Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 04:25 AM EDT

PDB ID	:	6SLE
Title	:	Structure of Reductive Aminase from Neosartorya fumigata in complex with NADP+
Authors	:	Sharma, M.; Mangas-Sanchez, J.; Turner, N.J.; Grogan, G.
Deposited on	:	2019-08-19
Resolution	:	2.77 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:

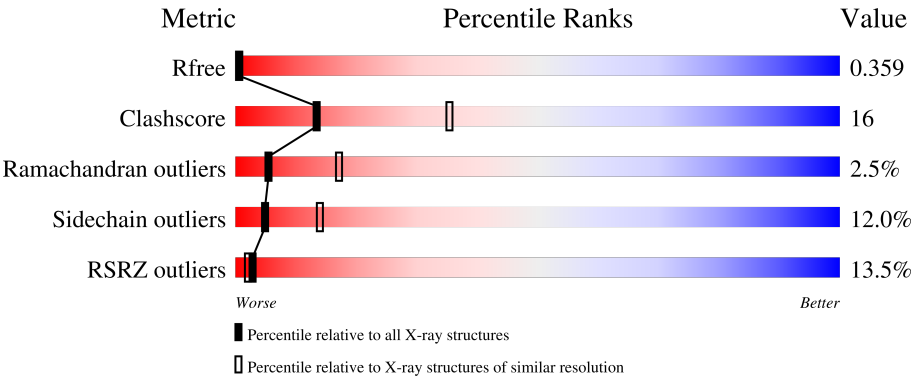
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.77 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.



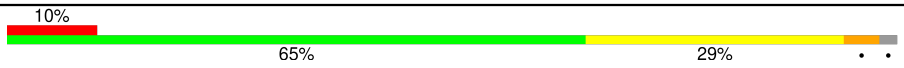
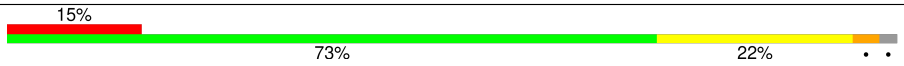
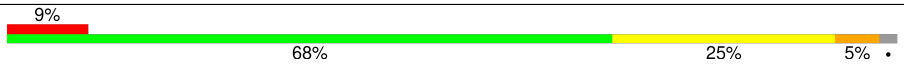
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	285	10% 65% 28% 6%
1	B	285	15% 71% 17% 8%
1	C	285	16% 74% 19%
1	D	285	11% 64% 28% 5%
1	E	285	18% 69% 21% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	285	
1	G	285	
1	H	285	

2 Entry composition (i)

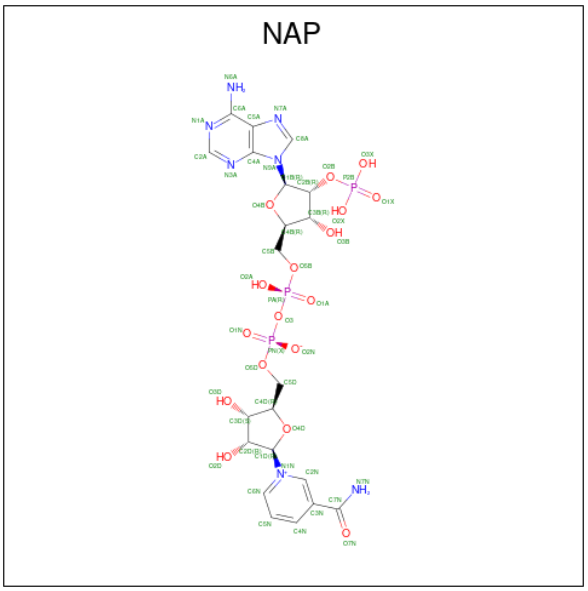
There are 3 unique types of molecules in this entry. The entry contains 15201 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Oxidoreductase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	1	0
			1951	1234	332	374	11			
1	B	261	Total	C	N	O	S	0	1	0
			1648	1032	286	320	10			
1	C	273	Total	C	N	O	S	0	0	0
			1820	1152	315	340	13			
1	D	278	Total	C	N	O	S	0	0	0
			1920	1222	320	367	11			
1	E	268	Total	C	N	O	S	0	0	0
			1708	1070	300	328	10			
1	F	280	Total	C	N	O	S	0	0	0
			1930	1221	326	372	11			
1	G	279	Total	C	N	O	S	0	0	0
			1820	1137	317	353	13			
1	H	278	Total	C	N	O	S	0	0	0
			1915	1210	322	372	11			

- Molecule 2 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
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	D	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		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	15	Total	O	0	0
			15	15		
3	C	8	Total	O	0	0
			8	8		
3	D	11	Total	O	0	0
			11	11		

Continued on next page...

Continued from previous page...

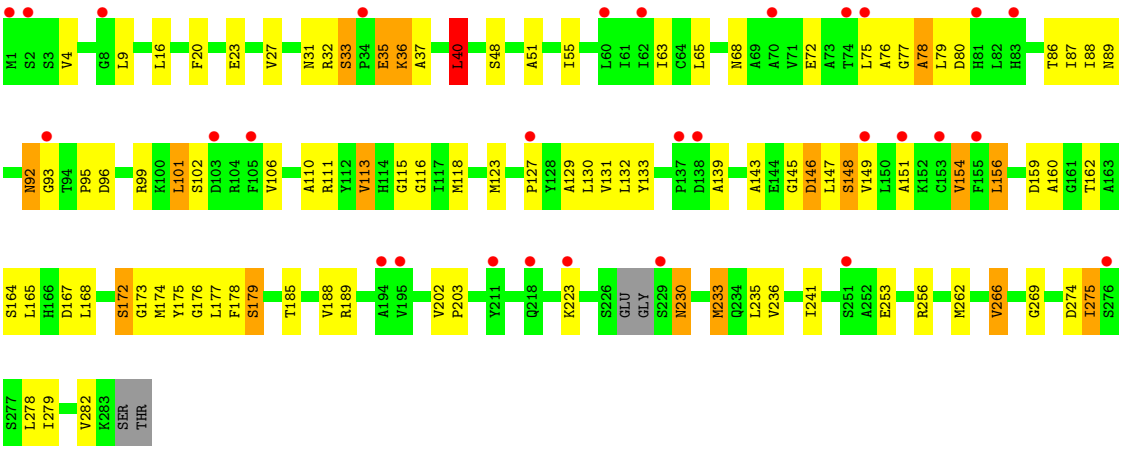
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	15	Total O 15 15	0	0
3	F	14	Total O 14 14	0	0
3	G	13	Total O 13 13	0	0
3	H	14	Total O 14 14	0	0

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.

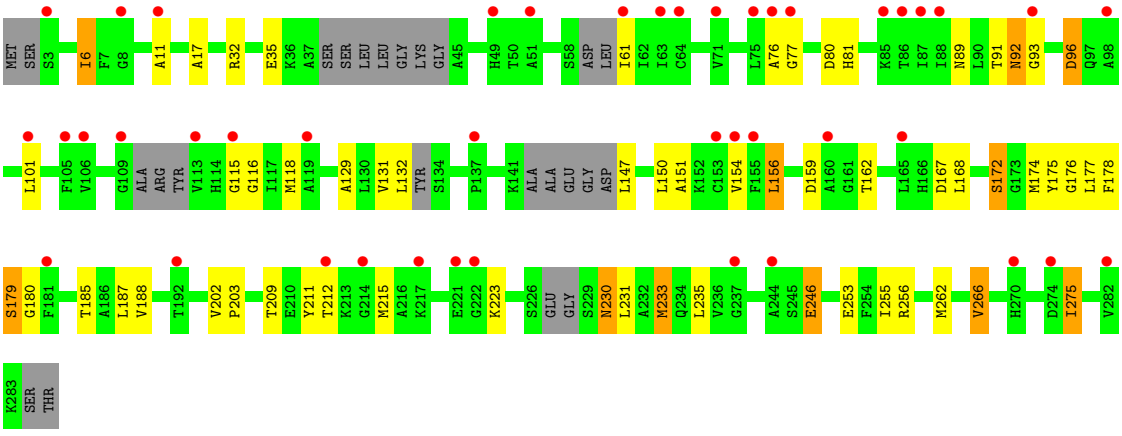
• Molecule 1: Oxidoreductase, putative

Chain A:



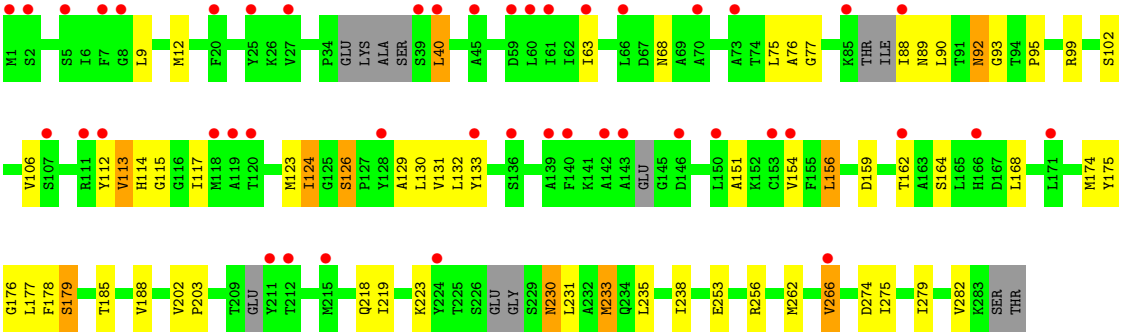
• Molecule 1: Oxidoreductase, putative

Chain B:



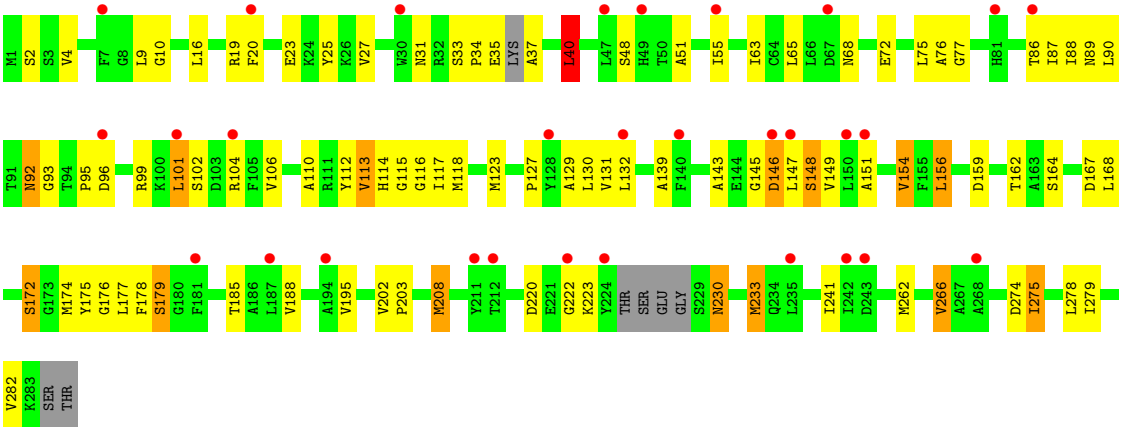
• Molecule 1: Oxidoreductase, putative

Chain C:



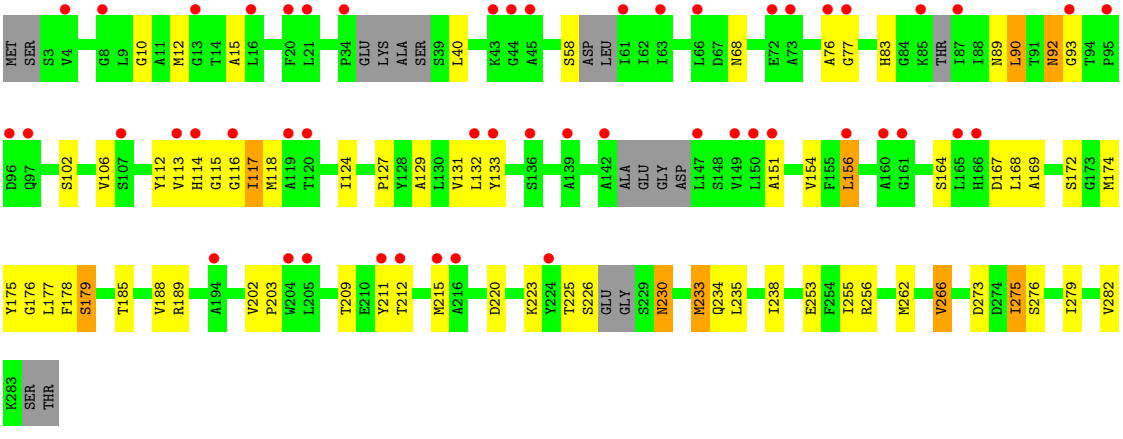
• Molecule 1: Oxidoreductase, putative

Chain D:



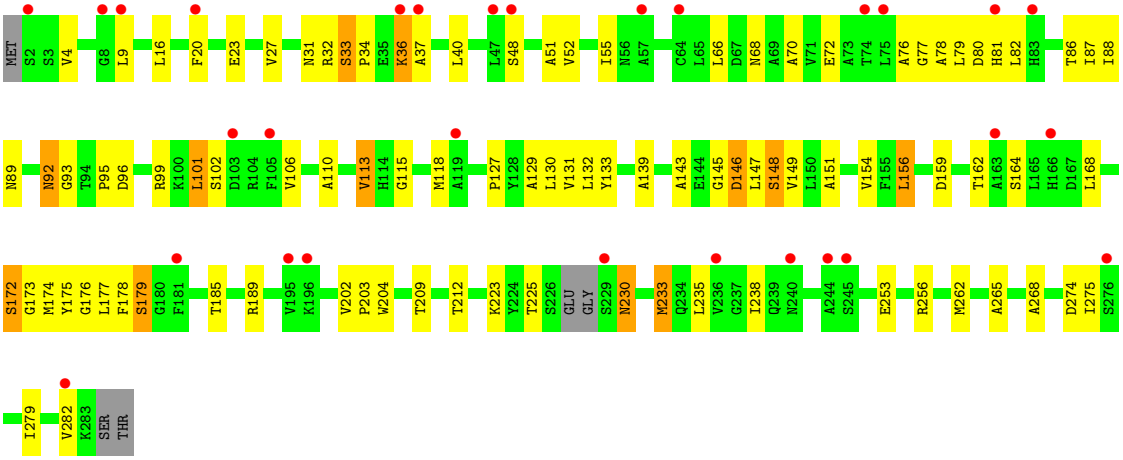
• Molecule 1: Oxidoreductase, putative

Chain E:



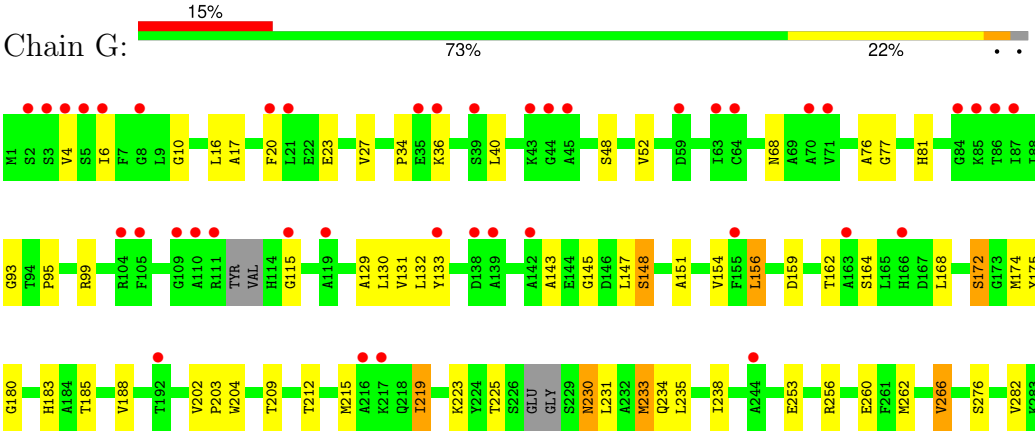
• Molecule 1: Oxidoreductase, putative

Chain F:



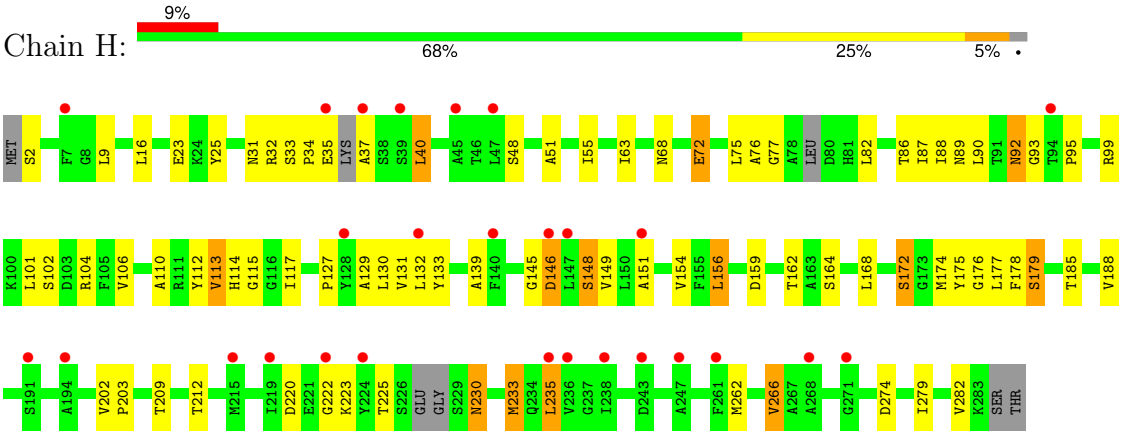
• Molecule 1: Oxidoreductase, putative

Chain G:



• Molecule 1: Oxidoreductase, putative

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.39Å 89.31Å 97.93Å 105.56° 90.00° 93.99°	Depositor
Resolution (Å)	48.28 – 2.77 48.28 – 2.77	Depositor EDS
% Data completeness (in resolution range)	79.0 (48.28-2.77) 79.1 (48.28-2.77)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.286 , 0.357 0.288 , 0.359	Depositor DCC
R_{free} test set	2665 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 32.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Reported twinning fraction	0.866 for H, K, L 0.134 for h,-k,-l	Depositor
Outliers	0 of 53895 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	15201	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5207e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.77	0/1986	0.85	0/2701
1	B	0.81	0/1671	0.84	0/2281
1	C	0.77	0/1846	0.82	0/2510
1	D	0.78	0/1952	0.85	0/2658
1	E	0.78	0/1729	0.83	0/2359
1	F	0.78	0/1962	0.83	0/2673
1	G	0.78	0/1848	0.84	0/2521
1	H	0.78	0/1945	0.85	0/2647
All	All	0.78	0/14939	0.84	0/20350

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1951	0	1816	77	0
1	B	1648	0	1353	47	0
1	C	1820	0	1620	41	0
1	D	1920	0	1801	67	0
1	E	1708	0	1434	70	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1930	0	1782	71	0
1	G	1820	0	1555	53	0
1	H	1915	0	1779	56	0
2	A	48	0	25	4	0
2	B	48	0	25	3	0
2	C	48	0	25	2	0
2	D	48	0	25	5	0
2	E	48	0	25	3	0
2	F	48	0	25	4	0
2	G	48	0	25	6	0
2	H	48	0	25	2	0
3	A	15	0	0	3	0
3	B	15	0	0	2	0
3	C	8	0	0	3	0
3	D	11	0	0	2	0
3	E	15	0	0	5	0
3	F	14	0	0	6	0
3	G	13	0	0	3	0
3	H	14	0	0	0	0
All	All	15201	0	13340	458	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 16.

