Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 09:39 PM EDT

PDB ID	:	6AQZ
Title	:	Crystal structure of a gdp-l-fucose synthetase from Naegleria fowleri bound to NADP
Authors	:	Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2017-08-21
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 ⓘ 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 ⓘ) were used in the production of this report:

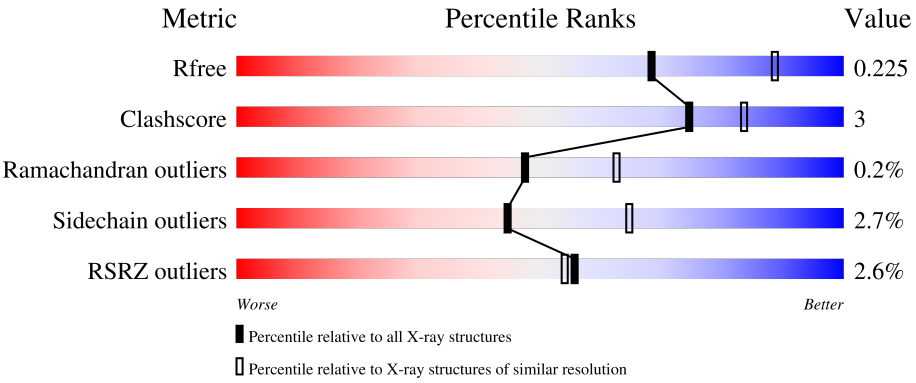
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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	341	90% 8% .
1	B	341	% 87% 7% 5%
1	C	341	88% 10% .
1	D	341	5% 82% 13% 5%

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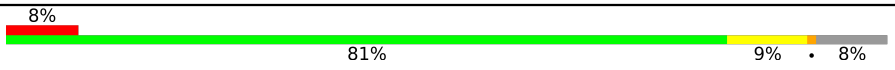
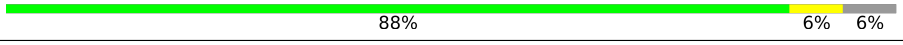
Mol	Chain	Length	Quality of chain
1	E	341	
1	F	341	

2 Entry composition (i)

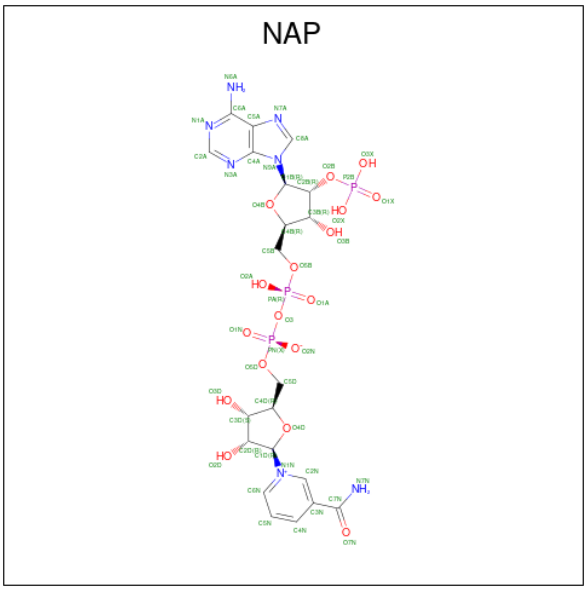
There are 4 unique types of molecules in this entry. The entry contains 15349 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 gdp-l-fucose synthetase.

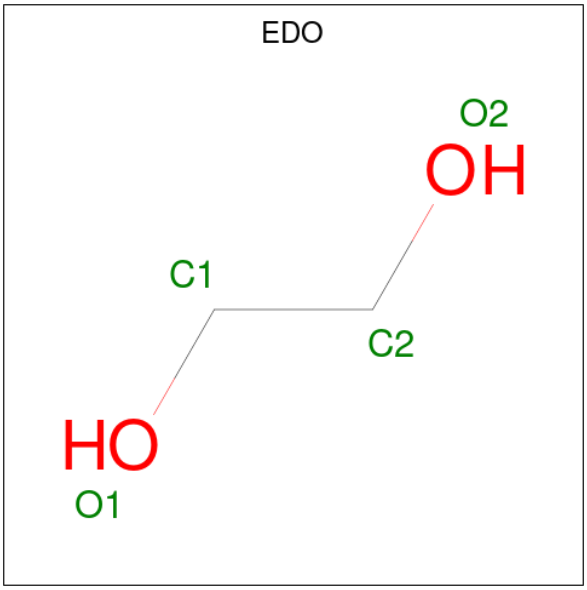
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2610	1675	432	485	18			
1	B	323	Total	C	N	O	S	0	0	0
			2488	1594	414	464	16			
1	C	334	Total	C	N	O	S	0	1	0
			2605	1665	432	489	19			
1	D	324	Total	C	N	O	S	0	0	0
			2398	1526	406	450	16			
1	E	313	Total	C	N	O	S	0	0	0
			2246	1436	377	418	15			
1	F	321	Total	C	N	O	S	0	0	0
			2508	1612	414	466	16			

- 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
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total	O	0	0
			70	70		
4	B	64	Total	O	0	0
			64	64		
4	C	51	Total	O	0	0
			51	51		
4	D	11	Total	O	0	0
			11	11		

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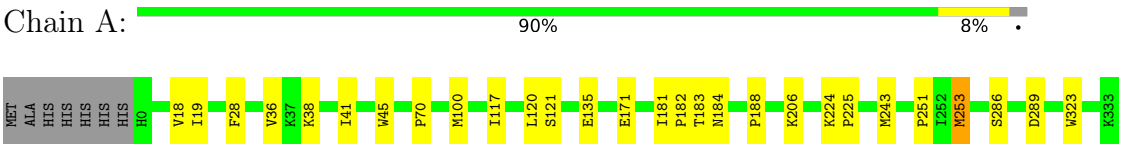
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	6	Total O 6 6	0	0
4	F	48	Total O 48 48	0	0

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.

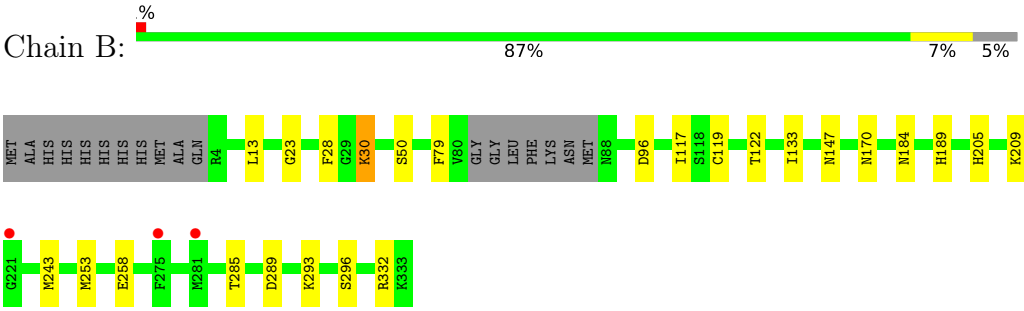
• Molecule 1: gdp-l-fucose synthetase

Chain A:



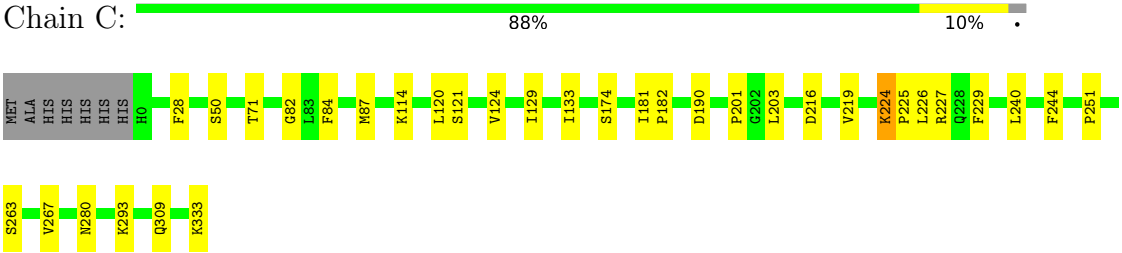
• Molecule 1: gdp-l-fucose synthetase

Chain B:



