Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 12:46 PM JST

PDB ID	:	8JFI
Title	:	Crystal structure of 3-oxoacyl-ACP reductase FabG in complex with NADP+ and 3-keto-hexanoyl-ACP from Helicobacter pylori
Authors	:	Zhou, J.S.; Zhang, L.
Deposited on	:	2023-05-18
Resolution	:	2.38 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:

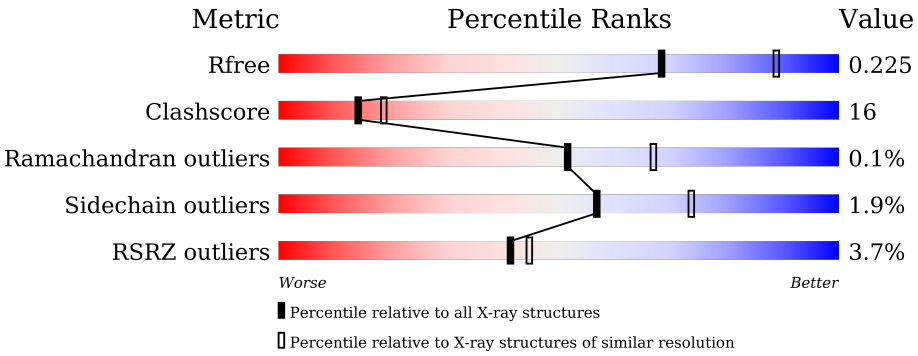
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	248	4% 76% 22% ·
1	B	248	74% 19% · ·
1	C	248	64% 31% 5%
1	D	248	4% 67% 29% ·
1	E	248	3% 65% 29% · ·
1	F	248	8% 58% 35% · 6%

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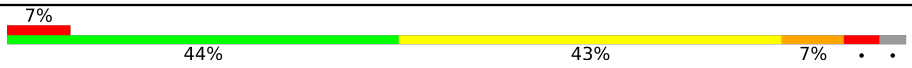
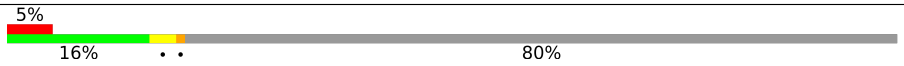
Mol	Chain	Length	Quality of chain
2	G	75	
2	H	75	
2	I	75	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11923 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 3-oxoacyl-[acyl-carrier-protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1875	1179	323	363	10			
1	B	237	Total	C	N	O	S	0	0	0
			1789	1128	309	343	9			
1	C	236	Total	C	N	O	S	0	0	0
			1782	1123	307	343	9			
1	D	237	Total	C	N	O	S	0	0	0
			1787	1126	308	344	9			
1	E	237	Total	C	N	O	S	0	0	0
			1790	1128	308	344	10			
1	F	233	Total	C	N	O	S	0	0	0
			1755	1106	304	336	9			

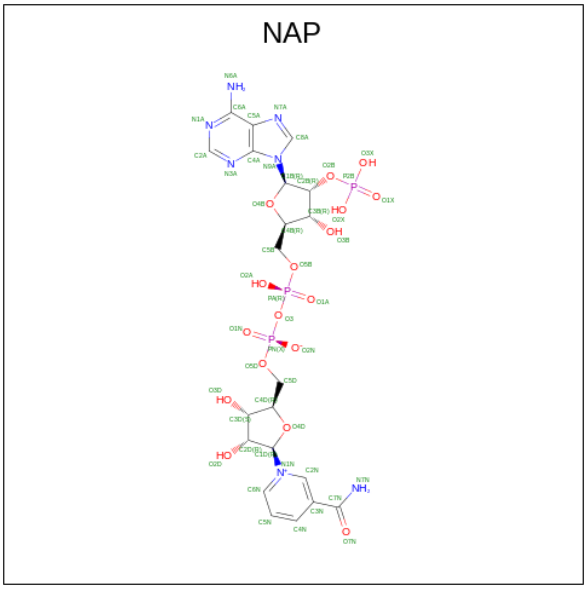
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP G2M827
B	0	SER	-	expression tag	UNP G2M827
C	0	SER	-	expression tag	UNP G2M827
D	0	SER	-	expression tag	UNP G2M827
E	0	SER	-	expression tag	UNP G2M827
F	0	SER	-	expression tag	UNP G2M827

- Molecule 2 is a protein called Acyl carrier protein.

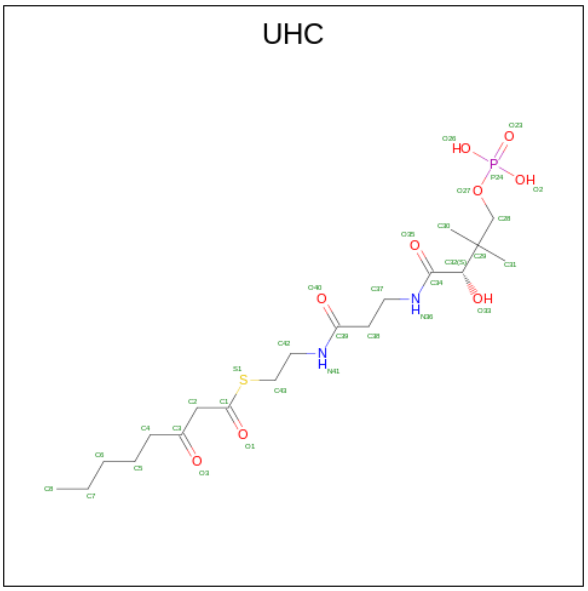
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	73	Total	C	N	O	S	0	0	0
			566	359	85	121	1			
2	H	15	Total	C	N	O	S	0	0	0
			110	71	16	22	1			
2	I	9	Total	C	N	O	S	0	0	0
			68	45	9	13	1			

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is {S}-[2-[3-[[(2 {S})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] 3-oxidanylideneoctanethioate (three-letter code: UHC) (formula: $C_{19}H_{35}N_2O_9PS$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 29 17 2 8 1 1	0	0

- Molecule 5 is water.

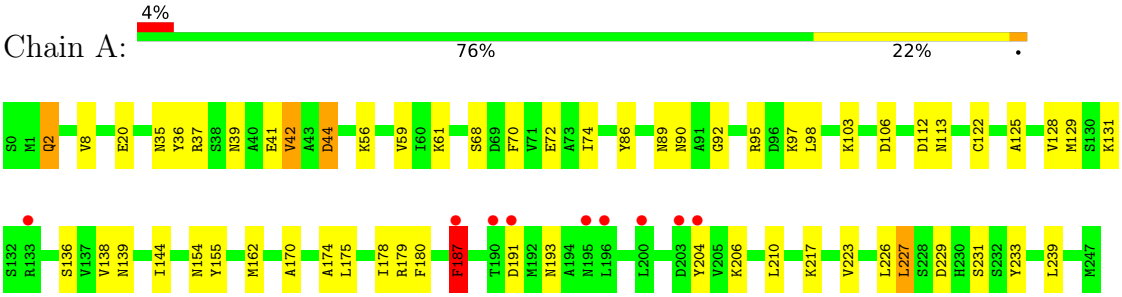
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	23	Total O 23 23	0	0
5	B	21	Total O 21 21	0	0
5	C	7	Total O 7 7	0	0
5	D	9	Total O 9 9	0	0
5	E	10	Total O 10 10	0	0
5	F	11	Total O 11 11	0	0
5	G	3	Total O 3 3	0	0

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.

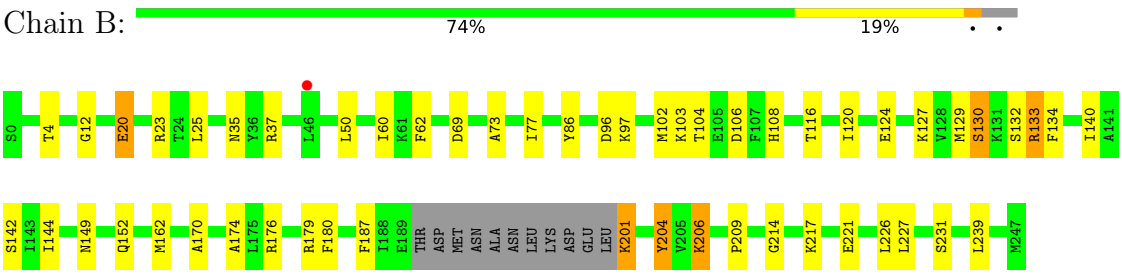
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

Chain A:



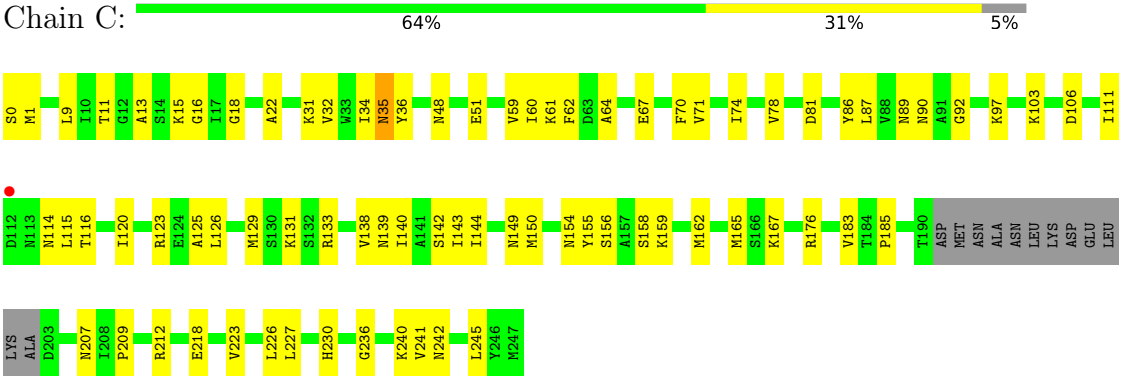
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

Chain B:



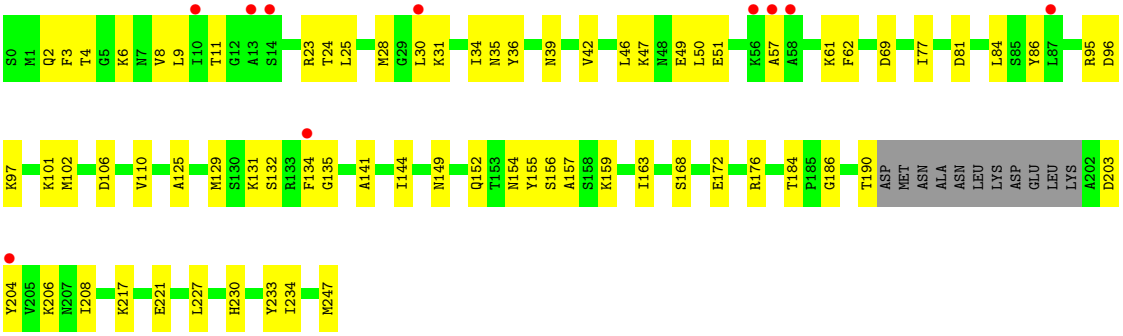
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

Chain C:



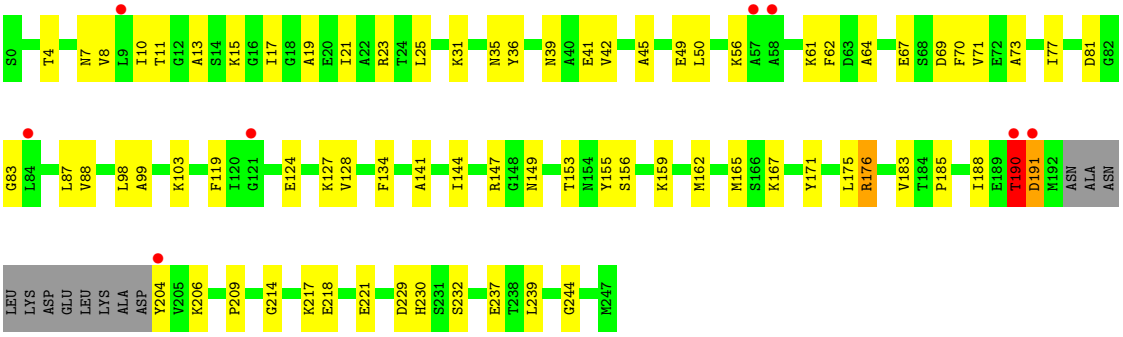
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

Chain D:



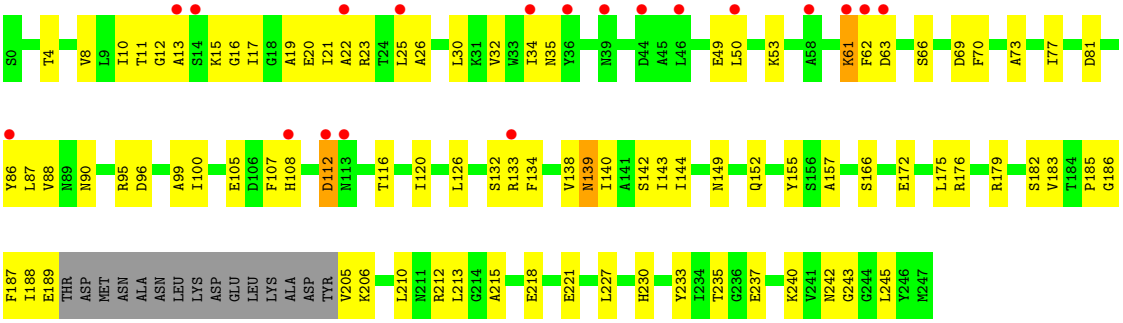
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

Chain E:



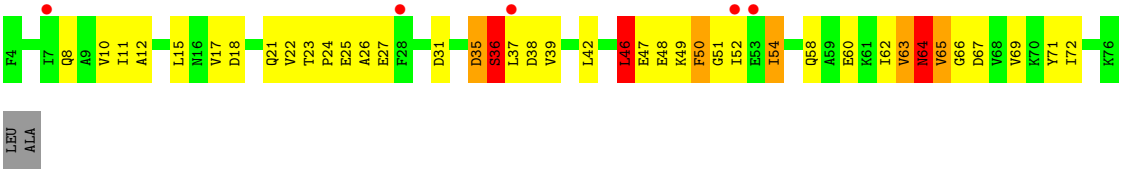
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

Chain F:



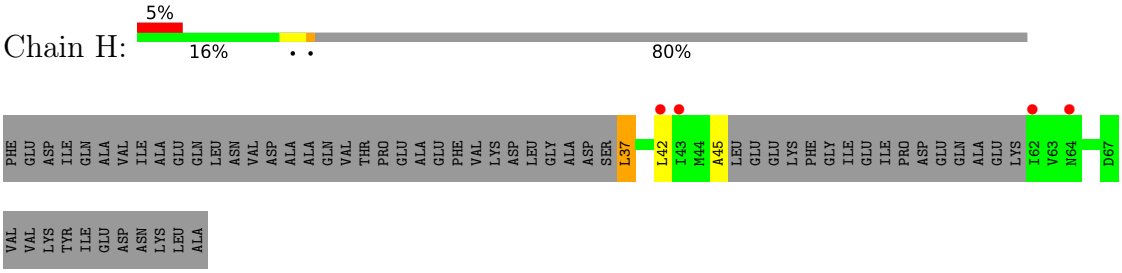
• Molecule 2: Acyl carrier protein

Chain G:



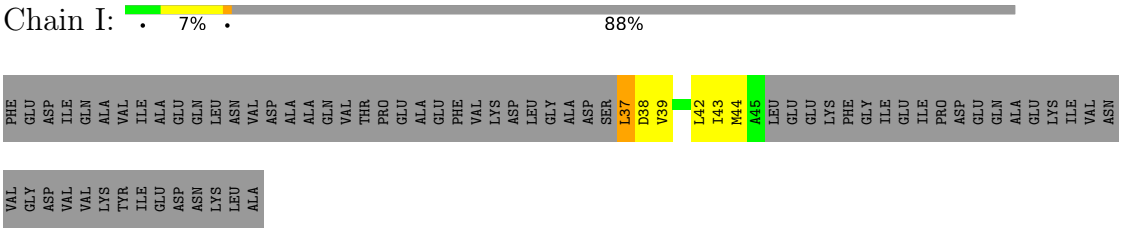
• Molecule 2: Acyl carrier protein

Chain H:



• Molecule 2: Acyl carrier protein

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	85.84Å 252.65Å 166.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.16 – 2.38 126.33 – 2.38	Depositor EDS
% Data completeness (in resolution range)	55.4 (63.16-2.38) 55.4 (126.33-2.38)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.206 , 0.225 0.206 , 0.225	Depositor DCC
R_{free} test set	2022 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	48.7	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11923	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: UHC, 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	0.64	2/1899 (0.1%)	0.78	5/2553 (0.2%)
1	B	0.74	6/1812 (0.3%)	0.76	1/2434 (0.0%)
1	C	0.64	3/1805 (0.2%)	0.67	0/2426
1	D	0.46	0/1810	0.67	1/2433 (0.0%)
1	E	0.55	1/1813 (0.1%)	0.73	4/2436 (0.2%)
1	F	0.76	6/1777 (0.3%)	0.84	4/2387 (0.2%)
2	G	1.22	5/571 (0.9%)	1.13	1/774 (0.1%)
2	H	0.37	0/108	1.05	1/145 (0.7%)
2	I	0.64	0/67	1.09	0/90
All	All	0.68	23/11662 (0.2%)	0.77	17/15678 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
2	G	0	2
All	All	0	4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	36	SER	CA-CB	-10.37	1.37	1.52
1	F	138	VAL	C-O	-8.03	1.08	1.23
1	F	183	VAL	C-O	-7.58	1.08	1.23
1	F	185	PRO	C-O	-7.37	1.08	1.23
1	B	130	SER	CA-CB	-7.20	1.42	1.52
2	G	60	GLU	CD-OE1	-7.04	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	41	GLU	CD-OE2	6.70	1.33	1.25
2	G	47	GLU	CD-OE1	-6.54	1.18	1.25
1	A	42	VAL	C-O	-6.37	1.11	1.23
1	B	129	MET	C-O	-6.26	1.11	1.23
1	C	138	VAL	C-O	-6.07	1.11	1.23
2	G	47	GLU	CD-OE2	-6.06	1.19	1.25
1	B	209	PRO	C-O	-6.02	1.11	1.23
1	C	142	SER	C-O	-5.97	1.12	1.23
2	G	36	SER	CB-OG	-5.87	1.34	1.42
1	B	133	ARG	C-O	-5.55	1.12	1.23
1	A	44	ASP	C-O	-5.37	1.13	1.23
1	F	182	SER	C-O	-5.28	1.13	1.23
1	F	140	ILE	C-O	-5.26	1.13	1.23
1	C	142	SER	CB-OG	-5.21	1.35	1.42
1	B	20	GLU	CG-CD	5.16	1.59	1.51
1	B	206	LYS	C-O	-5.11	1.13	1.23
1	F	139	ASN	C-O	-5.00	1.13	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	175	LEU	CB-CG-CD2	-13.59	87.90	111.00
1	F	175	LEU	CB-CG-CD1	9.23	126.70	111.00
1	A	37	ARG	CG-CD-NE	9.09	130.88	111.80
2	H	37	LEU	CB-CG-CD2	-8.13	97.18	111.00
1	E	41	GLU	CA-CB-CG	8.03	131.06	113.40
1	A	187	PHE	CB-CG-CD2	-7.42	115.61	120.80
1	D	176	ARG	NE-CZ-NH1	-6.27	117.16	120.30
1	E	103	LYS	CD-CE-NZ	-6.26	97.31	111.70
1	A	227	LEU	CA-CB-CG	6.21	129.57	115.30
1	F	187	PHE	CB-CA-C	6.18	122.75	110.40
2	G	51	GLY	N-CA-C	-5.96	98.20	113.10
1	E	190	THR	N-CA-CB	-5.76	99.35	110.30
1	B	204	TYR	CB-CA-C	-5.68	99.03	110.40
1	E	176	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	F	112	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	A	112	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	A	56	LYS	CA-CB-CG	5.08	124.58	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	PHE	Sidechain
1	F	142	SER	Mainchain
2	G	46	LEU	Mainchain
2	G	64	ASN	Mainchain