All (458) 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:127:PRO:HA	1:F:127:PRO:HA	1.20	1.16
1:A:127:PRO:HA	1:H:127:PRO:HA	1.26	1.09
1:A:40:LEU:HD23	1:A:40:LEU:O	1.58	1.02
1:A:111:ARG:CD	1:A:139:ALA:HB2	1.92	1.00
1:E:12:MET:SD	1:E:124:ILE:HD11	2.04	0.98
1:A:145:GLY:O	1:A:148:SER:OG	1.89	0.90
1:F:79:LEU:O	1:F:81:HIS:N	2.04	0.90
1:G:145:GLY:O	1:G:148:SER:OG	1.89	0.90
1:H:145:GLY:O	1:H:148:SER:OG	1.89	0.89
1:D:145:GLY:O	1:D:148:SER:OG	1.90	0.88
1:B:167:ASP:OD1	3:B:401:HOH:O	1.91	0.88
1:F:145:GLY:O	1:F:148:SER:OG	1.89	0.88
1:D:127:PRO:HA	1:F:127:PRO:CA	2.04	0.86
1:D:127:PRO:CA	1:F:127:PRO:HA	2.04	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:LEU:HD12	1:E:117:ILE:HG12	1.57	0.84
1:C:12:MET:SD	1:C:124:ILE:HD11	2.17	0.83
1:B:246[A]:GLU:OE1	1:B:246[A]:GLU:HA	1.78	0.83
1:D:19:ARG:HB2	3:D:401:HOH:O	1.81	0.79
3:F:409:HOH:O	1:G:282:VAL:CB	2.32	0.77
1:A:127:PRO:HA	1:H:127:PRO:CA	2.12	0.76
1:A:92:ASN:HB2	3:A:1102:HOH:O	1.85	0.76
1:A:127:PRO:CA	1:H:127:PRO:HA	2.11	0.75
1:D:63:ILE:HD11	1:D:75:LEU:HD11	1.70	0.73
1:E:234:GLN:NE2	3:E:401:HOH:O	1.91	0.73
1:A:32[B]:ARG:HG2	1:A:32[B]:ARG:HH21	1.53	0.73
1:H:63:ILE:HD11	1:H:75:LEU:HD11	1.73	0.71
1:E:90:LEU:CD1	1:E:117:ILE:HG12	2.20	0.70
1:F:4:VAL:HG11	1:F:20:PHE:CD2	2.26	0.70
1:D:4:VAL:HG11	1:D:20:PHE:CD2	2.26	0.70
1:F:175:TYR:O	1:F:179:SER:OG	2.09	0.70
1:D:90:LEU:HD13	1:D:117:ILE:HD11	1.74	0.69
1:B:253:GLU:OE1	1:B:256:ARG:NH1	2.24	0.69
1:C:63:ILE:HD11	1:C:75:LEU:HD11	1.75	0.69
1:D:145:GLY:HA3	3:D:410:HOH:O	1.92	0.69
1:D:175:TYR:O	1:D:179:SER:OG	2.10	0.68
1:H:90:LEU:HD13	1:H:117:ILE:HD11	1.75	0.68
1:H:82:LEU:HD22	1:H:87:ILE:HD11	1.76	0.68
1:D:175:TYR:CZ	1:E:238:ILE:HD11	2.28	0.67
1:A:175:TYR:O	1:A:179:SER:OG	2.10	0.67
1:A:63:ILE:HD11	1:A:75:LEU:HD11	1.75	0.67
1:A:4:VAL:HG11	1:A:20:PHE:CD2	2.29	0.67
1:D:72:GLU:HG3	1:D:101:LEU:HD11	1.77	0.67
1:C:90:LEU:HD13	1:C:117:ILE:HD11	1.76	0.67
1:G:4:VAL:HG11	1:G:20:PHE:CD2	2.31	0.66
1:E:175:TYR:O	1:E:179:SER:OG	2.10	0.66
1:F:82:LEU:HD22	1:F:87:ILE:HD11	1.76	0.66
1:F:175:TYR:CZ	1:G:238:ILE:HD11	2.31	0.65
1:B:175:TYR:O	1:B:179:SER:OG	2.11	0.65
1:G:81:HIS:HB2	3:G:410:HOH:O	1.96	0.65
1:E:215:MET:HG3	1:E:276:SER:HB3	1.79	0.65
1:C:175:TYR:O	1:C:179:SER:OG	2.11	0.65
1:B:92:ASN:HB3	2:B:301:NAP:O2D	1.98	0.64
1:G:175:TYR:O	1:G:179:SER:OG	2.11	0.64
1:A:253:GLU:OE2	1:A:256:ARG:NH1	2.31	0.63
1:F:9:LEU:HD12	1:F:31:ASN:HB2	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:ALA:O	1:E:172:SER:OG	2.13	0.63
1:F:253:GLU:OE2	1:F:256:ARG:NH1	2.32	0.63
1:H:9:LEU:HD12	1:H:31:ASN:HB2	1.81	0.63
1:A:9:LEU:HD12	1:A:31:ASN:HB2	1.81	0.63
1:G:52:VAL:HA	3:G:410:HOH:O	2.00	0.62
1:H:175:TYR:O	1:H:179:SER:OG	2.11	0.61
1:C:253:GLU:OE2	1:C:256:ARG:NH1	2.33	0.61
1:E:15:ALA:CB	1:E:124:ILE:HD12	2.30	0.61
1:H:235:LEU:HD22	1:H:262:MET:HB3	1.83	0.61
1:A:262:MET:HG3	1:A:278:LEU:HD21	1.82	0.61
1:G:253:GLU:OE2	1:G:256:ARG:NH1	2.32	0.61
1:E:253:GLU:OE2	1:E:256:ARG:NH1	2.34	0.61
1:E:238:ILE:HD13	1:E:262:MET:HE1	1.83	0.61
1:D:9:LEU:HD12	1:D:31:ASN:HB2	1.83	0.60
1:D:168:LEU:O	1:D:172:SER:OG	2.19	0.60
1:A:168:LEU:O	1:A:172:SER:OG	2.20	0.60
1:G:260:GLU:HG2	3:G:412:HOH:O	2.02	0.60
1:G:238:ILE:HD13	1:G:262:MET:HE1	1.83	0.59
1:F:168:LEU:O	1:F:172:SER:OG	2.20	0.59
1:H:168:LEU:O	1:H:172:SER:OG	2.20	0.59
1:A:72:GLU:HG3	1:A:101:LEU:HD11	1.84	0.59
1:F:72:GLU:HG3	1:F:101:LEU:HD11	1.85	0.59
1:D:31:ASN:ND2	1:D:37:ALA:HB3	2.18	0.58
1:D:51:ALA:O	1:D:55:ILE:HG12	2.03	0.58
1:A:51:ALA:O	1:A:55:ILE:HG12	2.02	0.58
1:F:33:SER:OG	2:F:301:NAP:O3X	2.22	0.58
1:F:51:ALA:O	1:F:55:ILE:HG12	2.02	0.58
1:G:168:LEU:O	1:G:172:SER:OG	2.21	0.58
1:G:215:MET:O	1:G:219:ILE:HD13	2.04	0.58
1:G:233:MET:HE2	1:G:233:MET:O	2.04	0.58
1:B:89:ASN:HD21	1:B:91:THR:HB	1.69	0.58
1:H:51:ALA:O	1:H:55:ILE:HG12	2.03	0.58
1:H:112:TYR:OH	1:H:114:HIS:HD2	1.87	0.58
1:H:115:GLY:HA2	1:H:132:LEU:O	2.04	0.57
1:C:112:TYR:OH	1:C:114:HIS:HD2	1.88	0.57
1:C:115:GLY:HA2	1:C:132:LEU:O	2.04	0.57
1:D:115:GLY:HA2	1:D:132:LEU:O	2.04	0.57
1:D:112:TYR:OH	1:D:114:HIS:HD2	1.87	0.57
1:F:31:ASN:ND2	2:F:301:NAP:O2X	2.31	0.57
1:A:35:GLU:OE1	1:A:36:LYS:N	2.38	0.57
1:D:130:LEU:HD21	1:D:154:VAL:HG21	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLY:HA2	1:B:132:LEU:O	2.05	0.57
1:E:115:GLY:HA2	1:E:132:LEU:O	2.05	0.57
1:B:233:MET:HE2	1:B:233:MET:O	2.04	0.56
1:E:112:TYR:OH	1:E:114:HIS:HD2	1.88	0.56
1:E:234:GLN:O	1:E:238:ILE:HD13	2.05	0.56
1:F:87:ILE:HD12	1:F:110:ALA:HB1	1.86	0.56
1:A:160:ALA:HB3	3:A:1105:HOH:O	2.06	0.56
1:B:168:LEU:O	1:B:172:SER:OG	2.22	0.56
1:G:115:GLY:HA2	1:G:132:LEU:O	2.05	0.56
1:A:65:LEU:HD22	2:A:1000:NAP:N3A	2.21	0.56
1:E:233:MET:HE2	1:E:233:MET:O	2.05	0.56
1:A:130:LEU:HD21	1:A:154:VAL:HG21	1.88	0.56
1:F:115:GLY:HA2	1:F:132:LEU:O	2.05	0.56
1:E:102:SER:O	1:E:106:VAL:HG13	2.06	0.55
1:C:92:ASN:N	3:C:402:HOH:O	2.39	0.55
1:B:96:ASP:OD1	1:B:96:ASP:C	2.45	0.55
1:C:92:ASN:CA	3:C:402:HOH:O	2.55	0.55
1:H:130:LEU:HD23	1:H:131:VAL:N	2.22	0.55
1:H:31:ASN:ND2	1:H:37:ALA:HB3	2.22	0.55
1:H:68:ASN:O	1:H:72:GLU:HG3	2.07	0.55
1:D:208:MET:HG3	1:E:174:MET:HG3	1.89	0.54
1:A:115:GLY:HA2	1:A:132:LEU:O	2.06	0.54
2:A:1000:NAP:O2D	1:B:233:MET:HE1	2.08	0.54
1:B:61:ILE:HD12	1:B:61:ILE:N	2.23	0.54
1:F:33:SER:HB2	1:F:36:LYS:CB	2.37	0.54
1:G:234:GLN:O	1:G:238:ILE:HD13	2.08	0.54
1:B:147:LEU:O	1:B:150:LEU:HG	2.08	0.54
1:A:87:ILE:HD12	1:A:110:ALA:HB1	1.90	0.54
1:A:33:SER:HB2	1:A:36:LYS:CB	2.39	0.53
2:A:1000:NAP:O2D	1:B:233:MET:CE	2.56	0.53
1:F:130:LEU:HD23	1:F:131:VAL:N	2.24	0.53
1:A:235:LEU:HD12	1:A:266:VAL:HG11	1.91	0.53
1:C:130:LEU:HD23	1:C:131:VAL:N	2.24	0.53
1:G:130:LEU:HD23	1:G:131:VAL:N	2.23	0.53
1:G:219:ILE:CD1	1:G:276:SER:HB2	2.39	0.53
1:H:72:GLU:CD	1:H:104:ARG:HH22	2.11	0.53
1:H:235:LEU:HD23	1:H:266:VAL:HG11	1.91	0.53
1:H:146:ASP:OD1	1:H:146:ASP:N	2.43	0.52
1:A:269:GLY:O	1:E:225:THR:CB	2.57	0.52
1:E:234:GLN:HG3	3:E:401:HOH:O	2.08	0.52
1:G:174:MET:HG2	1:G:178:PHE:CE2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:ILE:HD12	1:H:110:ALA:HB1	1.92	0.52
1:C:9:LEU:N	2:C:301:NAP:O3B	2.42	0.51
1:E:15:ALA:HB3	1:E:124:ILE:HD12	1.90	0.51
1:H:93:GLY:O	1:H:168:LEU:HD11	2.11	0.51
1:A:146:ASP:OD1	1:A:146:ASP:N	2.43	0.51
1:F:268:ALA:HA	3:F:404:HOH:O	2.10	0.51
1:B:89:ASN:ND2	1:B:91:THR:HB	2.25	0.51
1:B:235:LEU:HD12	1:B:266:VAL:HG11	1.92	0.51
1:E:15:ALA:HB1	1:E:124:ILE:HD12	1.92	0.51
1:A:32[B]:ARG:HG2	1:A:32[B]:ARG:NH2	2.24	0.51
1:A:174:MET:HG2	1:A:178:PHE:CE2	2.45	0.51
1:D:146:ASP:OD1	1:D:146:ASP:N	2.42	0.51
1:A:129:ALA:HB1	1:A:151:ALA:HB2	1.93	0.51
1:F:173:GLY:HA2	1:G:180:GLY:HA3	1.93	0.51
1:B:93:GLY:O	1:B:168:LEU:HD11	2.11	0.51
1:C:93:GLY:O	1:C:168:LEU:HD11	2.11	0.51
1:F:174:MET:HG2	1:F:178:PHE:CE2	2.46	0.51
1:A:102:SER:O	1:A:106:VAL:HG23	2.11	0.51
1:E:230:ASN:O	1:E:233:MET:HG3	2.11	0.51
1:B:174:MET:HG2	1:B:178:PHE:CE2	2.46	0.51
1:E:174:MET:HG2	1:E:178:PHE:CE2	2.46	0.51
1:D:174:MET:HG2	1:D:178:PHE:CE2	2.46	0.50
1:C:174:MET:HG2	1:C:178:PHE:CE2	2.46	0.50
1:D:95:PRO:O	1:D:99:ARG:HG3	2.12	0.50
1:G:230:ASN:O	1:G:233:MET:HG3	2.12	0.50
1:C:218:GLN:NE2	3:C:401:HOH:O	2.06	0.50
1:B:235:LEU:HA	1:B:262:MET:HE3	1.94	0.50
1:F:20:PHE:HB3	1:F:27:VAL:HG22	1.93	0.50
1:A:40:LEU:HD23	1:A:40:LEU:C	2.30	0.50
1:G:93:GLY:O	1:G:168:LEU:HD11	2.12	0.50
1:D:20:PHE:HB3	1:D:27:VAL:HG22	1.92	0.50
1:F:102:SER:O	1:F:106:VAL:HG23	2.12	0.50
1:A:116:GLY:C	1:A:118:MET:HE2	2.32	0.50
1:D:93:GLY:O	1:D:168:LEU:HD11	2.10	0.50
1:D:130:LEU:HD23	1:D:131:VAL:N	2.27	0.50
1:H:174:MET:HG2	1:H:178:PHE:CE2	2.47	0.50
1:C:102:SER:O	1:C:106:VAL:HG23	2.12	0.50
1:F:93:GLY:O	1:F:168:LEU:HD11	2.12	0.50
1:F:233:MET:HE3	2:G:301:NAP:H2D	1.94	0.50
1:H:95:PRO:O	1:H:99:ARG:HG3	2.12	0.50
1:A:20:PHE:HB3	1:A:27:VAL:HG22	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ALA:HB1	1:B:151:ALA:HB2	1.94	0.49
1:D:102:SER:O	1:D:106:VAL:HG23	2.12	0.49
1:B:230:ASN:O	1:B:233:MET:HG3	2.12	0.49
1:D:241:ILE:HG13	1:E:168:LEU:HD22	1.94	0.49
1:D:262:MET:HG3	1:D:278:LEU:HD21	1.93	0.49
1:G:20:PHE:HB3	1:G:27:VAL:CG2	2.42	0.49
1:E:116:GLY:O	1:E:118:MET:HE2	2.12	0.49
1:G:20:PHE:HB3	1:G:27:VAL:HG22	1.93	0.49
1:H:102:SER:O	1:H:106:VAL:HG23	2.13	0.49
1:H:230:ASN:O	1:H:233:MET:HG3	2.13	0.49
1:A:95:PRO:O	1:A:99:ARG:HG3	2.13	0.49
1:F:95:PRO:O	1:F:99:ARG:HG3	2.12	0.49
1:A:78:ALA:O	1:A:80:ASP:N	2.40	0.49
1:E:90:LEU:HB3	1:E:117:ILE:HD11	1.95	0.49
1:F:204:TRP:HE1	1:G:174:MET:HB2	1.78	0.49
1:B:211:TYR:CE2	1:B:215:MET:HE2	2.48	0.49
1:E:226:SER:HA	3:E:406:HOH:O	2.13	0.49
1:F:129:ALA:HB1	1:F:151:ALA:HB2	1.95	0.49
1:G:129:ALA:HB1	1:G:151:ALA:HB2	1.95	0.49
1:G:6:ILE:HD12	1:G:17:ALA:HB2	1.95	0.49
1:G:95:PRO:O	1:G:99:ARG:HG3	2.12	0.49
1:C:230:ASN:O	1:C:233:MET:HG3	2.13	0.49
1:G:183:HIS:HD1	1:G:183:HIS:C	2.16	0.49
1:A:20:PHE:HB3	1:A:27:VAL:CG2	2.43	0.48
1:C:95:PRO:O	1:C:99:ARG:HG3	2.13	0.48
1:D:146:ASP:O	1:D:149:VAL:HG22	2.13	0.48
1:E:129:ALA:HB1	1:E:151:ALA:HB2	1.94	0.48
1:E:238:ILE:N	1:E:238:ILE:HD12	2.27	0.48
1:E:235:LEU:HD12	1:E:266:VAL:HG11	1.94	0.48
1:F:88:ILE:CD1	1:F:113:VAL:HG13	2.43	0.48
1:F:146:ASP:O	1:F:149:VAL:HG22	2.14	0.48
1:A:159:ASP:HB3	1:A:162:THR:OG1	2.14	0.48
1:D:129:ALA:HB1	1:D:151:ALA:HB2	1.95	0.48
1:F:176:GLY:O	1:F:179:SER:OG	2.32	0.48
1:H:176:GLY:O	1:H:179:SER:OG	2.31	0.48
1:E:93:GLY:O	1:E:168:LEU:HD11	2.13	0.48
1:F:146:ASP:OD1	1:F:146:ASP:N	2.42	0.48
1:A:93:GLY:O	1:A:168:LEU:HD11	2.12	0.48
1:A:146:ASP:O	1:A:149:VAL:HG22	2.14	0.48
1:C:176:GLY:O	1:C:179:SER:OG	2.32	0.48
1:A:32[B]:ARG:HA	1:A:32[B]:ARG:NE	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HD23	1:A:131:VAL:N	2.29	0.48
1:F:20:PHE:HB3	1:F:27:VAL:CG2	2.44	0.48
1:F:235:LEU:HA	1:F:262:MET:HE3	1.95	0.48
1:A:230:ASN:O	1:A:233:MET:HG3	2.14	0.48
1:B:176:GLY:O	1:B:179:SER:OG	2.31	0.48
1:C:129:ALA:HB1	1:C:151:ALA:HB2	1.96	0.48
1:E:118:MET:HE3	1:E:167:ASP:HA	1.95	0.48
1:E:211:TYR:CE1	1:E:215:MET:HE1	2.49	0.48
1:C:185:THR:O	1:C:188:VAL:HG12	2.14	0.47
1:D:175:TYR:CB	1:E:255:ILE:HD11	2.44	0.47
1:A:173:GLY:HA2	1:B:180:GLY:HA3	1.97	0.47
1:F:233:MET:CE	2:G:301:NAP:O2D	2.62	0.47
1:G:176:GLY:O	1:G:179:SER:OG	2.32	0.47
1:B:116:GLY:O	1:B:118:MET:HE2	2.14	0.47
1:D:159:ASP:HB3	1:D:162:THR:OG1	2.14	0.47