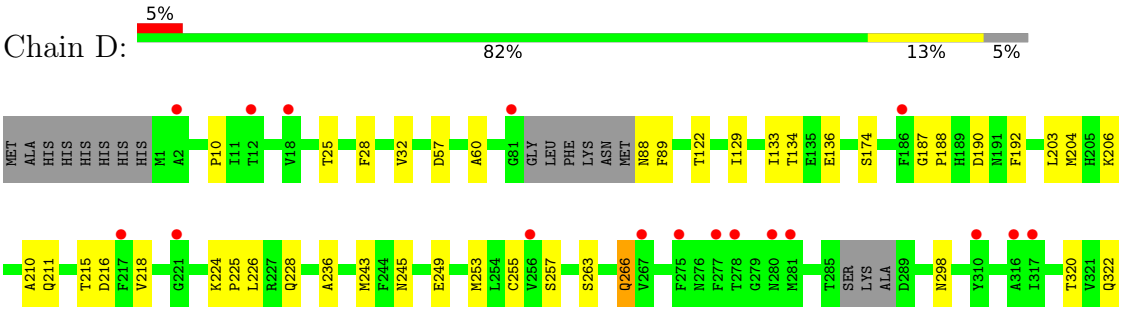
• Molecule 1: gdp-l-fucose synthetase

Chain C:



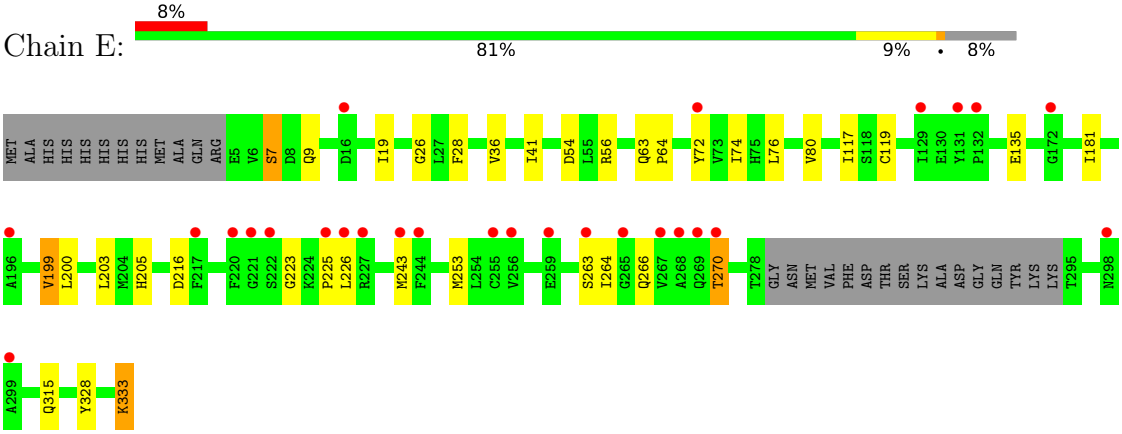
• Molecule 1: gdp-l-fucose synthetase

Chain D:



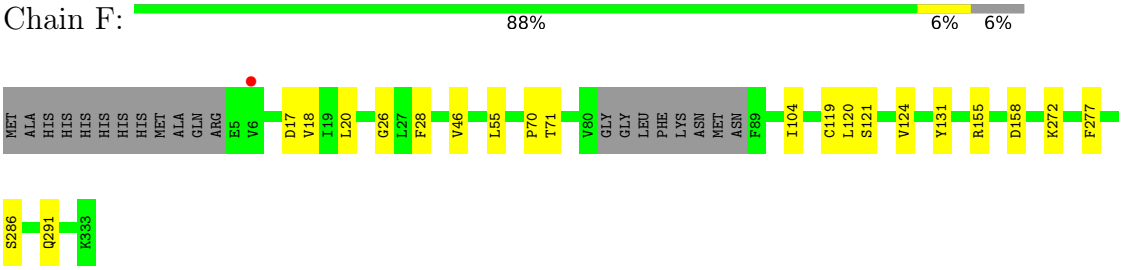
• Molecule 1: gdp-l-fucose synthetase

Chain E:



• Molecule 1: gdp-l-fucose synthetase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.37Å 104.03Å 120.17Å 90.00° 108.67° 90.00°	Depositor
Resolution (Å)	46.12 – 2.40 48.49 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.12-2.40) 98.9 (48.49-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.178 , 0.224 0.178 , 0.225	Depositor DCC
R_{free} test set	2041 reflections (2.32%)	wwPDB-VP
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15349	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, EDO

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	0.46	0/2681	0.60	2/3639 (0.1%)
1	B	0.45	1/2552 (0.0%)	0.57	0/3468
1	C	0.44	0/2675	0.57	0/3631
1	D	0.36	0/2460	0.54	0/3350
1	E	0.37	1/2306 (0.0%)	0.52	0/3155
1	F	0.44	1/2573 (0.0%)	0.58	0/3492
All	All	0.42	3/15247 (0.0%)	0.56	2/20735 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	119	CYS	CB-SG	-5.85	1.72	1.81
1	F	119	CYS	CB-SG	-5.66	1.72	1.81
1	B	119	CYS	CB-SG	-5.50	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	253	MET	CA-CB-CG	-6.26	102.66	113.30
1	A	100	MET	CG-SD-CE	5.55	109.08	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2610	0	2468	13	0
1	B	2488	0	2311	10	0
1	C	2605	0	2444	18	0
1	D	2398	0	2110	22	0
1	E	2246	0	1911	17	0
1	F	2508	0	2385	12	0
2	A	48	0	25	2	0
2	B	48	0	23	2	0
2	C	48	0	25	3	0
2	E	48	0	24	2	0
2	F	48	0	23	2	0
3	B	4	0	6	1	0
4	A	70	0	0	0	0
4	B	64	0	0	0	0
4	C	51	0	0	1	0
4	D	11	0	0	0	0
4	E	6	0	0	0	0
4	F	48	0	0	1	0
All	All	15349	0	13755	91	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 3.

