Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 06:49 am BST

PDB ID	:	6Q94
Title	:	Crystal structure of human GDP-D-mannose 4,6-dehydratase (S156D) in complex with GDP-Man
Authors	:	Pfeiffer, M.; Krojer, T.; Johansson, C.; von Delft, F.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; Nidetzky, B.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on	:	2018-12-17
Resolution	:	2.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

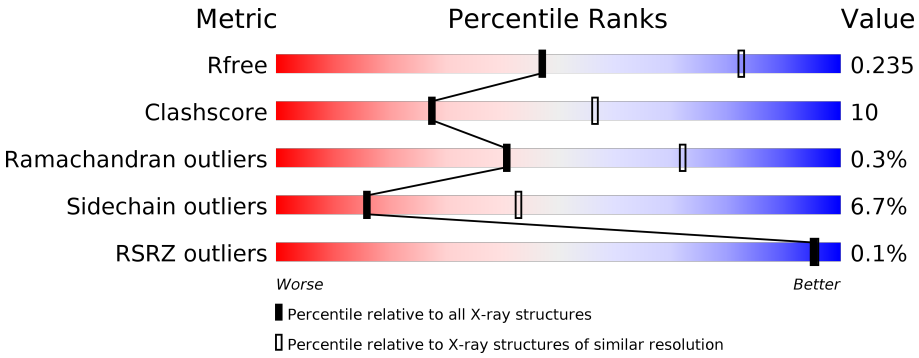
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	352	80% 17%
1	B	352	80% 16%
1	C	352	84% 15%
1	D	352	77% 19%
1	E	352	78% 18%
1	F	352	77% 19%

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Mol	Chain	Length	Quality of chain
1	G	352	
1	H	352	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22956 atoms, of which 176 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GDP-mannose 4,6 dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	344	Total	C	N	O	S	0	0	0
			2757	1757	475	515	10			
1	A	350	Total	C	N	O	S	0	0	0
			2778	1769	477	522	10			
1	C	348	Total	C	N	O	S	0	0	0
			2779	1771	479	519	10			
1	D	343	Total	C	N	O	S	0	0	0
			2739	1746	469	514	10			
1	E	350	Total	C	N	O	S	0	0	0
			2787	1777	481	519	10			
1	F	350	Total	C	N	O	S	0	0	0
			2784	1775	477	522	10			
1	G	350	Total	C	N	O	S	0	0	0
			2784	1775	481	518	10			
1	H	341	Total	C	N	O	S	0	0	0
			2720	1734	468	508	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	21	SER	-	expression tag	UNP O60547
B	22	MET	-	expression tag	UNP O60547
B	156	ASP	SER	engineered mutation	UNP O60547
A	21	SER	-	expression tag	UNP O60547
A	22	MET	-	expression tag	UNP O60547
A	156	ASP	SER	engineered mutation	UNP O60547
C	21	SER	-	expression tag	UNP O60547
C	22	MET	-	expression tag	UNP O60547
C	156	ASP	SER	engineered mutation	UNP O60547
D	21	SER	-	expression tag	UNP O60547
D	22	MET	-	expression tag	UNP O60547
D	156	ASP	SER	engineered mutation	UNP O60547
E	21	SER	-	expression tag	UNP O60547

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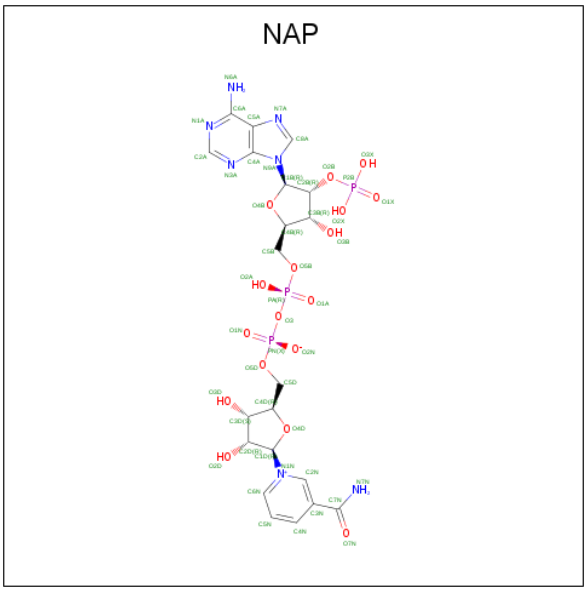
Chain	Residue	Modelled	Actual	Comment	Reference
E	22	MET	-	expression tag	UNP O60547
E	156	ASP	SER	engineered mutation	UNP O60547
F	21	SER	-	expression tag	UNP O60547
F	22	MET	-	expression tag	UNP O60547
F	156	ASP	SER	engineered mutation	UNP O60547
G	21	SER	-	expression tag	UNP O60547
G	22	MET	-	expression tag	UNP O60547
G	156	ASP	SER	engineered mutation	UNP O60547
H	21	SER	-	expression tag	UNP O60547
H	22	MET	-	expression tag	UNP O60547
H	156	ASP	SER	engineered mutation	UNP O60547

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	0
			59	15	19	6	16	3		
2	A	1	Total	C	H	N	O	P	0	0
			59	15	19	6	16	3		
2	C	1	Total	C	H	N	O	P	0	0
			59	15	19	6	16	3		
2	D	1	Total	C	H	N	O	P	0	0
			59	15	19	6	16	3		
2	E	1	Total	C	H	N	O	P	0	0
			59	15	19	6	16	3		

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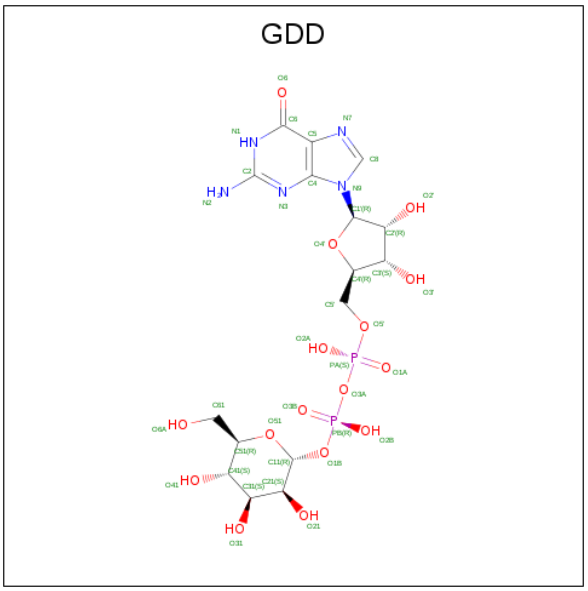
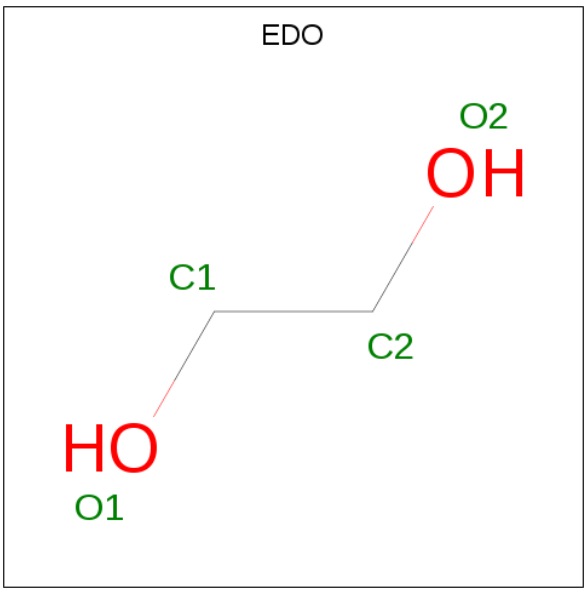
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	F	1	Total	C	H	N	O	P	0	0
			59	15	19	6	16	3		
2	G	1	Total	C	H	N	O	P	0	0
			59	15	19	6	16	3		
2	H	1	Total	C	H	N	O	P	0	0
			59	15	19	6	16	3		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE-ALPHA-D-MANNOSE (three-letter code: GDD) (formula: $C_{16}H_{25}N_5O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
3	A	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
3	C	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
3	D	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
3	E	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
3	F	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
3	G	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
3	H	1	Total	C	N	O	P	0	0
			39	16	5	16	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	G	1	Total	C	H	O	0	0
			10	2	6	2		
4	H	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is water.