1:D:20:PHE:HB3	1:D:27:VAL:CG2	2.44	0.47
1:D:116:GLY:O	1:D:118:MET:HE2	2.14	0.47
1:D:176:GLY:O	1:D:179:SER:OG	2.33	0.47
1:H:129:ALA:HB1	1:H:151:ALA:HB2	1.97	0.47
1:H:146:ASP:O	1:H:149:VAL:HG22	2.14	0.47
1:A:116:GLY:O	1:A:118:MET:HE2	2.15	0.47
1:B:233:MET:HE2	1:B:233:MET:C	2.35	0.47
1:E:116:GLY:C	1:E:118:MET:HE2	2.35	0.47
1:B:6:ILE:HD12	1:B:17:ALA:HB2	1.96	0.47
1:D:175:TYR:HB3	1:E:255:ILE:HD11	1.96	0.47
1:F:159:ASP:HB3	1:F:162:THR:OG1	2.15	0.47
1:F:185:THR:CG2	1:F:189:ARG:NH2	2.78	0.47
1:G:238:ILE:N	1:G:238:ILE:HD12	2.29	0.47
1:H:32:ARG:HB3	2:H:1001:NAP:O3X	2.15	0.47
1:H:159:ASP:HB3	1:H:162:THR:OG1	2.15	0.47
1:H:174:MET:O	1:H:177:LEU:HB3	2.15	0.47
1:E:176:GLY:O	1:E:179:SER:OG	2.32	0.47
1:H:235:LEU:CD2	1:H:262:MET:HB3	2.45	0.47
1:C:88:ILE:HD13	1:C:113:VAL:HG13	1.97	0.47
1:E:234:GLN:O	1:E:238:ILE:CD1	2.63	0.47
1:F:174:MET:O	1:F:177:LEU:HB3	2.15	0.46
1:D:208:MET:CG	1:E:174:MET:HG3	2.45	0.46
1:A:176:GLY:O	1:A:179:SER:OG	2.33	0.46
1:C:174:MET:O	1:C:177:LEU:HB3	2.15	0.46
1:E:185:THR:O	1:E:188:VAL:HG12	2.15	0.46
2:D:301:NAP:O2D	1:E:233:MET:HE1	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:MET:O	1:E:177:LEU:HB3	2.16	0.46
1:F:265:ALA:HB2	3:F:406:HOH:O	2.15	0.46
1:G:233:MET:HE2	1:G:233:MET:C	2.35	0.46
1:C:235:LEU:HA	1:C:262:MET:HE3	1.98	0.46
1:E:233:MET:HE2	1:E:233:MET:C	2.36	0.46
1:G:235:LEU:HD23	1:G:262:MET:HE3	1.97	0.46
1:A:31:ASN:ND2	1:A:37:ALA:HB3	2.31	0.46
1:F:86:THR:HG23	1:F:139:ALA:HB1	1.97	0.46
1:G:174:MET:O	1:G:177:LEU:HB3	2.16	0.46
1:G:185:THR:O	1:G:188:VAL:HG12	2.15	0.46
1:B:116:GLY:C	1:B:118:MET:HE2	2.36	0.46
1:B:185:THR:O	1:B:188:VAL:HG12	2.15	0.46
1:A:86:THR:HG23	1:A:139:ALA:HB1	1.98	0.46
1:B:159:ASP:HB3	1:B:162:THR:OG1	2.15	0.46
1:D:65:LEU:O	2:D:301:NAP:C3D	2.64	0.46
1:D:130:LEU:HD21	1:D:154:VAL:CG2	2.46	0.46
1:F:238:ILE:HD12	1:F:262:MET:HE2	1.97	0.46
1:C:159:ASP:HB3	1:C:162:THR:OG1	2.16	0.45
1:C:230:ASN:ND2	1:C:233:MET:H	2.15	0.45
1:D:174:MET:O	1:D:177:LEU:HB3	2.15	0.45
1:H:88:ILE:CD1	1:H:113:VAL:HG13	2.46	0.45
1:A:174:MET:O	1:A:177:LEU:HB3	2.16	0.45
1:C:235:LEU:HD12	1:C:266:VAL:HG11	1.97	0.45
1:E:102:SER:O	1:E:106:VAL:HG22	2.15	0.45
1:F:31:ASN:ND2	1:F:37:ALA:HB3	2.31	0.45
1:F:70:ALA:HB1	2:F:301:NAP:C2A	2.46	0.45
1:G:159:ASP:HB3	1:G:162:THR:OG1	2.16	0.45
1:A:88:ILE:CD1	1:A:113:VAL:HG13	2.46	0.45
1:H:185:THR:O	1:H:188:VAL:HG12	2.16	0.45
1:H:235:LEU:HD22	1:H:262:MET:HE3	1.99	0.45
1:A:173:GLY:HA2	1:B:180:GLY:CA	2.46	0.45
1:F:202:VAL:N	1:F:203:PRO:HD2	2.32	0.45
1:F:230:ASN:ND2	1:F:233:MET:H	2.15	0.45
1:F:233:MET:HE3	2:G:301:NAP:C2D	2.46	0.45
1:G:225:THR:CB	1:H:225:THR:CB	2.94	0.45
1:G:230:ASN:ND2	1:G:233:MET:H	2.15	0.45
1:G:235:LEU:HD12	1:G:266:VAL:HG11	1.98	0.45
1:F:265:ALA:CB	3:F:406:HOH:O	2.63	0.45
1:B:174:MET:O	1:B:177:LEU:HB3	2.16	0.45
1:D:87:ILE:HD12	1:D:110:ALA:HB1	1.97	0.45
1:D:230:ASN:ND2	1:D:233:MET:H	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:VAL:HG23	3:F:410:HOH:O	2.17	0.45
1:G:10:GLY:HA3	2:G:301:NAP:O1A	2.17	0.45
1:A:160:ALA:CB	3:A:1105:HOH:O	2.64	0.45
1:A:230:ASN:ND2	1:A:233:MET:H	2.15	0.45
1:E:12:MET:HG2	1:E:117:ILE:HD12	1.98	0.45
1:E:230:ASN:ND2	1:E:233:MET:H	2.15	0.45
1:A:55:ILE:HD11	1:A:75:LEU:HD21	1.99	0.45
1:B:230:ASN:ND2	1:B:233:MET:H	2.15	0.45
1:H:230:ASN:ND2	1:H:233:MET:H	2.15	0.45
1:B:266:VAL:HG21	3:B:413:HOH:O	2.16	0.45
1:E:202:VAL:N	1:E:203:PRO:HD2	2.32	0.45
1:F:143:ALA:O	1:F:147:LEU:HD12	2.17	0.45
1:H:86:THR:HG23	1:H:139:ALA:HB1	1.99	0.45
1:D:55:ILE:HD11	1:D:75:LEU:CD2	2.47	0.44
1:F:118:MET:HE3	1:G:204:TRP:CH2	2.52	0.44
1:A:165:LEU:HD11	1:B:187:LEU:O	2.17	0.44
1:E:118:MET:HE1	1:E:167:ASP:OD1	2.17	0.44
1:C:202:VAL:N	1:C:203:PRO:HD2	2.32	0.44
1:D:143:ALA:O	1:D:147:LEU:HD12	2.17	0.44
1:D:68:ASN:ND2	1:D:89:ASN:HD21	2.16	0.44
1:D:118:MET:HE3	1:D:167:ASP:HA	1.99	0.44
1:B:202:VAL:N	1:B:203:PRO:HD2	2.33	0.44
1:F:131:VAL:HG23	1:F:151:ALA:HB3	2.00	0.44
1:F:173:GLY:HA2	1:G:180:GLY:CA	2.47	0.44
1:H:202:VAL:N	1:H:203:PRO:HD2	2.33	0.44
1:D:88:ILE:CD1	1:D:113:VAL:HG13	2.47	0.44
1:D:86:THR:HG23	1:D:139:ALA:HB1	1.98	0.44
1:D:202:VAL:N	1:D:203:PRO:HD2	2.33	0.44
1:G:234:GLN:O	1:G:238:ILE:CD1	2.65	0.44
1:H:68:ASN:ND2	1:H:89:ASN:HD21	2.16	0.44
1:A:131:VAL:HG23	1:A:151:ALA:HB3	2.00	0.43
1:H:2:SER:HB3	1:H:25:TYR:CE2	2.53	0.43
1:H:92:ASN:OD1	1:H:92:ASN:C	2.56	0.43
1:A:202:VAL:N	1:A:203:PRO:HD2	2.33	0.43
1:C:92:ASN:OD1	1:C:92:ASN:C	2.56	0.43
1:F:101:LEU:HD12	1:F:101:LEU:HA	1.88	0.43
1:H:92:ASN:HB3	2:H:1001:NAP:O2D	2.18	0.43
1:D:92:ASN:C	1:D:92:ASN:OD1	2.56	0.43
1:A:118:MET:HE1	1:A:167:ASP:OD1	2.18	0.43
1:D:185:THR:O	1:D:188:VAL:HG12	2.17	0.43
1:D:195:VAL:HG23	1:E:220:ASP:OD2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:N	1:D:40:LEU:CD1	2.82	0.43
1:E:92:ASN:OD1	1:E:92:ASN:C	2.56	0.43
1:H:156:LEU:N	1:H:156:LEU:CD2	2.82	0.43
1:B:131:VAL:HG23	1:B:151:ALA:HB3	2.00	0.43
1:H:72:GLU:HB3	1:H:104:ARG:NH1	2.34	0.43
1:B:235:LEU:HA	1:B:235:LEU:HD23	1.89	0.43
1:D:275:ILE:HD13	1:D:275:ILE:O	2.19	0.43
1:E:131:VAL:HG23	1:E:151:ALA:HB3	2.00	0.43
1:D:262:MET:O	1:D:266:VAL:HG13	2.19	0.43
1:F:92:ASN:C	1:F:92:ASN:OD1	2.57	0.43
1:F:185:THR:HG22	1:F:189:ARG:NH2	2.33	0.43
1:F:209:THR:O	1:F:212:THR:OG1	2.36	0.43
1:F:233:MET:HE2	2:G:301:NAP:O2D	2.19	0.43
1:F:279:ILE:O	1:F:282:VAL:HG22	2.19	0.43
1:G:92:ASN:OD1	1:G:92:ASN:C	2.57	0.43
1:H:72:GLU:HG2	1:H:104:ARG:NH2	2.34	0.43
1:A:88:ILE:HD13	1:A:113:VAL:HG13	2.01	0.43
1:B:92:ASN:OD1	1:B:92:ASN:C	2.57	0.43
1:F:68:ASN:ND2	1:F:89:ASN:HD21	2.17	0.43
1:F:265:ALA:HA	3:F:406:HOH:O	2.18	0.43
1:A:92:ASN:C	1:A:92:ASN:OD1	2.57	0.43
1:A:241:ILE:HG13	1:B:168:LEU:HD22	2.01	0.43
1:C:88:ILE:CD1	1:C:113:VAL:HG13	2.49	0.43
1:F:88:ILE:HD13	1:F:113:VAL:HG13	2.00	0.42
1:G:68:ASN:ND2	1:G:89:ASN:HD21	2.17	0.42
1:A:174:MET:CG	1:A:178:PHE:CE2	3.02	0.42
1:A:262:MET:O	1:A:266:VAL:HG13	2.20	0.42
1:D:174:MET:CG	1:D:178:PHE:CE2	3.02	0.42
1:E:211:TYR:CE1	1:E:215:MET:CE	3.01	0.42
1:F:32:ARG:HB3	2:F:301:NAP:O3X	2.19	0.42
1:F:156:LEU:N	1:F:156:LEU:CD2	2.82	0.42
1:A:131:VAL:HB	1:A:133:TYR:CE1	2.54	0.42
1:D:65:LEU:HD22	2:D:301:NAP:N3A	2.34	0.42
2:D:301:NAP:O2D	1:E:233:MET:CE	2.67	0.42
1:G:202:VAL:N	1:G:203:PRO:HD2	2.34	0.42
1:G:209:THR:O	1:G:212:THR:OG1	2.37	0.42
1:A:130:LEU:HD21	1:A:154:VAL:CG2	2.49	0.42
1:C:68:ASN:ND2	1:C:89:ASN:HD21	2.17	0.42
1:D:2:SER:HB3	1:D:25:TYR:CE1	2.55	0.42
1:E:10:GLY:HA3	2:E:301:NAP:O1A	2.19	0.42
1:E:279:ILE:O	1:E:282:VAL:HG22	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:235:LEU:HD13	1:H:235:LEU:HA	1.82	0.42
1:A:185:THR:O	1:A:188:VAL:HG12	2.19	0.42
1:B:11:ALA:N	2:B:301:NAP:O2N	2.52	0.42
1:H:279:ILE:O	1:H:282:VAL:HG22	2.20	0.42
1:A:275:ILE:HD13	1:A:275:ILE:O	2.20	0.42
1:B:32:ARG:CB	2:B:301:NAP:O1X	2.67	0.42
1:D:156:LEU:CD2	1:D:156:LEU:N	2.82	0.42
1:C:123:MET:C	1:C:126:SER:HG	2.20	0.42
1:D:10:GLY:HA3	2:D:301:NAP:O1A	2.20	0.42
1:H:55:ILE:HD11	1:H:75:LEU:CD2	2.50	0.42
1:C:68:ASN:HD22	1:C:89:ASN:HD21	1.68	0.42
1:E:230:ASN:C	3:E:401:HOH:O	2.58	0.42
1:E:238:ILE:HD12	1:E:238:ILE:H	1.84	0.42
1:H:131:VAL:HG23	1:H:151:ALA:HB3	2.01	0.42
1:A:156:LEU:N	1:A:156:LEU:CD2	2.82	0.42
1:C:131:VAL:HG23	1:C:151:ALA:HB3	2.01	0.42
1:E:90:LEU:HD12	1:E:117:ILE:CG1	2.38	0.42
1:A:68:ASN:ND2	1:A:89:ASN:HD21	2.18	0.41
1:A:279:ILE:O	1:A:282:VAL:HG22	2.19	0.41
1:C:219:ILE:HD13	1:C:279:ILE:HD13	2.01	0.41
1:D:116:GLY:C	1:D:118:MET:HE2	2.39	0.41
1:E:127:PRO:HG3	3:E:412:HOH:O	2.19	0.41
1:F:131:VAL:HB	1:F:133:TYR:CE1	2.55	0.41
1:G:143:ALA:O	1:G:147:LEU:HD12	2.20	0.41
1:A:31:ASN:ND2	2:A:1000:NAP:O2X	2.41	0.41
1:E:275:ILE:O	1:E:275:ILE:HD13	2.20	0.41
1:A:32[B]:ARG:NE	1:A:32[B]:ARG:CA	2.83	0.41
1:C:238:ILE:HD12	1:C:262:MET:HE2	2.02	0.41
1:E:92:ASN:HB3	2:E:301:NAP:O2D	2.19	0.41
1:G:131:VAL:HG23	1:G:151:ALA:HB3	2.01	0.41
1:B:156:LEU:N	1:B:156:LEU:CD2	2.83	0.41
1:B:262:MET:O	1:B:266:VAL:HG13	2.21	0.41
1:C:75:LEU:HD23	1:C:75:LEU:HA	1.88	0.41
1:E:156:LEU:N	1:E:156:LEU:CD2	2.83	0.41
1:E:262:MET:O	1:E:266:VAL:HG13	2.21	0.41
1:E:68:ASN:ND2	1:E:89:ASN:HD21	2.17	0.41
1:E:174:MET:CG	1:E:178:PHE:CE2	3.04	0.41
1:E:209:THR:O	1:E:212:THR:OG1	2.37	0.41
1:H:174:MET:CG	1:H:178:PHE:CE2	3.04	0.41
1:H:262:MET:O	1:H:266:VAL:HG13	2.20	0.41
1:A:143:ALA:O	1:A:147:LEU:HD12	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:VAL:HB	1:C:133:TYR:CE1	2.56	0.41
1:E:68:ASN:HD22	1:E:89:ASN:HD21	1.68	0.41
1:G:156:LEU:N	1:G:156:LEU:CD2	2.83	0.41
1:C:123:MET:O	1:C:126:SER:OG	2.32	0.41
1:G:174:MET:CG	1:G:178:PHE:CE2	3.04	0.41
1:A:123:MET:O	1:A:129:ALA:HB2	2.20	0.41
1:B:275:ILE:HD13	1:B:275:ILE:O	2.21	0.41
1:C:9:LEU:H	2:C:301:NAP:HO3A	1.69	0.41
1:D:131:VAL:HG23	1:D:151:ALA:HB3	2.02	0.41
1:D:279:ILE:O	1:D:282:VAL:HG22	2.21	0.41
1:E:131:VAL:HB	1:E:133:TYR:CE1	2.56	0.41
1:E:235:LEU:HD23	1:E:262:MET:HE3	2.03	0.41
1:F:79:LEU:C	1:F:81:HIS:N	2.73	0.41
1:H:209:THR:O	1:H:212:THR:OG1	2.39	0.41
1:C:156:LEU:N	1:C:156:LEU:CD2	2.83	0.41
1:D:40:LEU:HD13	1:D:40:LEU:H	1.86	0.41
1:F:174:MET:CG	1:F:178:PHE:CE2	3.03	0.41
1:G:131:VAL:HB	1:G:133:TYR:CE1	2.56	0.41
1:C:279:ILE:O	1:C:282:VAL:HG22	2.22	0.40
1:F:87:ILE:HD12	1:F:110:ALA:CB	2.51	0.40
1:H:131:VAL:HB	1:H:133:TYR:CE1	2.56	0.40
1:E:117:ILE:HB	2:E:301:NAP:H5N	2.03	0.40
1:H:88:ILE:HD13	1:H:113:VAL:HG13	2.03	0.40
1:D:88:ILE:HD13	1:D:113:VAL:HG13	2.03	0.40
1:G:68:ASN:HD22	1:G:89:ASN:HD21	1.70	0.40
1:A:87:ILE:HD12	1:A:110:ALA:CB	2.52	0.40
1:D:123:MET:O	1:D:129:ALA:HB2	2.21	0.40
1:F:68:ASN:HD22	1:F:89:ASN:HD21	1.69	0.40
1:F:233:MET:CE	2:G:301:NAP:H2D	2.52	0.40
1:G:262:MET:O	1:G:266:VAL:HG13	2.21	0.40
1:B:174:MET:CG	1:B:178:PHE:CE2	3.04	0.40
1:B:209:THR:O	1:B:212:THR:OG1	2.38	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	278/285 (98%)	244 (88%)	26 (9%)	8 (3%)	4	14
1	B	248/285 (87%)	220 (89%)	22 (9%)	6 (2%)	6	18
1	C	261/285 (92%)	233 (89%)	23 (9%)	5 (2%)	8	23
1	D	272/285 (95%)	245 (90%)	20 (7%)	7 (3%)	5	16
1	E	256/285 (90%)	229 (90%)	22 (9%)	5 (2%)	7	22
1	F	276/285 (97%)	243 (88%)	24 (9%)	9 (3%)	4	11
1	G	273/285 (96%)	243 (89%)	23 (8%)	7 (3%)	5	16
1	H	270/285 (95%)	244 (90%)	19 (7%)	7 (3%)	5	16
All	All	2134/2280 (94%)	1901 (89%)	179 (8%)	54 (2%)	5	17