All (91) 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:263:SER:N	1:D:266:GLN:OE1	2.05	0.89
1:D:206:LYS:NZ	1:D:218:VAL:O	2.16	0.79
1:C:226:LEU:O	1:C:227:ARG:NH1	2.18	0.75
1:A:181:ILE:HB	1:A:253:MET:HG2	1.69	0.74
1:F:17:ASP:HB2	1:F:71:THR:OG1	1.87	0.74
1:E:328:TYR:O	1:E:333:LYS:NZ	2.23	0.70
1:A:18:VAL:HB	1:A:70:PRO:HA	1.74	0.69
1:F:131:TYR:OH	1:F:291:GLN:NE2	2.27	0.67
1:D:10:PRO:HG3	1:D:245:ASN:HD21	1.62	0.63
1:B:258:GLU:OE1	1:B:293:LYS:NZ	2.31	0.62
1:E:54:ASP:OD1	1:E:56:ARG:HG2	2.00	0.61
1:E:225:PRO:O	1:E:264:ILE:N	2.35	0.59
1:C:309:GLN:NE2	4:C:502:HOH:O	2.30	0.59
1:E:7:SER:OG	1:E:9:GLN:O	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:THR:HB	1:C:114:LYS:HE3	1.85	0.58
1:D:328:TYR:O	1:D:333:LYS:NZ	2.34	0.58
1:D:88:ASN:OD1	1:D:89:PHE:N	2.35	0.57
1:F:55:LEU:HD13	1:F:104:ILE:HD11	1.85	0.57
1:A:36:VAL:HA	1:A:41[A]:ILE:HD13	1.85	0.57
2:E:401:NAP:N7N	2:E:401:NAP:O2N	2.39	0.55
1:D:210:ALA:HA	1:D:215:THR:HG23	1.89	0.55
1:D:192:PHE:HE2	1:D:204:MET:HE2	1.73	0.54
1:F:18:VAL:HB	1:F:70:PRO:HA	1.89	0.54
1:F:120:LEU:O	2:F:401:NAP:H6N	2.08	0.53
1:B:30:LYS:HG2	1:B:189:HIS:CD2	2.45	0.52
1:C:121:SER:O	1:C:124:VAL:HG22	2.10	0.51
1:D:226:LEU:HA	1:D:263:SER:HA	1.93	0.51
1:E:135:GLU:HG3	1:E:253:MET:HG3	1.92	0.51
1:E:266:GLN:O	1:E:270:THR:OG1	2.28	0.51
1:C:203:LEU:HD22	1:C:219:VAL:HG12	1.93	0.50
1:B:205:HIS:O	1:B:209:LYS:HG3	2.12	0.49
1:F:20:LEU:HD12	1:F:46:VAL:HB	1.95	0.49
1:E:226:LEU:HA	1:E:263:SER:HA	1.95	0.48
1:B:117:ILE:HD11	1:B:243:MET:HA	1.95	0.48
1:B:293:LYS:O	1:F:286:SER:HB3	2.13	0.48
1:B:50:SER:OG	2:B:401:NAP:O2X	2.22	0.48
1:C:229:PHE:CE2	1:C:267:VAL:HG21	2.49	0.47
1:C:84:PHE:O	1:C:87:MET:HG2	2.15	0.47
1:C:190:ASP:OD2	1:C:201:PRO:HG3	2.15	0.47
1:B:133:ILE:HG22	1:B:253:MET:HE3	1.97	0.47
1:D:57:ASP:HB3	1:D:60:ALA:HB3	1.97	0.47
1:C:263:SER:O	1:C:267:VAL:HG23	2.15	0.46
1:A:117:ILE:HD11	1:A:243:MET:HA	1.96	0.46
1:D:215:THR:OG1	1:D:216:ASP:N	2.48	0.46
1:C:120:LEU:O	2:C:401:NAP:H6N	2.15	0.46
1:F:120:LEU:HD11	1:F:158:ASP:HB2	1.98	0.46
1:A:120:LEU:O	2:A:401:NAP:H6N	2.15	0.46
1:C:50:SER:HG	2:C:401:NAP:P2B	2.39	0.46
1:D:187:GLY:O	1:D:190:ASP:HB2	2.15	0.46
1:E:199:VAL:O	1:E:203:LEU:HD13	2.16	0.46
1:A:224:LYS:N	1:A:225:PRO:CD	2.79	0.46
1:E:181:ILE:HB	1:E:253:MET:HG2	1.99	0.45
1:F:272:LYS:HE2	1:F:277:PHE:O	2.17	0.45
1:C:82:GLY:HA3	1:C:87:MET:HG3	1.97	0.45
1:D:188:PRO:HB3	1:D:323:TRP:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:PRO:HB3	1:A:323:TRP:CG	2.52	0.45
1:C:240:LEU:O	1:C:244:PHE:HD1	1.99	0.44
1:D:210:ALA:HA	1:D:215:THR:CG2	2.47	0.44
1:D:192:PHE:CE2	1:D:204:MET:HE2	2.52	0.44
1:C:129:ILE:HD13	1:C:133:ILE:HG12	2.00	0.43
1:D:255:CYS:SG	1:D:298:ASN:HB3	2.58	0.43
1:B:79:PHE:CD2	1:B:96:ASP:HB3	2.53	0.43
1:D:32:VAL:HA	1:D:236:ALA:HB1	1.99	0.43
1:F:155:ARG:HD3	4:F:501:HOH:O	2.18	0.43
1:B:23:GLY:HA2	2:B:401:NAP:H1B	2.01	0.43
1:D:129:ILE:HD13	1:D:133:ILE:HD12	2.01	0.43
1:D:203:LEU:HD23	1:D:203:LEU:HA	1.89	0.43
1:C:216:ASP:OD1	1:C:280:ASN:HB2	2.18	0.42
1:E:205:HIS:CE1	1:E:333:LYS:HB2	2.54	0.42
1:E:74:ILE:HG22	1:E:76:LEU:HG	2.02	0.42
1:F:26:GLY:HA3	2:F:401:NAP:O5B	2.20	0.42
1:E:36:VAL:HA	1:E:41:ILE:HD13	2.00	0.42
1:C:182:PRO:HG2	2:C:401:NAP:C6N	2.49	0.42
1:E:117:ILE:HD11	1:E:243:MET:HA	2.01	0.42
1:E:63:GLN:HB2	1:E:64:PRO:HD3	2.01	0.42
1:E:223:GLY:C	1:E:225:PRO:HD3	2.39	0.42
1:A:135:GLU:HG3	1:A:253:MET:HG3	2.02	0.41
1:A:38:LYS:O	1:D:136:GLU:HG3	2.21	0.41
1:E:19:ILE:HG13	1:E:72:TYR:HB2	2.01	0.41
1:E:26:GLY:HA3	2:E:401:NAP:O5B	2.20	0.41
1:A:183:THR:HG23	1:A:184:ASN:N	2.36	0.41
1:D:204:MET:HE1	1:D:320:THR:HG22	2.02	0.41
1:F:121:SER:O	1:F:124:VAL:HG22	2.21	0.41
1:D:228:GLN:HE21	1:D:257:SER:C	2.23	0.41
1:D:225:PRO:O	1:D:263:SER:HA	2.21	0.41
1:A:19:ILE:HG21	1:A:45:TRP:CZ3	2.56	0.40
1:B:289:ASP:OD1	3:B:402:EDO:H22	2.21	0.40
1:C:224:LYS:N	1:C:225:PRO:CD	2.85	0.40
1:A:182:PRO:HG2	2:A:401:NAP:C6N	2.51	0.40
1:C:181:ILE:HD11	1:C:251:PRO:HB2	2.04	0.40
1:A:135:GLU:HG2	1:A:251:PRO:O	2.21	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	333/341 (98%)	327 (98%)	6 (2%)	0	100	100
1	B	319/341 (94%)	313 (98%)	5 (2%)	1 (0%)	41	55
1	C	333/341 (98%)	329 (99%)	3 (1%)	1 (0%)	41	55
1	D	318/341 (93%)	312 (98%)	5 (2%)	1 (0%)	41	55
1	E	309/341 (91%)	296 (96%)	13 (4%)	0	100	100
1	F	317/341 (93%)	312 (98%)	5 (2%)	0	100	100
All	All	1929/2046 (94%)	1889 (98%)	37 (2%)	3 (0%)	47	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	ASN
1	D	224	LYS
1	C	224	LYS

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	273/298 (92%)	267 (98%)	6 (2%)	52	71
1	B	255/298 (86%)	246 (96%)	9 (4%)	36	55
1	C	272/298 (91%)	268 (98%)	4 (2%)	65	80
1	D	227/298 (76%)	216 (95%)	11 (5%)	25	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	200/298 (67%)	191 (96%)	9 (4%)	27 44
1	F	265/298 (89%)	264 (100%)	1 (0%)	91 96
All	All	1492/1788 (83%)	1452 (97%)	40 (3%)	44 65

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	121	SER
1	A	171	GLU
1	A	206	LYS
1	A	286	SER
1	A	289	ASP
1	B	13	LEU
1	B	28	PHE
1	B	30	LYS
1	B	122	THR
1	B	147	ASN
1	B	170	ASN
1	B	285	THR
1	B	296	SER
1	B	332	ARG
1	C	28	PHE
1	C	174	SER
1	C	293	LYS
1	C	333	LYS
1	D	25	THR
1	D	28	PHE
1	D	122	THR
1	D	134	THR
1	D	174	SER
1	D	211	GLN
1	D	243	MET
1	D	249	GLU
1	D	253	MET
1	D	266	GLN
1	D	322	GLN
1	E	7	SER
1	E	28	PHE
1	E	80	VAL
1	E	199	VAL

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Mol	Chain	Res	Type
1	E	200	LEU
1	E	216	ASP
1	E	270	THR
1	E	315	GLN
1	E	333	LYS
1	F	28	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	189	HIS
1	B	211	GLN
1	C	291	GLN
1	D	212	GLN
1	D	245	ASN
1	F	269	GLN
1	F	291	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)

6 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	B	401	1	45,52,52	2.93	18 (40%)	56,80,80	1.98	17 (30%)
2	NAP	A	401	-	45,52,52	2.90	13 (28%)	56,80,80	1.88	14 (25%)
2	NAP	F	401	-	45,52,52	2.82	13 (28%)	56,80,80	1.89	12 (21%)
3	EDO	B	402	-	3,3,3	0.47	0	2,2,2	0.25	0
2	NAP	E	401	-	45,52,52	2.75	10 (22%)	56,80,80	2.00	16 (28%)
2	NAP	C	401	-	45,52,52	2.75	13 (28%)	56,80,80	1.83	13 (23%)

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	401	1	-	8/31/67/67	0/5/5/5
2	NAP	A	401	-	-	5/31/67/67	0/5/5/5
2	NAP	F	401	-	-	4/31/67/67	0/5/5/5
3	EDO	B	402	-	-	0/1/1/1	-
2	NAP	E	401	-	-	5/31/67/67	0/5/5/5
2	NAP	C	401	-	-	4/31/67/67	0/5/5/5