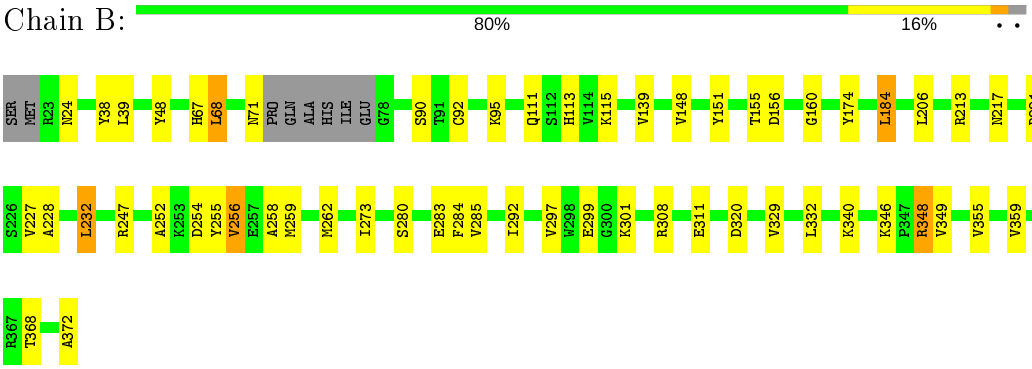
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			1	1		
5	C	1	Total	O	0	0
			1	1		
5	E	1	Total	O	0	0
			1	1		
5	G	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

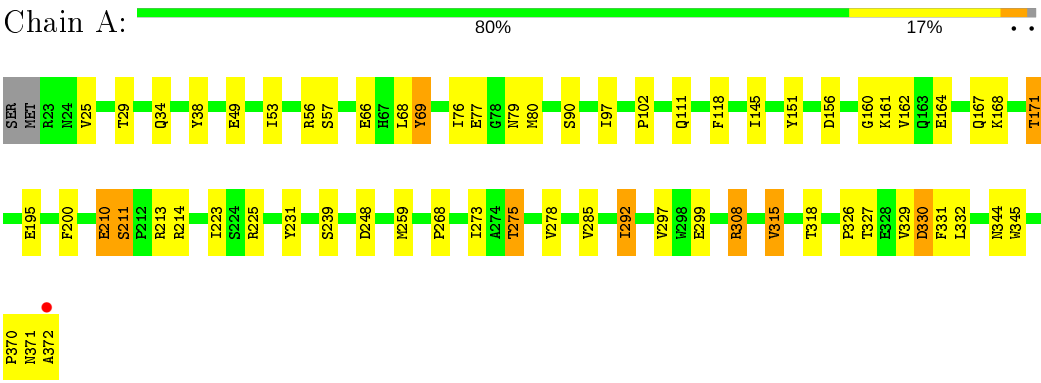
- Molecule 1: GDP-mannose 4,6 dehydratase

Chain B:



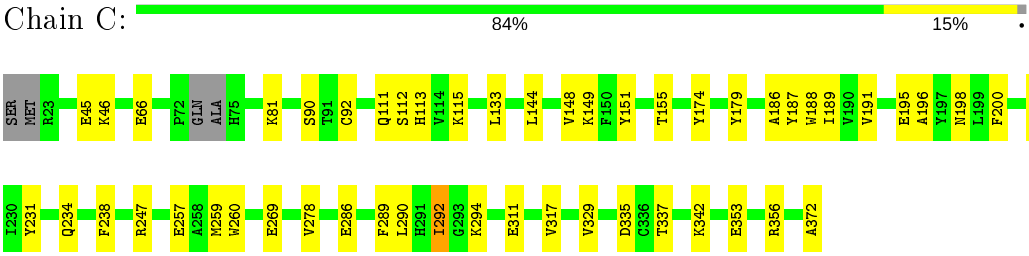
- Molecule 1: GDP-mannose 4,6 dehydratase

Chain A:



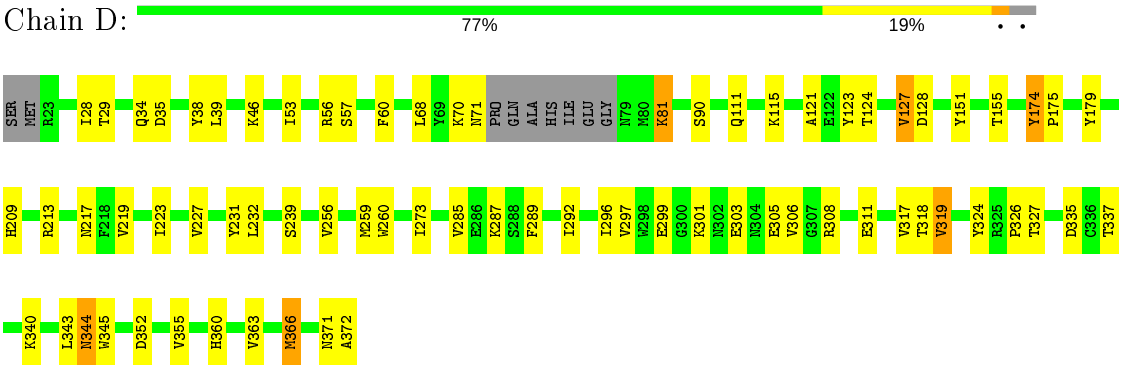
- Molecule 1: GDP-mannose 4,6 dehydratase

Chain C:



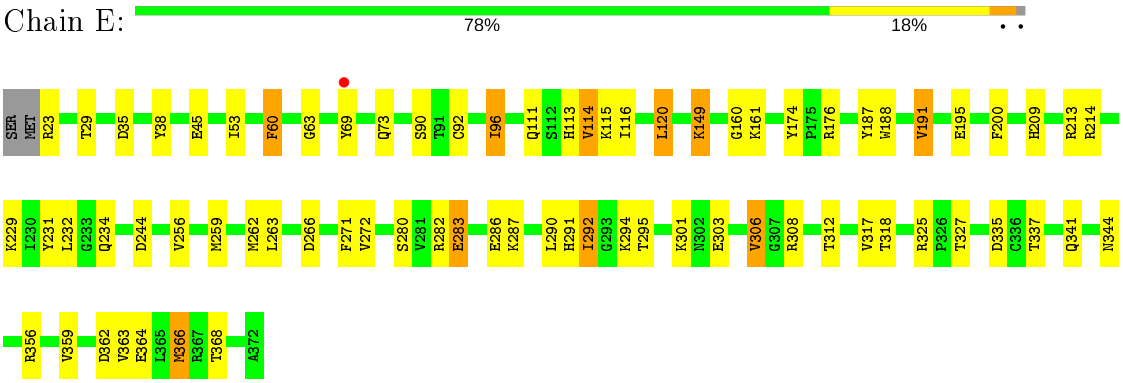
- Molecule 1: GDP-mannose 4,6 dehydratase

Chain D:



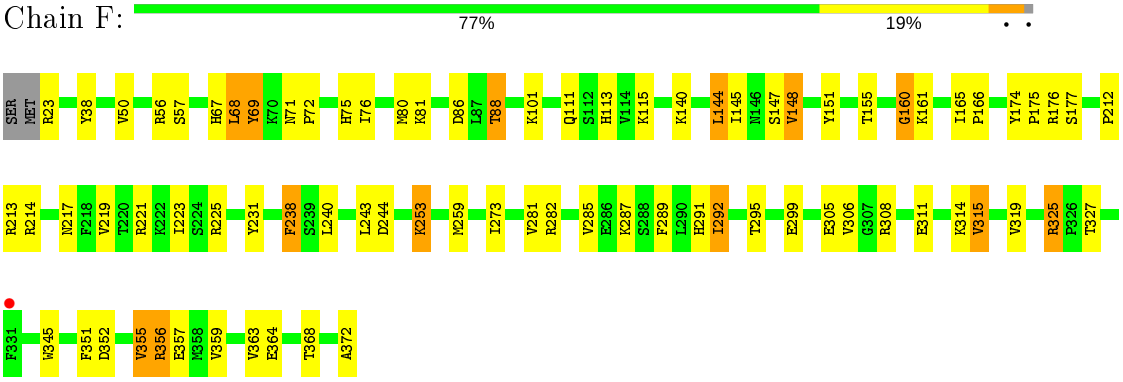
- Molecule 1: GDP-mannose 4,6 dehydratase

Chain E:



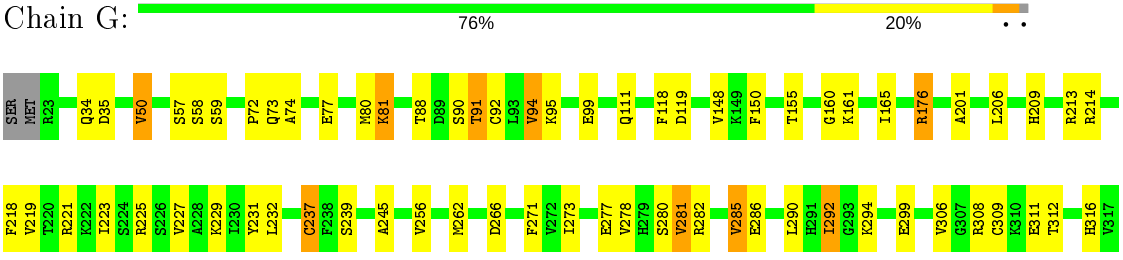
- Molecule 1: GDP-mannose 4,6 dehydratase

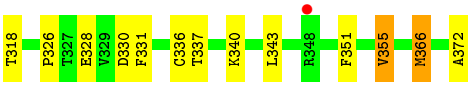
Chain F:



- Molecule 1: GDP-mannose 4,6 dehydratase

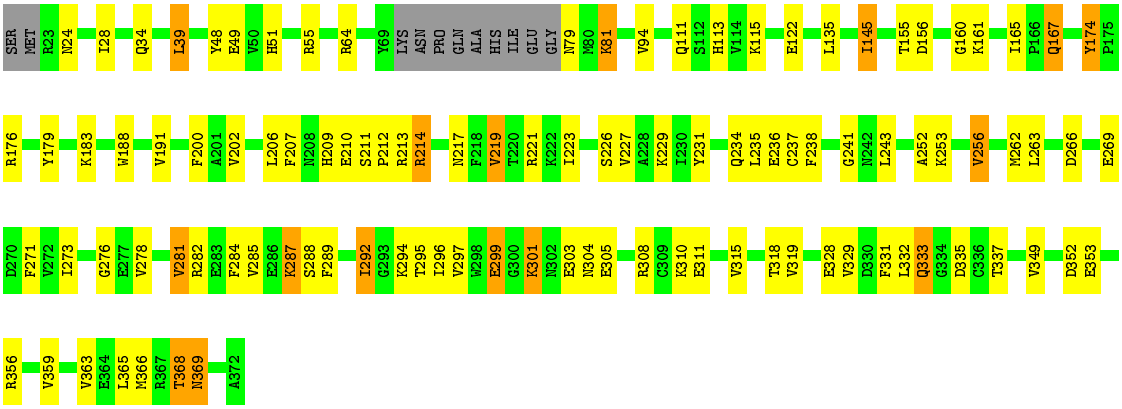
Chain G:





- Molecule 1: GDP-mannose 4,6 dehydratase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	101.62Å 231.06Å 383.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.53 – 2.80 115.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (115.53-2.80) 99.9 (115.53-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.186 , 0.235 0.186 , 0.235	Depositor DCC
R_{free} test set	5446 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	79.1	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22956	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.38	0/2839	0.54	0/3846
1	B	0.38	0/2817	0.56	0/3811
1	C	0.35	0/2840	0.53	0/3844
1	D	0.35	0/2799	0.53	0/3791
1	E	0.37	0/2849	0.54	0/3858
1	F	0.35	0/2846	0.52	0/3855
1	G	0.37	0/2847	0.53	0/3857
1	H	0.31	0/2779	0.48	0/3761
All	All	0.36	0/22616	0.53	0/30623

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	2778	0	2718	58	0
1	B	2757	0	2715	39	0
1	C	2779	0	2728	37	0
1	D	2739	0	2679	56	0
1	E	2787	0	2736	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2784	0	2725	60	0
1	G	2784	0	2728	66	0
1	H	2720	0	2673	99	0
2	A	40	19	19	2	0
2	B	40	19	19	0	0
2	C	40	19	19	0	0
2	D	40	19	19	1	0
2	E	40	19	19	0	0
2	F	40	19	19	1	0
2	G	40	19	19	0	0
2	H	40	19	19	3	0
3	A	39	0	23	2	0
3	B	39	0	23	0	0
3	C	39	0	23	2	0
3	D	39	0	23	0	0
3	E	39	0	23	1	0
3	F	39	0	23	1	0
3	G	39	0	23	2	0
3	H	39	0	23	5	0
4	D	8	12	12	0	0
4	G	4	6	6	0	0
4	H	4	6	6	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
All	All	22780	176	22062	450	0

