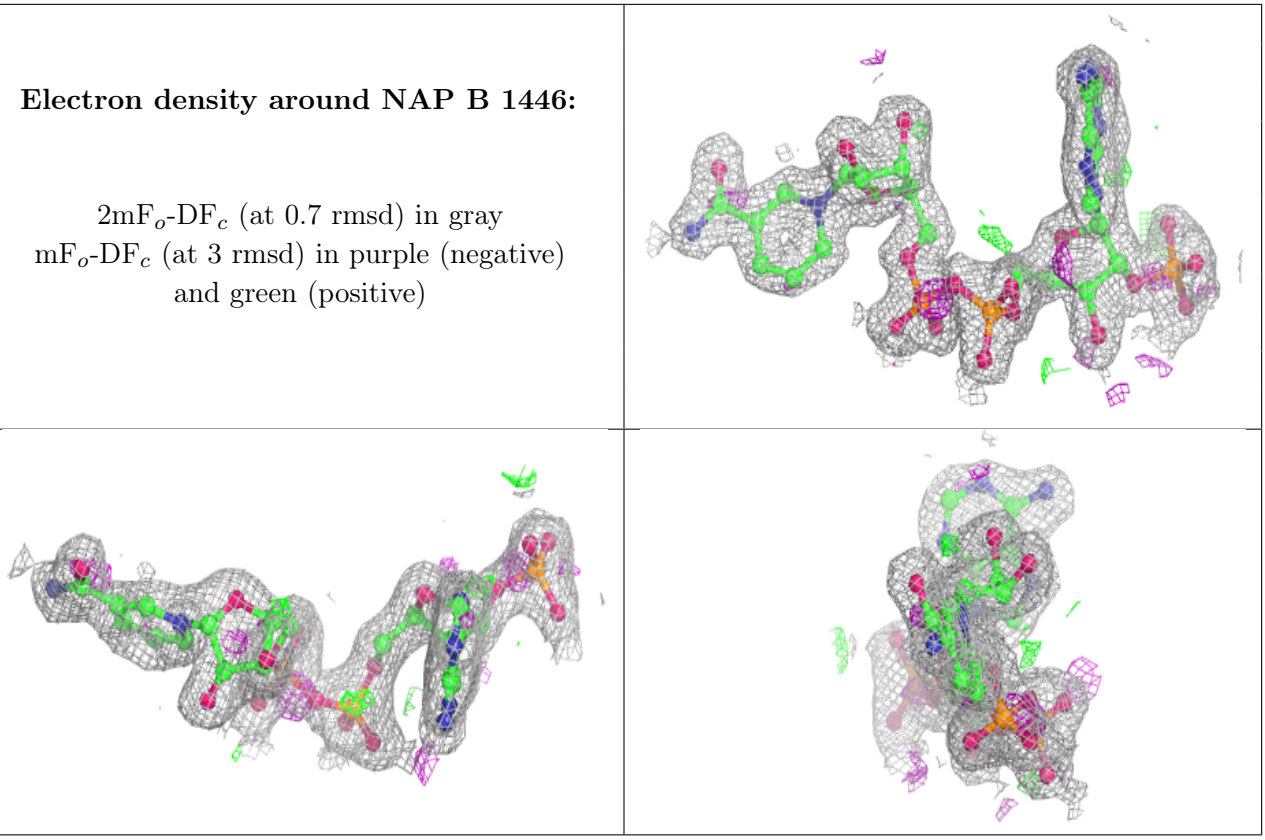
Electron density around NAP A 1447:

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



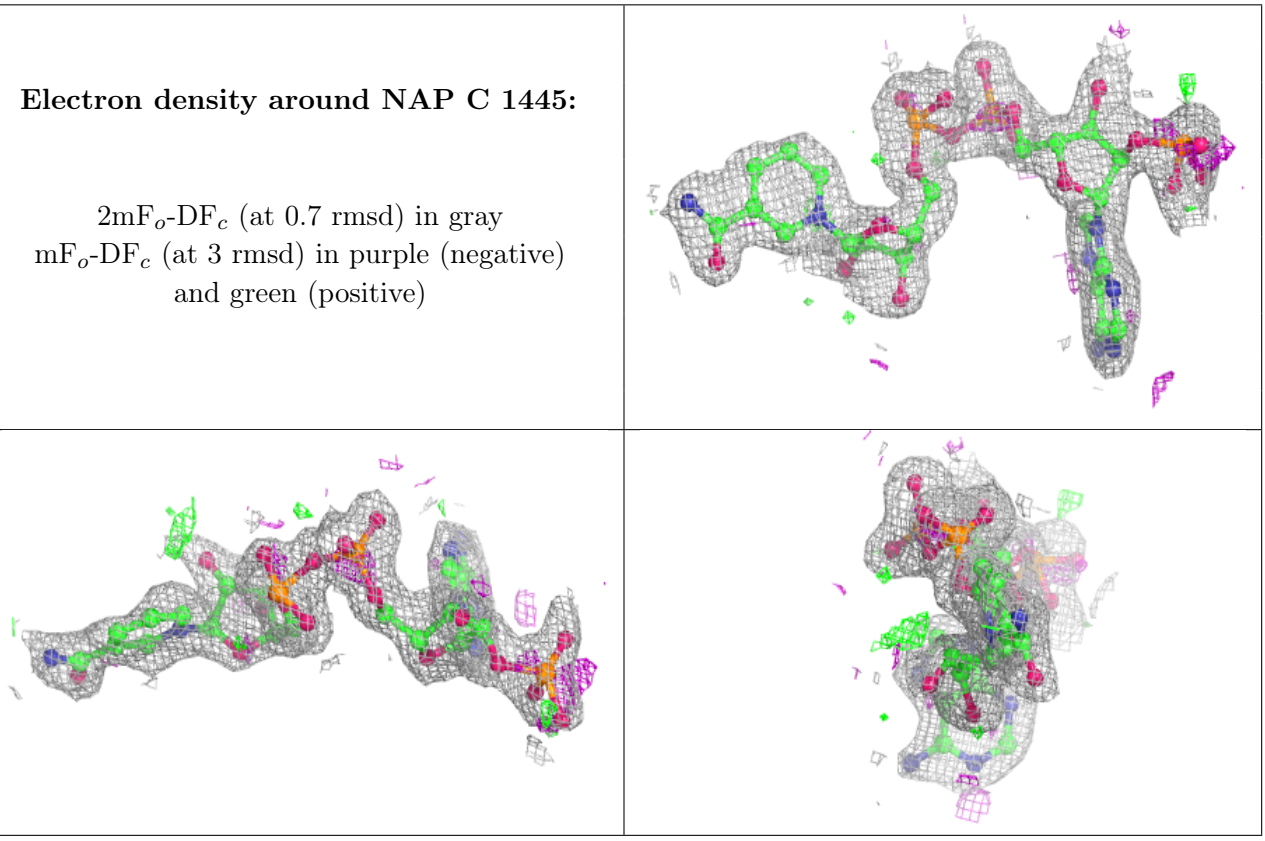
Electron density around NAP B 1446:

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



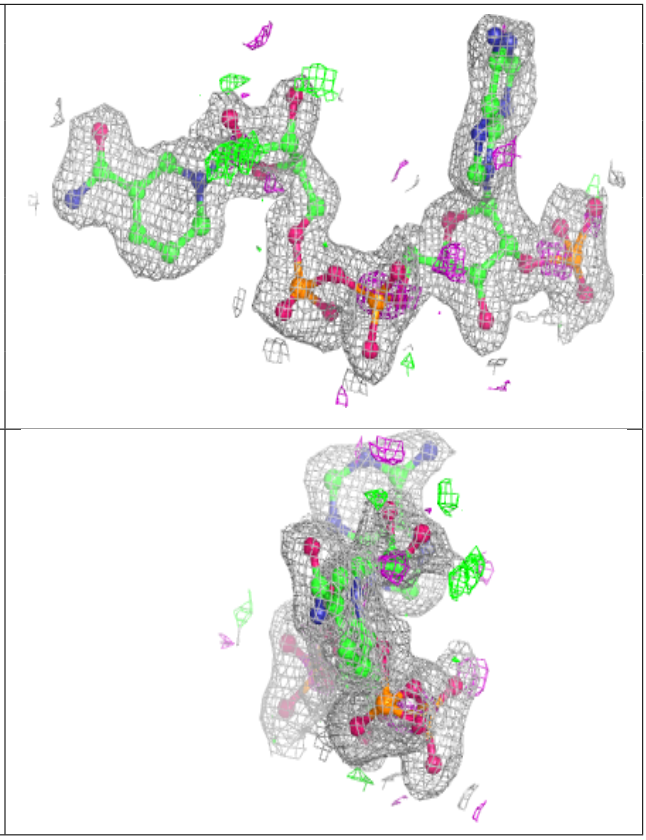
Electron density around NAP C 1445:

$2mF_o$-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 1445:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.