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	P2B-O2B	14.11	1.86	1.59
2	B	401	NAP	P2B-O2B	13.88	1.85	1.59
2	C	401	NAP	P2B-O2B	13.79	1.85	1.59
2	E	401	NAP	P2B-O2B	12.81	1.83	1.59
2	F	401	NAP	P2B-O2B	11.46	1.81	1.59
2	F	401	NAP	C2N-N1N	6.86	1.43	1.35
2	F	401	NAP	C4N-C3N	6.34	1.50	1.39
2	E	401	NAP	C4N-C3N	6.32	1.50	1.39
2	F	401	NAP	C5N-C4N	5.80	1.51	1.38
2	C	401	NAP	C4N-C3N	5.65	1.49	1.39
2	A	401	NAP	C4N-C3N	5.40	1.48	1.39
2	A	401	NAP	C5N-C4N	5.22	1.49	1.38
2	B	401	NAP	C4N-C3N	5.22	1.48	1.39
2	B	401	NAP	PN-O5D	4.72	1.78	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAP	C5N-C4N	4.41	1.48	1.38
2	E	401	NAP	C5N-C4N	4.40	1.48	1.38
2	E	401	NAP	PN-O5D	4.34	1.76	1.59
2	B	401	NAP	C3N-C7N	-4.34	1.44	1.50
2	A	401	NAP	C2N-N1N	4.26	1.40	1.35
2	C	401	NAP	C2N-N1N	4.13	1.40	1.35
2	B	401	NAP	C2N-N1N	4.04	1.39	1.35
2	A	401	NAP	PN-O5D	3.98	1.75	1.59
2	E	401	NAP	C7N-N7N	3.95	1.40	1.33
2	A	401	NAP	C7N-N7N	3.88	1.40	1.33
2	B	401	NAP	C5N-C4N	3.62	1.46	1.38
2	F	401	NAP	C6N-N1N	3.43	1.43	1.35
2	F	401	NAP	C7N-N7N	3.36	1.39	1.33
2	F	401	NAP	O4D-C1D	3.33	1.45	1.41
2	F	401	NAP	C3D-C4D	3.27	1.61	1.53
2	E	401	NAP	O2D-C2D	-3.26	1.35	1.43
2	B	401	NAP	C7N-N7N	3.11	1.38	1.33
2	C	401	NAP	O4B-C1B	3.05	1.45	1.41
2	A	401	NAP	C3D-C4D	3.04	1.60	1.53
2	B	401	NAP	C2A-N1A	2.99	1.39	1.33
2	F	401	NAP	PN-O5D	2.97	1.71	1.59
2	E	401	NAP	C2D-C1D	2.83	1.58	1.53
2	A	401	NAP	C6N-N1N	2.81	1.42	1.35
2	E	401	NAP	C2N-N1N	2.81	1.38	1.35
2	A	401	NAP	O2B-C2B	-2.80	1.33	1.44
2	C	401	NAP	PN-O5D	2.80	1.70	1.59
2	F	401	NAP	O3D-C3D	-2.75	1.36	1.43
2	E	401	NAP	O2B-C2B	-2.73	1.34	1.44
2	B	401	NAP	O2B-C2B	-2.69	1.34	1.44
2	F	401	NAP	O2D-C2D	-2.69	1.36	1.43
2	B	401	NAP	C3D-C4D	2.68	1.59	1.53
2	C	401	NAP	O2D-C2D	-2.57	1.36	1.43
2	F	401	NAP	O2B-C2B	-2.50	1.35	1.44
2	C	401	NAP	O2B-C2B	-2.48	1.35	1.44
2	B	401	NAP	O4B-C1B	2.40	1.44	1.41
2	B	401	NAP	C3B-C4B	2.37	1.59	1.53
2	B	401	NAP	C6A-N6A	2.36	1.42	1.34
2	C	401	NAP	C6N-C5N	-2.28	1.33	1.38
2	B	401	NAP	C2D-C1D	2.27	1.57	1.53
2	B	401	NAP	PA-O5B	2.24	1.68	1.59
2	A	401	NAP	C3B-C4B	2.23	1.58	1.53
2	C	401	NAP	C6N-N1N	2.18	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	NAP	O5D-C5D	-2.17	1.36	1.44
2	C	401	NAP	C3D-C4D	2.17	1.58	1.53
2	E	401	NAP	C2A-N1A	2.16	1.37	1.33
2	A	401	NAP	O2D-C2D	-2.16	1.37	1.43
2	B	401	NAP	C4A-N3A	2.15	1.38	1.35
2	B	401	NAP	C6N-C5N	-2.12	1.33	1.38
2	A	401	NAP	C6N-C5N	-2.12	1.33	1.38
2	C	401	NAP	C7N-N7N	2.12	1.37	1.33
2	A	401	NAP	C2A-N3A	2.10	1.35	1.32
2	C	401	NAP	O5D-C5D	-2.04	1.36	1.44
2	B	401	NAP	O2D-C2D	-2.01	1.38	1.43

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	NAP	C5N-C4N-C3N	-6.70	112.42	120.34
2	B	401	NAP	C5N-C4N-C3N	-6.64	112.48	120.34
2	E	401	NAP	PN-O3-PA	-5.96	112.36	132.83
2	A	401	NAP	C5N-C4N-C3N	-5.89	113.37	120.34
2	B	401	NAP	PN-O3-PA	-5.80	112.92	132.83
2	A	401	NAP	PN-O3-PA	-5.57	113.70	132.83
2	F	401	NAP	PN-O3-PA	-5.32	114.56	132.83
2	C	401	NAP	C5N-C4N-C3N	-5.24	114.14	120.34
2	C	401	NAP	PN-O3-PA	-5.23	114.87	132.83
2	F	401	NAP	C5N-C4N-C3N	-5.14	114.26	120.34
2	B	401	NAP	C2N-C3N-C4N	4.66	123.54	118.26
2	C	401	NAP	O7N-C7N-N7N	-4.47	116.22	122.58
2	A	401	NAP	C2N-C3N-C4N	3.71	122.46	118.26
2	F	401	NAP	O2B-P2B-O1X	-3.65	95.29	109.39
2	F	401	NAP	O7N-C7N-N7N	-3.62	117.44	122.58
2	E	401	NAP	C2N-C3N-C4N	3.62	122.36	118.26
2	F	401	NAP	O7N-C7N-C3N	3.48	123.80	119.63
2	C	401	NAP	O7N-C7N-C3N	3.42	123.72	119.63
2	E	401	NAP	O2B-P2B-O1X	-3.30	96.67	109.39
2	F	401	NAP	C2N-C3N-C4N	3.21	121.90	118.26
2	A	401	NAP	O7N-C7N-N7N	-3.15	118.11	122.58
2	E	401	NAP	O7N-C7N-C3N	3.10	123.34	119.63
2	B	401	NAP	C6N-N1N-C2N	-3.00	119.24	121.97
2	C	401	NAP	O2B-P2B-O1X	-2.94	98.06	109.39
2	B	401	NAP	O2B-P2B-O1X	-2.90	98.18	109.39
2	E	401	NAP	C2A-N1A-C6A	-2.90	113.80	118.75
2	E	401	NAP	PA-O5B-C5B	-2.75	105.53	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	NAP	O7N-C7N-N7N	-2.72	118.71	122.58
2	B	401	NAP	PA-O5B-C5B	-2.70	105.82	121.68
2	A	401	NAP	C3B-C2B-C1B	-2.68	97.85	102.89
2	C	401	NAP	C2N-C3N-C4N	2.68	121.30	118.26
2	E	401	NAP	O2N-PN-O1N	2.62	125.19	112.24
2	A	401	NAP	O7N-C7N-C3N	2.60	122.75	119.63
2	A	401	NAP	O2B-P2B-O1X	-2.60	99.37	109.39
2	A	401	NAP	O3X-P2B-O2X	2.58	117.49	107.64
2	F	401	NAP	O3X-P2B-O2X	2.57	117.48	107.64
2	B	401	NAP	O7N-C7N-C3N	2.55	122.69	119.63
2	E	401	NAP	C6N-N1N-C2N	-2.54	119.66	121.97
2	C	401	NAP	O3X-P2B-O2X	2.54	117.35	107.64
2	B	401	NAP	O3X-P2B-O2X	2.53	117.32	107.64
2	A	401	NAP	C6N-N1N-C2N	-2.52	119.68	121.97
2	A	401	NAP	C2A-N1A-C6A	-2.52	114.45	118.75
2	A	401	NAP	PA-O5B-C5B	-2.49	107.10	121.68
2	B	401	NAP	C2A-N1A-C6A	-2.47	114.53	118.75
2	B	401	NAP	O5D-PN-O1N	-2.47	99.44	109.07
2	B	401	NAP	PN-O5D-C5D	-2.46	107.25	121.68
2	C	401	NAP	PA-O5B-C5B	-2.42	107.48	121.68
2	E	401	NAP	PN-O5D-C5D	-2.39	107.67	121.68
2	E	401	NAP	O3X-P2B-O2X	2.37	116.70	107.64
2	C	401	NAP	O4B-C4B-C3B	2.36	109.79	105.11
2	E	401	NAP	C3B-C2B-C1B	-2.36	98.46	102.89
2	B	401	NAP	O7N-C7N-N7N	-2.34	119.25	122.58
2	C	401	NAP	O2N-PN-O1N	2.32	123.71	112.24
2	B	401	NAP	O2N-PN-O1N	2.32	123.69	112.24
2	F	401	NAP	O5D-PN-O1N	-2.29	100.12	109.07
2	F	401	NAP	C2A-N1A-C6A	-2.25	114.91	118.75
2	F	401	NAP	PA-O5B-C5B	-2.25	108.51	121.68
2	F	401	NAP	O4B-C4B-C3B	2.23	109.52	105.11
2	B	401	NAP	O4B-C4B-C3B	2.19	109.45	105.11
2	E	401	NAP	O2N-PN-O5D	-2.19	97.59	107.75
2	E	401	NAP	O4B-C4B-C3B	2.18	109.42	105.11
2	A	401	NAP	O2N-PN-O1N	2.13	122.80	112.24
2	C	401	NAP	C6N-N1N-C2N	-2.13	120.03	121.97
2	B	401	NAP	O3X-P2B-O2B	-2.11	96.53	105.99
2	A	401	NAP	O5D-PN-O1N	-2.09	100.89	109.07
2	E	401	NAP	O5D-PN-O1N	-2.08	100.93	109.07
2	F	401	NAP	C6N-N1N-C2N	-2.07	120.09	121.97
2	C	401	NAP	C2A-N1A-C6A	-2.06	115.23	118.75
2	A	401	NAP	O2N-PN-O5D	-2.03	98.33	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	NAP	O5D-PN-O1N	-2.02	101.17	109.07
2	B	401	NAP	C2N-N1N-C1D	2.01	123.62	119.14
2	B	401	NAP	C6N-C5N-C4N	2.01	122.36	119.44