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

All (450) 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:G:225:ARG:HH22	1:G:372:ALA:HB1	1.15	1.06
1:A:66:GLU:HA	1:A:69:TYR:HE2	1.20	1.03
1:H:81:LYS:HA	1:H:81:LYS:HE2	1.42	0.99
1:H:212:PRO:O	1:H:221:ARG:NH1	1.99	0.95
1:H:206:LEU:HD22	1:H:273:ILE:HB	1.50	0.94
1:D:289:PHE:CB	1:D:296:ILE:HD11	1.99	0.93
1:C:231:TYR:HB2	1:C:292:ILE:HD11	1.47	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77:GLU:CB	1:G:81:LYS:HE3	1.99	0.92
1:G:81:LYS:HA	1:G:81:LYS:HE2	1.54	0.90
1:H:231:TYR:HB2	1:H:292:ILE:HD11	1.51	0.90
1:G:206:LEU:HD22	1:G:273:ILE:HB	1.54	0.88
1:D:343:LEU:O	1:D:344:ASN:ND2	2.07	0.87
1:C:292:ILE:HG23	1:C:294:LYS:HG3	1.58	0.85
1:E:244:ASP:OD1	1:E:282:ARG:NH1	2.11	0.84
1:H:227:VAL:HG12	1:H:292:ILE:HD12	1.60	0.83
1:H:231:TYR:HB2	1:H:292:ILE:CD1	2.07	0.83
1:E:176:ARG:O	1:E:327:THR:HG21	1.79	0.82
1:A:66:GLU:HA	1:A:69:TYR:CE2	2.12	0.82
1:E:335:ASP:OD1	1:E:337:THR:HG23	1.80	0.81
1:G:227:VAL:HG12	1:G:292:ILE:HD12	1.61	0.81
1:E:256:VAL:HG12	1:E:259:MET:HE1	1.62	0.80
1:A:330:ASP:HB2	1:A:331:PHE:CD1	2.17	0.80
1:G:225:ARG:NH2	1:G:372:ALA:HB1	1.95	0.80
1:H:276:GLY:O	1:H:333:GLN:NE2	2.15	0.79
1:H:28:ILE:HD13	1:H:39:LEU:HD23	1.64	0.79
1:C:231:TYR:HB2	1:C:292:ILE:CD1	2.12	0.79
1:B:206:LEU:HD22	1:B:273:ILE:HB	1.65	0.79
1:H:64:ARG:NH1	1:H:213:ARG:O	2.16	0.78
1:H:81:LYS:HA	1:H:81:LYS:CE	2.13	0.78
1:F:225:ARG:NH2	1:F:372:ALA:O	2.16	0.78
1:B:247:ARG:NH2	1:B:329:VAL:O	2.17	0.77
1:C:231:TYR:CB	1:C:292:ILE:HD11	2.14	0.77
1:C:289:PHE:O	1:C:292:ILE:HG22	1.85	0.77
1:H:167:GLN:HE22	1:H:333:GLN:H	1.31	0.76
1:C:225:ARG:HH22	1:C:372:ALA:HA	1.49	0.76
1:G:231:TYR:HB2	1:G:292:ILE:CD1	2.16	0.76
1:D:151:TYR:CZ	1:D:259:MET:HG2	2.21	0.76
1:D:287:LYS:NZ	1:D:352:ASP:OD2	2.13	0.76
1:A:168:LYS:H	1:A:171:THR:CG2	1.98	0.75
1:A:176:ARG:O	1:A:327:THR:HG21	1.86	0.75
1:H:349:VAL:HG13	1:H:353:GLU:HG3	1.68	0.74
1:E:195:GLU:OE1	1:F:174:TYR:OH	2.05	0.73
1:H:223:ILE:HD13	1:H:285:VAL:HG22	1.69	0.73
1:F:359:VAL:O	1:F:363:VAL:HG23	1.87	0.73
1:E:29:THR:HG22	1:E:53:ILE:HD12	1.71	0.73
1:B:228:ALA:O	1:B:232:LEU:HD12	1.89	0.73
1:G:155:THR:OG1	3:G:402:GDD:H611	1.90	0.72
1:H:145:ILE:HD12	1:H:145:ILE:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:206:LEU:CD2	1:H:273:ILE:HB	2.20	0.72
1:E:92:CYS:O	1:E:96:ILE:HG12	1.91	0.71
1:H:331:PHE:O	1:H:332:LEU:HD23	1.91	0.71
1:D:289:PHE:CG	1:D:296:ILE:HD11	2.26	0.71
1:G:281:VAL:O	1:G:285:VAL:HG12	1.90	0.71
1:H:262:MET:CE	1:H:271:PHE:HB2	2.21	0.71
1:H:349:VAL:HG13	1:H:353:GLU:CG	2.21	0.71
1:G:165:ILE:HD13	1:G:331:PHE:HD2	1.55	0.70
1:H:231:TYR:CB	1:H:292:ILE:HD11	2.21	0.70
1:F:243:LEU:HD11	1:F:319:VAL:HG22	1.74	0.70
1:D:296:ILE:N	1:D:296:ILE:HD12	2.08	0.69
1:G:221:ARG:O	1:G:225:ARG:HG3	1.93	0.69
1:B:113:HIS:CE1	1:B:115:LYS:HB3	2.28	0.69
1:G:292:ILE:HG22	1:G:294:LYS:HG3	1.75	0.69
1:G:58:SER:O	1:H:64:ARG:NH2	2.26	0.69
1:F:72:PRO:HB2	1:F:76:ILE:HA	1.74	0.69
1:H:161:LYS:HB2	1:H:176:ARG:HD2	1.75	0.68
1:G:231:TYR:HB2	1:G:292:ILE:HD13	1.75	0.68
1:A:34:GLN:HB3	2:A:401:NAP:O1N	1.94	0.68
1:B:225:ARG:NH2	1:B:372:ALA:O	2.27	0.68
1:F:231:TYR:HB2	1:F:292:ILE:HD11	1.76	0.68
1:A:25:VAL:HG22	1:A:102:PRO:HA	1.76	0.68
1:H:335:ASP:OD1	1:H:337:THR:OG1	2.10	0.68
1:D:289:PHE:HB2	1:D:296:ILE:HD11	1.77	0.67
1:F:238:PHE:CE2	1:F:240:LEU:HD11	2.29	0.67
1:H:292:ILE:CG2	1:H:294:LYS:HG3	2.24	0.67
1:G:299:GLU:OE1	1:G:308:ARG:NE	2.18	0.67
1:G:271:PHE:CZ	1:G:343:LEU:HD11	2.30	0.66
1:A:225:ARG:HH22	1:A:372:ALA:HB2	1.60	0.66
1:A:29:THR:HG22	1:A:53:ILE:HD12	1.77	0.66
1:D:28:ILE:HD13	1:D:39:LEU:HD23	1.77	0.66
1:H:289:PHE:HB3	1:H:296:ILE:HD11	1.78	0.66
1:H:34:GLN:HB3	2:H:401:NAP:O1N	1.96	0.66
1:H:289:PHE:CB	1:H:296:ILE:HD11	2.26	0.65
1:H:179:TYR:HH	3:H:402:GDD:HE	1.42	0.65
1:D:366:MET:HA	1:D:366:MET:HE3	1.79	0.65
1:H:368:THR:O	1:H:369:ASN:HB3	1.96	0.65
1:F:56:ARG:HD3	1:F:57:SER:N	2.13	0.64
1:F:287:LYS:NZ	1:F:352:ASP:OD1	2.31	0.64
1:D:227:VAL:HG13	1:D:292:ILE:HD13	1.80	0.64
1:B:366:MET:HE3	1:B:366:MET:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:364:GLU:O	1:E:368:THR:HG23	1.98	0.63
1:H:296:ILE:HD12	1:H:296:ILE:N	2.14	0.63
1:H:156:ASP:OD2	1:H:207:PHE:HA	1.99	0.63
1:D:335:ASP:OD1	1:D:337:THR:OG1	2.16	0.63
1:H:295:THR:OG1	1:H:310:LYS:HG2	1.97	0.63
1:F:289:PHE:O	1:F:292:ILE:HG22	1.99	0.62
1:H:28:ILE:CD1	1:H:39:LEU:HD23	2.29	0.62
1:H:241:GLY:O	1:H:243:LEU:HD12	1.98	0.62
1:H:262:MET:HE1	1:H:271:PHE:HB2	1.80	0.62
1:H:289:PHE:CG	1:H:296:ILE:HD11	2.35	0.62
1:D:56:ARG:HG2	1:D:57:SER:N	2.13	0.62
1:D:289:PHE:HB3	1:D:296:ILE:HD11	1.82	0.62
1:A:364:GLU:O	1:A:368:THR:HG23	2.00	0.62
1:D:70:LYS:O	1:D:71:ASN:HB2	2.00	0.62
1:C:231:TYR:CA	1:C:292:ILE:HD11	2.30	0.61
1:H:359:VAL:O	1:H:363:VAL:HG23	2.00	0.61
1:H:284:PHE:O	1:H:288:SER:OG	2.13	0.61
1:H:303:GLU:O	1:H:319:VAL:HG13	2.00	0.61
1:F:151:TYR:CZ	1:F:259:MET:HG2	2.36	0.61
1:G:165:ILE:HD13	1:G:331:PHE:CD2	2.35	0.61
1:D:303:GLU:HA	1:D:319:VAL:HG22	1.83	0.61
1:H:200:PHE:HE1	1:H:263:LEU:HD22	1.66	0.61
1:H:179:TYR:OH	3:H:402:GDD:O41	2.15	0.61
1:A:56:ARG:HD3	1:A:57:SER:N	2.17	0.60
1:A:79:ASN:OD1	1:E:308:ARG:NH2	2.34	0.60
1:G:74:ALA:HB2	1:H:235:LEU:HD23	1.83	0.60
1:C:144:LEU:O	1:C:148:VAL:HG12	2.01	0.60
1:D:289:PHE:HB2	1:D:296:ILE:CD1	2.32	0.60
1:H:243:LEU:O	1:H:281:VAL:HG13	2.01	0.60
1:G:81:LYS:HA	1:G:81:LYS:CE	2.29	0.60
1:B:227:VAL:HG13	1:B:292:ILE:HD13	1.82	0.60
1:E:231:TYR:HB2	1:E:292:ILE:CG1	2.32	0.60
1:A:161:LYS:HD2	1:A:176:ARG:NH2	2.18	0.59
1:F:306:VAL:HG11	1:F:315:VAL:HG21	1.83	0.59
1:F:356:ARG:HG3	1:F:357:GLU:N	2.15	0.59
1:A:308:ARG:HH21	1:A:308:ARG:CB	2.15	0.59
1:E:38:TYR:OH	1:E:213:ARG:HD2	2.02	0.58
1:A:225:ARG:HH22	1:A:372:ALA:CB	2.16	0.58
1:B:39:LEU:HD13	1:B:256:VAL:HG12	1.84	0.58
1:F:231:TYR:CD1	1:F:292:ILE:HG13	2.38	0.58
3:A:402:GDD:O3B	3:A:402:GDD:H5'1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:HIS:CE1	1:C:115:LYS:HB3	2.39	0.58
1:C:247:ARG:NH2	1:C:329:VAL:O	2.36	0.58
1:G:306:VAL:HG23	1:G:318:THR:HG22	1.84	0.58
1:H:301:LYS:N	1:H:301:LYS:HD3	2.19	0.58
1:C:353:GLU:HG3	1:C:356:ARG:HH12	1.67	0.58
1:H:226:SER:HB3	1:H:238:PHE:CD2	2.38	0.58
1:B:359:VAL:O	1:B:363:VAL:HG23	2.03	0.58
1:C:238:PHE:O	1:C:317:VAL:HA	2.03	0.58
1:D:366:MET:CE	1:D:366:MET:HA	2.33	0.57
1:E:231:TYR:CG	1:E:292:ILE:HD11	2.39	0.57
1:C:179:TYR:HH	3:C:402:GDD:HE	1.52	0.57
1:F:281:VAL:O	1:F:285:VAL:HG23	2.04	0.57
1:H:202:VAL:HG13	1:H:269:GLU:O	2.05	0.57
1:B:113:HIS:HE1	1:B:115:LYS:HB3	1.69	0.57
1:F:38:TYR:CD1	1:F:253:LYS:HG2	2.40	0.57
1:D:299:GLU:OE1	1:D:308:ARG:NH1	2.38	0.56
1:E:38:TYR:CZ	1:E:213:ARG:HD2	2.40	0.56
1:A:69:TYR:H	1:A:69:TYR:HD2	1.52	0.56
1:F:221:ARG:O	1:F:225:ARG:HG3	2.06	0.56
1:H:310:LYS:HG3	1:H:311:GLU:N	2.20	0.56
1:G:231:TYR:CD1	1:G:292:ILE:HG12	2.41	0.56
1:H:113:HIS:CE1	1:H:115:LYS:HB3	2.40	0.56