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	1875	0	1894	43	0
1	B	1789	0	1811	38	1
1	C	1782	0	1800	72	0
1	D	1787	0	1805	56	0
1	E	1790	0	1808	59	0
1	F	1755	0	1780	78	0
2	G	566	0	553	34	1
2	H	110	0	115	3	0
2	I	68	0	74	18	0
3	A	48	0	24	6	0
3	B	48	0	24	5	0
3	C	48	0	24	5	0
3	D	48	0	24	3	0
3	E	48	0	23	3	0
3	F	48	0	24	1	0
4	A	29	0	0	3	0
5	A	23	0	0	2	0
5	B	21	0	0	2	0
5	C	7	0	0	0	0
5	D	9	0	0	3	0
5	E	10	0	0	2	0
5	F	11	0	0	1	0
5	G	3	0	0	0	0
All	All	11923	0	11783	369	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (369) 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)
4:A:302:UHC:P24	2:G:36:SER:OG	1.97	1.23
1:B:201:LYS:HD2	5:B:403:HOH:O	0.99	1.15
1:C:176:ARG:NH2	2:I:37:LEU:HD12	1.65	1.10
1:C:176:ARG:CZ	2:I:37:LEU:HD12	1.87	1.05
1:C:176:ARG:NH1	2:I:37:LEU:HD12	1.73	1.04
1:C:176:ARG:HH22	2:I:37:LEU:HD12	1.22	1.03
1:C:133:ARG:HG2	1:C:176:ARG:HD2	1.40	1.00
1:F:105:GLU:HA	1:F:108:HIS:HD2	1.28	0.97
2:I:38:ASP:O	2:I:42:LEU:HD13	1.64	0.96
1:F:15:LYS:HA	1:F:19:ALA:HB2	1.49	0.95
1:C:176:ARG:NH2	2:I:37:LEU:CD1	2.29	0.94
1:C:176:ARG:HH22	2:I:37:LEU:CD1	1.85	0.89
1:C:176:ARG:NH1	2:I:37:LEU:CD1	2.36	0.89
1:C:176:ARG:HH12	2:I:37:LEU:HD12	1.32	0.89
1:E:7:ASN:ND2	1:E:83:GLY:O	2.10	0.84
1:C:176:ARG:CZ	2:I:37:LEU:CD1	2.54	0.84
1:E:176:ARG:HH12	2:H:37:LEU:HD21	1.42	0.83
1:F:105:GLU:HA	1:F:108:HIS:CD2	2.13	0.83
2:G:25:GLU:OE1	2:G:64:ASN:ND2	2.11	0.83
1:A:179:ARG:NH1	1:A:231:SER:O	2.12	0.83
1:E:176:ARG:NH1	2:H:37:LEU:HD21	1.96	0.81
1:F:12:GLY:H	1:F:35:ASN:HD22	1.27	0.80
1:C:176:ARG:HH12	2:I:37:LEU:CD1	1.94	0.79
1:F:17:ILE:HD11	1:F:188:ILE:HG21	1.65	0.77
1:E:191:ASP:OD1	1:E:191:ASP:N	2.18	0.77
1:E:229:ASP:O	1:E:232:SER:OG	2.03	0.76
1:F:86:TYR:HB3	1:F:227:LEU:HD22	1.69	0.75
1:E:230:HIS:HB3	1:F:221:GLU:HB3	1.69	0.75
1:D:190:THR:HB	3:D:301:NAP:H72N	1.51	0.74
1:E:221:GLU:OE1	1:F:230:HIS:ND1	2.16	0.74
3:C:301:NAP:N7N	3:C:301:NAP:O1N	2.20	0.74
1:E:218:GLU:OE1	1:F:233:TYR:HB2	1.90	0.72
1:B:37:ARG:HH12	3:B:301:NAP:P2B	2.13	0.72
1:A:36:TYR:HE1	1:A:61:LYS:HD2	1.55	0.72
1:C:67:GLU:OE2	1:C:123:ARG:NH2	2.20	0.70
1:E:45:ALA:O	1:E:49:GLU:HG2	1.90	0.70
1:A:128:VAL:O	5:A:401:HOH:O	2.10	0.69
2:G:62:ILE:HD13	2:G:67:ASP:HB2	1.75	0.69
1:F:144:ILE:HD12	1:F:149:ASN:HB2	1.75	0.68
2:G:36:SER:O	2:G:37:LEU:C	2.32	0.68
1:E:39:ASN:N	1:E:39:ASN:OD1	2.26	0.68
1:A:68:SER:O	1:A:72:GLU:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:64:ASN:ND2	2:G:64:ASN:O	2.27	0.68
1:A:191:ASP:HB3	3:A:301:NAP:O1A	1.93	0.67
1:F:8:VAL:HG13	1:F:10:ILE:HD11	1.74	0.67
1:F:144:ILE:HG21	1:F:155:TYR:HD2	1.58	0.67
1:C:242:ASN:OD1	1:C:245:LEU:N	2.28	0.67
1:E:73:ALA:O	1:E:77:ILE:HD12	1.95	0.67
1:D:141:ALA:HB3	1:D:184:THR:HG22	1.78	0.66
2:G:48:GLU:HG3	2:G:48:GLU:O	1.95	0.66
1:B:62:PHE:HB2	1:B:69:ASP:HB3	1.77	0.66
1:D:102:MET:HE1	1:D:154:ASN:HB3	1.79	0.65
1:B:144:ILE:HD12	1:B:149:ASN:HB2	1.78	0.64
1:E:36:TYR:CE2	1:E:61:LYS:HE3	2.32	0.64
2:G:66:GLY:O	2:G:69:VAL:HG22	1.98	0.64
1:F:12:GLY:H	1:F:35:ASN:ND2	1.95	0.64
1:B:217:LYS:O	1:B:221:GLU:HG3	1.97	0.64
2:G:12:ALA:HB1	2:G:17:VAL:O	1.97	0.64
1:F:15:LYS:CA	1:F:19:ALA:HB2	2.26	0.64
1:F:108:HIS:O	1:F:112:ASP:HB2	1.97	0.64
1:F:20:GLU:O	1:F:23:ARG:N	2.32	0.63
2:I:39:VAL:O	2:I:43:ILE:HG12	1.99	0.62
1:A:89:ASN:HD22	1:A:139:ASN:HD21	1.48	0.62
1:E:209:PRO:HG2	1:E:244:GLY:HA3	1.81	0.62
1:D:8:VAL:HG11	1:D:25:LEU:HD23	1.81	0.62
1:A:36:TYR:CE1	1:A:61:LYS:HD2	2.35	0.61
1:F:149:ASN:ND2	1:F:152:GLN:OE1	2.27	0.61
4:A:302:UHC:P24	2:G:36:SER:CB	2.87	0.61
1:B:73:ALA:O	1:B:77:ILE:HD12	2.01	0.61
1:E:124:GLU:O	1:E:128:VAL:HG12	2.01	0.61
2:G:36:SER:O	2:G:39:VAL:N	2.31	0.61
1:A:90:ASN:ND2	3:A:301:NAP:H4D	2.15	0.60
1:C:241:VAL:HG12	1:D:233:TYR:HD2	1.66	0.60
1:F:139:ASN:HD22	1:F:166:SER:HB2	1.66	0.60
1:F:112:ASP:O	1:F:116:THR:HB	2.02	0.60
1:D:204:TYR:O	1:D:208:ILE:HG13	2.01	0.60
1:D:46:LEU:O	1:D:49:GLU:HG2	2.01	0.60
1:D:203:ASP:HA	1:D:206:LYS:NZ	2.16	0.60
1:C:144:ILE:HG22	1:C:156:SER:HB3	1.83	0.59
1:A:206:LYS:NZ	5:A:402:HOH:O	2.28	0.59
1:D:155:TYR:CE1	1:D:159:LYS:HE2	2.37	0.59
1:A:89:ASN:HD22	1:A:139:ASN:ND2	2.00	0.59
1:F:95:ARG:NH1	5:F:401:HOH:O	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ARG:NH2	1:C:218:GLU:OE2	2.31	0.59
1:A:97:LYS:NZ	1:A:106:ASP:OD2	2.26	0.59
2:G:10:VAL:HG11	2:G:46:LEU:HD11	1.84	0.58
2:G:49:LYS:O	2:G:49:LYS:HG2	2.03	0.58
1:E:23:ARG:HG3	1:E:50:LEU:HD21	1.84	0.58
1:F:63:ASP:HB3	1:F:66:SER:OG	2.04	0.58
2:G:36:SER:C	2:G:38:ASP:N	2.52	0.58
1:E:64:ALA:HA	1:E:70:PHE:HD2	1.69	0.58
1:B:60:ILE:HD13	1:B:77:ILE:HD11	1.85	0.57
2:G:11:ILE:HD11	2:G:22:VAL:HG22	1.86	0.57
1:D:36:TYR:CZ	1:D:61:LYS:HB2	2.39	0.57
2:G:11:ILE:HG22	2:G:42:LEU:HD11	1.86	0.57
1:C:133:ARG:HG2	1:C:176:ARG:CD	2.25	0.57
1:C:64:ALA:HA	1:C:70:PHE:HD2	1.70	0.56
1:D:31:LYS:NZ	1:D:81:ASP:OD1	2.37	0.56
1:D:190:THR:HB	3:D:301:NAP:N7N	2.20	0.56
1:E:8:VAL:HG21	1:E:25:LEU:HD13	1.87	0.56
1:F:25:LEU:O	1:F:30:LEU:HB2	2.05	0.56
3:B:301:NAP:H52A	3:B:301:NAP:H52N	1.87	0.56
1:B:187:PHE:CE2	1:B:204:TYR:HD2	2.24	0.56
1:E:144:ILE:HD12	1:E:149:ASN:HB2	1.88	0.56
1:D:131:LYS:HG3	1:D:132:SER:N	2.20	0.56
1:E:39:ASN:HD22	1:E:42:VAL:CG2	2.19	0.56
1:D:42:VAL:HG23	5:D:408:HOH:O	2.06	0.55
1:A:20:GLU:OE1	1:A:217:LYS:HE3	2.05	0.55
2:G:10:VAL:HG11	2:G:46:LEU:CD1	2.36	0.55
1:B:37:ARG:NH1	3:B:301:NAP:O1X	2.38	0.55
1:A:144:ILE:HD11	1:A:155:TYR:HD2	1.70	0.55
1:D:34:ILE:HD13	1:D:46:LEU:HD23	1.88	0.55
2:I:38:ASP:O	2:I:42:LEU:CD1	2.48	0.55
1:C:35:ASN:ND2	1:C:62:PHE:CZ	2.74	0.55
1:C:90:ASN:OD1	3:C:301:NAP:H4D	2.06	0.55
1:F:189:GLU:OE1	1:F:215:ALA:HA	2.06	0.55
1:F:16:GLY:O	1:F:19:ALA:HB3	2.06	0.55
1:C:15:LYS:NZ	3:C:301:NAP:H3B	2.22	0.55
1:F:20:GLU:OE1	1:F:21:ILE:N	2.39	0.55
2:G:54:ILE:HG13	2:G:54:ILE:O	2.06	0.55
1:C:0:SER:O	1:C:1:MET:HG3	2.07	0.54
1:C:86:TYR:HB3	1:C:227:LEU:HD22	1.89	0.54
1:E:237:GLU:OE1	1:F:240:LYS:HE3	2.05	0.54
1:F:210:LEU:HD12	1:F:243:GLY:HA2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:58:GLN:HG3	2:G:71:TYR:CD1	2.42	0.54
1:F:35:ASN:HD21	3:F:301:NAP:H2A	1.72	0.54
2:G:50:PHE:HD1	2:G:50:PHE:O	1.90	0.54
1:C:165:MET:HB2	1:F:157:ALA:HB2	1.89	0.54
1:F:143:ILE:CG2	1:F:186:GLY:HA2	2.37	0.54
1:B:96:ASP:O	1:B:97:LYS:HG3	2.08	0.54
2:G:8:GLN:HG3	2:G:22:VAL:HB	1.89	0.54
1:D:141:ALA:O	3:D:301:NAP:H6N	2.08	0.53
1:B:187:PHE:CE2	1:B:204:TYR:CD2	2.97	0.53
1:B:174:ALA:C	1:B:176:ARG:H	2.11	0.53
1:F:22:ALA:O	1:F:32:VAL:HG11	2.08	0.53
1:C:150:MET:HG3	1:F:172:GLU:HG2	1.91	0.53
1:D:217:LYS:O	1:D:221:GLU:HG3	2.09	0.53
2:G:36:SER:O	2:G:38:ASP:N	2.42	0.53
1:F:73:ALA:O	1:F:77:ILE:HD12	2.09	0.52
1:C:11:THR:O	1:C:90:ASN:HB3	2.10	0.52
1:C:144:ILE:HD12	1:C:149:ASN:HB2	1.90	0.52
1:D:110:VAL:HG21	1:D:154:ASN:ND2	2.24	0.52
1:B:4:THR:HB	1:B:134:PHE:CZ	2.45	0.52
1:B:142:SER:HB2	3:B:301:NAP:H5N	1.90	0.52
1:D:47:LYS:O	1:D:51:GLU:HG2	2.09	0.52
1:D:101:LYS:O	1:D:101:LYS:HG2	2.10	0.52
1:A:2:GLN:OE1	1:A:229:ASP:OD2	2.27	0.52
1:F:143:ILE:HG21	1:F:186:GLY:HA2	1.92	0.52
1:F:23:ARG:HA	1:F:50:LEU:HD21	1.92	0.51
1:B:124:GLU:OE1	1:B:127:LYS:HD2	2.09	0.51
1:C:176:ARG:NH2	2:I:37:LEU:HD13	2.21	0.51
1:D:168:SER:O	1:D:172:GLU:HG3	2.10	0.51
1:F:20:GLU:HA	1:F:23:ARG:HE	1.74	0.51
1:C:176:ARG:NH1	2:I:37:LEU:HD11	2.21	0.51
1:B:103:LYS:O	1:B:106:ASP:N	2.43	0.51
1:F:21:ILE:O	1:F:25:LEU:HD23	2.10	0.51
1:A:35:ASN:OD1	1:A:36:TYR:N	2.44	0.51
3:A:301:NAP:H51N	3:A:301:NAP:H52A	1.91	0.51
1:B:201:LYS:C	1:B:201:LYS:HD3	2.31	0.51
1:C:116:THR:O	1:C:120:ILE:HG12	2.11	0.51
1:D:3:PHE:HE2	1:D:28:MET:HB3	1.76	0.51
1:E:4:THR:HB	1:E:134:PHE:CZ	2.46	0.51
1:A:187:PHE:HD2	1:A:204:TYR:CD2	2.29	0.51
1:B:201:LYS:CD	5:B:403:HOH:O	1.87	0.51
1:E:31:LYS:NZ	1:E:81:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:TYR:HB3	1:D:227:LEU:HD22	1.93	0.50
1:D:4:THR:HB	1:D:134:PHE:CZ	2.47	0.50
1:C:115:LEU:CD2	1:F:107:PHE:HZ	2.24	0.50
1:A:125:ALA:HB1	1:A:129:MET:CE	2.41	0.50
1:C:35:ASN:OD1	1:C:35:ASN:C	2.50	0.50
1:E:144:ILE:HG22	1:E:156:SER:HB3	1.93	0.50
1:E:39:ASN:ND2	1:E:42:VAL:HB	2.27	0.50
1:F:12:GLY:N	1:F:35:ASN:HD22	2.03	0.49
2:G:24:PRO:O	2:G:65:VAL:HG13	2.12	0.49
1:C:115:LEU:HD22	1:F:107:PHE:CZ	2.47	0.49
1:D:47:LYS:HG2	1:D:57:ALA:CB	2.41	0.49
1:F:116:THR:O	1:F:120:ILE:HG13	2.12	0.49
1:D:62:PHE:HB2	1:D:69:ASP:HB3	1.94	0.49
1:B:104:THR:HG22	1:B:108:HIS:CD2	2.47	0.49
1:C:236:GLY:HA3	1:D:247:MET:HE2	1.94	0.49
1:F:10:ILE:HG12	1:F:21:ILE:HG22	1.95	0.49
1:B:179:ARG:NH1	1:B:231:SER:O	2.46	0.49
1:E:141:ALA:O	3:E:301:NAP:H6N	2.13	0.49
1:F:62:PHE:CE2	1:F:70:PHE:CD1	3.01	0.48
1:A:179:ARG:NH2	1:A:226:LEU:O	2.47	0.48
1:E:147:ARG:NH2	5:E:401:HOH:O	2.36	0.48
1:B:86:TYR:HB3	1:B:227:LEU:HD22	1.94	0.48
1:F:77:ILE:O	1:F:81:ASP:HB2	2.12	0.48
1:C:89:ASN:HB2	1:C:139:ASN:HD22	1.78	0.48
1:F:100:ILE:O	2:I:44:MET:HE1	2.12	0.48
1:F:205:VAL:HG22	1:F:213:LEU:HD21	1.95	0.48
1:A:154:ASN:OD1	1:A:155:TYR:N	2.45	0.48
1:C:115:LEU:HD22	1:F:107:PHE:HZ	1.79	0.48
1:A:70:PHE:HE1	1:A:74:ILE:HD11	1.78	0.47
1:A:187:PHE:HB2	4:A:302:UHC:C6	2.44	0.47
1:E:35:ASN:OD1	1:E:36:TYR:N	2.47	0.47
1:F:212:ARG:NH2	1:F:218:GLU:OE2	2.33	0.47
2:G:50:PHE:O	2:G:50:PHE:CD1	2.67	0.47
1:A:39:ASN:OD1	1:A:39:ASN:N	2.42	0.47
1:D:144:ILE:HG22	1:D:156:SER:HB3	1.97	0.47
1:E:39:ASN:HD22	1:E:42:VAL:HG23	1.79	0.47
1:F:49:GLU:O	1:F:53:LYS:HG3	2.15	0.47
1:A:239:LEU:HD13	1:B:239:LEU:HD13	1.96	0.47
1:E:87:LEU:HD12	1:E:88:VAL:H	1.79	0.47
1:C:230:HIS:HA	1:D:221:GLU:OE1	2.14	0.47
1:E:62:PHE:HB2	1:E:69:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:PHE:HE2	1:E:70:PHE:CD2	2.32	0.47
1:E:67:GLU:O	1:E:71:VAL:HG23	2.15	0.47
1:C:62:PHE:HE2	1:C:70:PHE:CD2	2.33	0.47
1:C:48:ASN:O	1:C:51:GLU:N	2.48	0.47
1:D:9:LEU:HD22	1:D:77:ILE:HD12	1.97	0.47
1:F:61:LYS:O	1:F:62:PHE:HB3	2.15	0.47
1:D:11:THR:HA	1:D:35:ASN:HB3	1.98	0.46
1:F:139:ASN:ND2	1:F:166:SER:HB2	2.28	0.46
2:G:35:ASP:OD1	2:G:36:SER:N	2.49	0.46
1:D:95:ARG:NH1	1:D:106:ASP:HA	2.30	0.46
1:F:87:LEU:HG	1:F:88:VAL:N	2.30	0.46
1:A:89:ASN:HB2	1:A:139:ASN:HD22	1.81	0.46
3:B:301:NAP:H2N	3:B:301:NAP:O1N	2.15	0.46
1:A:95:ARG:NH1	1:A:106:ASP:OD1	2.49	0.46
1:C:92:GLY:HA2	1:C:114:ASN:OD1	2.16	0.46
1:D:97:LYS:HG2	1:D:101:LYS:HD3	1.98	0.46
1:A:122:CYS:O	1:A:125:ALA:HB3	2.16	0.45
1:F:144:ILE:HD12	1:F:149:ASN:CB	2.45	0.45
1:E:99:ALA:HB2	1:E:153:THR:HG21	1.98	0.45
1:C:18:GLY:HA3	1:C:90:ASN:ND2	2.30	0.45
1:E:190:THR:HG21	3:E:301:NAP:H72N	1.82	0.45
1:C:15:LYS:HZ3	3:C:301:NAP:H3B	1.82	0.45
1:C:207:ASN:O	1:C:209:PRO:HD3	2.17	0.45
1:E:217:LYS:O	1:E:221:GLU:HG3	2.16	0.45
2:I:38:ASP:OD1	2:I:38:ASP:N	2.48	0.45
1:B:201:LYS:C	1:B:201:LYS:CD	2.85	0.45
1:F:20:GLU:CD	1:F:20:GLU:C	2.74	0.45
1:B:23:ARG:HA	1:B:50:LEU:HD21	1.98	0.45
1:E:119:PHE:HB2	1:E:165:MET:SD	2.56	0.45
1:A:8:VAL:HA	1:A:86:TYR:O	2.16	0.45
1:E:31:LYS:HG3	1:E:56:LYS:HB3	1.98	0.45
1:F:132:SER:O	1:F:133:ARG:HG2	2.17	0.45
1:C:74:ILE:O	1:C:78:VAL:HG23	2.17	0.45
2:G:27:GLU:O	2:G:31:ASP:HB2	2.17	0.45
1:F:25:LEU:HD12	1:F:30:LEU:HD12	1.99	0.45
1:A:175:LEU:O	1:A:175:LEU:HD23	2.17	0.45
1:A:187:PHE:CE1	1:A:193:ASN:CG	2.91	0.45
1:D:129:MET:HB3	1:D:134:PHE:O	2.17	0.45
1:C:67:GLU:O	1:C:71:VAL:HG23	2.17	0.44
1:E:204:TYR:C	1:E:206:LYS:H	2.19	0.44
1:D:96:ASP:OD1	1:D:152:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:THR:O	1:F:90:ASN:HB3	2.17	0.44
1:C:240:LYS:HB3	1:C:242:ASN:HD22	1.82	0.44
1:A:92:GLY:HA3	3:A:301:NAP:H3D	1.99	0.44
1:C:176:ARG:NH2	2:I:38:ASP:OD1	2.50	0.44
1:F:4:THR:HB	1:F:134:PHE:CZ	2.52	0.44
1:C:36:TYR:CZ	1:C:61:LYS:HB2	2.52	0.44
2:G:49:LYS:HE2	2:G:49:LYS:HB2	1.79	0.44
1:A:113:ASN:HD22	3:A:301:NAP:H61A	1.64	0.44
1:F:206:LYS:HD2	1:F:206:LYS:N	2.32	0.44
1:E:155:TYR:CZ	1:E:159:LYS:HE3	2.53	0.44
1:F:144:ILE:HD13	1:F:144:ILE:HA	1.70	0.44
1:C:183:VAL:HG12	1:C:185:PRO:HD3	1.99	0.44
1:E:188:ILE:HG23	1:E:214:GLY:O	2.18	0.44
1:A:41:GLU:H	1:A:41:GLU:HG3	1.61	0.43
1:B:102:MET:HG2	1:B:106:ASP:HB2	2.00	0.43
1:D:125:ALA:O	1:D:129:MET:HG3	2.18	0.43
1:E:87:LEU:HD12	1:E:88:VAL:N	2.32	0.43
1:D:24:THR:O	1:D:28:MET:HG3	2.18	0.43
1:C:159:LYS:HD3	1:C:162:MET:HE2	1.99	0.43
1:E:141:ALA:HA	1:E:162:MET:HE1	2.00	0.43
1:E:183:VAL:O	1:E:185:PRO:HD3	2.18	0.43
1:A:90:ASN:HD21	3:A:301:NAP:H4D	1.82	0.43
1:A:103:LYS:O	1:A:106:ASP:N	2.52	0.43
1:D:47:LYS:HG2	1:D:57:ALA:HB1	2.00	0.43
1:E:175:LEU:HD12	1:E:175:LEU:H	1.83	0.43
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.69	0.43
1:A:170:ALA:O	1:A:174:ALA:HB2	2.18	0.43
1:B:116:THR:O	1:B:120:ILE:HD12	2.19	0.43
1:C:226:LEU:HA	1:C:226:LEU:HD23	1.71	0.43
1:D:157:ALA:HB2	1:E:165:MET:HB2	2.00	0.43
1:C:13:ALA:HB3	1:C:34:ILE:HG23	2.01	0.42
2:G:64:ASN:ND2	2:G:64:ASN:C	2.72	0.42
1:B:96:ASP:OD1	1:B:152:GLN:HG2	2.18	0.42
1:C:125:ALA:HB1	1:C:129:MET:SD	2.59	0.42
1:A:44:ASP:OD1	1:A:59:VAL:HG21	2.19	0.42
1:C:9:LEU:O	1:C:87:LEU:HD12	2.19	0.42
1:E:175:LEU:O	1:E:176:ARG:HG3	2.19	0.42
1:B:37:ARG:NH1	1:B:37:ARG:HB3	2.33	0.42
1:C:97:LYS:HE3	1:C:97:LYS:HB2	1.81	0.42
1:E:15:LYS:HA	1:E:19:ALA:HB2	2.00	0.42
1:E:98:LEU:HD23	1:E:98:LEU:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:ASP:OD1	1:F:152:GLN:HG2	2.19	0.42
1:F:176:ARG:HG3	1:F:176:ARG:O	2.18	0.42
2:G:17:VAL:HB	2:G:21:GLN:HG3	2.02	0.42
1:C:36:TYR:HE1	1:C:59:VAL:CG1	2.32	0.42
1:F:212:ARG:HH22	1:F:218:GLU:CD	2.20	0.42
1:A:139:ASN:HB3	1:A:162:MET:SD	2.60	0.42
1:B:25:LEU:HD21	1:B:227:LEU:CD1	2.49	0.42
1:C:35:ASN:HA	1:C:60:ILE:O	2.19	0.42
1:E:127:LYS:NZ	5:E:405:HOH:O	2.45	0.42
1:D:217:LYS:HG2	1:D:221:GLU:OE2	2.19	0.42
1:F:144:ILE:HG21	1:F:155:TYR:CD2	2.46	0.42
1:B:226:LEU:HD23	1:B:226:LEU:HA	1.87	0.42
1:C:22:ALA:O	1:C:32:VAL:HG11	2.20	0.42
1:C:111:ILE:HD13	1:C:158:SER:HB3	2.01	0.42
1:C:131:LYS:HA	1:C:131:LYS:HD3	1.75	0.42
1:C:154:ASN:OD1	1:C:155:TYR:N	2.53	0.42
1:C:167:LYS:HG2	1:D:247:MET:HB3	2.02	0.42
1:D:39:ASN:HB3	5:D:408:HOH:O	2.19	0.42
1:E:17:ILE:O	1:E:21:ILE:HG13	2.19	0.42
1:F:66:SER:OG	1:F:69:ASP:HB3	2.19	0.42
1:F:144:ILE:CD1	1:F:149:ASN:HB2	2.49	0.42
1:F:179:ARG:HB3	1:F:235:THR:HG22	2.01	0.42
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.88	0.42
1:E:190:THR:HG21	3:E:301:NAP:N7N	2.34	0.42
2:G:23:THR:CG2	2:G:26:ALA:HB2	2.50	0.42
2:G:46:LEU:HA	2:G:46:LEU:HD12	1.69	0.42
2:G:72:ILE:HD13	2:G:72:ILE:HA	1.90	0.42
1:C:35:ASN:ND2	1:C:62:PHE:CE2	2.88	0.42
1:F:126:LEU:HD23	1:F:126:LEU:HA	1.90	0.42
1:D:144:ILE:HD12	1:D:149:ASN:HB2	2.02	0.41
1:F:210:LEU:O	1:F:212:ARG:HG2	2.20	0.41
1:B:170:ALA:HB2	1:B:180:PHE:HB2	2.01	0.41
1:E:232:SER:HB2	1:F:218:GLU:OE2	2.21	0.41
1:F:17:ILE:O	1:F:21:ILE:HD12	2.20	0.41
1:A:178:ILE:HG22	1:A:180:PHE:CE1	2.55	0.41
1:C:241:VAL:HG22	1:D:234:ILE:HD11	2.01	0.41
2:H:42:LEU:HA	2:H:45:ALA:HB3	2.03	0.41
1:B:20:GLU:HA	1:B:20:GLU:OE1	2.19	0.41
1:C:140:ILE:O	1:C:162:MET:HE1	2.19	0.41
1:D:6:LYS:HA	1:D:30:LEU:HD22	2.03	0.41
1:C:240:LYS:HB3	1:C:242:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:ARG:HG2	1:F:50:LEU:HD21	2.02	0.41
1:D:84:LEU:HD12	1:D:84:LEU:HA	1.82	0.41
1:D:131:LYS:HG3	1:D:132:SER:H	1.85	0.41
1:E:62:PHE:HE2	1:E:70:PHE:CE2	2.38	0.41
1:E:167:LYS:O	1:E:171:TYR:HD1	2.03	0.41
1:B:140:ILE:O	1:B:162:MET:HE1	2.21	0.41
1:F:13:ALA:HB3	1:F:34:ILE:HG23	2.03	0.41
1:B:174:ALA:C	1:B:176:ARG:N	2.74	0.41
1:D:97:LYS:HE2	1:D:101:LYS:NZ	2.36	0.41
2:G:18:ASP:OD1	2:G:18:ASP:N	2.54	0.41
1:A:233:TYR:CE2	1:B:214:GLY:HA3	2.55	0.41
1:B:23:ARG:HE	1:B:23:ARG:HB2	1.52	0.41
1:C:126:LEU:HD12	1:F:99:ALA:HB3	2.02	0.41
1:D:23:ARG:HA	1:D:50:LEU:HD11	2.03	0.41
1:D:203:ASP:OD1	5:D:401:HOH:O	2.22	0.41
1:E:11:THR:HA	1:E:35:ASN:HD22	1.86	0.41
1:F:17:ILE:CD1	1:F:188:ILE:HG21	2.44	0.41
1:F:242:ASN:OD1	1:F:245:LEU:N	2.53	0.41
2:G:49:LYS:O	2:G:49:LYS:CG	2.69	0.41
1:C:16:GLY:HA3	3:C:301:NAP:O2N	2.21	0.41
1:C:31:LYS:NZ	1:C:81:ASP:OD1	2.51	0.41
1:D:47:LYS:HD2	1:D:47:LYS:C	2.40	0.41
1:D:154:ASN:OD1	1:D:155:TYR:N	2.54	0.41
2:G:63:VAL:O	2:G:63:VAL:CG2	2.69	0.41
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.65	0.40
1:B:37:ARG:HB3	1:B:37:ARG:HH11	1.86	0.40
1:C:183:VAL:HG21	1:C:223:VAL:HG22	2.02	0.40
1:D:2:GLN:HB3	1:D:230:HIS:CE1	2.56	0.40
1:E:10:ILE:HG22	1:E:13:ALA:HB2	2.02	0.40
1:A:138:VAL:HG11	1:A:223:VAL:HG22	2.03	0.40
1:B:12:GLY:N	1:B:35:ASN:OD1	2.45	0.40
1:E:239:LEU:HD12	1:F:237:GLU:HG2	2.04	0.40
1:E:190:THR:O	1:E:190:THR:CG2	2.66	0.40
1:A:136:SER:OG	1:A:227:LEU:HA	2.21	0.40
1:D:34:ILE:HD12	1:D:47:LYS:HB2	2.03	0.40
1:D:134:PHE:CD1	1:D:135:GLY:N	2.89	0.40
1:D:159:LYS:O	1:D:163:ILE:HG13	2.21	0.40
1:E:204:TYR:C	1:E:206:LYS:N	2.75	0.40
1:C:103:LYS:O	1:C:106:ASP:N	2.54	0.40
1:F:26:ALA:HA	1:F:30:LEU:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ARG:NH2	2:G:37:LEU:CD1[3_455]	1.64	0.56