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	NAP	C5D-O5D-PN-O3
2	B	401	NAP	O4D-C4D-C5D-O5D
2	B	401	NAP	C3D-C4D-C5D-O5D
2	E	401	NAP	O4D-C4D-C5D-O5D
2	A	401	NAP	O4D-C4D-C5D-O5D
2	E	401	NAP	C3D-C4D-C5D-O5D
2	C	401	NAP	PN-O3-PA-O1A
2	F	401	NAP	PN-O3-PA-O1A
2	B	401	NAP	O4B-C4B-C5B-O5B
2	A	401	NAP	O4B-C4B-C5B-O5B
2	B	401	NAP	C5D-O5D-PN-O1N
2	B	401	NAP	C5D-O5D-PN-O2N
2	F	401	NAP	O4D-C4D-C5D-O5D
2	B	401	NAP	PN-O3-PA-O2A
2	E	401	NAP	PN-O3-PA-O1A
2	A	401	NAP	PN-O3-PA-O1A
2	A	401	NAP	PN-O3-PA-O2A
2	B	401	NAP	PN-O3-PA-O1A
2	E	401	NAP	PN-O3-PA-O2A
2	F	401	NAP	PN-O3-PA-O2A
2	A	401	NAP	C3D-C4D-C5D-O5D
2	C	401	NAP	O4D-C4D-C5D-O5D
2	C	401	NAP	O4B-C4B-C5B-O5B
2	C	401	NAP	PN-O3-PA-O2A
2	E	401	NAP	O4B-C4B-C5B-O5B
2	F	401	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NAP	2	0
2	A	401	NAP	2	0

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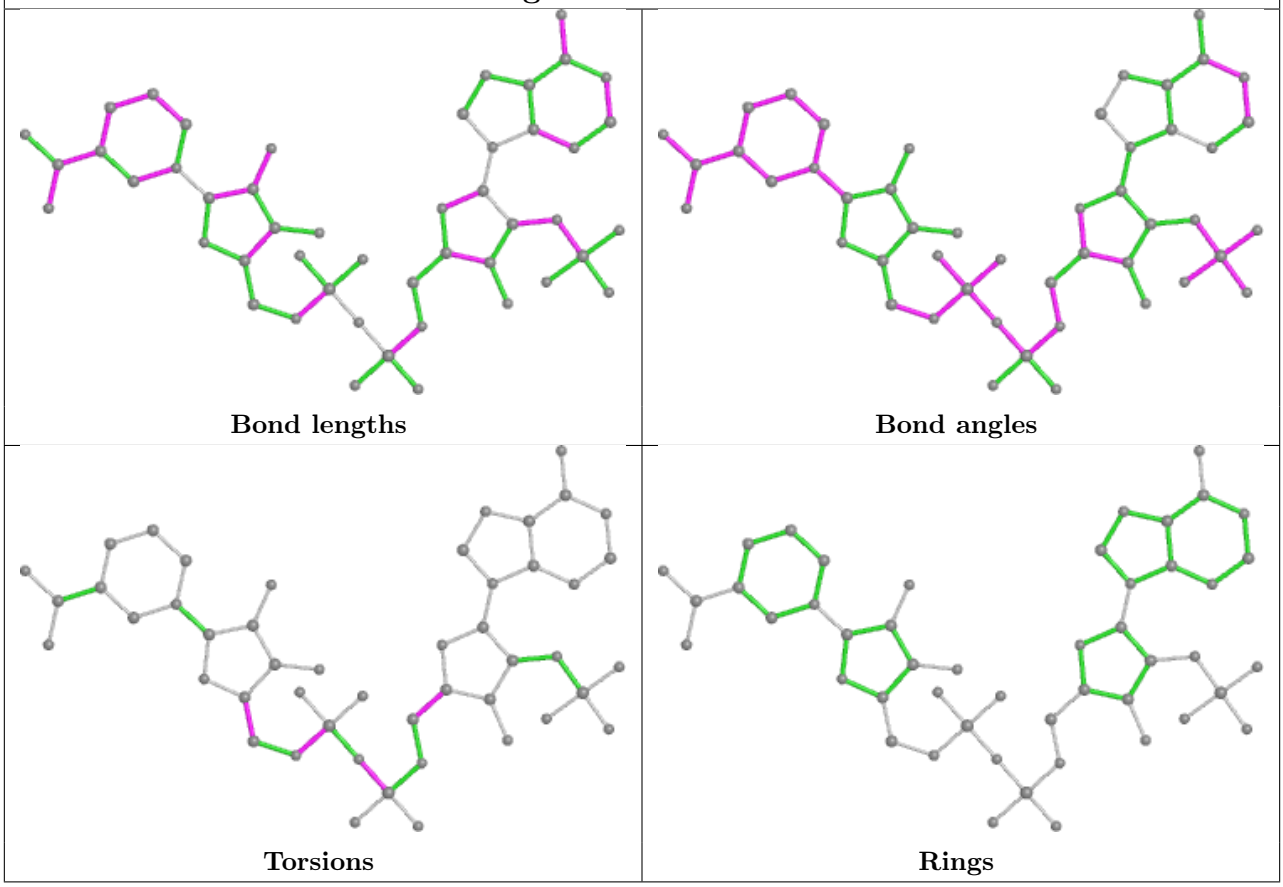
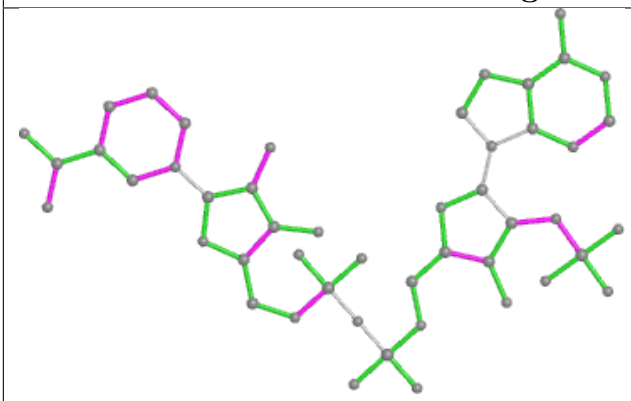
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	NAP	2	0
3	B	402	EDO	1	0
2	E	401	NAP	2	0
2	C	401	NAP	3	0

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.