1:G:219:VAL:O	1:G:223:ILE:HG13	2.06	0.56
1:C:229:LYS:HE3	1:C:234:GLN:OE1	2.06	0.56
1:A:329:VAL:HG11	1:A:332:LEU:HD11	1.87	0.56
1:D:231:TYR:HD2	1:D:292:ILE:HB	1.71	0.55
1:F:231:TYR:CB	1:F:292:ILE:HD11	2.36	0.55
1:G:73:GLN:O	1:H:229:LYS:HE2	2.05	0.55
1:A:168:LYS:O	1:A:171:THR:HG23	2.06	0.55
1:D:289:PHE:CB	1:D:296:ILE:CD1	2.80	0.55
1:A:248:ASP:OD1	1:A:275:THR:HG22	2.06	0.55
1:A:56:ARG:C	1:A:56:ARG:HD3	2.27	0.55
1:B:38:TYR:CE2	1:B:213:ARG:HD2	2.41	0.55
1:F:113:HIS:CD2	1:F:217:ASN:HB3	2.42	0.55
1:F:223:ILE:HD13	1:F:285:VAL:HG22	1.89	0.55
1:E:362:ASP:O	1:E:366:MET:HG2	2.07	0.55
1:A:38:TYR:CE2	1:A:213:ARG:HD2	2.42	0.55
1:F:291:HIS:NE2	1:F:356:ARG:HB2	2.22	0.55
1:E:231:TYR:CD2	1:E:292:ILE:HD11	2.42	0.55
1:H:301:LYS:HE2	1:H:304:ASN:HB2	1.87	0.55
1:E:149:LYS:HE2	1:E:263:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:VAL:CG1	1:F:315:VAL:HG21	2.37	0.55
1:H:165:ILE:N	1:H:165:ILE:HD12	2.22	0.55
1:B:364:GLU:O	1:B:368:THR:HG23	2.06	0.55
1:D:303:GLU:HA	1:D:319:VAL:CG2	2.36	0.55
1:G:229:LYS:HD2	1:G:366:MET:CE	2.37	0.55
1:C:335:ASP:OD1	1:C:337:THR:OG1	2.22	0.54
1:F:223:ILE:CD1	1:F:285:VAL:HG22	2.37	0.54
1:H:289:PHE:HB3	1:H:296:ILE:CD1	2.37	0.54
1:D:39:LEU:CA	1:D:256:VAL:HG21	2.38	0.54
1:A:308:ARG:HG3	1:A:315:VAL:HB	1.88	0.54
2:A:401:NAP:O4D	2:A:401:NAP:O2N	2.24	0.54
1:E:291:HIS:NE2	1:E:356:ARG:HG3	2.22	0.54
1:A:248:ASP:OD1	1:A:275:THR:CG2	2.55	0.54
1:A:299:GLU:OE1	1:A:308:ARG:NH2	2.41	0.54
1:F:115:LYS:HD3	1:F:115:LYS:O	2.08	0.54
1:H:289:PHE:CB	1:H:296:ILE:CD1	2.86	0.54
1:H:262:MET:HE2	1:H:271:PHE:HB2	1.90	0.54
1:E:231:TYR:HB2	1:E:292:ILE:HG12	1.88	0.54
1:C:311:GLU:N	1:C:311:GLU:OE1	2.39	0.53
1:E:256:VAL:HA	1:E:259:MET:HE2	1.90	0.53
1:H:299:GLU:CD	1:H:308:ARG:HH21	2.11	0.53
1:E:114:VAL:HG11	3:E:402:GDD:O3B	2.08	0.53
1:B:311:GLU:OE1	1:B:311:GLU:N	2.40	0.53
1:B:39:LEU:HB2	1:B:256:VAL:CG1	2.38	0.53
1:H:223:ILE:CD1	1:H:285:VAL:HG22	2.38	0.53
1:B:24:ASN:HB3	1:B:48:TYR:CD2	2.44	0.53
1:E:359:VAL:O	1:E:363:VAL:HG23	2.09	0.53
1:H:39:LEU:HB2	1:H:256:VAL:HG12	1.90	0.53
1:B:151:TYR:CZ	1:B:259:MET:HG2	2.44	0.53
1:D:273:ILE:HG23	1:D:345:TRP:CH2	2.44	0.53
1:G:118:PHE:CD1	1:G:326:PRO:HG2	2.44	0.53
1:F:71:ASN:N	1:F:72:PRO:HD3	2.24	0.53
1:G:282:ARG:O	1:G:285:VAL:HG13	2.09	0.53
1:G:227:VAL:CG1	1:G:292:ILE:HD12	2.36	0.53
1:G:237:CYS:HB2	1:G:316:HIS:HA	1.91	0.53
1:A:168:LYS:H	1:A:171:THR:HG23	1.72	0.53
1:C:286:GLU:O	1:C:290:LEU:HD13	2.09	0.53
1:H:160:GLY:HA3	1:H:174:TYR:O	2.09	0.53
1:E:291:HIS:CD2	1:E:356:ARG:HG3	2.44	0.52
1:A:68:LEU:HB2	1:A:80:MET:HE1	1.90	0.52
1:D:301:LYS:HA	1:D:301:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LEU:HD22	1:B:273:ILE:CB	2.37	0.52
1:H:206:LEU:HD22	1:H:273:ILE:CB	2.32	0.52
1:C:231:TYR:CD1	1:C:292:ILE:HG12	2.45	0.52
1:H:353:GLU:OE2	1:H:356:ARG:NH2	2.42	0.52
1:G:292:ILE:O	1:G:292:ILE:HG23	2.10	0.52
1:G:311:GLU:N	1:G:311:GLU:OE1	2.39	0.52
1:A:118:PHE:HZ	1:A:327:THR:HG22	1.73	0.52
1:A:118:PHE:CZ	1:A:327:THR:HG22	2.45	0.52
1:A:371:ASN:O	1:A:372:ALA:HB2	2.10	0.51
1:D:155:THR:HG21	1:D:179:TYR:OH	2.10	0.51
1:D:311:GLU:OE1	1:D:311:GLU:N	2.41	0.51
1:G:286:GLU:O	1:G:290:LEU:HD13	2.10	0.51
1:H:39:LEU:N	1:H:256:VAL:HG11	2.24	0.51
1:C:231:TYR:HB2	1:C:292:ILE:CG1	2.39	0.51
1:H:188:TRP:O	1:H:191:VAL:HG22	2.10	0.51
1:H:318:THR:HG22	1:H:319:VAL:N	2.25	0.51
1:F:144:LEU:O	1:F:148:VAL:HG13	2.08	0.51
1:H:183:LYS:HE3	2:H:401:NAP:O2D	2.09	0.51
1:G:262:MET:HG2	1:G:271:PHE:CD2	2.45	0.51
1:C:151:TYR:CZ	1:C:259:MET:HG2	2.45	0.51
1:F:176:ARG:NH1	1:F:327:THR:HB	2.26	0.51
1:H:305:GLU:O	1:H:319:VAL:HG12	2.11	0.51
1:G:309:CYS:SG	1:G:312:THR:OG1	2.69	0.51
1:H:167:GLN:NE2	1:H:333:GLN:O	2.44	0.51
1:B:301:LYS:HA	1:B:301:LYS:HE2	1.92	0.51
1:G:90:SER:O	1:G:94:VAL:HG12	2.11	0.51
1:H:253:LYS:O	1:H:256:VAL:HG23	2.11	0.51
1:A:168:LYS:H	1:A:171:THR:HG21	1.74	0.51
1:C:196:ALA:HB1	1:D:326:PRO:HB2	1.93	0.50
1:F:160:GLY:HA3	1:F:174:TYR:O	2.11	0.50
1:G:328:GLU:OE1	1:G:328:GLU:HA	2.11	0.50
1:C:269:GLU:OE2	1:C:342:LYS:NZ	2.39	0.50
1:D:35:ASP:OD2	1:D:209:HIS:NE2	2.41	0.50
1:F:243:LEU:HD11	1:F:319:VAL:CG2	2.40	0.50
1:H:165:ILE:HG23	1:H:331:PHE:HE2	1.76	0.50
1:G:229:LYS:HD2	1:G:366:MET:HE2	1.92	0.50
1:H:113:HIS:HE1	1:H:115:LYS:HB3	1.75	0.50
1:H:214:ARG:NH2	3:H:402:GDD:O21	2.43	0.50
1:B:227:VAL:CG1	1:B:292:ILE:HD13	2.42	0.50
1:C:186:ALA:O	1:C:189:ILE:HG22	2.12	0.50
1:F:161:LYS:HB2	1:F:176:ARG:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:245:ALA:O	1:G:280:SER:HA	2.12	0.50
1:H:292:ILE:HG23	1:H:292:ILE:O	2.11	0.50
1:B:39:LEU:CA	1:B:256:VAL:HG11	2.42	0.49
1:D:306:VAL:HG13	1:D:318:THR:HG22	1.94	0.49
1:D:340:LYS:O	1:D:344:ASN:HA	2.10	0.49
1:F:295:THR:HG23	1:F:311:GLU:OE1	2.12	0.49
1:D:56:ARG:NH2	2:F:402:NAP:O2A	2.45	0.49
1:G:206:LEU:HD22	1:G:273:ILE:CB	2.36	0.49
1:C:188:TRP:CD2	1:D:175:PRO:HD2	2.46	0.49
1:B:280:SER:OG	1:B:283:GLU:HG3	2.13	0.49
1:G:214:ARG:HD2	1:G:218:PHE:CD2	2.47	0.49
1:C:225:ARG:O	1:C:229:LYS:HG3	2.13	0.49
1:H:227:VAL:HG12	1:H:292:ILE:CD1	2.38	0.49
1:A:231:TYR:CD1	1:A:292:ILE:HG13	2.47	0.49
1:B:254:ASP:OD1	1:B:348:ARG:HG2	2.12	0.49
1:G:88:THR:HG22	1:G:88:THR:O	2.13	0.49
1:H:229:LYS:HE3	1:H:234:GLN:NE2	2.27	0.49
1:F:144:LEU:HB3	1:F:148:VAL:CG1	2.42	0.49
1:B:299:GLU:OE1	1:B:308:ARG:NH1	2.46	0.48
1:H:296:ILE:N	1:H:296:ILE:CD1	2.75	0.48
1:H:292:ILE:HG23	1:H:294:LYS:HG3	1.94	0.48
1:G:161:LYS:HD2	1:G:176:ARG:NH2	2.28	0.48
1:B:258:ALA:O	1:B:262:MET:HG3	2.12	0.48
1:E:161:LYS:HD2	1:E:176:ARG:NH2	2.29	0.48
1:F:56:ARG:C	1:F:56:ARG:HD3	2.33	0.48
1:H:229:LYS:HE3	1:H:234:GLN:HE21	1.78	0.48
1:B:156:ASP:OD2	1:B:332:LEU:HD13	2.13	0.48
1:F:144:LEU:HB3	1:F:148:VAL:HG13	1.95	0.48
1:H:235:LEU:HD13	1:H:236:GLU:N	2.27	0.48
1:A:273:ILE:HG23	1:A:345:TRP:CH2	2.48	0.48
1:G:231:TYR:HB2	1:G:292:ILE:HD11	1.95	0.48
1:F:231:TYR:HB2	1:F:292:ILE:CG1	2.44	0.47
1:G:221:ARG:HG3	1:G:225:ARG:HD2	1.96	0.47
1:G:292:ILE:O	1:G:292:ILE:CG2	2.62	0.47
1:A:167:GLN:HA	1:A:171:THR:HG21	1.96	0.47
1:D:360:HIS:O	1:D:363:VAL:HG22	2.13	0.47
1:E:306:VAL:HG23	1:E:318:THR:HG22	1.95	0.47
1:F:231:TYR:HB2	1:F:292:ILE:CD1	2.41	0.47
1:F:67:HIS:CD2	1:F:68:LEU:HD13	2.50	0.47
1:G:57:SER:HB3	1:G:59:SER:O	2.15	0.47
1:A:308:ARG:HH21	1:A:308:ARG:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:LYS:HG2	1:G:366:MET:HG2	1.96	0.47
1:F:306:VAL:HG12	1:F:315:VAL:HG23	1.97	0.47
1:D:81:LYS:HD2	1:D:81:LYS:HA	1.58	0.47
1:G:150:PHE:O	1:G:201:ALA:HA	2.15	0.47
1:C:292:ILE:CG2	1:C:294:LYS:HG3	2.39	0.47
1:C:188:TRP:CE3	1:D:175:PRO:HD2	2.50	0.47
1:E:188:TRP:CE3	1:F:175:PRO:HD2	2.50	0.47
1:F:351:PHE:O	1:F:355:VAL:HG12	2.15	0.47
1:H:311:GLU:OE1	1:H:311:GLU:N	2.39	0.47
1:B:320:ASP:OD2	1:E:301:LYS:HD2	2.14	0.47
1:G:91:THR:OG1	1:H:122:GLU:OE1	2.33	0.47
1:H:223:ILE:HD13	1:H:285:VAL:CG2	2.41	0.46
1:A:210:GLU:O	1:A:211:SER:HB3	2.14	0.46
1:F:50:VAL:O	1:F:80:MET:HA	2.15	0.46