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	GLU
1	E	40	LEU
1	F	80	ASP
1	G	40	LEU
1	H	40	LEU
1	A	40	LEU
1	C	40	LEU
1	D	40	LEU
1	F	40	LEU
1	H	77	GLY
1	A	36	LYS
1	A	78	ALA
1	B	77	GLY
1	C	76	ALA
1	E	76	ALA
1	F	36	LYS
1	F	78	ALA
1	G	76	ALA
1	A	76	ALA
1	A	154	VAL
1	B	76	ALA
1	B	154	VAL
1	B	223	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	154	VAL
1	D	76	ALA
1	D	154	VAL
1	D	223	LYS
1	E	154	VAL
1	F	76	ALA
1	F	154	VAL
1	F	223	LYS
1	G	36	LYS
1	G	154	VAL
1	G	223	LYS
1	H	76	ALA
1	H	154	VAL
1	H	223	LYS
1	A	79	LEU
1	A	223	LYS
1	C	223	LYS
1	E	223	LYS
1	B	80	ASP
1	E	77	GLY
1	C	77	GLY
1	D	77	GLY
1	D	34	PRO
1	G	77	GLY
1	H	34	PRO
1	A	77	GLY
1	D	222	GLY
1	F	34	PRO
1	F	77	GLY
1	H	222	GLY
1	G	34	PRO