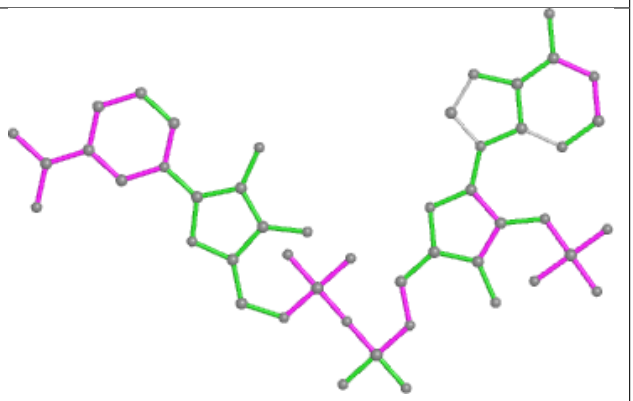
Ligand NAP B 401



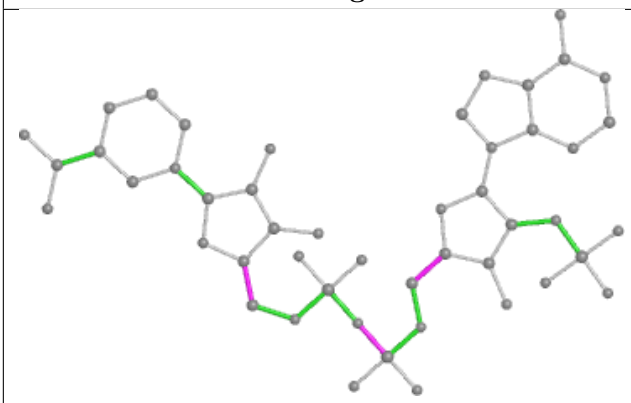
Ligand NAP A 401



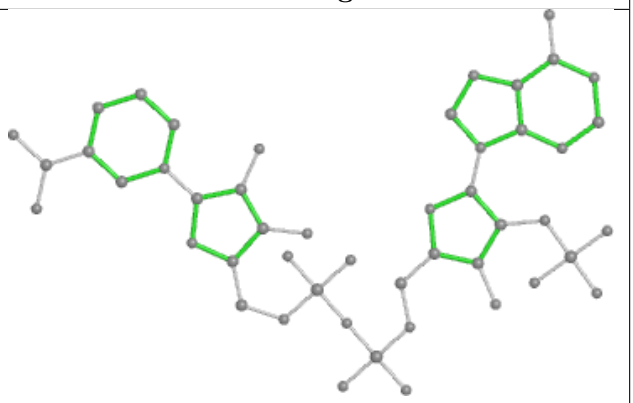
Bond lengths



Bond angles

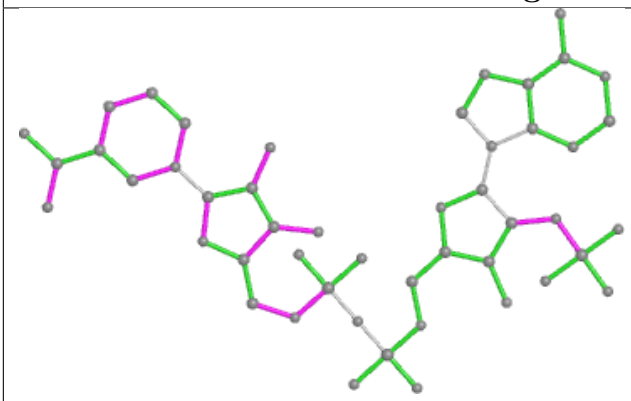


Torsions

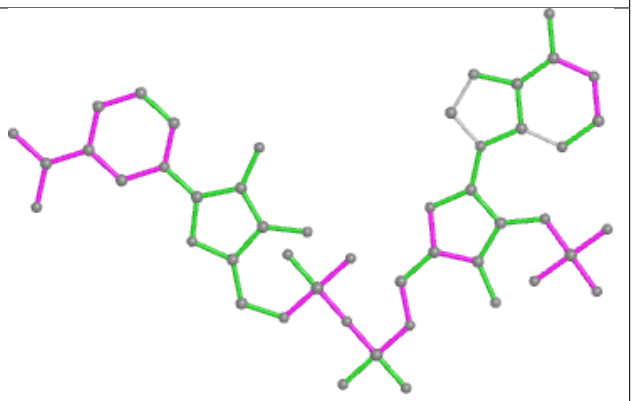


Rings

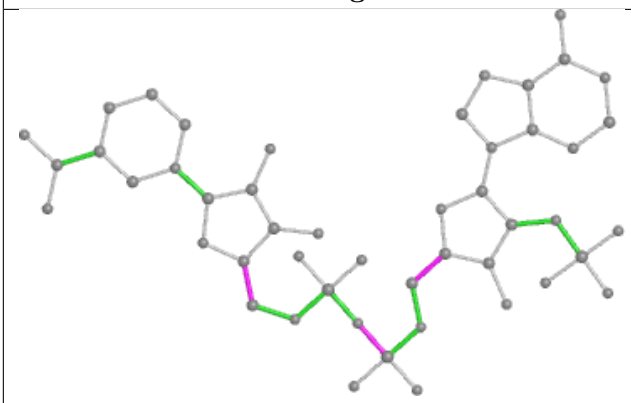
Ligand NAP F 401



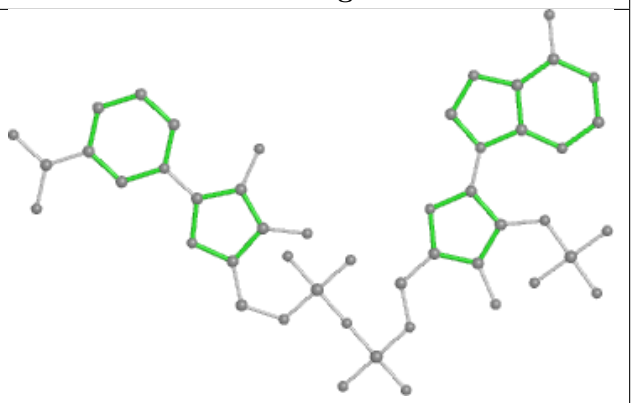
Bond lengths



Bond angles

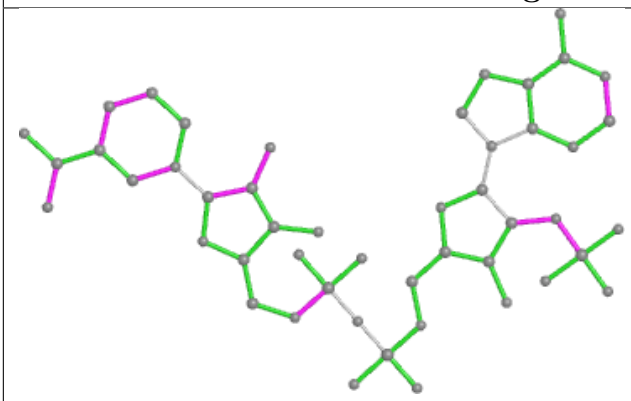


Torsions

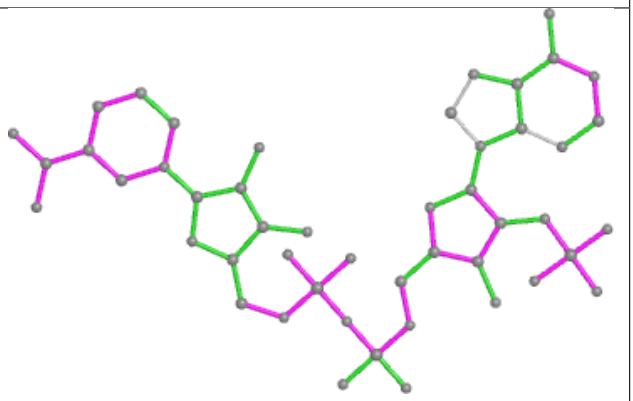


Rings

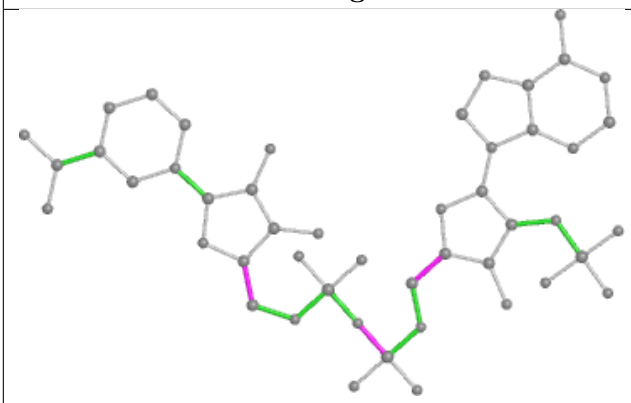
Ligand NAP E 401



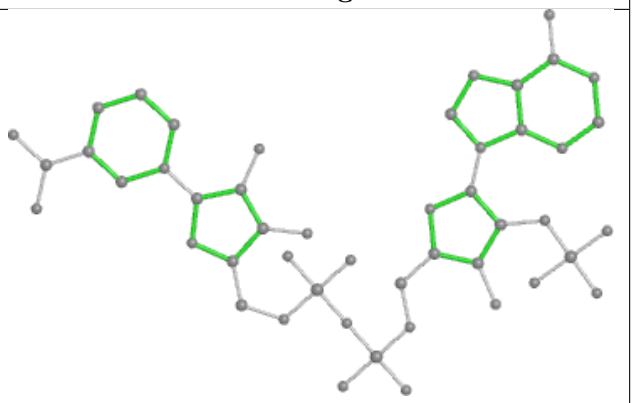
Bond lengths



Bond angles

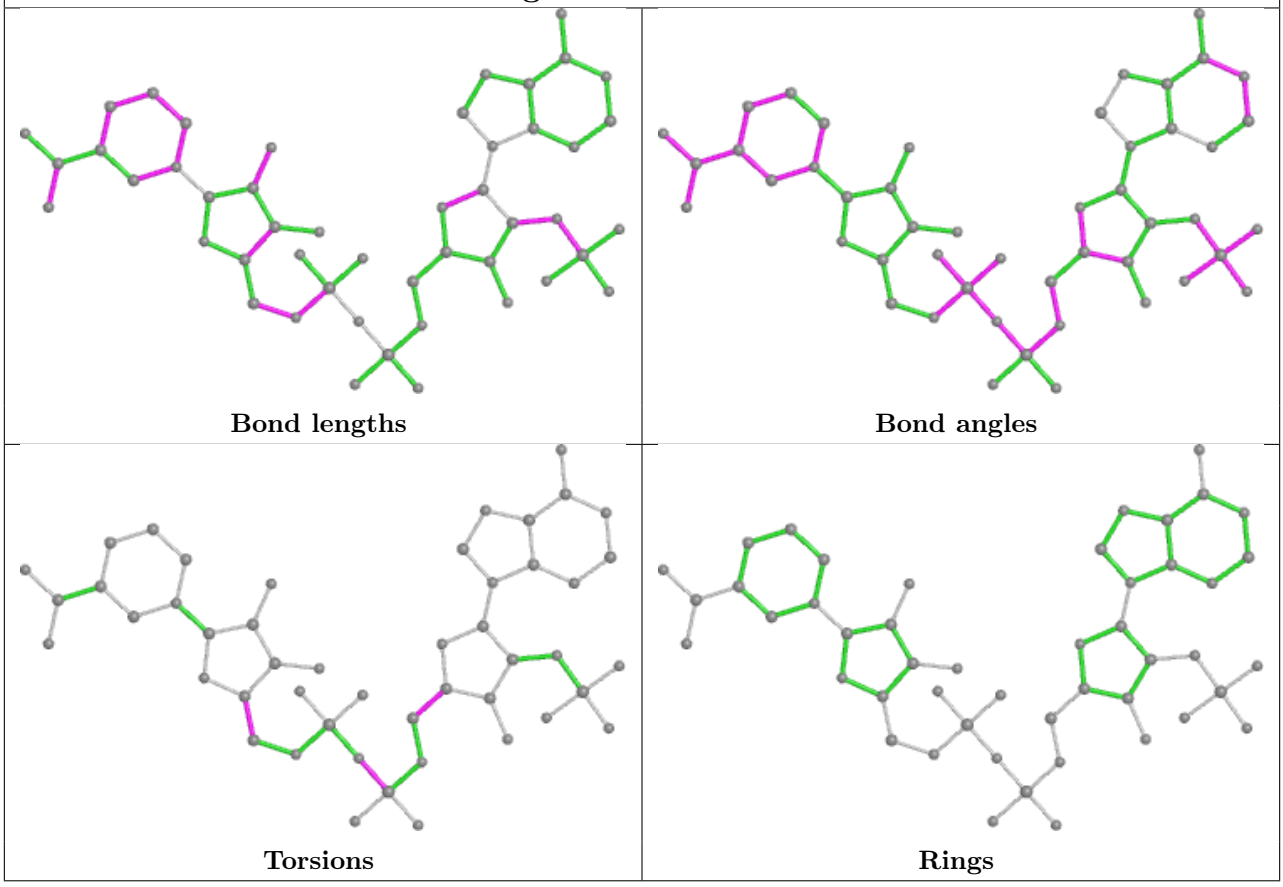


Torsions



Rings

Ligand NAP C 401



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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	334/341 (97%)	-0.27	0 100 100	32, 56, 83, 105	0
1	B	323/341 (94%)	-0.09	5 (1%) 73 72	34, 57, 104, 141	0
1	C	334/341 (97%)	-0.24	0 100 100	38, 55, 86, 112	0
1	D	324/341 (95%)	0.22	17 (5%) 27 26	46, 84, 112, 145	0
1	E	313/341 (91%)	0.38	27 (8%) 10 9	52, 90, 130, 170	0
1	F	321/341 (94%)	-0.31	1 (0%) 94 93	36, 58, 85, 106	0
All	All	1949/2046 (95%)	-0.06	50 (2%) 56 54	32, 65, 108, 170	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	225	PRO	6.1