1:B:67:HIS:CD2	1:B:68:LEU:HD13	2.51	0.46
1:D:239:SER:HA	1:D:318:THR:O	2.16	0.46
1:G:336:CYS:O	1:G:340:LYS:HG3	2.15	0.46
1:F:308:ARG:HA	1:F:315:VAL:HA	1.97	0.46
1:G:271:PHE:CE1	1:G:343:LEU:HD11	2.50	0.46
1:A:200:PHE:CE2	1:A:268:PRO:HD3	2.51	0.46
1:A:162:VAL:CG1	1:A:164:GLU:O	2.63	0.46
1:C:46:LYS:HE3	1:C:260:TRP:CH2	2.51	0.46
1:D:34:GLN:HB3	2:D:401:NAP:O2N	2.16	0.46
1:H:24:ASN:HB3	1:H:48:TYR:CD2	2.51	0.46
1:B:284:PHE:CE2	1:B:355:VAL:HG22	2.51	0.46
1:D:371:ASN:O	1:D:372:ALA:HB2	2.15	0.46
1:A:25:VAL:CG2	1:A:102:PRO:HA	2.44	0.46
1:C:353:GLU:CG	1:C:356:ARG:HH12	2.29	0.46
1:D:39:LEU:HD13	1:D:259:MET:HE2	1.97	0.46
1:F:219:VAL:HB	3:F:401:GDD:N3	2.30	0.46
1:B:206:LEU:HD13	1:B:255:TYR:HB3	1.99	0.45
1:A:223:ILE:HD13	1:A:285:VAL:HG22	1.98	0.45
1:B:366:MET:HE3	1:B:372:ALA:HB3	1.98	0.45
1:D:343:LEU:C	1:D:344:ASN:HD22	2.13	0.45
1:H:282:ARG:NH1	1:H:305:GLU:OE1	2.47	0.45
1:E:115:LYS:CG	1:E:325:ARG:HG2	2.47	0.45
1:F:243:LEU:O	1:F:282:ARG:HG3	2.17	0.45
1:F:282:ARG:NH1	1:F:305:GLU:OE2	2.42	0.45
1:G:91:THR:O	1:G:94:VAL:HG13	2.16	0.45
1:H:183:LYS:HE3	2:H:401:NAP:HO2N	1.80	0.45
1:A:191:VAL:O	1:A:195:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PHE:CD1	1:A:326:PRO:HG2	2.51	0.45
1:H:51:HIS:HA	1:H:81:LYS:O	2.16	0.45
1:A:151:TYR:CZ	1:A:259:MET:HG2	2.52	0.45
1:C:149:LYS:HD3	1:C:200:PHE:CE1	2.52	0.45
1:A:25:VAL:HB	1:A:49:GLU:HG2	1.98	0.45
1:A:292:ILE:HG23	1:A:292:ILE:O	2.17	0.45
1:A:308:ARG:NH2	1:A:308:ARG:HB3	2.33	0.44
1:G:34:GLN:OE1	1:G:214:ARG:HB2	2.17	0.44
1:A:161:LYS:HD2	1:A:176:ARG:HH22	1.81	0.44
1:D:231:TYR:CD2	1:D:292:ILE:HB	2.52	0.44
1:A:369:ASN:HA	1:A:370:PRO:HD3	1.87	0.44
1:H:135:LEU:HA	1:H:135:LEU:HD12	1.84	0.44
1:H:145:ILE:H	1:H:145:ILE:CD1	2.16	0.44
1:H:235:LEU:HD13	1:H:237:CYS:N	2.33	0.44
1:A:225:ARG:HH12	1:A:372:ALA:HB1	1.83	0.44
1:C:46:LYS:HE3	1:C:260:TRP:CZ3	2.53	0.44
1:D:39:LEU:HA	1:D:256:VAL:HG21	1.99	0.44
1:D:46:LYS:HE3	1:D:260:TRP:CH2	2.52	0.44
1:F:140:LYS:HB2	1:F:145:ILE:HD11	1.98	0.44
1:H:252:ALA:O	1:H:256:VAL:HG22	2.18	0.44
1:H:295:THR:C	1:H:296:ILE:HD12	2.38	0.44
1:D:115:LYS:NZ	1:D:324:TYR:O	2.45	0.44
1:A:156:ASP:OD2	1:A:332:LEU:HD13	2.18	0.44
1:C:187:TYR:O	1:C:191:VAL:HG23	2.18	0.44
1:F:244:ASP:OD1	1:F:282:ARG:NE	2.43	0.44
1:G:239:SER:HB3	1:G:318:THR:OG1	2.17	0.44
1:G:351:PHE:O	1:G:355:VAL:HG12	2.18	0.44
1:G:95:LYS:NZ	1:G:99:GLU:OE2	2.46	0.44
1:A:292:ILE:HD12	1:A:292:ILE:HA	1.56	0.43
1:D:305:GLU:O	1:D:319:VAL:CG1	2.66	0.43
1:E:292:ILE:HG23	1:E:294:LYS:HG3	1.99	0.43
1:F:306:VAL:CG1	1:F:315:VAL:CG2	2.96	0.43
1:D:29:THR:HG22	1:D:53:ILE:HD12	2.01	0.43
1:G:214:ARG:NH2	3:G:402:GDD:O21	2.35	0.43
1:F:88:THR:O	1:F:88:THR:HG23	2.18	0.43
1:D:39:LEU:HB2	1:D:256:VAL:CG2	2.48	0.43
1:F:71:ASN:N	1:F:72:PRO:CD	2.81	0.43
1:H:281:VAL:O	1:H:285:VAL:HG23	2.18	0.43
1:D:124:THR:O	1:D:128:ASP:HB2	2.19	0.43
1:E:35:ASP:OD2	1:E:209:HIS:NE2	2.34	0.43
1:E:280:SER:OG	1:E:283:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ARG:O	1:B:225:ARG:HG3	2.18	0.43
1:F:212:PRO:O	1:F:221:ARG:NH1	2.52	0.43
1:G:91:THR:HA	1:G:94:VAL:CG1	2.48	0.43
1:E:344:ASN:OD1	1:G:73:GLN:NE2	2.47	0.43
1:H:243:LEU:HD12	1:H:243:LEU:N	2.34	0.43
1:E:38:TYR:CZ	1:E:213:ARG:CD	3.01	0.42
1:F:88:THR:O	1:F:88:THR:CG2	2.67	0.42
1:G:262:MET:CE	1:G:271:PHE:HB2	2.49	0.42
1:H:287:LYS:HE3	1:H:352:ASP:OD1	2.19	0.42
1:F:23:ARG:NH2	1:F:101:LYS:O	2.51	0.42
1:F:165:ILE:HA	1:F:166:PRO:HA	1.88	0.42
1:G:161:LYS:HD2	1:G:176:ARG:HH22	1.84	0.42
1:G:150:PHE:HB3	1:G:201:ALA:HB2	2.01	0.42
1:G:50:VAL:CG2	1:G:80:MET:HG3	2.50	0.42
1:A:223:ILE:HD13	1:A:285:VAL:CG2	2.49	0.42
1:A:329:VAL:CG1	1:A:332:LEU:HD11	2.49	0.42
1:B:24:ASN:HB3	1:B:48:TYR:CE2	2.54	0.42
1:C:196:ALA:HB2	1:D:327:THR:HG23	2.00	0.42
1:F:273:ILE:HG23	1:F:345:TRP:CH2	2.54	0.42
1:E:120:LEU:HD12	1:E:120:LEU:HA	1.70	0.42
1:A:156:ASP:OD1	3:A:402:GDD:H612	2.20	0.42
1:E:262:MET:HG2	1:E:271:PHE:CD2	2.54	0.42
1:H:155:THR:HG21	1:H:179:TYR:HH	1.85	0.42
1:A:231:TYR:CG	1:A:292:ILE:HG13	2.55	0.42
1:A:69:TYR:N	1:A:69:TYR:CD2	2.88	0.42
1:E:292:ILE:CG2	1:E:294:LYS:HG3	2.50	0.42
3:H:402:GDD:H5'1	3:H:402:GDD:O3B	2.19	0.42
1:C:195:GLU:OE1	1:D:174:TYR:OH	2.37	0.42
1:E:60:PHE:HZ	1:E:63:GLY:HA2	1.83	0.42
1:F:306:VAL:HG12	1:F:315:VAL:CG2	2.50	0.42
1:G:271:PHE:CE2	1:G:343:LEU:HD11	2.54	0.42
1:E:113:HIS:HB3	1:E:116:ILE:HB	2.01	0.42
1:B:223:ILE:HD13	1:B:285:VAL:HG22	2.02	0.41
1:D:38:TYR:CE1	1:D:213:ARG:NH1	2.88	0.41
1:H:219:VAL:HG23	3:H:402:GDD:C4	2.50	0.41
1:E:286:GLU:O	1:E:290:LEU:HD13	2.19	0.41
1:H:188:TRP:HA	1:H:191:VAL:HG22	2.02	0.41
1:E:283:GLU:OE2	1:E:287:LYS:HE3	2.21	0.41
1:C:113:HIS:HE1	1:C:115:LYS:HB3	1.82	0.41
1:D:123:TYR:O	1:D:127:VAL:HG13	2.21	0.41
1:E:149:LYS:HD2	1:E:200:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:PHE:CZ	1:E:63:GLY:HA2	2.56	0.41
1:F:38:TYR:CE1	1:F:253:LYS:HG2	2.55	0.41
1:B:252:ALA:O	1:B:256:VAL:HG23	2.20	0.41
1:E:96:ILE:H	1:E:96:ILE:HG12	1.61	0.41
1:E:341:GLN:HB3	1:G:72:PRO:HD2	2.02	0.41
1:H:211:SER:HB2	1:H:212:PRO:HD2	2.02	0.41
1:H:328:GLU:HG3	1:H:329:VAL:N	2.34	0.41
1:H:200:PHE:CE1	1:H:263:LEU:HD22	2.50	0.41
1:A:239:SER:HA	1:A:318:THR:O	2.20	0.41
1:B:348:ARG:HG3	1:B:349:VAL:HG23	2.03	0.41
1:C:112:SER:O	3:C:402:GDD:O31	2.31	0.41
1:D:223:ILE:HD13	1:D:285:VAL:HG22	2.02	0.41
1:G:35:ASP:OD2	1:G:209:HIS:NE2	2.48	0.41
1:B:139:VAL:HG11	1:B:148:VAL:HG11	2.03	0.41
1:E:188:TRP:HA	1:E:191:VAL:HG13	2.01	0.41
1:B:366:MET:CE	1:B:366:MET:HA	2.47	0.41
1:F:86:ASP:C	1:F:88:THR:H	2.25	0.41
1:C:133:LEU:HD21	1:D:121:ALA:HB1	2.03	0.41
1:E:187:TYR:O	1:E:191:VAL:CG1	2.69	0.41
1:E:232:LEU:HD11	1:E:363:VAL:HG13	2.03	0.41
1:E:366:MET:HE3	1:E:366:MET:HA	2.03	0.41
1:F:115:LYS:HB2	1:F:325:ARG:NH2	2.35	0.41
1:F:69:TYR:HD1	1:F:69:TYR:HA	1.76	0.41
1:A:330:ASP:HB2	1:A:331:PHE:HD1	1.77	0.40
1:A:68:LEU:HB2	1:A:80:MET:CE	2.50	0.40
1:B:39:LEU:N	1:B:256:VAL:HG11	2.36	0.40
1:B:184:LEU:HA	1:B:184:LEU:HD23	1.87	0.40
1:E:229:LYS:HB3	1:E:234:GLN:HB2	2.03	0.40
1:D:232:LEU:HA	1:D:232:LEU:HD23	1.87	0.40
1:D:46:LYS:HE3	1:D:260:TRP:CZ3	2.56	0.40
1:H:331:PHE:C	1:H:332:LEU:HD23	2.41	0.40
1:G:231:TYR:CD2	1:G:232:LEU:HD23	2.57	0.40
1:H:207:PHE:O	1:H:209:HIS:ND1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	348/352 (99%)	335 (96%)	10 (3%)	3 (1%)	17	46
1	B	340/352 (97%)	326 (96%)	13 (4%)	1 (0%)	41	72
1	C	344/352 (98%)	334 (97%)	10 (3%)	0	100	100
1	D	339/352 (96%)	326 (96%)	13 (4%)	0	100	100
1	E	348/352 (99%)	330 (95%)	17 (5%)	1 (0%)	41	72
1	F	348/352 (99%)	332 (95%)	14 (4%)	2 (1%)	25	56
1	G	348/352 (99%)	335 (96%)	12 (3%)	1 (0%)	41	72
1	H	337/352 (96%)	323 (96%)	13 (4%)	1 (0%)	41	72
All	All	2752/2816 (98%)	2641 (96%)	102 (4%)	9 (0%)	41	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	GLY
1	E	160	GLY
1	G	160	GLY
1	F	75	HIS
1	H	369	ASN
1	F	160	GLY
1	B	160	GLY
1	A	211	SER
1	A	76	ILE