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	246/248 (99%)	234 (95%)	12 (5%)	0	100 100
1	B	233/248 (94%)	220 (94%)	13 (6%)	0	100 100
1	C	232/248 (94%)	219 (94%)	13 (6%)	0	100 100
1	D	233/248 (94%)	214 (92%)	18 (8%)	1 (0%)	34 46
1	E	233/248 (94%)	211 (91%)	22 (9%)	0	100 100
1	F	229/248 (92%)	210 (92%)	19 (8%)	0	100 100
2	G	71/75 (95%)	59 (83%)	11 (16%)	1 (1%)	11 14
2	H	11/75 (15%)	10 (91%)	1 (9%)	0	100 100
2	I	7/75 (9%)	6 (86%)	1 (14%)	0	100 100
All	All	1495/1713 (87%)	1383 (92%)	110 (7%)	2 (0%)	51 67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	35	ASP
1	D	186	GLY

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	197/197 (100%)	194 (98%)	3 (2%)	65 79
1	B	187/197 (95%)	182 (97%)	5 (3%)	44 62
1	C	187/197 (95%)	185 (99%)	2 (1%)	73 86
1	D	187/197 (95%)	187 (100%)	0	100 100
1	E	188/197 (95%)	186 (99%)	2 (1%)	73 86
1	F	184/197 (93%)	183 (100%)	1 (0%)	88 95
2	G	62/63 (98%)	53 (86%)	9 (14%)	3 3
2	H	13/63 (21%)	13 (100%)	0	100 100
2	I	8/63 (13%)	7 (88%)	1 (12%)	4 5
All	All	1213/1371 (88%)	1190 (98%)	23 (2%)	57 73

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

Mol	Chain	Res	Type
1	A	2	GLN
1	A	42	VAL
1	A	131	LYS
1	B	130	SER
1	B	132	SER
1	B	133	ARG
1	B	201	LYS
1	B	206	LYS
1	C	35	ASN
1	C	143	ILE
1	E	190	THR
1	E	191	ASP
1	F	61	LYS
2	G	15	LEU
2	G	36	SER
2	G	46	LEU
2	G	50	PHE
2	G	52	ILE
2	G	54	ILE
2	G	63	VAL
2	G	64	ASN
2	G	65	VAL
2	I	37	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	113	ASN
1	A	139	ASN
1	A	177	ASN
1	C	2	GLN
1	C	39	ASN
1	C	89	ASN
1	C	139	ASN
1	D	2	GLN
1	F	35	ASN
1	F	108	HIS
2	G	64	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

7 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	D	301	-	45,52,52	1.14	4 (8%)	56,80,80	1.85	11 (19%)
3	NAP	A	301	-	45,52,52	1.20	4 (8%)	56,80,80	1.97	13 (23%)
3	NAP	B	301	-	45,52,52	1.24	5 (11%)	56,80,80	2.10	17 (30%)
3	NAP	E	301	1	45,52,52	1.10	3 (6%)	56,80,80	1.97	14 (25%)
3	NAP	C	301	-	45,52,52	1.28	5 (11%)	56,80,80	2.00	19 (33%)
3	NAP	F	301	-	45,52,52	1.32	6 (13%)	56,80,80	2.00	13 (23%)
4	UHC	A	302	-	21,28,31	1.00	2 (9%)	26,36,41	1.86	7 (26%)

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	D	301	-	-	13/31/67/67	0/5/5/5
3	NAP	A	301	-	-	8/31/67/67	0/5/5/5
3	NAP	B	301	-	-	11/31/67/67	0/5/5/5
3	NAP	E	301	1	-	8/31/67/67	0/5/5/5
3	NAP	C	301	-	-	11/31/67/67	0/5/5/5
3	NAP	F	301	-	-	14/31/67/67	0/5/5/5
4	UHC	A	302	-	-	19/33/36/39	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	NAP	C3N-C7N	3.91	1.56	1.50
3	F	301	NAP	C6N-N1N	-3.58	1.26	1.35
3	E	301	NAP	C6N-N1N	-3.54	1.26	1.35
3	F	301	NAP	C2N-N1N	3.54	1.39	1.35
3	C	301	NAP	C2D-C1D	3.52	1.59	1.53
3	B	301	NAP	C2D-C1D	3.49	1.59	1.53
3	C	301	NAP	C2N-N1N	3.41	1.39	1.35
3	A	301	NAP	C2N-N1N	3.34	1.39	1.35
3	A	301	NAP	C6N-N1N	-3.33	1.27	1.35
3	B	301	NAP	C6N-N1N	-3.33	1.27	1.35
3	D	301	NAP	C6N-N1N	-3.20	1.27	1.35
3	F	301	NAP	C2D-C1D	3.06	1.58	1.53
3	B	301	NAP	C2N-N1N	2.96	1.38	1.35
3	A	301	NAP	C2D-C1D	2.95	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	NAP	C6N-N1N	-2.92	1.28	1.35
3	D	301	NAP	C2N-N1N	2.82	1.38	1.35
3	D	301	NAP	C2D-C1D	2.80	1.58	1.53
3	F	301	NAP	C3N-C7N	2.78	1.54	1.50
3	E	301	NAP	C2N-N1N	2.66	1.38	1.35
3	A	301	NAP	C8A-N7A	-2.44	1.30	1.34
3	F	301	NAP	C8A-N7A	-2.44	1.30	1.34
3	E	301	NAP	O4D-C4D	-2.34	1.39	1.45
3	B	301	NAP	C3N-C7N	2.29	1.54	1.50
3	B	301	NAP	C8A-N7A	-2.26	1.30	1.34
3	C	301	NAP	O4B-C1B	2.23	1.44	1.41
4	A	302	UHC	O3-C3	-2.19	1.18	1.21
3	F	301	NAP	C2N-C3N	2.15	1.42	1.39
3	D	301	NAP	C8A-N7A	-2.13	1.30	1.34
4	A	302	UHC	O1-C1	-2.02	1.17	1.21