1	E	226	LEU	5.9
1	E	220	PHE	4.9
1	E	269	GLN	4.8
1	E	265	GLY	3.7
1	D	275	PHE	3.7
1	D	278	THR	3.6
1	D	217	PHE	3.6
1	E	256	VAL	3.5
1	D	280	ASN	3.4
1	F	6	VAL	3.2
1	E	222	SER	3.1
1	D	221	GLY	3.1
1	E	270	THR	3.1
1	E	244	PHE	3.0
1	E	263	SER	3.0
1	E	221	GLY	3.0
1	E	267	VAL	2.9
1	E	255	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	217	PHE	2.8
1	D	281	MET	2.8
1	D	316	ALA	2.7
1	D	18	VAL	2.7
1	D	2	ALA	2.6
1	D	81	GLY	2.6
1	E	299	ALA	2.5
1	D	277	PHE	2.5
1	D	12	THR	2.5
1	E	217	PHE	2.4
1	B	221	GLY	2.4
1	D	267	VAL	2.4
1	E	196	ALA	2.4
1	D	256	VAL	2.4
1	D	186	PHE	2.4
1	D	310	TYR	2.3
1	B	214	GLY	2.3
1	E	243	MET	2.2
1	D	317	ILE	2.2
1	E	129	ILE	2.2
1	E	259	GLU	2.2
1	E	227	ARG	2.2
1	E	16	ASP	2.2
1	E	268	ALA	2.2
1	E	72	TYR	2.2
1	E	298	ASN	2.2
1	E	132	PRO	2.2
1	E	172	GLY	2.2
1	B	275	PHE	2.1
1	B	281	MET	2.0
1	E	131	TYR	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

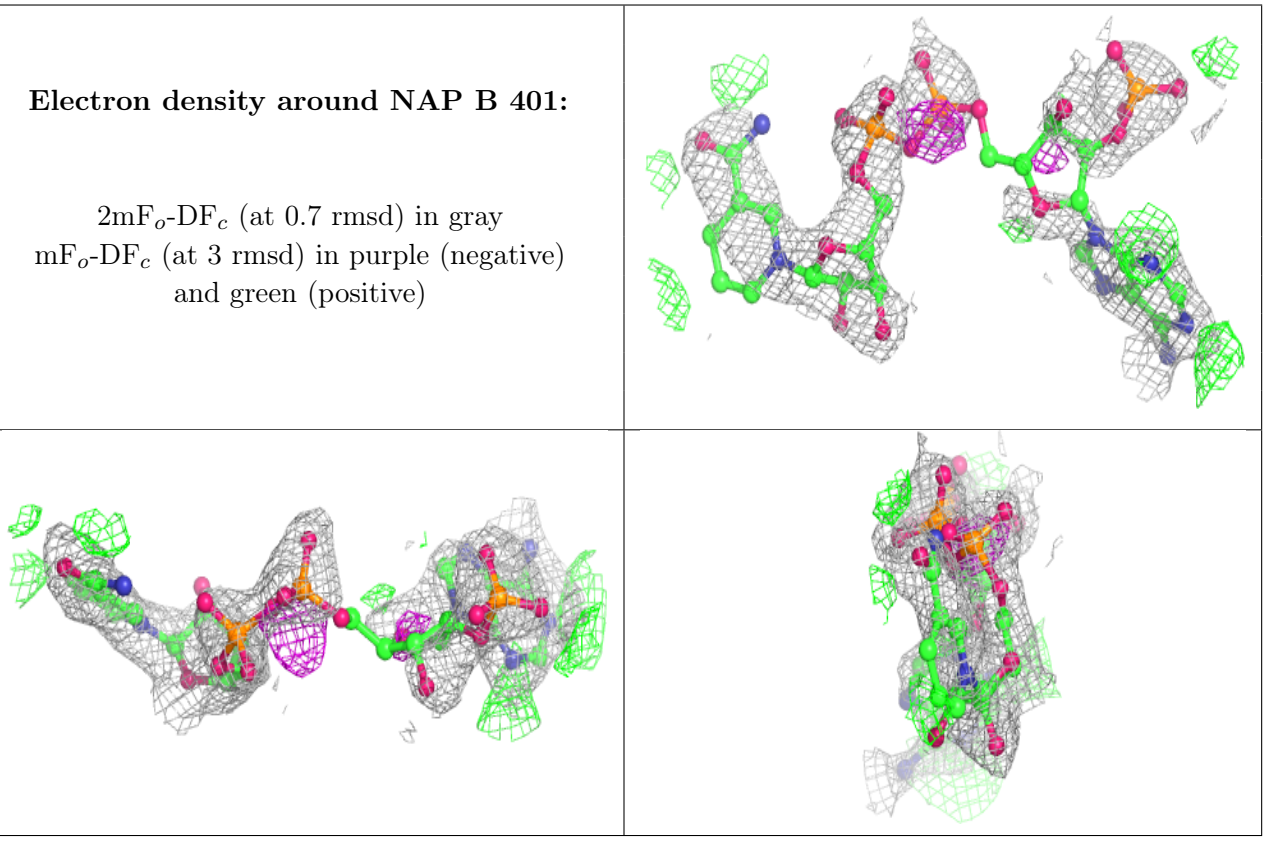
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NAP	B	401	48/48	0.75	0.32	43,74,87,90	48
3	EDO	B	402	4/4	0.92	0.48	81,81,81,81	0
2	NAP	E	401	48/48	0.95	0.13	51,68,81,94	0
2	NAP	A	401	48/48	0.98	0.13	34,46,58,59	0
2	NAP	F	401	48/48	0.98	0.14	39,45,55,67	0
2	NAP	C	401	48/48	0.98	0.14	39,47,57,59	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.