5.3.2 Protein sidechains (i)

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	177/221 (80%)	154 (87%)	23 (13%)	4 11
1	B	116/221 (52%)	100 (86%)	16 (14%)	3 10
1	C	147/221 (66%)	133 (90%)	14 (10%)	8 23
1	D	176/221 (80%)	152 (86%)	24 (14%)	3 10
1	E	125/221 (57%)	110 (88%)	15 (12%)	5 14
1	F	173/221 (78%)	153 (88%)	20 (12%)	5 15
1	G	142/221 (64%)	128 (90%)	14 (10%)	8 21
1	H	176/221 (80%)	154 (88%)	22 (12%)	4 13
All	All	1232/1768 (70%)	1084 (88%)	148 (12%)	5 14

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	23	GLU
1	A	33	SER
1	A	35	GLU
1	A	40	LEU
1	A	48	SER
1	A	92	ASN
1	A	96	ASP
1	A	101	LEU
1	A	113	VAL
1	A	146	ASP
1	A	148	SER
1	A	156	LEU
1	A	164	SER
1	A	172	SER
1	A	179	SER
1	A	189	ARG
1	A	230	ASN
1	A	233	MET
1	A	236	VAL
1	A	266	VAL
1	A	274	ASP
1	A	275	ILE
1	B	6	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	81	HIS
1	B	92	ASN
1	B	96	ASP
1	B	101	LEU
1	B	156	LEU
1	B	172	SER
1	B	179	SER
1	B	230	ASN
1	B	231	LEU
1	B	233	MET
1	B	246[A]	GLU
1	B	246[B]	GLU
1	B	255	ILE
1	B	266	VAL
1	B	275	ILE
1	C	40	LEU
1	C	92	ASN
1	C	113	VAL
1	C	124	ILE
1	C	126	SER
1	C	156	LEU
1	C	164	SER
1	C	179	SER
1	C	230	ASN
1	C	231	LEU
1	C	233	MET
1	C	266	VAL
1	C	274	ASP
1	C	275	ILE
1	D	16	LEU
1	D	23	GLU
1	D	33	SER
1	D	35	GLU
1	D	40	LEU
1	D	48	SER
1	D	92	ASN
1	D	96	ASP
1	D	101	LEU
1	D	104	ARG
1	D	113	VAL
1	D	146	ASP
1	D	148	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	156	LEU
1	D	164	SER
1	D	172	SER
1	D	179	SER
1	D	208	MET
1	D	220	ASP
1	D	230	ASN
1	D	233	MET
1	D	266	VAL
1	D	274	ASP
1	D	275	ILE
1	E	58	SER
1	E	83	HIS
1	E	90	LEU
1	E	92	ASN
1	E	113	VAL
1	E	117	ILE
1	E	156	LEU
1	E	164	SER
1	E	179	SER
1	E	189	ARG
1	E	230	ASN
1	E	233	MET
1	E	266	VAL
1	E	273	ASP
1	E	275	ILE
1	F	16	LEU
1	F	23	GLU
1	F	33	SER
1	F	48	SER
1	F	66	LEU
1	F	92	ASN
1	F	96	ASP
1	F	101	LEU
1	F	113	VAL
1	F	146	ASP
1	F	148	SER
1	F	156	LEU
1	F	164	SER
1	F	172	SER
1	F	179	SER
1	F	225	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	230	ASN
1	F	233	MET
1	F	274	ASP
1	F	275	ILE
1	G	16	LEU
1	G	23	GLU
1	G	48	SER
1	G	92	ASN
1	G	148	SER
1	G	156	LEU
1	G	164	SER
1	G	172	SER
1	G	179	SER
1	G	219	ILE
1	G	230	ASN
1	G	231	LEU
1	G	233	MET
1	G	266	VAL
1	H	16	LEU
1	H	23	GLU
1	H	33	SER
1	H	35	GLU
1	H	40	LEU
1	H	48	SER
1	H	72	GLU
1	H	92	ASN
1	H	101	LEU
1	H	113	VAL
1	H	146	ASP
1	H	148	SER
1	H	156	LEU
1	H	164	SER
1	H	172	SER
1	H	179	SER
1	H	220	ASP
1	H	230	ASN
1	H	233	MET
1	H	235	LEU
1	H	266	VAL
1	H	274	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	68	ASN
1	A	218	GLN
1	A	230	ASN
1	B	89	ASN
1	B	218	GLN
1	B	230	ASN
1	B	248	GLN
1	C	56	ASN
1	C	68	ASN
1	C	114	HIS
1	C	230	ASN
1	D	56	ASN
1	D	68	ASN
1	D	114	HIS
1	D	218	GLN
1	D	230	ASN
1	D	248	GLN
1	E	56	ASN
1	E	68	ASN
1	E	114	HIS
1	E	218	GLN
1	E	230	ASN
1	E	248	GLN
1	F	56	ASN
1	F	68	ASN
1	F	218	GLN
1	F	230	ASN
1	G	56	ASN
1	G	68	ASN
1	G	218	GLN
1	G	230	ASN
1	G	248	GLN
1	H	56	ASN
1	H	68	ASN
1	H	114	HIS
1	H	218	GLN
1	H	230	ASN
1	H	248	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	F	301	-	46,52,52	1.38	5 (10%)	61,80,80	2.08	16 (26%)
2	NAP	H	1001	-	46,52,52	1.54	8 (17%)	61,80,80	2.10	14 (22%)
2	NAP	B	301	-	46,52,52	1.17	4 (8%)	61,80,80	1.43	10 (16%)
2	NAP	A	1000	-	46,52,52	1.54	7 (15%)	61,80,80	2.02	18 (29%)
2	NAP	C	301	-	46,52,52	0.92	2 (4%)	61,80,80	1.40	8 (13%)
2	NAP	E	301	-	46,52,52	0.97	3 (6%)	61,80,80	1.23	6 (9%)
2	NAP	D	301	-	46,52,52	1.39	7 (15%)	61,80,80	2.19	17 (27%)
2	NAP	G	301	-	46,52,52	1.15	4 (8%)	61,80,80	1.49	9 (14%)

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	F	301	-	-	14/31/67/67	0/5/5/5
2	NAP	H	1001	-	-	11/31/67/67	0/5/5/5
2	NAP	B	301	-	-	11/31/67/67	0/5/5/5
2	NAP	A	1000	-	-	7/31/67/67	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	C	301	-	-	12/31/67/67	0/5/5/5
2	NAP	E	301	-	-	14/31/67/67	0/5/5/5
2	NAP	D	301	-	-	2/31/67/67	0/5/5/5
2	NAP	G	301	-	-	7/31/67/67	0/5/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NAP	O4B-C1B	5.00	1.47	1.40
2	A	1000	NAP	PN-O3	4.32	1.64	1.59
2	H	1001	NAP	O4B-C1B	4.23	1.46	1.40
2	D	301	NAP	O4B-C1B	4.17	1.46	1.40
2	A	1000	NAP	O4D-C1D	4.06	1.46	1.40
2	F	301	NAP	O4D-C1D	4.04	1.46	1.40
2	H	1001	NAP	C2N-N1N	-3.86	1.30	1.35
2	B	301	NAP	O4D-C1D	3.70	1.45	1.40
2	A	1000	NAP	O4B-C1B	3.43	1.45	1.40
2	H	1001	NAP	O4D-C1D	3.29	1.45	1.40
2	D	301	NAP	C4N-C3N	-3.20	1.34	1.39
2	G	301	NAP	O4B-C1B	3.16	1.45	1.40
2	A	1000	NAP	PA-O3	3.15	1.62	1.59
2	H	1001	NAP	P2B-O2B	3.06	1.64	1.59
2	A	1000	NAP	C2N-N1N	2.89	1.38	1.35
2	H	1001	NAP	C3N-C7N	-2.87	1.46	1.50
2	C	301	NAP	O4B-C1B	2.71	1.44	1.40
2	E	301	NAP	O4D-C1D	2.70	1.44	1.40
2	B	301	NAP	C2A-N3A	2.65	1.36	1.32
2	H	1001	NAP	C8A-N7A	2.63	1.39	1.34
2	B	301	NAP	PN-O3	-2.63	1.56	1.59
2	G	301	NAP	C2A-N3A	2.51	1.36	1.32
2	G	301	NAP	P2B-O2B	2.50	1.63	1.59
2	D	301	NAP	O4D-C1D	2.37	1.44	1.40
2	A	1000	NAP	C2A-N3A	2.36	1.35	1.32
2	D	301	NAP	C8A-N7A	2.36	1.39	1.34
2	D	301	NAP	PN-O3	2.33	1.62	1.59
2	D	301	NAP	C6A-C5A	2.30	1.52	1.43
2	A	1000	NAP	PA-O1A	2.30	1.58	1.50
2	E	301	NAP	C2A-N3A	2.28	1.35	1.32
2	C	301	NAP	P2B-O2B	2.25	1.63	1.59
2	B	301	NAP	P2B-O2B	2.21	1.63	1.59
2	H	1001	NAP	C6A-C5A	2.21	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1001	NAP	C2A-N3A	2.19	1.35	1.32
2	F	301	NAP	C7N-N7N	2.18	1.37	1.33
2	E	301	NAP	O4B-C1B	2.14	1.43	1.40
2	D	301	NAP	PA-O3	2.10	1.61	1.59
2	F	301	NAP	C2D-C3D	-2.07	1.47	1.53
2	F	301	NAP	P2B-O1X	2.05	1.56	1.50
2	G	301	NAP	PA-O3	2.01	1.61	1.59