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	301	NAP	O2B-C2B-C3B	6.83	136.43	111.68
3	E	301	NAP	O2B-C2B-C3B	6.78	136.27	111.68
3	A	301	NAP	O2B-C2B-C3B	6.65	135.79	111.68
3	C	301	NAP	O2B-C2B-C3B	6.64	135.76	111.68
3	D	301	NAP	O2B-C2B-C3B	6.42	134.94	111.68
3	F	301	NAP	C3D-C2D-C1D	-6.39	91.36	100.98
3	B	301	NAP	O2B-C2B-C3B	6.21	134.20	111.68
3	A	301	NAP	O2D-C2D-C1D	5.80	132.26	110.85
3	B	301	NAP	O2D-C2D-C1D	5.68	131.84	110.85
3	D	301	NAP	O2D-C2D-C1D	5.57	131.41	110.85
4	A	302	UHC	C30-C29-C32	5.49	118.34	108.82
3	F	301	NAP	O2D-C2D-C1D	5.41	130.84	110.85
3	C	301	NAP	O2D-C2D-C1D	5.20	130.06	110.85
3	D	301	NAP	C3D-C2D-C1D	-5.13	93.26	100.98
3	A	301	NAP	C6N-N1N-C2N	-5.11	117.31	121.97
3	B	301	NAP	C6N-N1N-C2N	-4.58	117.80	121.97
3	E	301	NAP	O2D-C2D-C1D	4.36	126.94	110.85
3	A	301	NAP	C3D-C2D-C1D	-4.35	94.43	100.98
3	B	301	NAP	O2X-P2B-O2B	-3.88	88.63	105.99
3	C	301	NAP	O2D-C2D-C3D	-3.87	99.30	111.82
3	E	301	NAP	C3N-C2N-N1N	-3.83	116.68	120.43
3	E	301	NAP	O2D-C2D-C3D	-3.67	99.96	111.82
3	C	301	NAP	O7N-C7N-N7N	-3.60	117.46	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	301	NAP	C3D-C2D-C1D	-3.58	95.58	100.98
3	F	301	NAP	C3N-C2N-N1N	-3.58	116.92	120.43
3	B	301	NAP	C3D-C2D-C1D	-3.44	95.80	100.98
3	C	301	NAP	C2N-C3N-C4N	-3.42	114.38	118.26
3	A	301	NAP	C5N-C4N-C3N	-3.39	116.33	120.34
3	B	301	NAP	C5N-C4N-C3N	-3.38	116.35	120.34
3	E	301	NAP	C6N-N1N-C2N	-3.31	118.95	121.97
4	A	302	UHC	O3-C3-C2	-3.30	115.24	120.83
3	B	301	NAP	C3N-C2N-N1N	-3.26	117.24	120.43
3	B	301	NAP	O3D-C3D-C4D	3.25	120.46	111.05
3	D	301	NAP	O3D-C3D-C4D	3.25	120.45	111.05
3	C	301	NAP	PA-O5B-C5B	-3.22	102.82	121.68
3	B	301	NAP	O4B-C1B-C2B	-3.18	101.08	106.59
3	B	301	NAP	O2B-C2B-C1B	3.07	121.17	110.10
3	C	301	NAP	C1B-N9A-C4A	-3.06	121.26	126.64
3	D	301	NAP	O2D-C2D-C3D	-3.03	102.01	111.82
3	E	301	NAP	O2X-P2B-O2B	-3.01	92.52	105.99
3	F	301	NAP	O2D-C2D-C3D	-2.96	102.24	111.82
3	C	301	NAP	C3B-C2B-C1B	-2.95	97.34	102.89
3	E	301	NAP	C2D-C3D-C4D	2.93	108.33	102.64
3	A	301	NAP	C6N-C5N-C4N	-2.91	115.21	119.44
4	A	302	UHC	C30-C29-C28	-2.91	103.48	108.23
3	D	301	NAP	O2X-P2B-O2B	-2.89	93.04	105.99
3	F	301	NAP	O2B-C2B-C1B	2.82	120.25	110.10
3	A	301	NAP	O2X-P2B-O2B	-2.81	93.39	105.99
3	B	301	NAP	O2D-C2D-C3D	-2.80	102.76	111.82
3	B	301	NAP	O7N-C7N-C3N	2.78	122.96	119.63
3	A	301	NAP	O2D-C2D-C3D	-2.76	102.90	111.82
3	E	301	NAP	O5D-C5D-C4D	2.69	118.25	108.99
4	A	302	UHC	C31-C29-C28	-2.67	103.87	108.23
3	A	301	NAP	C4A-C5A-N7A	2.65	112.17	109.40
3	D	301	NAP	O2A-PA-O1A	2.62	125.19	112.24
3	F	301	NAP	O4B-C1B-C2B	-2.62	102.05	106.59
3	C	301	NAP	O2B-C2B-C1B	2.61	119.51	110.10
3	F	301	NAP	O2X-P2B-O2B	-2.61	94.30	105.99
3	D	301	NAP	C6N-N1N-C2N	-2.59	119.61	121.97
3	F	301	NAP	O3D-C3D-C4D	2.57	118.49	111.05
3	C	301	NAP	O3D-C3D-C4D	2.54	118.41	111.05
3	B	301	NAP	C2B-C3B-C4B	-2.54	96.48	101.99
3	A	301	NAP	O5D-C5D-C4D	2.52	117.67	108.99
3	E	301	NAP	O3D-C3D-C4D	2.49	118.23	111.05
4	A	302	UHC	C6-C5-C4	-2.45	102.21	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	301	NAP	PA-O5B-C5B	-2.42	107.52	121.68
3	E	301	NAP	O4B-C1B-C2B	-2.39	102.44	106.59
3	E	301	NAP	O2B-C2B-C1B	2.39	118.69	110.10
3	A	301	NAP	O2B-C2B-C1B	2.36	118.61	110.10
3	C	301	NAP	O2X-P2B-O2B	-2.36	95.42	105.99
3	D	301	NAP	O4B-C4B-C3B	2.34	109.75	105.11
3	B	301	NAP	O3X-P2B-O2X	2.34	116.57	107.64
4	A	302	UHC	C37-C38-C39	-2.32	108.50	112.36
3	C	301	NAP	O3X-P2B-O2X	2.31	116.45	107.64
4	A	302	UHC	C43-S1-C1	-2.28	94.77	101.87
3	B	301	NAP	C2N-C3N-C4N	-2.27	115.69	118.26
3	D	301	NAP	O4D-C1D-C2D	-2.25	103.64	106.93
3	F	301	NAP	C5N-C6N-N1N	-2.25	117.18	120.40
3	B	301	NAP	C3B-C2B-C1B	-2.24	98.67	102.89
3	B	301	NAP	O2A-PA-O1A	2.24	123.31	112.24
3	C	301	NAP	O2A-PA-O1A	2.22	123.19	112.24
3	F	301	NAP	C6N-C5N-C4N	-2.18	116.27	119.44
3	A	301	NAP	O3D-C3D-C4D	2.18	117.34	111.05
3	C	301	NAP	O7N-C7N-C3N	2.16	122.22	119.63
3	C	301	NAP	C3N-C7N-N7N	2.14	120.32	117.75
3	F	301	NAP	C6N-N1N-C2N	-2.14	120.02	121.97
3	C	301	NAP	C6N-N1N-C2N	-2.14	120.02	121.97
3	C	301	NAP	C3D-C2D-C1D	-2.12	97.78	100.98
3	E	301	NAP	O7N-C7N-C3N	2.12	122.17	119.63
3	C	301	NAP	O4B-C1B-C2B	2.09	110.22	106.59
3	C	301	NAP	O5D-C5D-C4D	2.08	116.16	108.99
3	A	301	NAP	O2A-PA-O1A	2.04	122.35	112.24
3	F	301	NAP	C4A-C5A-N7A	2.03	111.51	109.40
3	E	301	NAP	O3D-C3D-C2D	-2.02	105.28	111.82

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	NAP	C3B-C2B-O2B-P2B
3	A	301	NAP	O4D-C1D-N1N-C2N
3	B	301	NAP	C3B-C2B-O2B-P2B
3	B	301	NAP	C5D-O5D-PN-O3
3	B	301	NAP	O4D-C4D-C5D-O5D
3	B	301	NAP	C3D-C4D-C5D-O5D
3	B	301	NAP	O4D-C1D-N1N-C2N
3	C	301	NAP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	C	301	NAP	C3B-C2B-O2B-P2B
3	C	301	NAP	C5D-O5D-PN-O3
3	C	301	NAP	C5D-O5D-PN-O1N
3	D	301	NAP	C5B-O5B-PA-O2A
3	D	301	NAP	O4B-C4B-C5B-O5B
3	D	301	NAP	C3B-C2B-O2B-P2B
3	D	301	NAP	C5D-O5D-PN-O3
3	D	301	NAP	C5D-O5D-PN-O1N
3	D	301	NAP	C3D-C4D-C5D-O5D
3	E	301	NAP	C3B-C2B-O2B-P2B
3	E	301	NAP	O4D-C4D-C5D-O5D
3	E	301	NAP	C3D-C4D-C5D-O5D
3	F	301	NAP	C3B-C2B-O2B-P2B
3	F	301	NAP	C5D-O5D-PN-O3
3	F	301	NAP	O4D-C4D-C5D-O5D
3	F	301	NAP	C3D-C4D-C5D-O5D
3	F	301	NAP	O4D-C1D-N1N-C2N
3	F	301	NAP	O4D-C1D-N1N-C6N
4	A	302	UHC	O1-C1-S1-C43
4	A	302	UHC	C2-C1-S1-C43
4	A	302	UHC	C42-C43-S1-C1
4	A	302	UHC	C3-C4-C5-C6
4	A	302	UHC	C28-C29-C32-O33
4	A	302	UHC	C28-C29-C32-C34
4	A	302	UHC	C30-C29-C32-O33
4	A	302	UHC	C30-C29-C32-C34
4	A	302	UHC	C31-C29-C32-O33
4	A	302	UHC	C31-C29-C32-C34
4	A	302	UHC	N41-C42-C43-S1
4	A	302	UHC	C38-C39-N41-C42
3	A	301	NAP	O4D-C4D-C5D-O5D
3	A	301	NAP	C3D-C4D-C5D-O5D
3	D	301	NAP	O4D-C4D-C5D-O5D
4	A	302	UHC	O3-C3-C4-C5
4	A	302	UHC	C2-C3-C4-C5
4	A	302	UHC	O40-C39-N41-C42
3	C	301	NAP	O4D-C4D-C5D-O5D
3	C	301	NAP	C1B-C2B-O2B-P2B
3	C	301	NAP	C3B-C4B-C5B-O5B
3	D	301	NAP	C3B-C4B-C5B-O5B
4	A	302	UHC	O33-C32-C34-O35
3	C	301	NAP	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
3	C	301	NAP	O4B-C4B-C5B-O5B
3	E	301	NAP	C4D-C5D-O5D-PN
3	E	301	NAP	C2B-O2B-P2B-O1X
4	A	302	UHC	N36-C37-C38-C39
3	D	301	NAP	C5B-O5B-PA-O3
3	B	301	NAP	PA-O3-PN-O2N
3	B	301	NAP	C5D-O5D-PN-O1N
3	B	301	NAP	C5D-O5D-PN-O2N
3	D	301	NAP	C5D-O5D-PN-O2N
3	F	301	NAP	C5D-O5D-PN-O1N
3	F	301	NAP	C5D-O5D-PN-O2N
4	A	302	UHC	C1-C2-C3-O3
3	E	301	NAP	C4N-C3N-C7N-O7N
3	E	301	NAP	C4N-C3N-C7N-N7N
3	F	301	NAP	O4B-C4B-C5B-O5B
4	A	302	UHC	O1-C1-C2-C3
3	A	301	NAP	PA-O3-PN-O1N
3	D	301	NAP	PA-O3-PN-O1N
3	F	301	NAP	PA-O3-PN-O2N
3	D	301	NAP	C1B-C2B-O2B-P2B
3	B	301	NAP	O4B-C4B-C5B-O5B
3	F	301	NAP	C2B-O2B-P2B-O1X
3	A	301	NAP	C2D-C1D-N1N-C2N
3	B	301	NAP	C2D-C1D-N1N-C2N
3	C	301	NAP	C5B-O5B-PA-O3
3	F	301	NAP	C2B-O2B-P2B-O2X
3	F	301	NAP	C2D-C1D-N1N-C6N
3	A	301	NAP	O4B-C4B-C5B-O5B
3	E	301	NAP	O4B-C4B-C5B-O5B
3	B	301	NAP	PA-O3-PN-O1N
3	F	301	NAP	PA-O3-PN-O1N
3	A	301	NAP	C5D-O5D-PN-O1N
3	C	301	NAP	C5D-O5D-PN-O2N
3	D	301	NAP	C5B-O5B-PA-O1A

There are no ring outliers.