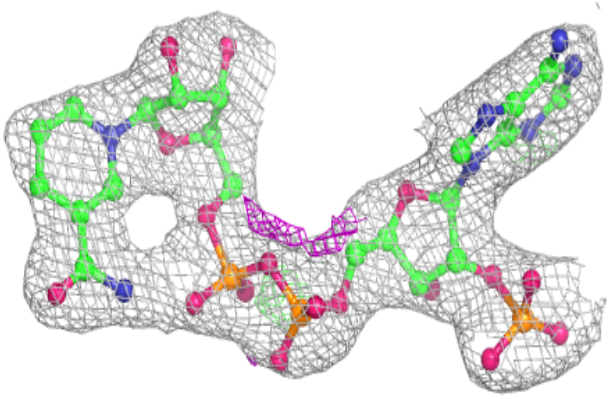
Electron density around NAP B 401:

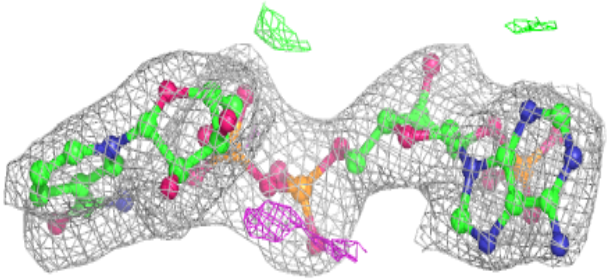
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

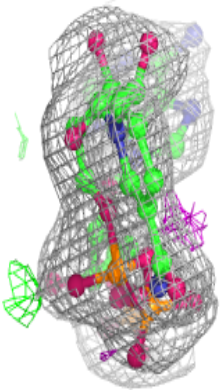


Electron density around NAP E 401:

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

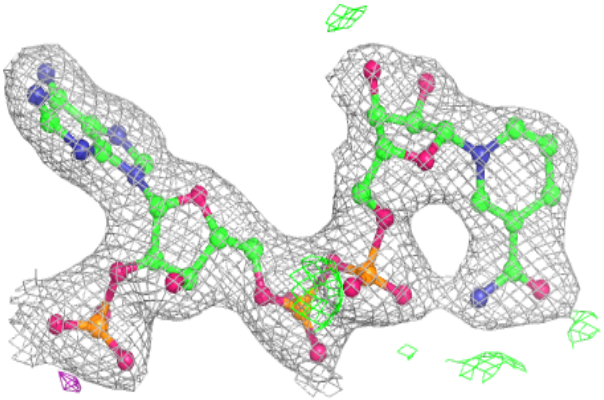


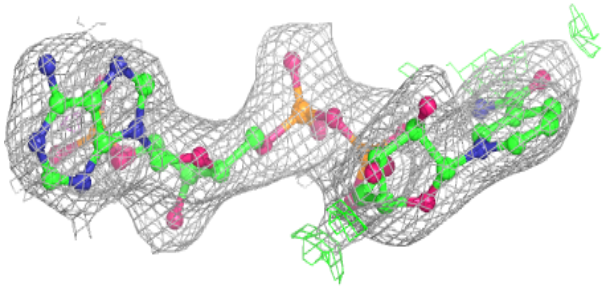


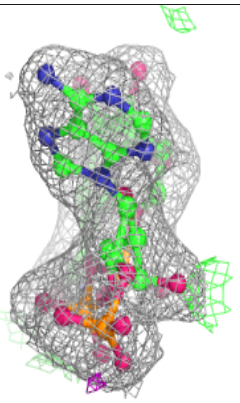


Electron density around NAP A 401:

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

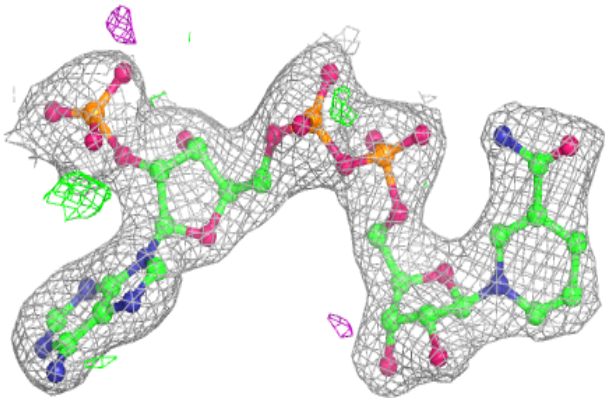


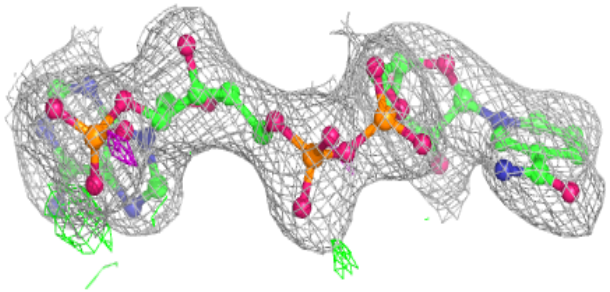


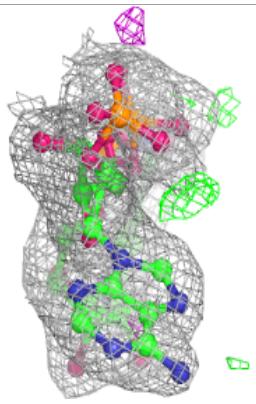


Electron density around NAP F 401:

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

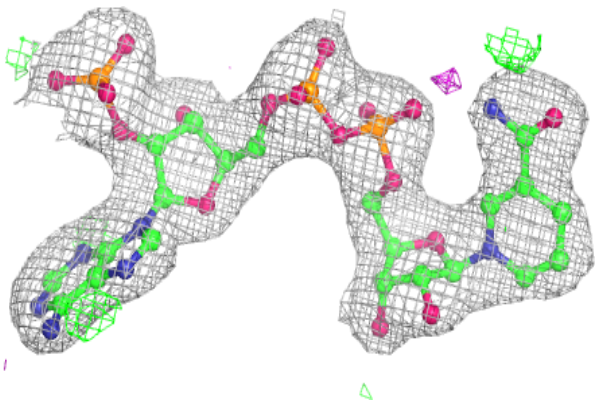


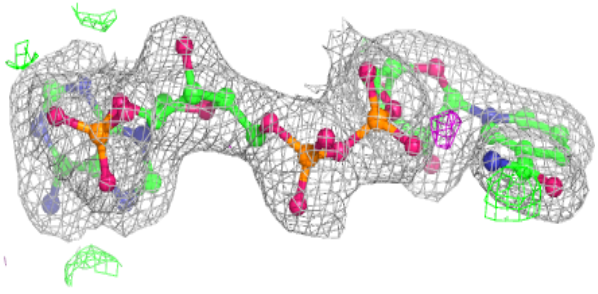


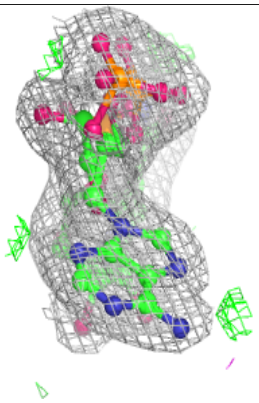


Electron density around NAP C 401:

$2mF_o$-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.