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1001	NAP	O4B-C1B-N9A	9.26	121.03	108.75
2	D	301	NAP	O4B-C1B-N9A	7.45	118.63	108.75
2	D	301	NAP	O3B-C3B-C4B	-6.43	92.60	111.08
2	H	1001	NAP	C4D-O4D-C1D	-6.00	104.43	109.92
2	F	301	NAP	O4B-C1B-N9A	5.55	116.10	108.75
2	A	1000	NAP	O4B-C1B-N9A	5.43	115.95	108.75
2	F	301	NAP	C6N-N1N-C2N	-5.25	117.41	121.88
2	F	301	NAP	N3A-C2A-N1A	-5.19	121.63	128.67
2	A	1000	NAP	N3A-C2A-N1A	-4.98	121.91	128.67
2	C	301	NAP	N3A-C2A-N1A	-4.43	122.67	128.67
2	H	1001	NAP	C5N-C4N-C3N	-4.38	116.06	120.36
2	D	301	NAP	N3A-C2A-N1A	-4.35	122.77	128.67
2	D	301	NAP	O3-PN-O1N	-4.34	97.65	110.70
2	A	1000	NAP	O2N-PN-O1N	4.30	132.46	112.44
2	F	301	NAP	P2B-O2B-C2B	-4.23	112.12	123.43
2	D	301	NAP	C6N-N1N-C2N	-4.07	118.42	121.88
2	A	1000	NAP	O2A-PA-O3	3.98	118.02	107.27
2	A	1000	NAP	O2D-C2D-C3D	-3.80	99.64	111.82
2	A	1000	NAP	O4B-C1B-C2B	-3.78	100.15	106.61
2	F	301	NAP	C4D-O4D-C1D	-3.71	106.53	109.92
2	G	301	NAP	C4B-O4B-C1B	3.69	113.31	109.92
2	F	301	NAP	O3X-P2B-O2X	3.69	121.64	107.80
2	F	301	NAP	C4A-C5A-N7A	-3.69	105.44	109.34
2	D	301	NAP	C5N-C4N-C3N	-3.65	116.78	120.36
2	D	301	NAP	C5B-C4B-C3B	-3.59	102.30	115.21
2	G	301	NAP	N3A-C2A-N1A	-3.54	123.87	128.67
2	B	301	NAP	N3A-C2A-N1A	-3.52	123.90	128.67
2	B	301	NAP	C4B-O4B-C1B	3.45	113.08	109.92
2	H	1001	NAP	C4A-C5A-N7A	-3.40	105.74	109.34
2	H	1001	NAP	O3-PA-O1A	-3.40	100.48	110.70
2	H	1001	NAP	N3A-C2A-N1A	-3.37	124.10	128.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	NAP	O4B-C1B-N9A	3.34	113.17	108.75
2	G	301	NAP	C4A-C5A-N7A	-3.28	105.87	109.34
2	A	1000	NAP	O5B-PA-O1A	3.21	121.66	108.94
2	A	1000	NAP	P2B-O2B-C2B	-3.21	114.86	123.43
2	D	301	NAP	C4A-C5A-N7A	-3.19	105.97	109.34
2	B	301	NAP	O2D-C2D-C3D	-3.18	101.62	111.82
2	A	1000	NAP	O3B-C3B-C4B	-3.14	102.07	111.08
2	B	301	NAP	C4A-C5A-N7A	-3.13	106.03	109.34
2	F	301	NAP	C5N-C4N-C3N	-3.11	117.31	120.36
2	E	301	NAP	N3A-C2A-N1A	-3.11	124.45	128.67
2	D	301	NAP	O2N-PN-O1N	3.10	126.86	112.44
2	F	301	NAP	O4D-C4D-C3D	3.10	111.30	105.15
2	G	301	NAP	O7N-C7N-N7N	-3.07	118.17	122.62
2	E	301	NAP	O4B-C1B-N9A	3.02	112.75	108.75
2	D	301	NAP	O3B-C3B-C2B	3.00	119.58	111.19
2	E	301	NAP	C4A-C5A-N7A	-2.98	106.19	109.34
2	F	301	NAP	C5A-C6A-N6A	2.97	124.84	120.31
2	H	1001	NAP	C2B-C1B-N9A	-2.96	105.97	112.56
2	B	301	NAP	O7N-C7N-N7N	-2.95	118.35	122.62
2	D	301	NAP	O4B-C4B-C5B	2.93	118.72	109.33
2	B	301	NAP	O7N-C7N-C3N	2.92	123.17	119.60
2	A	1000	NAP	O2X-P2B-O2B	-2.92	94.47	105.85
2	E	301	NAP	C6N-N1N-C2N	-2.89	119.42	121.88
2	B	301	NAP	O4D-C4D-C5D	-2.82	100.31	109.33
2	G	301	NAP	C3N-C7N-N7N	2.81	121.21	117.74
2	A	1000	NAP	O2X-P2B-O1X	2.81	121.77	110.83
2	H	1001	NAP	O7N-C7N-C3N	-2.77	116.22	119.60
2	A	1000	NAP	C4D-O4D-C1D	-2.76	107.40	109.92
2	C	301	NAP	C4A-C5A-N7A	-2.70	106.49	109.34
2	A	1000	NAP	N6A-C6A-N1A	2.68	124.07	118.33
2	F	301	NAP	O3B-C3B-C4B	-2.68	103.37	111.08
2	A	1000	NAP	O3X-P2B-O2X	2.66	117.77	107.80
2	C	301	NAP	O4D-C4D-C3D	2.63	110.38	105.15
2	F	301	NAP	O2D-C2D-C3D	-2.59	103.53	111.82
2	A	1000	NAP	C5D-C4D-C3D	-2.59	105.90	115.21
2	C	301	NAP	O4B-C1B-C2B	-2.56	102.25	106.61
2	F	301	NAP	O3B-C3B-C2B	-2.55	104.06	111.19
2	C	301	NAP	O3D-C3D-C2D	2.53	119.93	111.82
2	A	1000	NAP	O3-PN-O1N	-2.53	103.11	110.70
2	H	1001	NAP	O4D-C4D-C3D	2.52	110.16	105.15
2	H	1001	NAP	O5B-C5B-C4B	2.50	117.52	108.99
2	F	301	NAP	O2X-P2B-O2B	-2.50	96.10	105.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	NAP	O7N-C7N-N7N	-2.45	119.08	122.62
2	G	301	NAP	C2B-C3B-C4B	2.41	107.17	101.99
2	D	301	NAP	O2A-PA-O3	2.40	113.76	107.27
2	H	1001	NAP	C5A-C6A-N6A	2.38	123.94	120.31
2	D	301	NAP	O3X-P2B-O2B	-2.38	96.59	105.85
2	E	301	NAP	C4B-O4B-C1B	2.35	112.08	109.92
2	D	301	NAP	C6N-C5N-C4N	2.31	122.77	119.45
2	C	301	NAP	C4D-O4D-C1D	-2.30	107.81	109.92
2	B	301	NAP	P2B-O2B-C2B	-2.26	117.38	123.43
2	D	301	NAP	C1B-N9A-C4A	-2.26	122.66	126.64
2	B	301	NAP	C6N-N1N-C2N	-2.19	120.01	121.88
2	F	301	NAP	C5A-C6A-N1A	-2.18	115.02	120.23
2	D	301	NAP	O2D-C2D-C3D	2.16	118.74	111.82
2	G	301	NAP	O2X-P2B-O1X	2.16	119.24	110.83
2	H	1001	NAP	O2N-PN-O1N	2.15	122.43	112.44
2	C	301	NAP	C4B-O4B-C1B	2.12	111.87	109.92
2	G	301	NAP	O4B-C4B-C3B	-2.12	100.94	105.15
2	E	301	NAP	O3X-P2B-O2X	2.11	115.73	107.80
2	F	301	NAP	O7N-C7N-C3N	-2.10	117.03	119.60
2	A	1000	NAP	C1B-N9A-C4A	-2.09	122.96	126.64
2	D	301	NAP	O3X-P2B-O2X	2.09	115.65	107.80
2	B	301	NAP	C3B-C2B-C1B	2.07	106.77	102.81
2	H	1001	NAP	O2N-PN-O3	2.07	112.87	107.27
2	H	1001	NAP	O7N-C7N-N7N	2.05	125.58	122.62
2	A	1000	NAP	O2B-P2B-O1X	-2.02	102.13	109.33

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	NAP	C5B-O5B-PA-O1A
2	A	1000	NAP	C5B-O5B-PA-O2A
2	A	1000	NAP	C5B-O5B-PA-O3
2	A	1000	NAP	O4D-C1D-N1N-C2N
2	A	1000	NAP	O4D-C1D-N1N-C6N
2	B	301	NAP	C5B-O5B-PA-O1A
2	B	301	NAP	C5B-O5B-PA-O2A
2	B	301	NAP	C5B-O5B-PA-O3
2	B	301	NAP	C5D-O5D-PN-O2N
2	C	301	NAP	C5B-O5B-PA-O1A
2	C	301	NAP	C5B-O5B-PA-O3
2	C	301	NAP	O4B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	301	NAP	C3B-C4B-C5B-O5B
2	C	301	NAP	C5D-O5D-PN-O3
2	C	301	NAP	C5D-O5D-PN-O2N
2	C	301	NAP	O4D-C1D-N1N-C2N
2	D	301	NAP	O4D-C1D-N1N-C2N
2	E	301	NAP	C5B-O5B-PA-O3
2	E	301	NAP	C5D-O5D-PN-O3
2	E	301	NAP	C5D-O5D-PN-O1N
2	E	301	NAP	C5D-O5D-PN-O2N
2	E	301	NAP	O4D-C1D-N1N-C2N
2	E	301	NAP	O4D-C1D-N1N-C6N
2	E	301	NAP	C2D-C1D-N1N-C2N
2	E	301	NAP	C2D-C1D-N1N-C6N
2	F	301	NAP	C5B-O5B-PA-O3
2	F	301	NAP	PN-O3-PA-O5B
2	F	301	NAP	O4B-C4B-C5B-O5B
2	F	301	NAP	C5D-O5D-PN-O3
2	F	301	NAP	O4D-C1D-N1N-C2N
2	G	301	NAP	C5B-O5B-PA-O1A
2	G	301	NAP	C5B-O5B-PA-O2A
2	G	301	NAP	O4D-C1D-N1N-C2N
2	H	1001	NAP	C5B-O5B-PA-O1A
2	H	1001	NAP	C5B-O5B-PA-O2A
2	H	1001	NAP	O4D-C1D-N1N-C2N
2	B	301	NAP	O4D-C4D-C5D-O5D
2	F	301	NAP	C3B-C4B-C5B-O5B
2	A	1000	NAP	O4B-C4B-C5B-O5B
2	A	1000	NAP	C3B-C4B-C5B-O5B
2	H	1001	NAP	C3B-C2B-O2B-P2B
2	E	301	NAP	C3B-C4B-C5B-O5B
2	E	301	NAP	O4B-C4B-C5B-O5B
2	H	1001	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	C3B-C4B-C5B-O5B
2	G	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	O4B-C4B-C5B-O5B
2	H	1001	NAP	C1B-C2B-O2B-P2B
2	F	301	NAP	O4D-C4D-C5D-O5D
2	E	301	NAP	PN-O3-PA-O5B
2	B	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	C5D-O5D-PN-O1N
2	C	301	NAP	C5D-O5D-PN-O1N
2	E	301	NAP	C5B-O5B-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	301	NAP	C5B-O5B-PA-O1A
2	F	301	NAP	C5D-O5D-PN-O1N
2	G	301	NAP	C5B-O5B-PA-O3
2	H	1001	NAP	C5B-O5B-PA-O3
2	B	301	NAP	PA-O3-PN-O2N
2	C	301	NAP	PA-O3-PN-O2N
2	F	301	NAP	PA-O3-PN-O2N
2	H	1001	NAP	C3B-C4B-C5B-O5B
2	C	301	NAP	C2B-O2B-P2B-O3X
2	F	301	NAP	C3B-C2B-O2B-P2B
2	B	301	NAP	O4D-C1D-N1N-C6N
2	C	301	NAP	O4D-C1D-N1N-C6N
2	D	301	NAP	O4D-C1D-N1N-C6N
2	F	301	NAP	O4D-C1D-N1N-C6N
2	H	1001	NAP	O4D-C1D-N1N-C6N
2	E	301	NAP	PA-O3-PN-O2N
2	G	301	NAP	O4D-C4D-C5D-O5D
2	C	301	NAP	PA-O3-PN-O1N
2	F	301	NAP	PA-O3-PN-O1N
2	H	1001	NAP	C2B-O2B-P2B-O3X
2	F	301	NAP	C1B-C2B-O2B-P2B
2	E	301	NAP	PA-O3-PN-O1N
2	G	301	NAP	PN-O3-PA-O2A
2	H	1001	NAP	PN-O3-PA-O2A

There are no ring outliers.

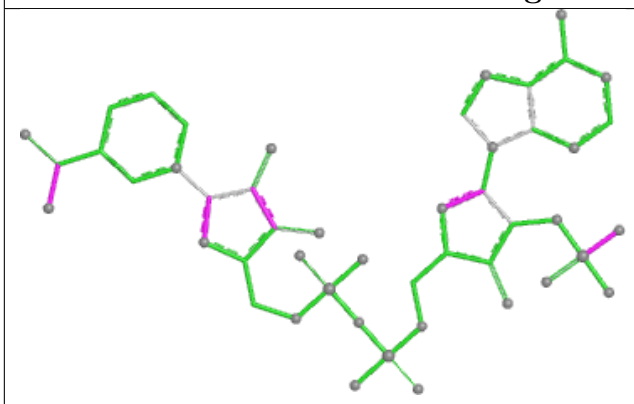
8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	NAP	4	0
2	H	1001	NAP	2	0
2	B	301	NAP	3	0
2	A	1000	NAP	4	0
2	C	301	NAP	2	0
2	E	301	NAP	3	0
2	D	301	NAP	5	0
2	G	301	NAP	6	0

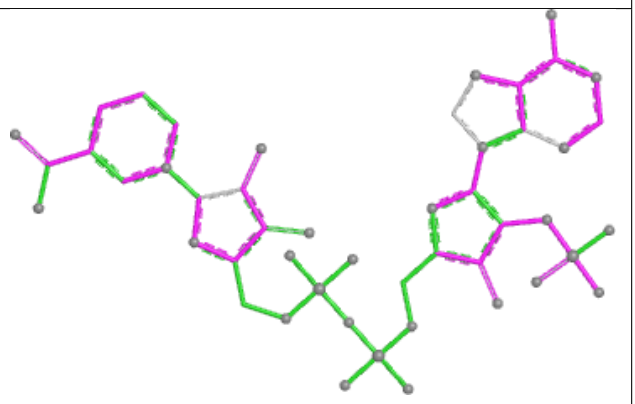
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