5.3.2 Protein sidechains

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	295/304 (97%)	278 (94%)	17 (6%)	20 50
1	B	296/304 (97%)	279 (94%)	17 (6%)	20 50
1	C	297/304 (98%)	284 (96%)	13 (4%)	28 61
1	D	293/304 (96%)	278 (95%)	15 (5%)	24 55
1	E	296/304 (97%)	272 (92%)	24 (8%)	11 33
1	F	296/304 (97%)	273 (92%)	23 (8%)	12 35
1	G	296/304 (97%)	274 (93%)	22 (7%)	13 37
1	H	291/304 (96%)	263 (90%)	28 (10%)	8 24
All	All	2360/2432 (97%)	2201 (93%)	159 (7%)	16 43

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	68	LEU
1	B	71	ASN
1	B	90	SER
1	B	92	CYS
1	B	95	LYS
1	B	111	GLN
1	B	155	THR
1	B	174	TYR
1	B	184	LEU
1	B	217	ASN
1	B	232	LEU
1	B	256	VAL
1	B	297	VAL
1	B	340	LYS
1	B	346	LYS
1	B	348	ARG
1	B	366	MET
1	A	69	TYR
1	A	77	GLU
1	A	90	SER
1	A	97	ILE
1	A	111	GLN
1	A	145	ILE
1	A	171	THR
1	A	210	GLU

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Mol	Chain	Res	Type
1	A	214	ARG
1	A	275	THR
1	A	278	VAL
1	A	292	ILE
1	A	297	VAL
1	A	308	ARG
1	A	315	VAL
1	A	330	ASP
1	A	344	ASN
1	C	45	GLU
1	C	66	GLU
1	C	81	LYS
1	C	90	SER
1	C	92	CYS
1	C	111	GLN
1	C	155	THR
1	C	174	TYR
1	C	198	ASN
1	C	217	ASN
1	C	257	GLU
1	C	278	VAL
1	C	292	ILE
1	D	60	PHE
1	D	68	LEU
1	D	81	LYS
1	D	90	SER
1	D	111	GLN
1	D	127	VAL
1	D	174	TYR
1	D	217	ASN
1	D	219	VAL
1	D	297	VAL
1	D	317	VAL
1	D	319	VAL
1	D	344	ASN
1	D	355	VAL
1	D	366	MET
1	E	23	ARG
1	E	45	GLU
1	E	60	PHE
1	E	69	TYR
1	E	73	GLN

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Mol	Chain	Res	Type
1	E	90	SER
1	E	96	ILE
1	E	111	GLN
1	E	114	VAL
1	E	120	LEU
1	E	149	LYS
1	E	174	TYR
1	E	191	VAL
1	E	214	ARG
1	E	266	ASP
1	E	272	VAL
1	E	283	GLU
1	E	292	ILE
1	E	295	THR
1	E	303	GLU
1	E	306	VAL
1	E	312	THR
1	E	317	VAL
1	E	366	MET
1	F	68	LEU
1	F	69	TYR
1	F	81	LYS
1	F	88	THR
1	F	111	GLN
1	F	144	LEU
1	F	147	SER
1	F	148	VAL
1	F	155	THR
1	F	177	SER
1	F	213	ARG
1	F	214	ARG
1	F	238	PHE
1	F	253	LYS
1	F	292	ILE
1	F	299	GLU
1	F	314	LYS
1	F	315	VAL
1	F	325	ARG
1	F	355	VAL
1	F	356	ARG
1	F	364	GLU
1	F	368	THR

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Mol	Chain	Res	Type
1	G	50	VAL
1	G	81	LYS
1	G	91	THR
1	G	92	CYS
1	G	94	VAL
1	G	111	GLN
1	G	119	ASP
1	G	148	VAL
1	G	176	ARG
1	G	213	ARG
1	G	237	CYS
1	G	256	VAL
1	G	266	ASP
1	G	277	GLU
1	G	278	VAL
1	G	281	VAL
1	G	285	VAL
1	G	292	ILE
1	G	330	ASP
1	G	337	THR
1	G	355	VAL
1	G	366	MET
1	H	39	LEU
1	H	49	GLU
1	H	55	ARG
1	H	79	ASN
1	H	81	LYS
1	H	94	VAL
1	H	111	GLN
1	H	145	ILE
1	H	167	GLN
1	H	174	TYR
1	H	210	GLU
1	H	214	ARG
1	H	217	ASN
1	H	219	VAL
1	H	256	VAL
1	H	266	ASP
1	H	278	VAL
1	H	281	VAL
1	H	287	LYS
1	H	292	ILE

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Mol	Chain	Res	Type
1	H	297	VAL
1	H	299	GLU
1	H	301	LYS
1	H	315	VAL
1	H	333	GLN
1	H	365	LEU
1	H	366	MET
1	H	368	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	HIS
1	A	371	ASN
1	G	234	GLN
1	H	167	GLN
1	H	234	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

20 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	GDD	E	402	-	35,42,42	0.77	1 (2%)	47,65,65	1.72	6 (12%)
2	NAP	F	402	-	36,43,52	0.60	0	44,67,80	0.82	1 (2%)
2	NAP	G	401	-	36,43,52	0.68	0	44,67,80	0.73	1 (2%)
3	GDD	H	402	-	35,42,42	0.84	1 (2%)	47,65,65	3.06	8 (17%)
2	NAP	C	401	-	36,43,52	0.65	0	44,67,80	0.94	2 (4%)
3	GDD	F	401	-	35,42,42	0.83	2 (5%)	47,65,65	1.72	6 (12%)
2	NAP	E	401	-	36,43,52	0.81	1 (2%)	44,67,80	0.99	3 (6%)
4	EDO	H	403	-	3,3,3	0.64	0	2,2,2	0.17	0
3	GDD	A	402	-	35,42,42	1.05	3 (8%)	47,65,65	3.18	17 (36%)
2	NAP	A	401	-	36,43,52	0.70	0	44,67,80	1.00	3 (6%)
3	GDD	C	402	-	35,42,42	0.87	2 (5%)	47,65,65	2.13	9 (19%)
2	NAP	H	401	-	36,43,52	0.61	0	44,67,80	0.95	2 (4%)
3	GDD	D	402	-	35,42,42	0.82	1 (2%)	47,65,65	2.33	10 (21%)
3	GDD	G	402	-	35,42,42	0.82	2 (5%)	47,65,65	2.85	9 (19%)
2	NAP	D	401	-	36,43,52	0.64	0	44,67,80	0.87	2 (4%)
4	EDO	D	403	-	3,3,3	0.65	0	2,2,2	0.12	0
3	GDD	B	402	-	35,42,42	0.84	1 (2%)	47,65,65	2.21	12 (25%)
4	EDO	D	404	-	3,3,3	0.67	0	2,2,2	0.20	0
2	NAP	B	401	-	36,43,52	0.75	1 (2%)	44,67,80	2.12	5 (11%)
4	EDO	G	403	-	3,3,3	0.68	0	2,2,2	0.08	0