7 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	NAP	3	0
3	A	301	NAP	6	0
3	B	301	NAP	5	0

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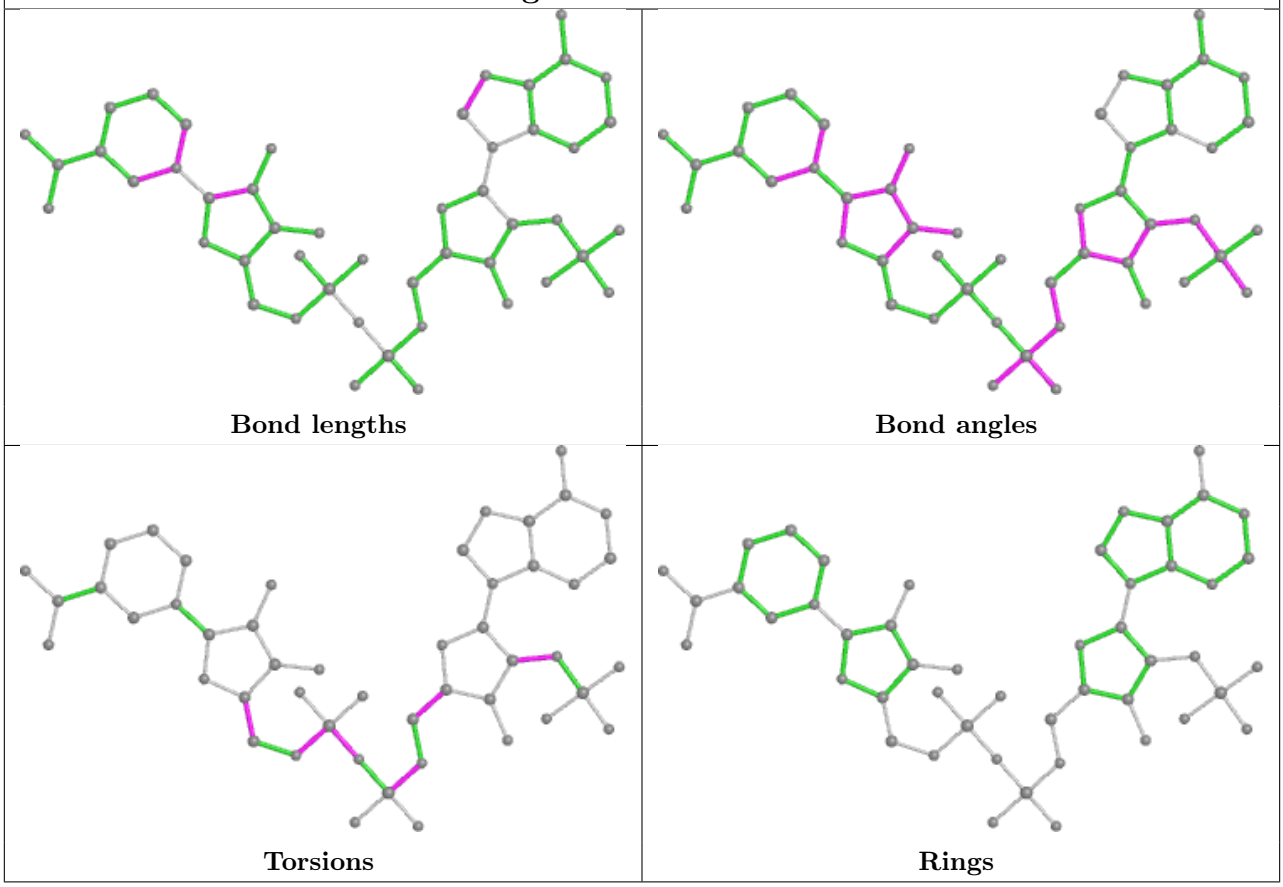
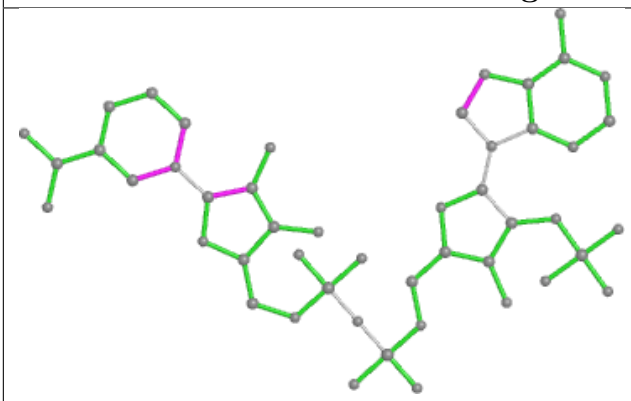
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	301	NAP	3	0
3	C	301	NAP	5	0
3	F	301	NAP	1	0
4	A	302	UHC	3	0

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.