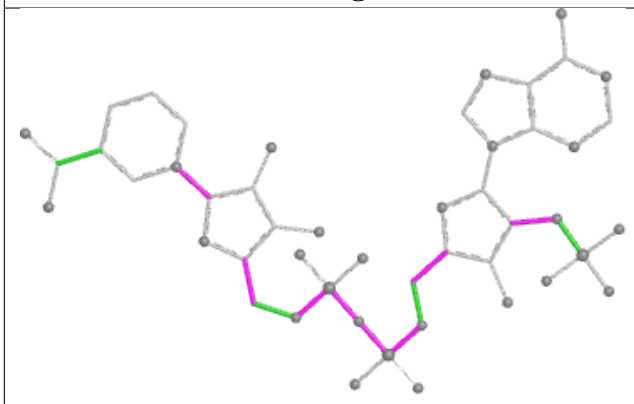
Ligand NAP F 301



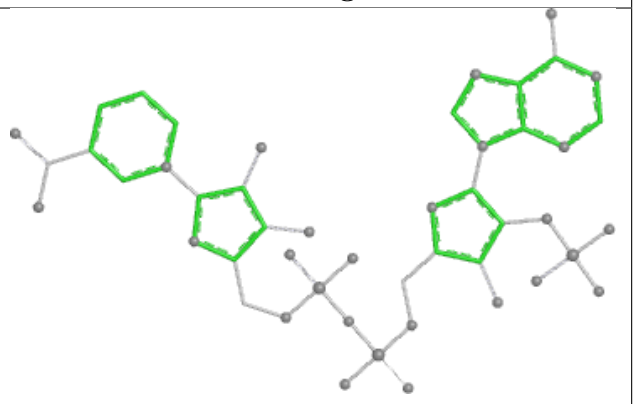
Bond lengths



Bond angles

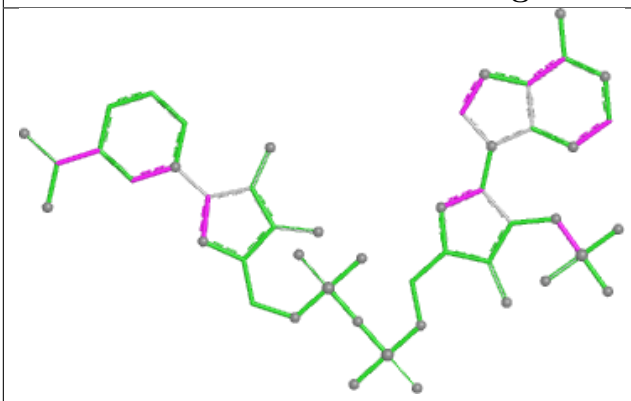


Torsions

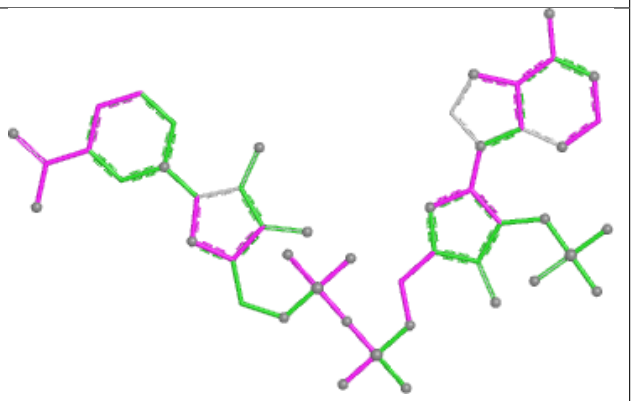


Rings

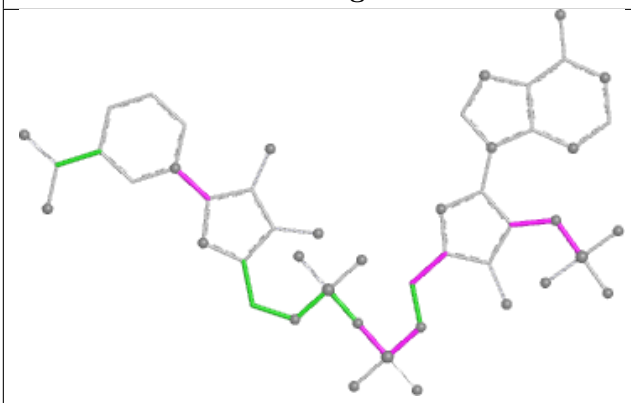
Ligand NAP H 1001



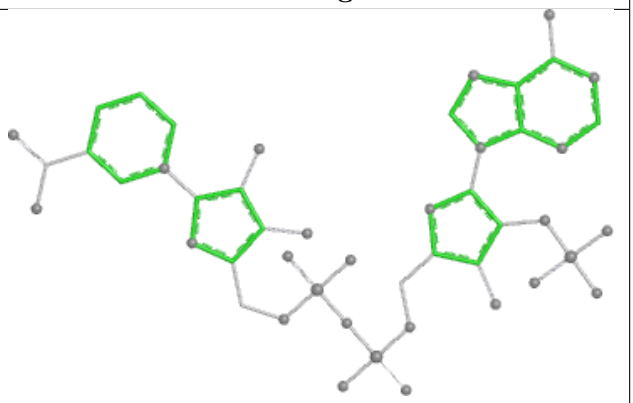
Bond lengths



Bond angles

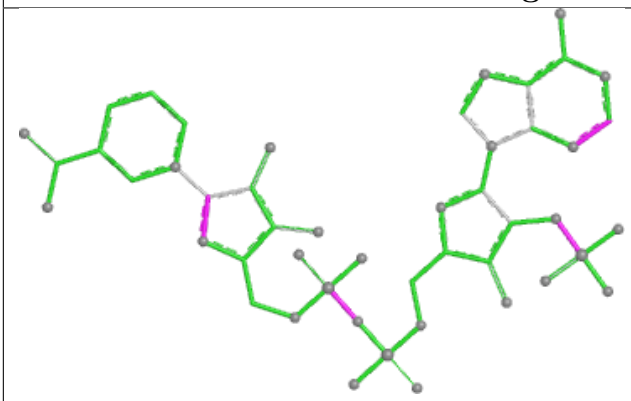


Torsions

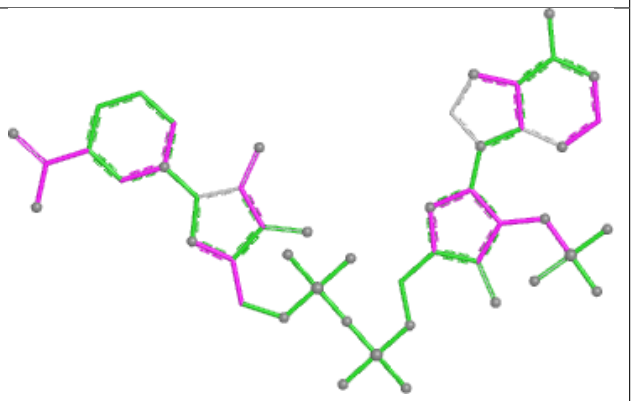


Rings

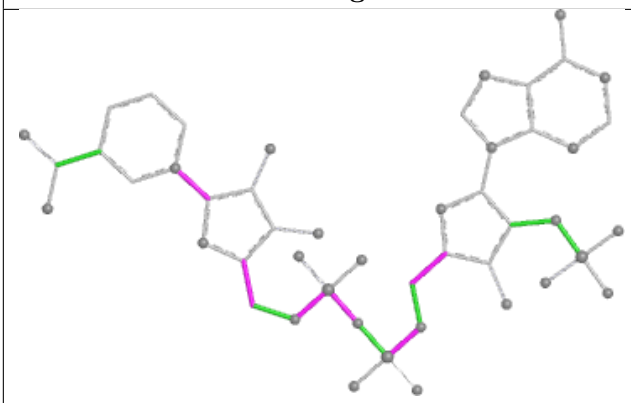
Ligand NAP B 301



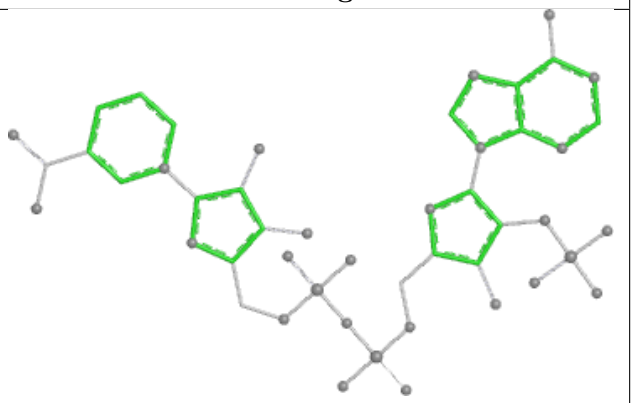
Bond lengths



Bond angles

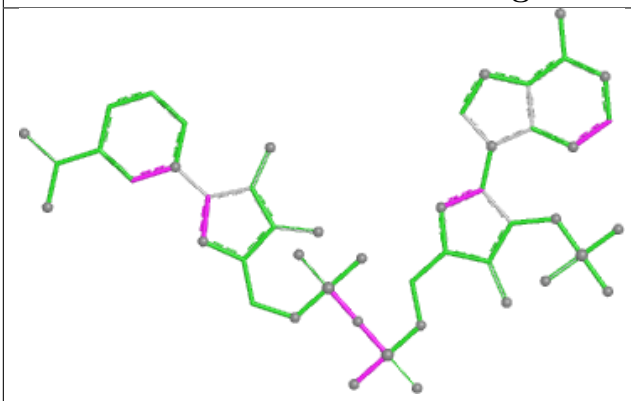


Torsions

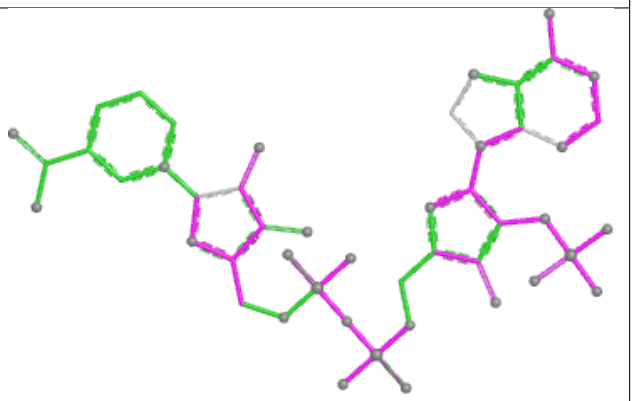


Rings

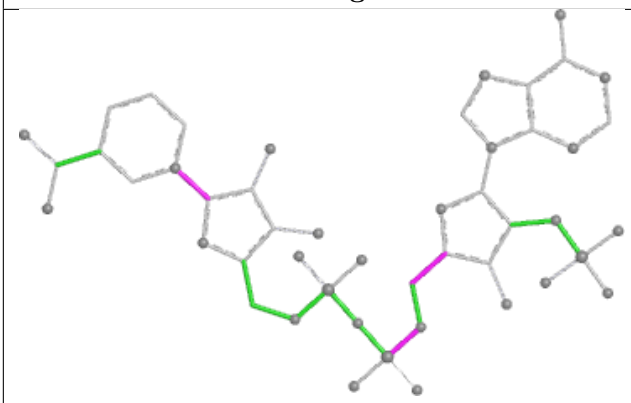
Ligand NAP A 1000



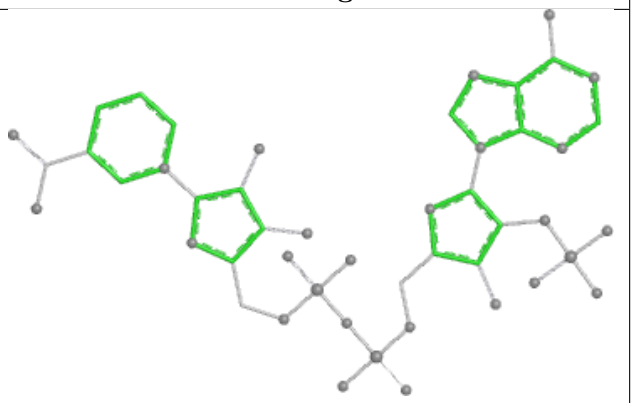
Bond lengths



Bond angles

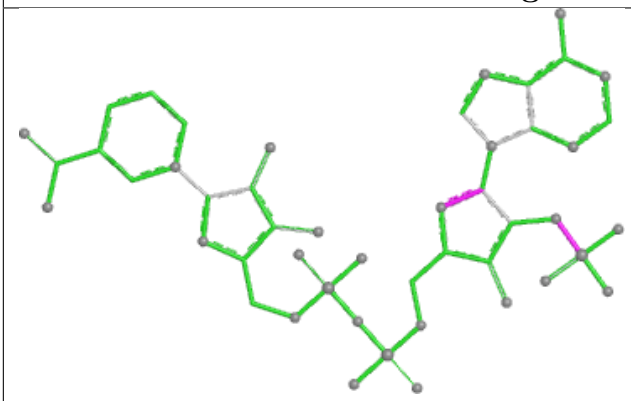


Torsions

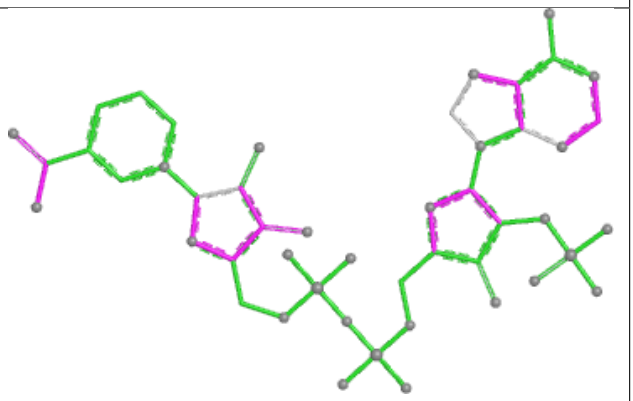


Rings

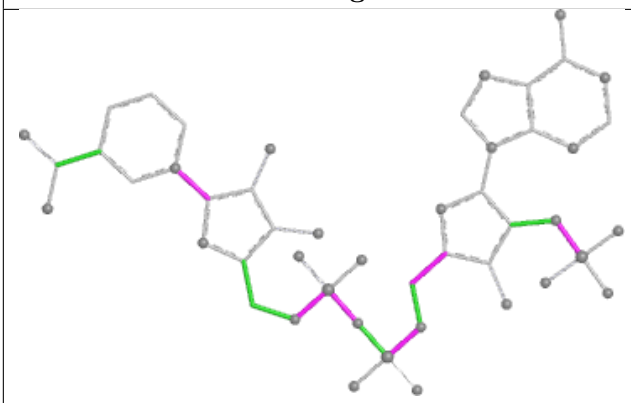
Ligand NAP C 301



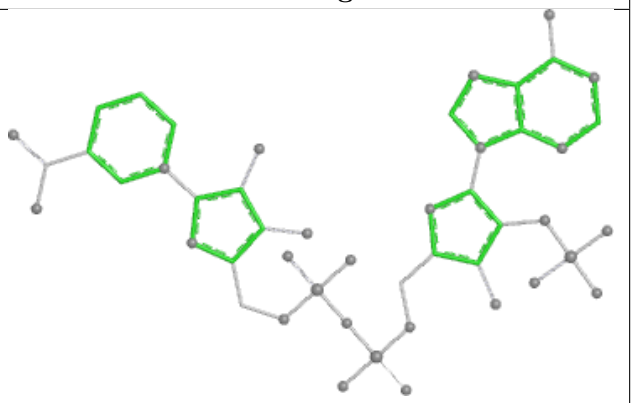
Bond lengths



Bond angles

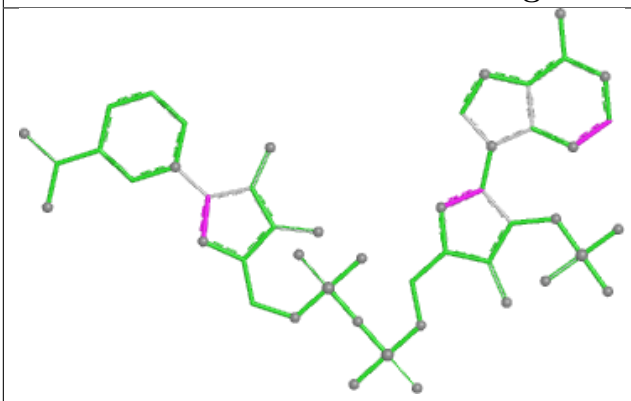


Torsions

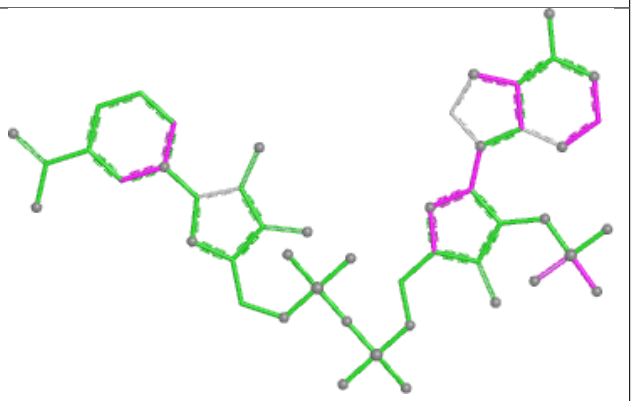


Rings

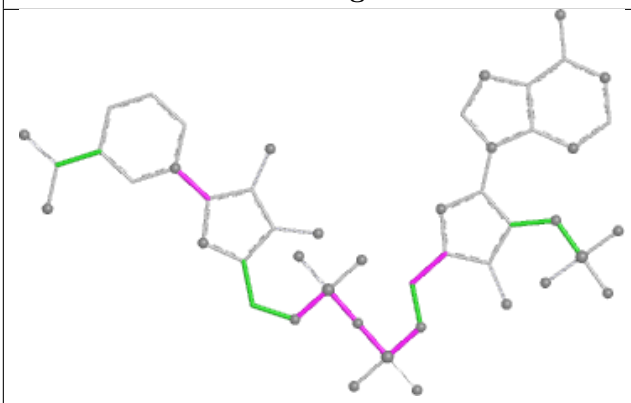
Ligand NAP E 301



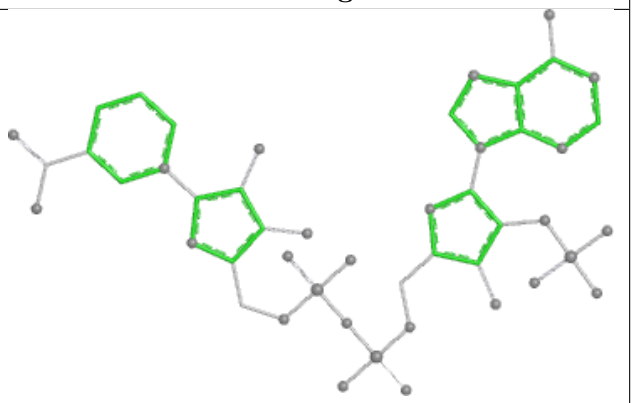
Bond lengths



Bond angles

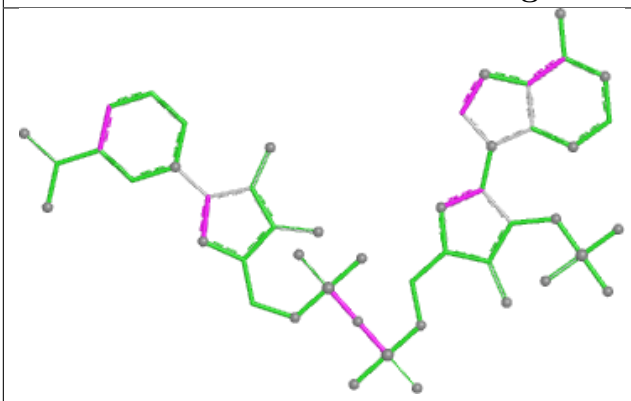


Torsions

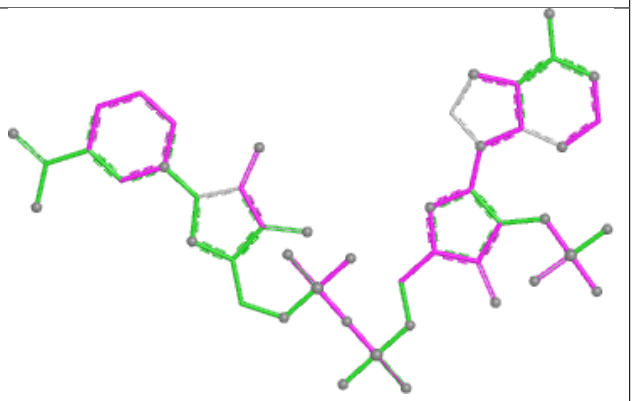


Rings

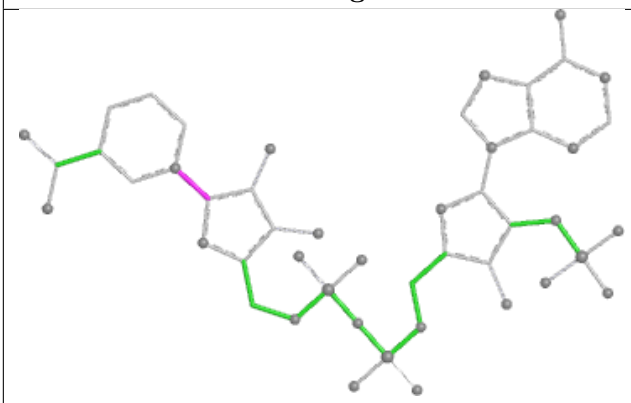
Ligand NAP D 301



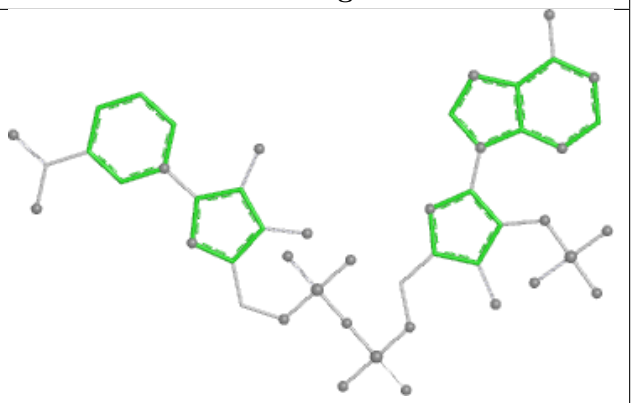
Bond lengths



Bond angles

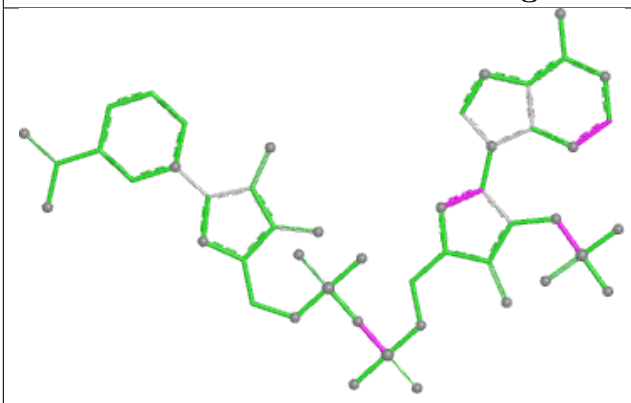


Torsions

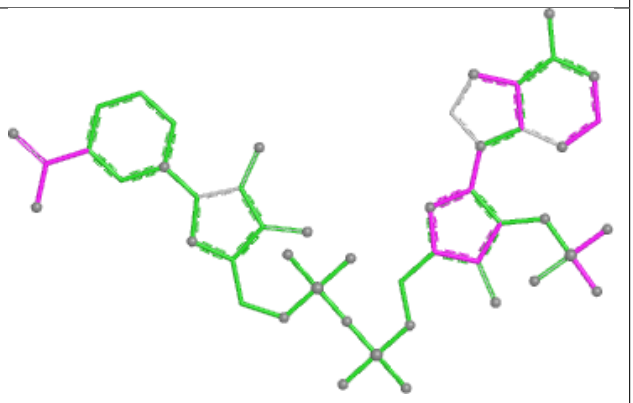


Rings

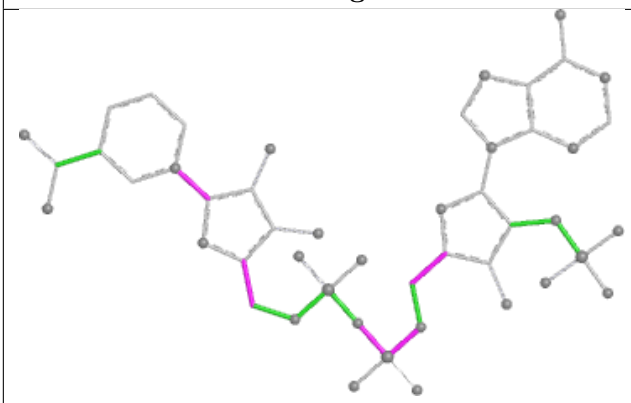
Ligand NAP G 301



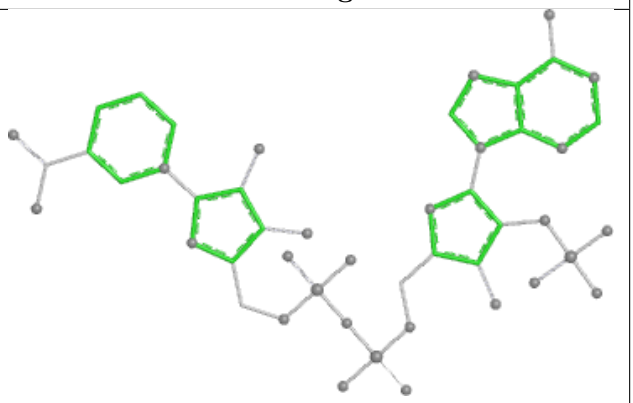
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	281/285 (98%)	0.55	29 (10%)	6	4	17, 46, 76, 100	0
1	B	261/285 (91%)	0.96	43 (16%)	1	1	21, 74, 118, 152	0
1	C	273/285 (95%)	0.90	45 (16%)	1	1	23, 71, 107, 126	0
1	D	278/285 (97%)	0.59	30 (10%)	5	4	17, 45, 70, 99	0
1	E	268/285 (94%)	0.95	51 (19%)	1	1	22, 69, 111, 134	0
1	F	280/285 (98%)	0.58	29 (10%)	6	4	16, 47, 79, 101	0
1	G	279/285 (97%)	0.86	43 (15%)	2	1	23, 68, 106, 127	0
1	H	278/285 (97%)	0.64	27 (9%)	7	5	18, 46, 76, 100	0
All	All	2198/2280 (96%)	0.75	297 (13%)	3	2	16, 53, 104, 152	0

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	36	LYS	11.9
1	C	119	ALA	10.9
1	B	87	ILE	10.8
1	G	105	PHE	9.9
1	B	86	THR	9.7
1	G	87	ILE	9.2
1	G	86	THR	8.2
1	C	140	PHE	8.1
1	G	64	CYS	8.1
1	E	45	ALA	7.8
1	G	142	ALA	7.7
1	F	81	HIS	6.9
1	C	59	ASP	6.8
1	C	8	GLY	6.4
1	E	119	ALA	6.2
1	G	44	GLY	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	60	LEU	5.9
1	F	37	ALA	5.9
1	B	64	CYS	5.9
1	C	85	LYS	5.8
1	E	76	ALA	5.8
1	C	61	ILE	5.7
1	A	137	PRO	5.7
1	G	111	ARG	5.7
1	E	224	TYR	5.5
1	B	105	PHE	5.4
1	E	215	MET	5.2
1	H	147	LEU	5.2
1	F	240	ASN	5.1
1	H	128	TYR	4.9
1	D	194	ALA	4.8
1	D	47	LEU	4.8
1	E	97	GLN	4.8
1	B	217	LYS	4.7
1	E	147	LEU	4.7
1	B	88	ILE	4.7
1	C	2	SER	4.6
1	E	16	LEU	4.6
1	C	146	ASP	4.6
1	B	61	ILE	4.6
1	A	8	GLY	4.5
1	F	83	HIS	4.5
1	B	109	GLY	4.5
1	B	113	VAL	4.5
1	C	143	ALA	4.5
1	H	151	ALA	4.5
1	H	37	ALA	4.4
1	G	35	GLU	4.4
1	H	224	TYR	4.3
1	F	166	HIS	4.3
1	G	217	LYS	4.2
1	E	61	ILE	4.2
1	C	139	ALA	4.2
1	G	43	LYS	4.2
1	H	194	ALA	4.1
1	C	25	TYR	4.1
1	A	195	VAL	4.1
1	E	21	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	98	ALA	4.0
1	E	66	LEU	3.9
1	B	153	CYS	3.9
1	F	75	LEU	3.9
1	E	113	VAL	3.8
1	F	36	LYS	3.8
1	D	20	PHE	3.8
1	A	1	MET	3.8
1	C	70	ALA	3.8
1	C	150	LEU	3.8
1	B	71	VAL	3.7
1	B	76	ALA	3.7
1	C	1	MET	3.7
1	G	166	HIS	3.7
1	E	8	GLY	3.7
1	E	77	GLY	3.7
1	G	109	GLY	3.6
1	B	192	THR	3.6
1	A	138	ASP	3.6
1	D	146	ASP	3.6
1	B	155	PHE	3.6
1	D	128	TYR	3.6
1	B	221	GLU	3.6
1	G	90	LEU	3.6
1	C	166	HIS	3.6
1	B	11	ALA	3.6
1	D	147	LEU	3.6
1	B	222	GLY	3.5
1	C	73	ALA	3.5
1	A	127	PRO	3.5
1	B	244	ALA	3.5
1	E	139	ALA	3.5
1	E	96	ASP	3.5
1	E	150	LEU	3.5
1	C	45	ALA	3.4
1	F	103	ASP	3.4
1	B	119	ALA	3.4
1	G	138	ASP	3.4
1	H	215	MET	3.4
1	E	95	PRO	3.4
1	F	8	GLY	3.4
1	C	88	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	87	ILE	3.4
1	H	7	PHE	3.4
1	E	216	ALA	3.4
1	D	222	GLY	3.4
1	C	120	THR	3.3
1	F	276	SER	3.3
1	E	194	ALA	3.3
1	G	3	SER	3.3
1	B	77	GLY	3.3
1	E	160	ALA	3.3
1	C	153	CYS	3.3
1	H	268	ALA	3.3
1	E	44	GLY	3.3
1	H	146	ASP	3.2
1	F	48	SER	3.2
1	B	63	ILE	3.2
1	D	151	ALA	3.2
1	A	83	HIS	3.2
1	G	119	ALA	3.2
1	H	235	LEU	3.2
1	G	115	GLY	3.2
1	B	274	ASP	3.2
1	G	8	GLY	3.2
1	B	93	GLY	3.2
1	G	163	ALA	3.2
1	E	107	SER	3.2
1	B	115	GLY	3.1
1	D	224	TYR	3.1
1	H	47	LEU	3.1
1	H	45	ALA	3.1
1	G	85	LYS	3.1
1	B	237	GLY	3.1
1	C	215	MET	3.1
1	B	165	LEU	3.1
1	E	161	GLY	3.1
1	A	229	SER	3.1
1	C	133	TYR	3.1
1	G	139	ALA	3.1
1	G	71	VAL	3.1
1	A	251	SER	3.0
1	D	55	ILE	3.0
1	E	120	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	112	TYR	3.0
1	D	212	THR	3.0
1	C	111	ARG	3.0
1	B	137	PRO	3.0
1	G	133	TYR	2.9
1	D	187	LEU	2.9
1	D	211	TYR	2.9
1	E	211	TYR	2.9
1	B	85	LYS	2.9
1	D	243	ASP	2.9
1	D	242	ILE	2.9
1	A	75	LEU	2.9
1	E	212	THR	2.9
1	G	45	ALA	2.9
1	H	35	GLU	2.9
1	C	212	THR	2.8
1	G	89	ASN	2.8
1	F	47	LEU	2.8
1	E	43	LYS	2.8
1	A	194	ALA	2.8
1	E	166	HIS	2.8
1	F	236	VAL	2.8
1	A	2	SER	2.8
1	B	101	LEU	2.8
1	C	154	VAL	2.8
1	E	149	VAL	2.8
1	C	39	SER	2.8
1	H	132	LEU	2.7
1	A	151	ALA	2.7
1	A	105	PHE	2.7
1	A	60	LEU	2.7
1	C	107	SER	2.7
1	E	116	GLY	2.7
1	E	165	LEU	2.7
1	E	20	PHE	2.6
1	E	136	SER	2.6
1	F	57	ALA	2.6
1	H	222	GLY	2.6
1	E	73	ALA	2.6
1	B	49	HIS	2.6
1	C	224	TYR	2.6
1	B	51	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	140	PHE	2.6
1	C	66	LEU	2.6
1	G	5	SER	2.6
1	E	4	VAL	2.6
1	F	181	PHE	2.6
1	C	7	PHE	2.5
1	F	20	PHE	2.5
1	B	3	SER	2.5
1	C	171	LEU	2.5
1	G	21	LEU	2.5
1	A	81	HIS	2.5
1	D	67	ASP	2.5
1	G	63	ILE	2.5
1	H	236	VAL	2.5
1	H	94	THR	2.5
1	H	243	ASP	2.5
1	A	276	SER	2.5
1	G	20	PHE	2.5
1	F	74	THR	2.5
1	G	39	SER	2.5
1	B	270	HIS	2.5
1	E	63	ILE	2.5
1	A	149	VAL	2.4
1	C	211	TYR	2.4
1	D	181	PHE	2.4
1	B	8	GLY	2.4
1	C	142	ALA	2.4
1	D	150	LEU	2.4
1	F	163	ALA	2.4
1	E	13	GLY	2.4
1	A	153	CYS	2.4
1	F	244	ALA	2.4
1	A	103	ASP	2.4
1	A	155	PHE	2.4
1	D	49	HIS	2.4
1	C	266	VAL	2.4
1	G	4	VAL	2.4
1	B	160	ALA	2.4
1	D	235	LEU	2.4
1	G	6	ILE	2.4
1	D	132	LEU	2.3
1	F	196	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	104	ARG	2.3
1	C	118	MET	2.3
1	D	81	HIS	2.3
1	E	85	LYS	2.3
1	D	7	PHE	2.3
1	H	261	PHE	2.3
1	E	114	HIS	2.3
1	E	132	LEU	2.3
1	F	245	SER	2.3
1	G	2	SER	2.3
1	E	133	TYR	2.3
1	D	101	LEU	2.3
1	D	268	ALA	2.3
1	G	216	ALA	2.3
1	H	191	SER	2.3
1	C	128	TYR	2.3
1	G	192	THR	2.3
1	A	62	ILE	2.3
1	D	96	ASP	2.3
1	H	219	ILE	2.3
1	A	70	ALA	2.2
1	E	142	ALA	2.2
1	A	223	LYS	2.2
1	F	195	VAL	2.2
1	F	282	VAL	2.2
1	G	84	GLY	2.2
1	F	229	SER	2.2
1	B	75	LEU	2.2
1	G	244	ALA	2.2
1	F	64	CYS	2.2
1	A	34	PRO	2.2
1	D	86	THR	2.2
1	B	106	VAL	2.2
1	C	136	SER	2.2
1	H	39	SER	2.2
1	E	156	LEU	2.2
1	A	74	THR	2.2
1	E	93	GLY	2.2
1	A	211	TYR	2.2
1	C	40	LEU	2.1
1	H	271	GLY	2.1
1	E	151	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	72	GLU	2.1
1	G	155	PHE	2.1
1	H	247	ALA	2.1
1	B	212	THR	2.1
1	C	5	SER	2.1
1	B	282	VAL	2.1
1	A	93	GLY	2.1
1	F	105	PHE	2.1
1	D	104	ARG	2.1
1	G	59	ASP	2.1
1	F	9	LEU	2.1
1	D	30	TRP	2.1
1	E	205	LEU	2.1
1	E	204	TRP	2.1
1	A	218	GLN	2.1
1	C	63	ILE	2.1
1	E	34	PRO	2.1
1	G	110	ALA	2.1
1	B	214	GLY	2.1
1	B	154	VAL	2.0
1	H	238	ILE	2.0
1	F	119	ALA	2.0
1	G	70	ALA	2.0
1	C	20	PHE	2.0
1	C	27	VAL	2.0
1	B	181	PHE	2.0
1	F	2	SER	2.0
1	C	162	THR	2.0
1	H	140	PHE	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)