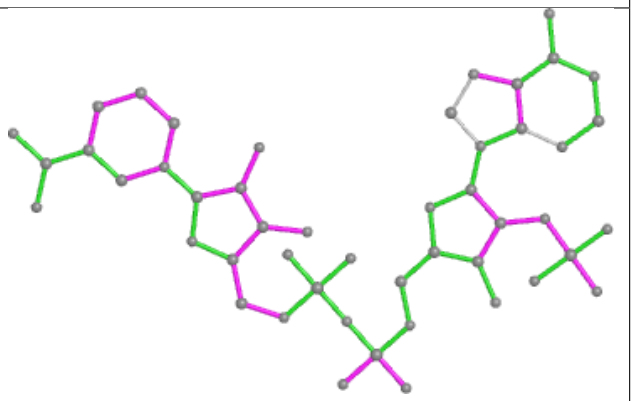
Ligand NAP D 301



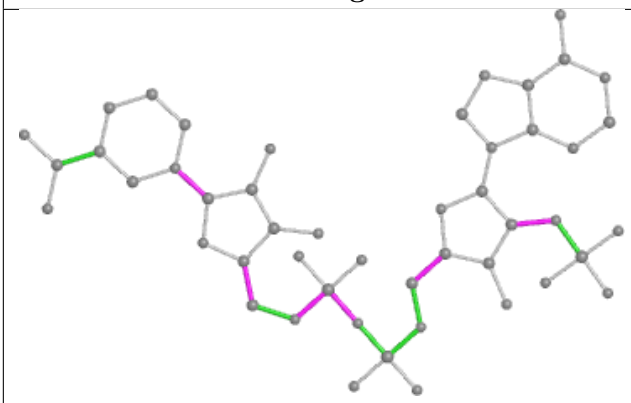
Ligand NAP A 301



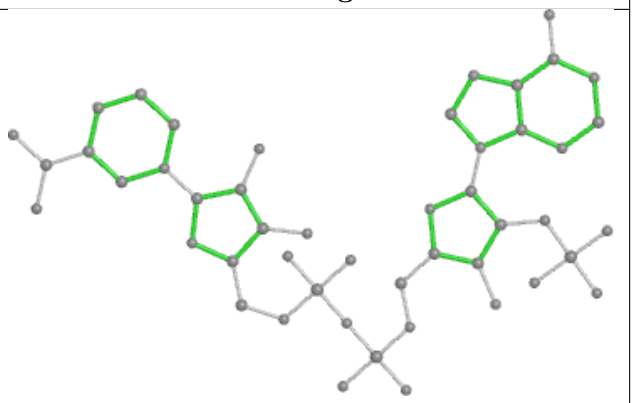
Bond lengths



Bond angles

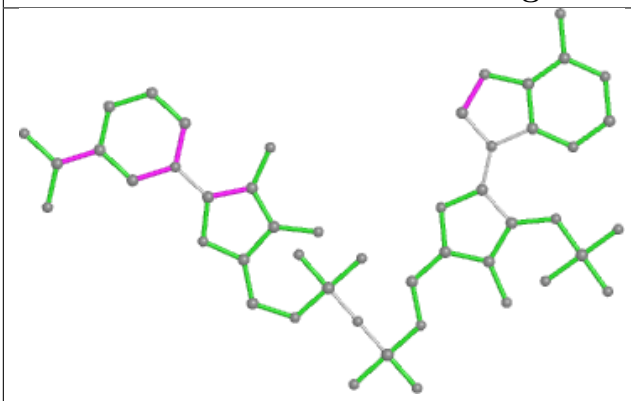


Torsions

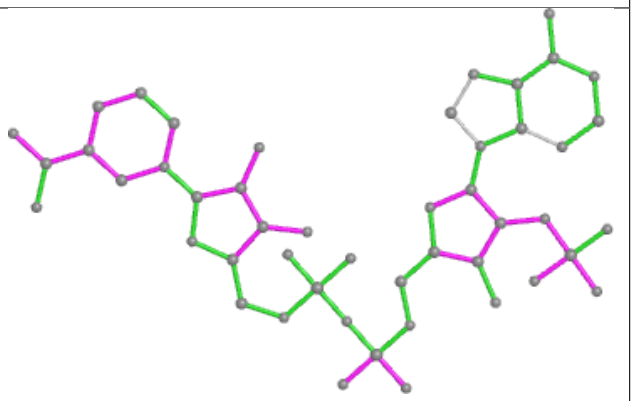


Rings

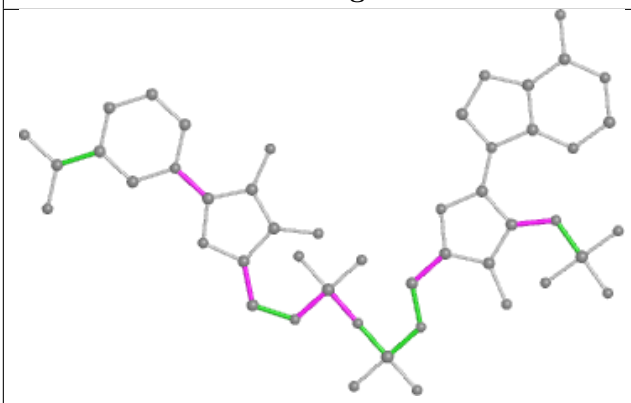
Ligand NAP B 301



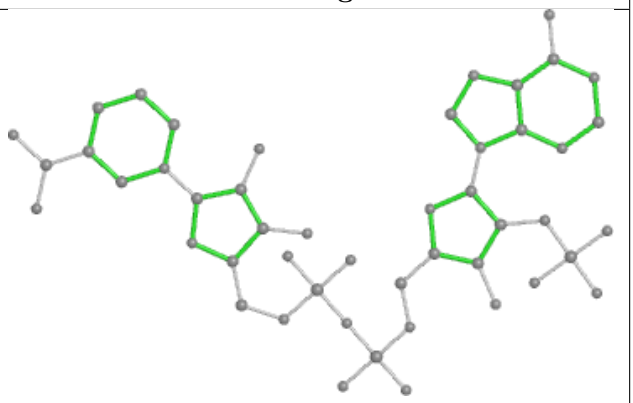
Bond lengths



Bond angles

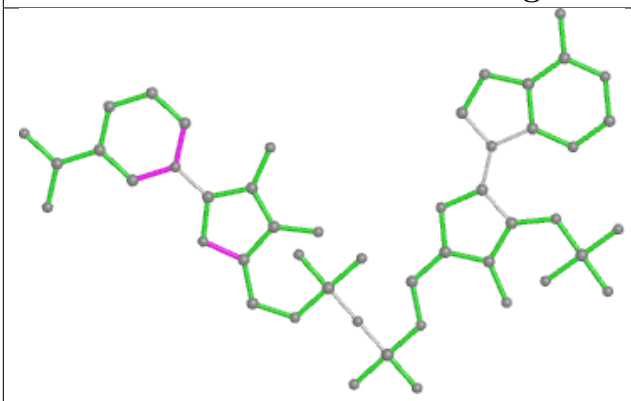


Torsions

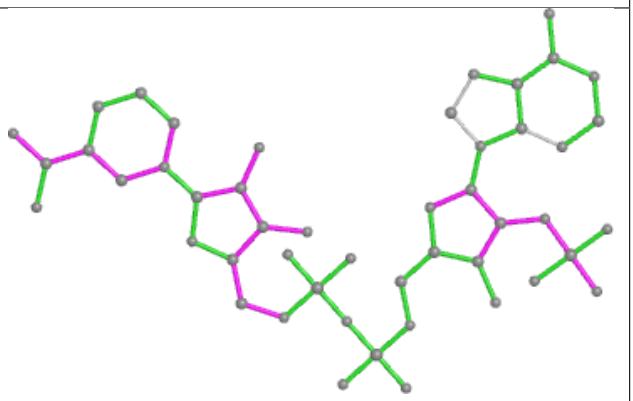


Rings

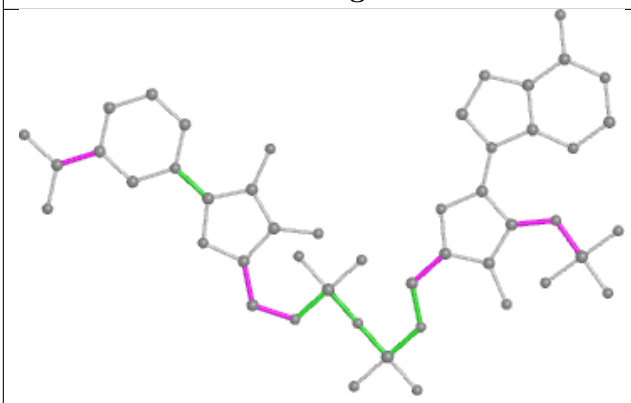
Ligand NAP E 301



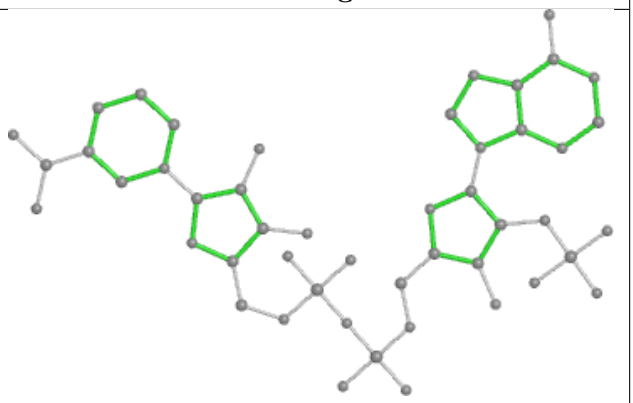
Bond lengths



Bond angles

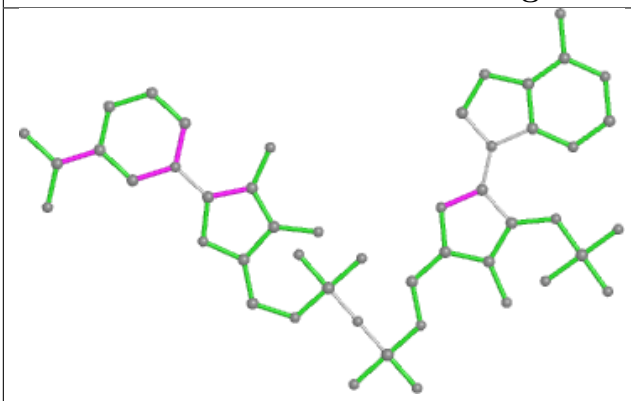


Torsions

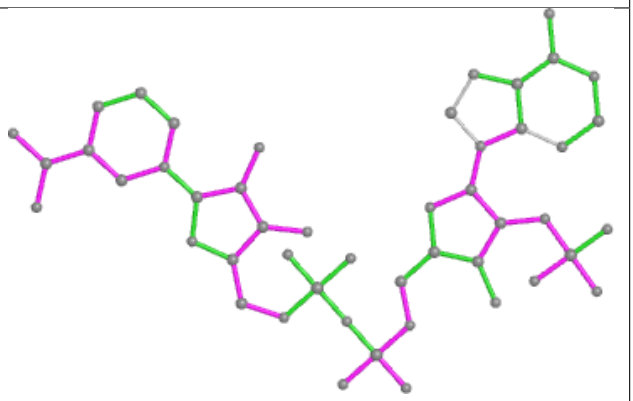


Rings

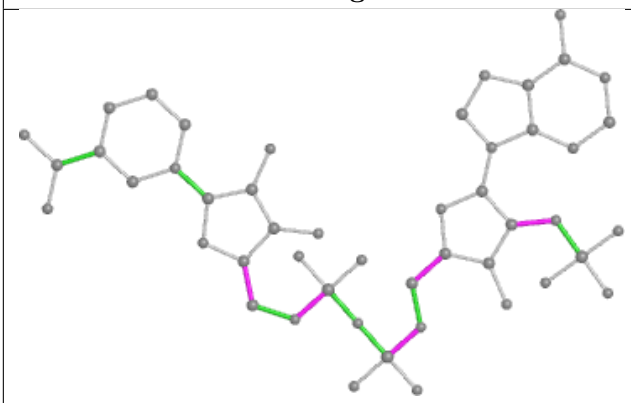
Ligand NAP C 301



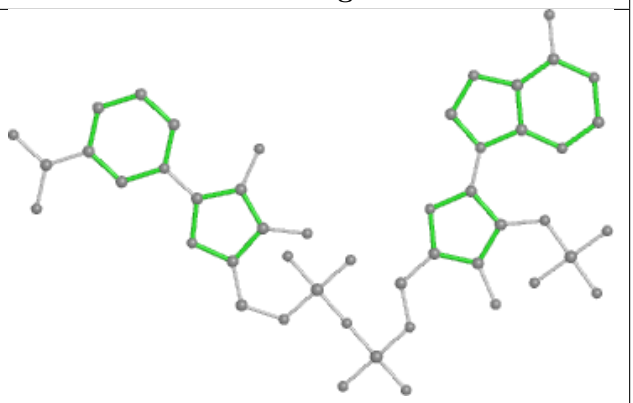
Bond lengths



Bond angles

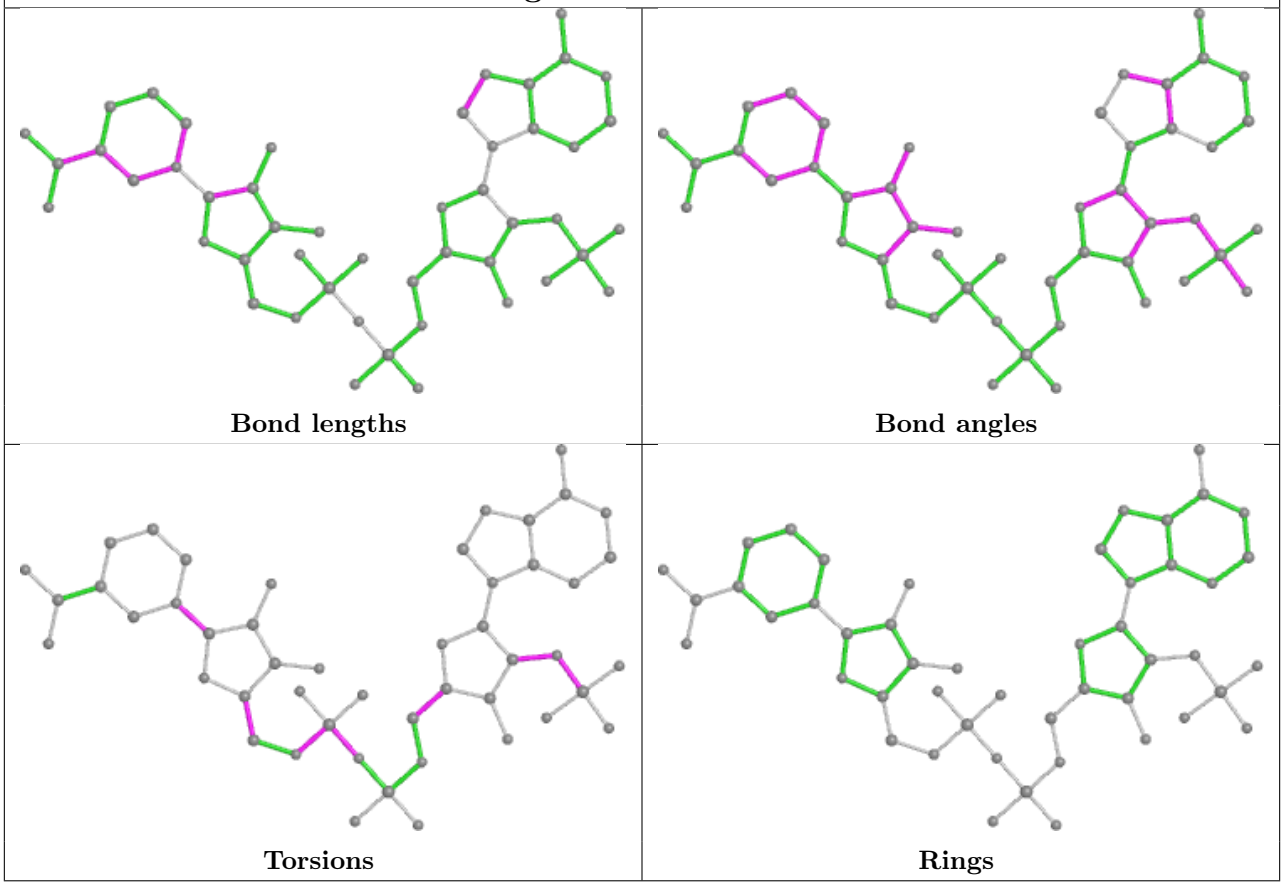


Torsions

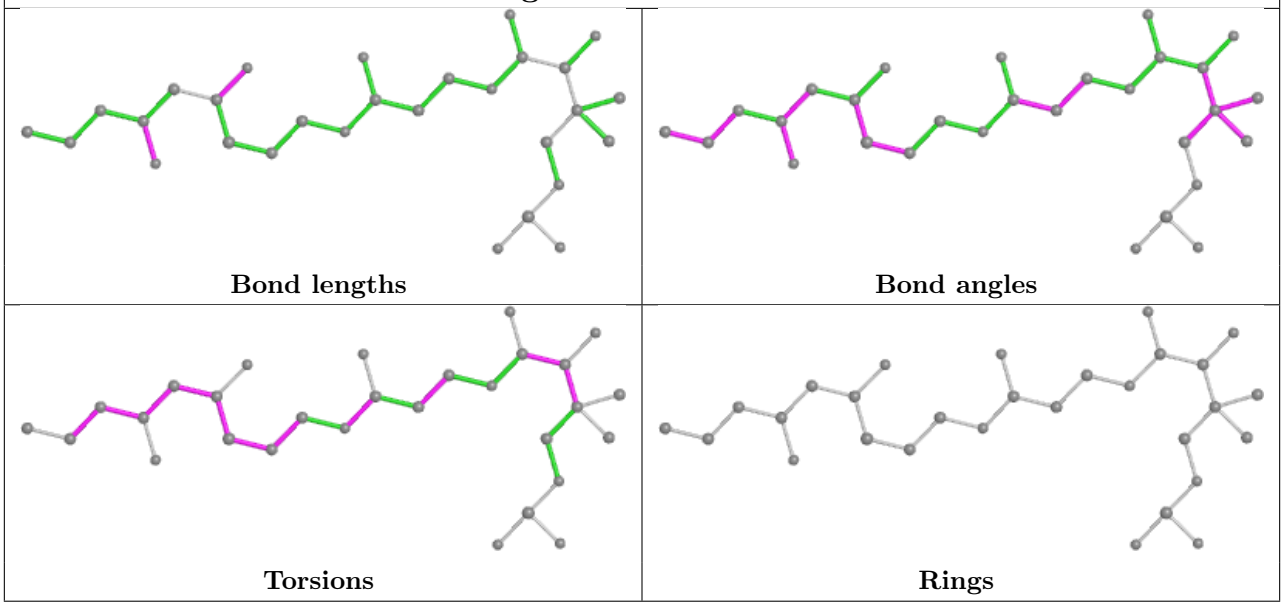


Rings

Ligand NAP F 301



Ligand UHC A 302



5.7 Other polymers

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	248/248 (100%)	0.31	9 (3%) 42 46	20, 35, 74, 103	0
1	B	237/248 (95%)	0.19	1 (0%) 92 93	21, 38, 59, 79	0
1	C	236/248 (95%)	0.18	1 (0%) 92 93	24, 42, 62, 76	0
1	D	237/248 (95%)	0.35	10 (4%) 36 39	30, 50, 68, 92	0
1	E	237/248 (95%)	0.45	8 (3%) 45 48	31, 48, 69, 91	0
1	F	233/248 (93%)	0.53	19 (8%) 11 12	33, 52, 78, 97	0
2	G	73/75 (97%)	0.42	5 (6%) 17 18	53, 76, 91, 102	0
2	H	15/75 (20%)	1.29	4 (26%) 0 0	78, 89, 100, 107	0
2	I	9/75 (12%)	0.95	0 100 100	74, 79, 86, 86	0
All	All	1525/1713 (89%)	0.35	57 (3%) 41 45	20, 45, 78, 107	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	191	ASP	6.5
1	D	57	ALA	6.1
1	A	196	LEU	5.2
2	G	53	GLU	5.1
2	G	7	ILE	4.1
2	G	52	ILE	4.0
1	D	30	LEU	3.8
1	F	112	ASP	3.8
2	H	64	ASN	3.7
1	F	22	ALA	3.6
1	F	58	ALA	3.6
1	A	187	PHE	3.4
1	A	195	ASN	3.4
1	E	190	THR	3.4
1	E	204	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	13	ALA	3.1
1	F	44	ASP	3.1
1	F	50	LEU	3.1
1	E	121	GLY	3.1
1	F	46	LEU	3.0
1	A	190	THR	3.0
1	D	204	TYR	3.0
1	A	200	LEU	2.9
1	A	191	ASP	2.9
1	F	25	LEU	2.8
1	E	57	ALA	2.8
2	H	62	ILE	2.7
1	A	203	ASP	2.6
2	G	28	PHE	2.6
1	C	112	ASP	2.6
1	F	61	LYS	2.5
1	F	63	ASP	2.5
1	F	36	TYR	2.4
1	F	113	ASN	2.4
1	D	87	LEU	2.4
1	D	56	LYS	2.4
1	F	86	TYR	2.4
1	A	204	TYR	2.4
1	E	84	LEU	2.4
1	F	108	HIS	2.4
1	B	46	LEU	2.3
2	G	37	LEU	2.3
1	D	10	ILE	2.3
1	E	58	ALA	2.3
1	F	62	PHE	2.3
1	E	9	LEU	2.3
1	F	14	SER	2.3
1	F	39	ASN	2.2
1	F	34	ILE	2.2
1	A	133	ARG	2.2
1	F	133	ARG	2.2
1	D	134	PHE	2.2
1	F	13	ALA	2.2
2	H	42	LEU	2.1
1	D	14	SER	2.1
2	H	43	ILE	2.0
1	D	58	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)

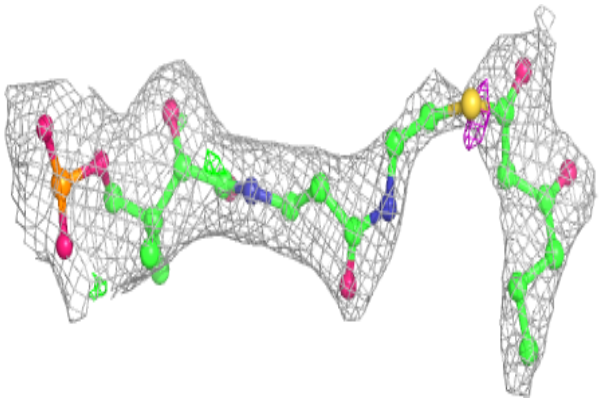
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

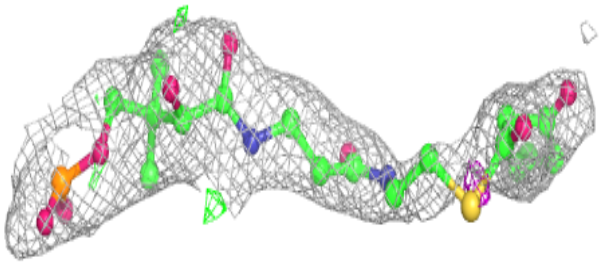
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	UHC	A	302	29/32	0.84	0.23	45,59,91,102	0
3	NAP	C	301	48/48	0.91	0.23	42,63,82,98	0
3	NAP	F	301	48/48	0.92	0.21	50,65,87,102	0
3	NAP	B	301	48/48	0.94	0.14	34,53,73,83	0
3	NAP	D	301	48/48	0.94	0.18	46,58,79,83	0
3	NAP	E	301	48/48	0.96	0.15	38,49,62,71	0
3	NAP	A	301	48/48	0.97	0.14	29,37,48,53	0

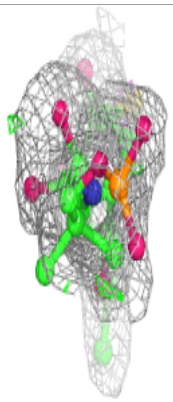
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UHC A 302:

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

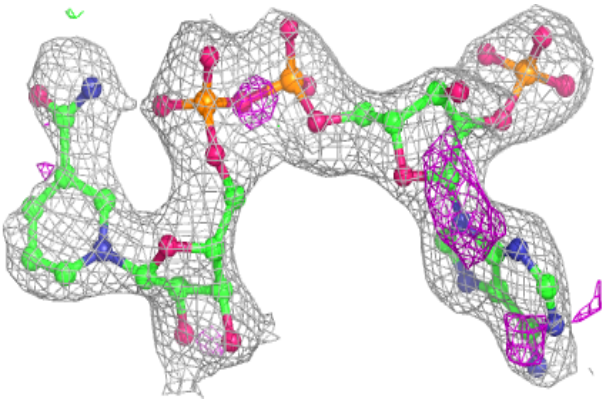


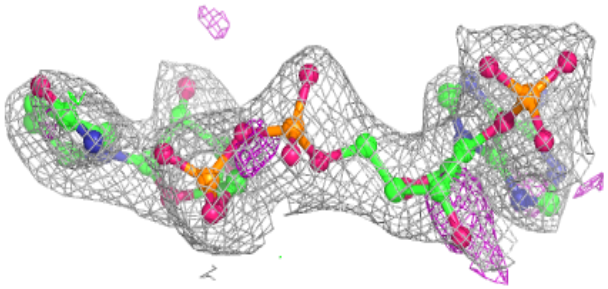


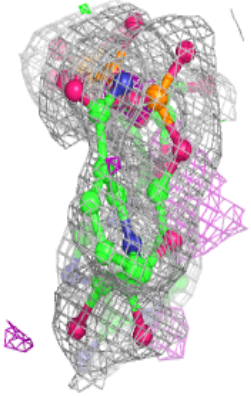


Electron density around NAP C 301:

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

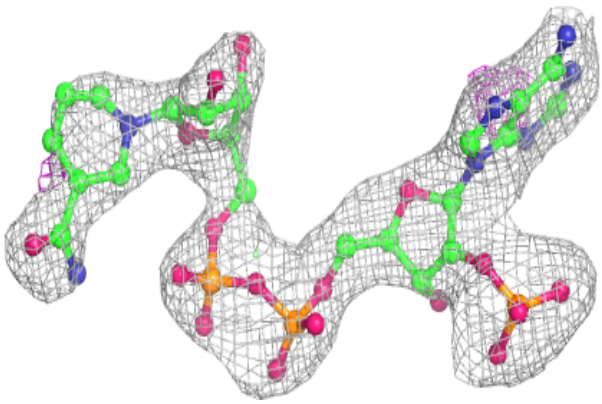


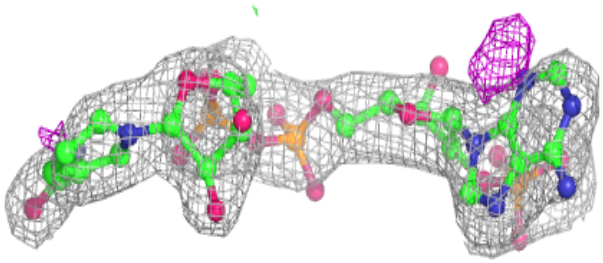


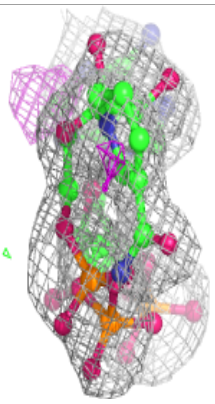


Electron density around NAP F 301:

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

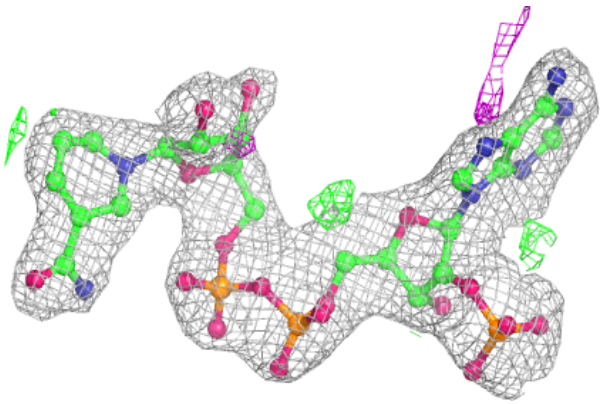


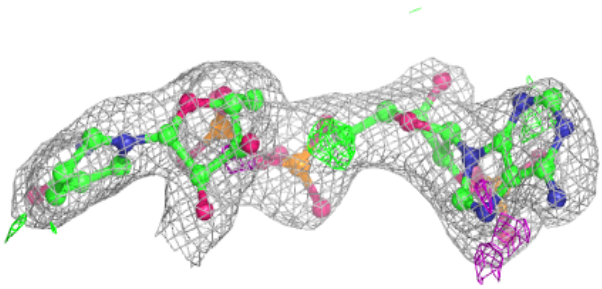


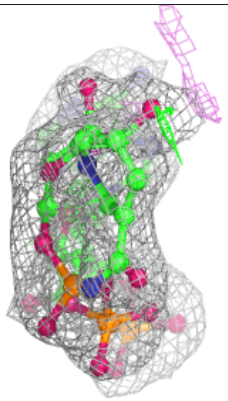


Electron density around NAP B 301:

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

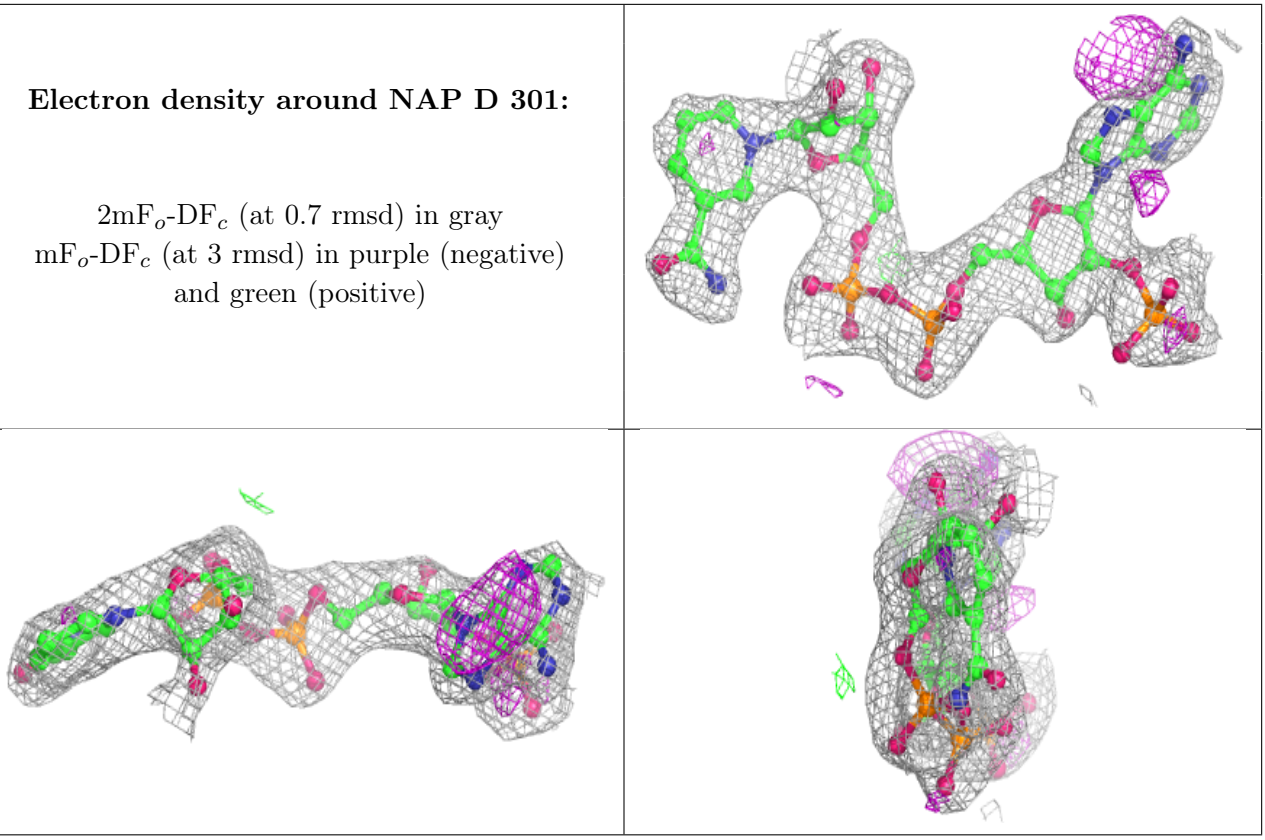






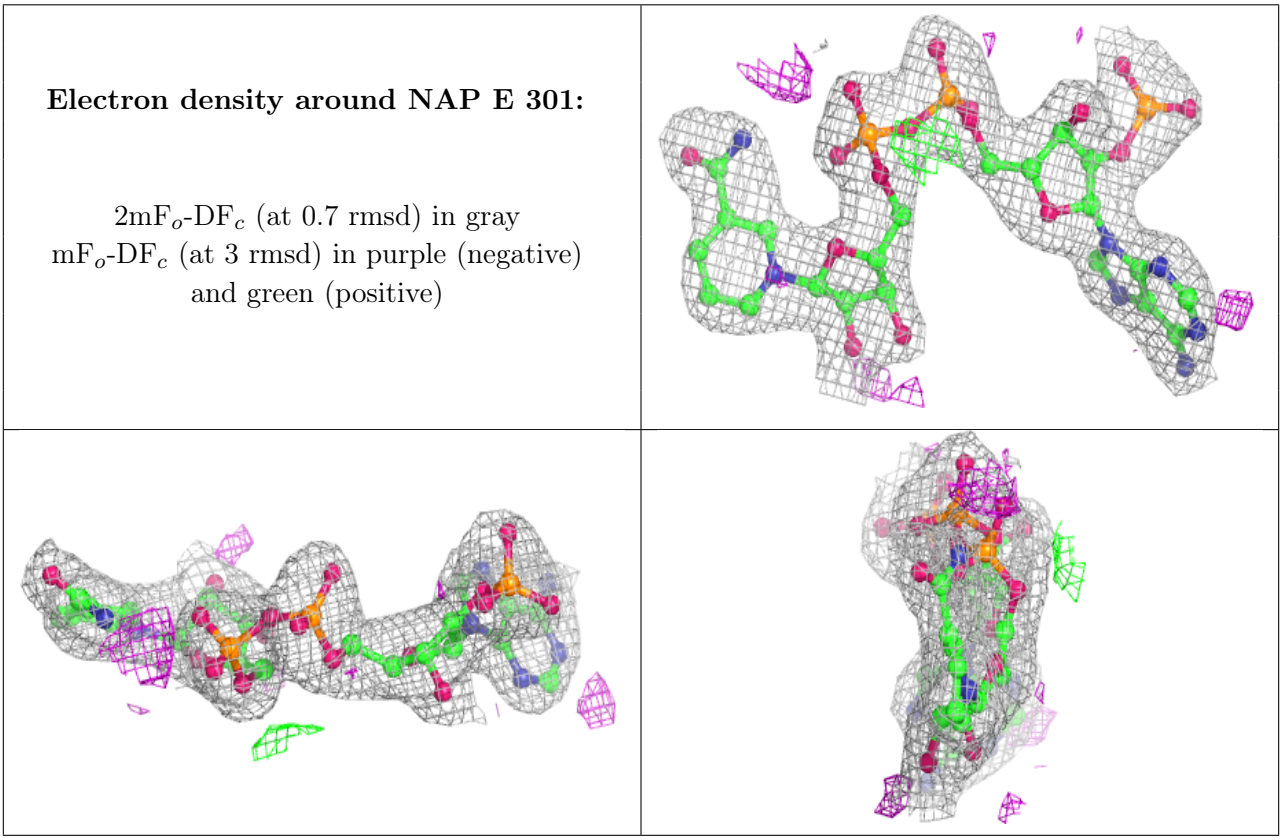
Electron density around NAP D 301:

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



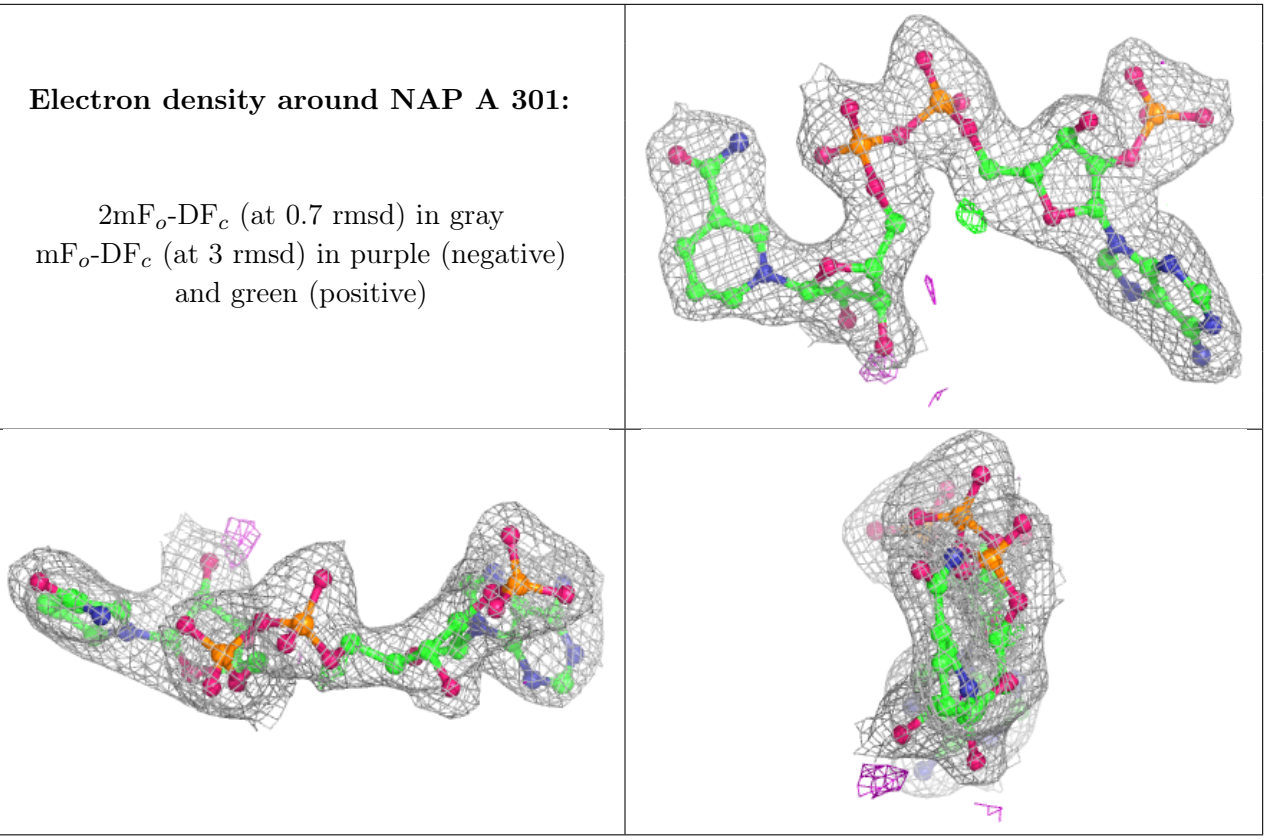
Electron density around NAP E 301:

$2mF_o$-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 301:

$2mF_o$-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.