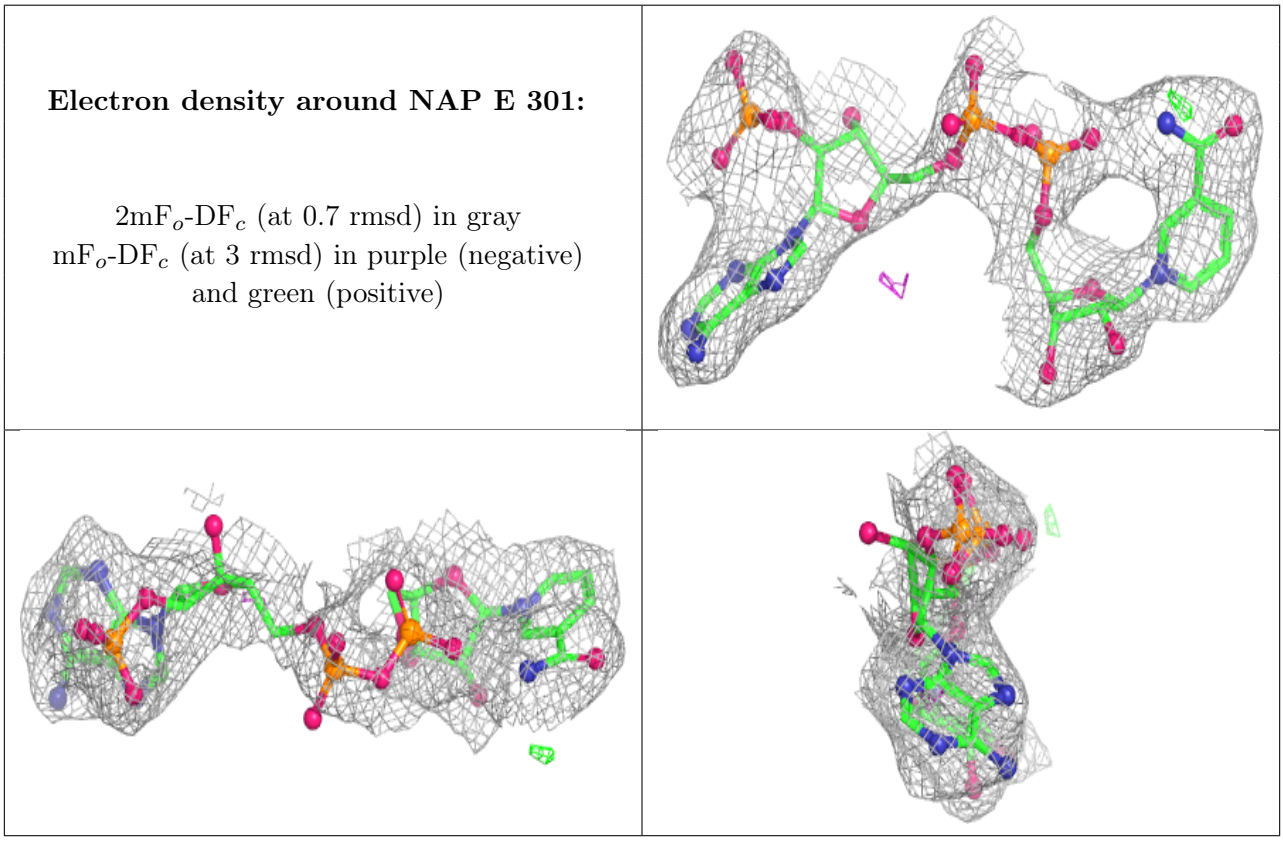
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NAP	E	301	48/48	0.85	0.20	35,66,93,100	0
2	NAP	C	301	48/48	0.86	0.21	26,51,81,93	0
2	NAP	A	1000	48/48	0.91	0.17	19,25,35,45	0
2	NAP	B	301	48/48	0.91	0.13	26,51,66,68	0
2	NAP	F	301	48/48	0.91	0.16	17,32,36,46	0
2	NAP	G	301	48/48	0.91	0.14	31,47,56,67	0
2	NAP	D	301	48/48	0.94	0.14	12,19,29,33	0
2	NAP	H	1001	48/48	0.95	0.12	16,21,37,40	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.

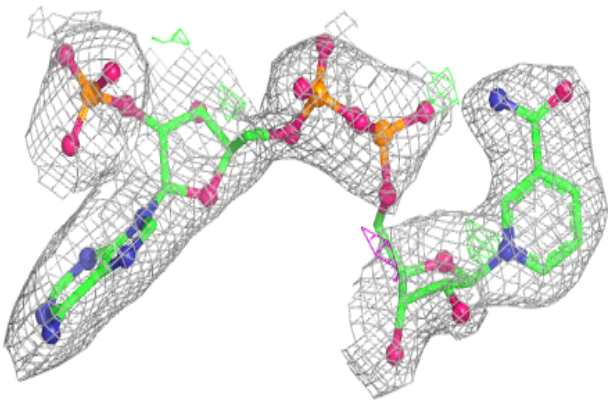
Electron density around NAP E 301:

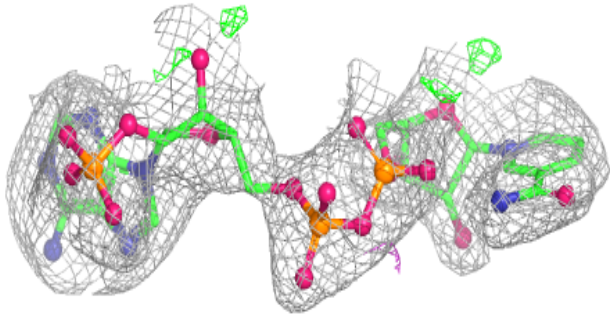
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

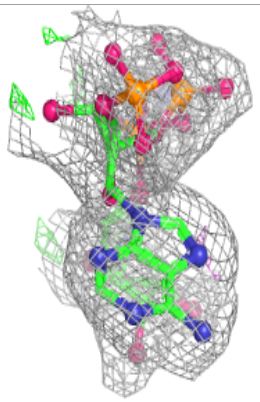


Electron density around NAP C 301:

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

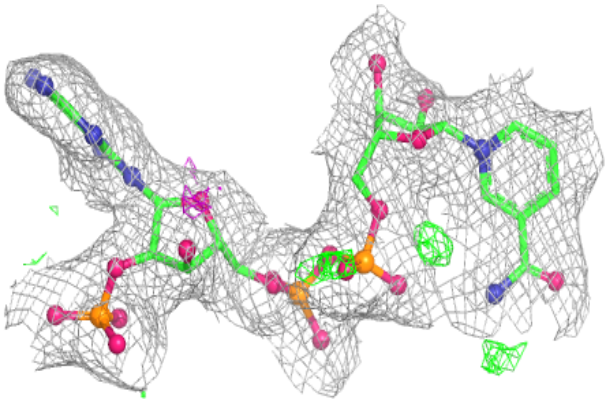


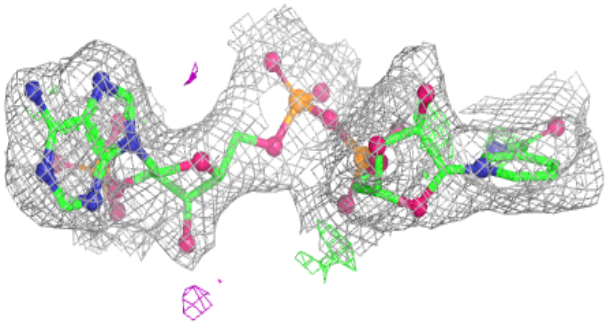


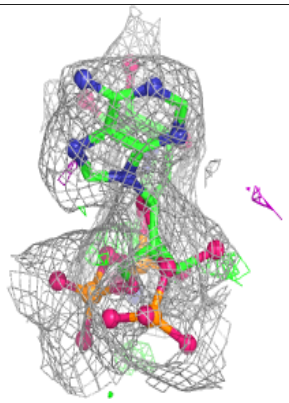


Electron density around NAP A 1000:

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

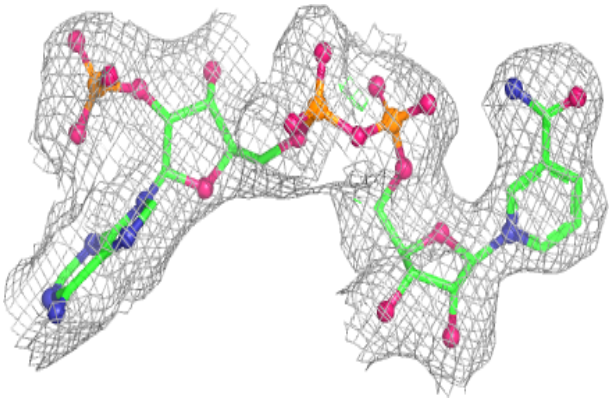


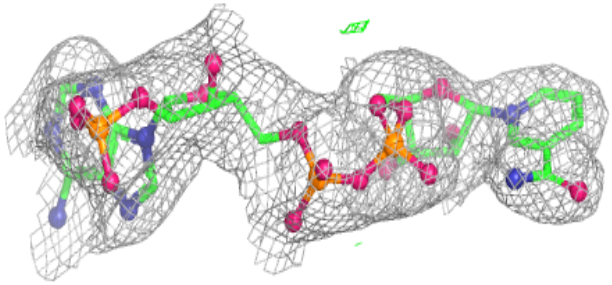


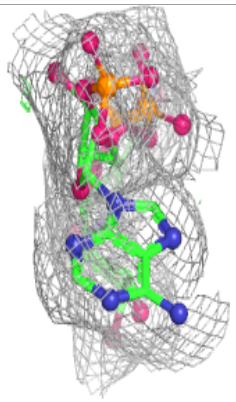


Electron density around NAP B 301:

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

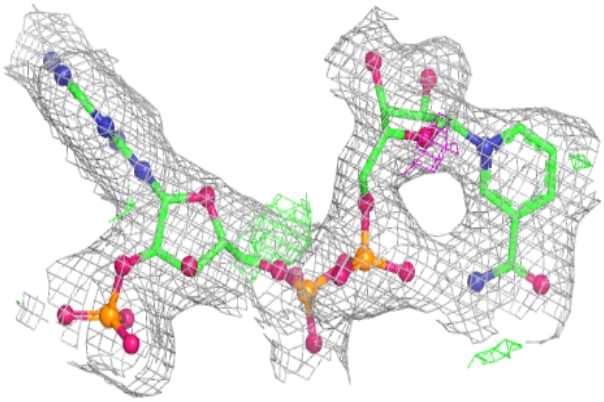


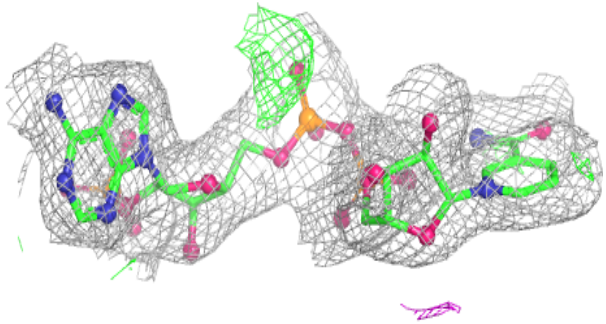


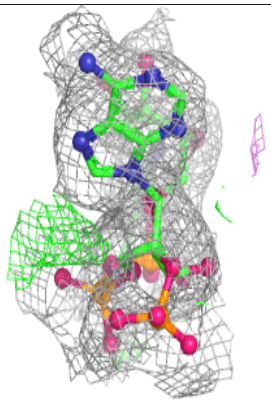


Electron density around NAP F 301:

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

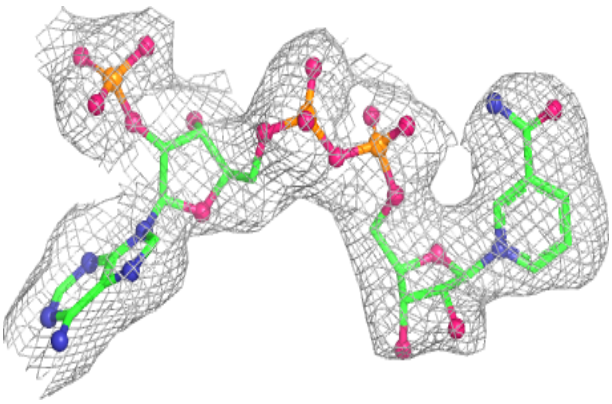


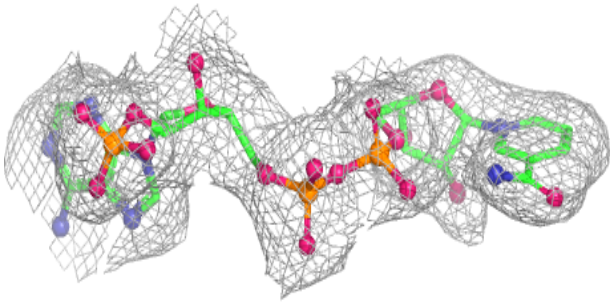


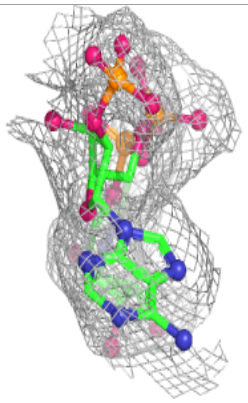


Electron density around NAP G 301:

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

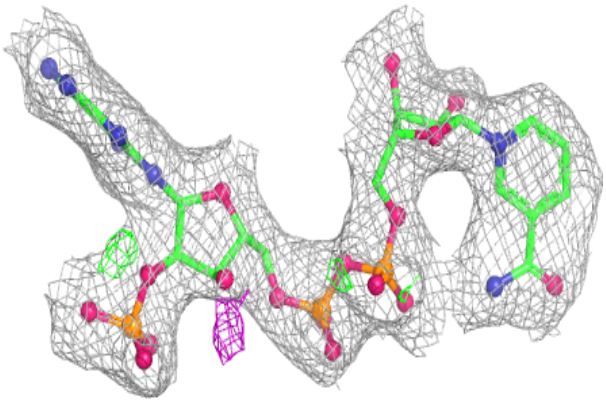


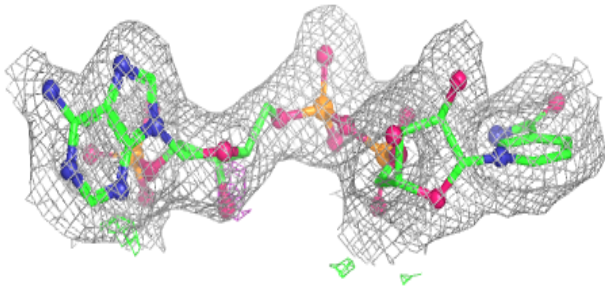


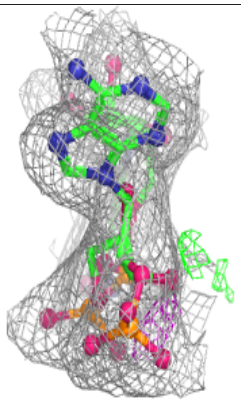


Electron density around NAP D 301:

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

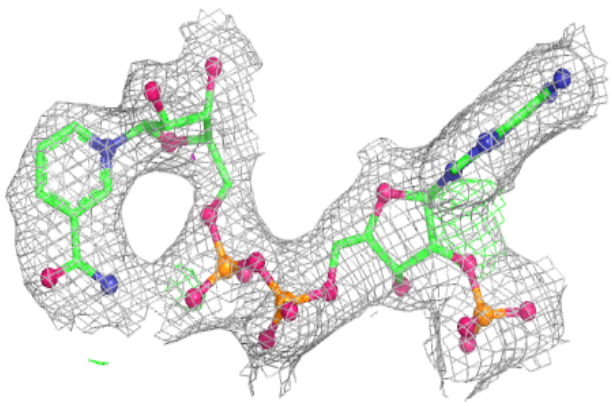


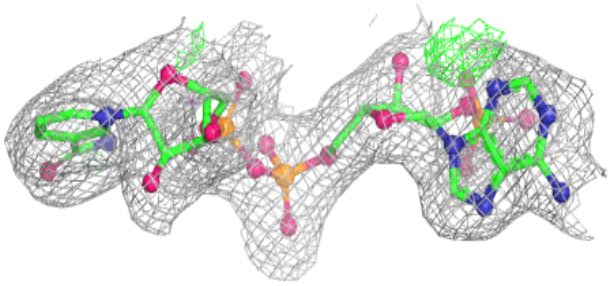


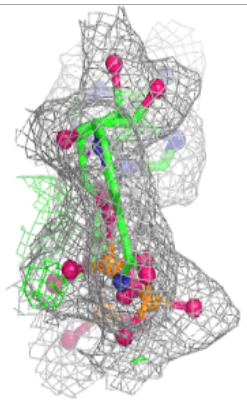


Electron density around NAP H 1001:

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







6.5 Other polymers (i)

There are no such residues in this entry.