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	GDD	E	402	-	-	1/19/59/59	0/4/4/4
2	NAP	F	402	-	-	13/23/59/67	0/4/4/5
2	NAP	G	401	-	-	8/23/59/67	0/4/4/5
3	GDD	H	402	-	-	3/19/59/59	0/4/4/4
2	NAP	C	401	-	-	9/23/59/67	0/4/4/5
3	GDD	F	401	-	-	5/19/59/59	0/4/4/4
2	NAP	E	401	-	-	8/23/59/67	0/4/4/5
4	EDO	H	403	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDD	A	402	-	-	8/19/59/59	0/4/4/4
2	NAP	A	401	-	-	3/23/59/67	0/4/4/5
3	GDD	C	402	-	-	3/19/59/59	0/4/4/4
2	NAP	H	401	-	-	7/23/59/67	0/4/4/5
3	GDD	D	402	-	-	3/19/59/59	0/4/4/4
3	GDD	G	402	-	-	8/19/59/59	0/4/4/4
2	NAP	D	401	-	-	9/23/59/67	0/4/4/5
4	EDO	D	403	-	-	1/1/1/1	-
3	GDD	B	402	-	-	3/19/59/59	0/4/4/4
4	EDO	D	404	-	-	1/1/1/1	-
2	NAP	B	401	-	-	8/23/59/67	0/4/4/5
4	EDO	G	403	-	-	0/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	GDD	C6-N1	3.42	1.39	1.33
3	F	401	GDD	C6-N1	3.42	1.39	1.33
3	A	402	GDD	PB-O1B	3.39	1.69	1.60
3	G	402	GDD	C6-N1	3.38	1.38	1.33
3	E	402	GDD	C6-N1	3.28	1.38	1.33
3	C	402	GDD	C6-N1	3.24	1.38	1.33
3	H	402	GDD	C6-N1	3.22	1.38	1.33
3	B	402	GDD	C6-N1	3.21	1.38	1.33
3	D	402	GDD	C6-N1	3.15	1.38	1.33
3	C	402	GDD	PB-O1B	2.24	1.66	1.60
2	E	401	NAP	P2B-O2B	2.20	1.63	1.59
3	A	402	GDD	PA-O5'	2.10	1.67	1.59
2	B	401	NAP	PA-O5B	2.08	1.67	1.59
3	G	402	GDD	PB-O1B	2.04	1.65	1.60
3	F	401	GDD	C6-C5	2.03	1.44	1.41

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	402	GDD	O3A-PB-O1B	-16.49	69.24	102.48
3	G	402	GDD	O3A-PB-O1B	-13.22	75.82	102.48
2	B	401	NAP	O2A-PA-O1A	-9.54	65.09	112.24
3	A	402	GDD	O51-C11-O1B	-8.79	99.87	111.36
3	A	402	GDD	O3A-PB-O1B	-8.62	85.10	102.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	GDD	C5-C6-N1	-8.42	111.92	123.43
3	D	402	GDD	O3A-PB-O1B	-8.36	85.63	102.48
3	G	402	GDD	C5-C6-N1	-8.34	112.02	123.43
3	A	402	GDD	C5-C6-N1	-8.31	112.06	123.43
3	F	401	GDD	C5-C6-N1	-8.26	112.13	123.43
3	H	402	GDD	C5-C6-N1	-8.25	112.15	123.43
3	D	402	GDD	C5-C6-N1	-8.23	112.18	123.43
3	C	402	GDD	C5-C6-N1	-8.10	112.35	123.43
3	E	402	GDD	C5-C6-N1	-8.07	112.39	123.43
3	A	402	GDD	O5'-PA-O1A	-7.96	77.95	109.07
2	B	401	NAP	O5B-PA-O1A	-7.84	78.43	109.07
3	G	402	GDD	C6-N1-C2	5.82	125.18	115.93
3	F	401	GDD	C6-N1-C2	5.80	125.14	115.93
3	A	402	GDD	C6-N1-C2	5.79	125.13	115.93
3	H	402	GDD	C6-N1-C2	5.79	125.13	115.93
3	B	402	GDD	C6-N1-C2	5.79	125.12	115.93
3	C	402	GDD	C6-N1-C2	5.79	125.12	115.93
3	D	402	GDD	C6-N1-C2	5.75	125.06	115.93
3	E	402	GDD	C6-N1-C2	5.67	124.94	115.93
3	A	402	GDD	PB-O3A-PA	5.56	151.90	132.83
3	G	402	GDD	O1B-PB-O3B	5.25	129.17	109.47
3	C	402	GDD	C11-O51-C51	4.91	123.33	113.69
3	G	402	GDD	PB-O1B-C11	4.79	138.27	119.74
3	B	402	GDD	C11-O51-C51	4.79	123.08	113.69
3	D	402	GDD	C11-O51-C51	4.78	123.07	113.69
3	B	402	GDD	O3A-PB-O1B	-4.75	92.90	102.48
3	H	402	GDD	O1B-PB-O3B	4.52	126.43	109.47
3	G	402	GDD	O51-C11-O1B	4.26	116.94	111.36
3	A	402	GDD	C11-O51-C51	4.23	122.00	113.69
3	A	402	GDD	O2A-PA-O5'	-4.00	89.18	107.75
3	B	402	GDD	PB-O3A-PA	3.70	145.53	132.83
3	C	402	GDD	O3A-PB-O1B	-3.63	95.17	102.48
3	A	402	GDD	O51-C51-C41	3.56	116.16	109.69
3	C	402	GDD	O51-C51-C41	3.53	116.10	109.69
3	C	402	GDD	PB-O1B-C11	3.27	132.38	119.74
2	B	401	NAP	O2A-PA-O5B	3.15	122.40	107.75
3	B	402	GDD	PB-O1B-C11	3.13	131.83	119.74
3	A	402	GDD	PB-O1B-C11	3.11	131.78	119.74
3	B	402	GDD	O51-C51-C41	3.02	115.18	109.69
3	E	402	GDD	N3-C2-N1	-3.00	123.22	127.22
3	A	402	GDD	O2B-PB-O3B	2.90	126.57	112.24
3	C	402	GDD	N3-C2-N1	-2.86	123.41	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	402	GDD	O51-C51-C41	2.85	114.88	109.69
3	G	402	GDD	N3-C2-N1	-2.81	123.47	127.22
3	H	402	GDD	N3-C2-N1	-2.80	123.49	127.22
3	D	402	GDD	N3-C2-N1	-2.77	123.53	127.22
3	F	401	GDD	N3-C2-N1	-2.77	123.53	127.22
3	A	402	GDD	N3-C2-N1	-2.75	123.55	127.22
3	B	402	GDD	N3-C2-N1	-2.75	123.56	127.22
2	E	401	NAP	O3D-C3D-C4D	-2.64	103.42	111.05
2	B	401	NAP	C3B-C2B-C1B	-2.64	97.93	102.89
3	A	402	GDD	O1B-PB-O3B	2.54	119.01	109.47
3	E	402	GDD	PB-O1B-C11	2.51	129.44	119.74
3	B	402	GDD	O51-C11-C21	2.51	115.65	110.35
2	F	402	NAP	C5A-C6A-N6A	2.47	124.11	120.35
2	A	401	NAP	C5A-C6A-N6A	2.47	124.11	120.35
3	A	402	GDD	C6-C5-C4	-2.45	118.46	120.80
3	F	401	GDD	C6-C5-C4	-2.45	118.46	120.80
2	C	401	NAP	C5A-C6A-N6A	2.44	124.06	120.35
3	A	402	GDD	O51-C11-C21	2.43	115.50	110.35
3	F	401	GDD	PB-O1B-C11	2.43	129.13	119.74
3	C	402	GDD	C6-C5-C4	-2.42	118.49	120.80
3	G	402	GDD	C2-N3-C4	-2.41	112.60	115.36
3	H	402	GDD	C6-C5-C4	-2.41	118.50	120.80
3	E	402	GDD	C2-N3-C4	-2.39	112.63	115.36
3	B	402	GDD	C6-C5-C4	-2.37	118.53	120.80
3	D	402	GDD	C6-C5-C4	-2.36	118.54	120.80
3	D	402	GDD	PB-O1B-C11	2.33	128.76	119.74
3	D	402	GDD	O51-C11-C21	2.32	115.26	110.35
2	D	401	NAP	C5A-C6A-N6A	2.32	123.87	120.35
2	H	401	NAP	C5A-C6A-N6A	2.31	123.86	120.35
2	C	401	NAP	O3D-C3D-C4D	-2.31	104.38	111.05
3	E	402	GDD	C6-C5-C4	-2.29	118.61	120.80
3	B	402	GDD	O2B-PB-O1B	2.28	115.80	106.78
2	G	401	NAP	C5A-C6A-N6A	2.27	123.81	120.35
3	C	402	GDD	C2-N3-C4	-2.27	112.76	115.36
2	B	401	NAP	C5A-C6A-N6A	2.26	123.78	120.35
3	H	402	GDD	C2-N3-C4	-2.25	112.79	115.36
2	E	401	NAP	C5A-C6A-N6A	2.23	123.75	120.35
3	A	402	GDD	O2A-PA-O1A	2.23	123.25	112.24
3	D	402	GDD	C2-N3-C4	-2.21	112.84	115.36
2	A	401	NAP	O2D-C2D-C3D	-2.19	104.75	111.82
3	F	401	GDD	C2-N3-C4	-2.18	112.86	115.36
3	G	402	GDD	C6-C5-C4	-2.18	118.72	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	402	GDD	O2B-PB-O1B	2.17	115.33	106.78
3	B	402	GDD	C2-N3-C4	-2.16	112.89	115.36
3	A	402	GDD	C2-N3-C4	-2.15	112.91	115.36
2	A	401	NAP	C3B-C2B-C1B	-2.09	98.95	102.89
2	D	401	NAP	C3B-C2B-C1B	-2.05	99.04	102.89
2	E	401	NAP	C3B-C2B-C1B	-2.03	99.07	102.89
2	H	401	NAP	O2D-C2D-C1D	2.02	116.76	110.02

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	402	GDD	C5'-O5'-PA-O1A
2	F	402	NAP	C5B-O5B-PA-O1A
2	F	402	NAP	C5B-O5B-PA-O2A
2	F	402	NAP	O4B-C4B-C5B-O5B
2	F	402	NAP	C2B-O2B-P2B-O1X
2	F	402	NAP	C2B-O2B-P2B-O2X
2	F	402	NAP	C5D-O5D-PN-O1N
2	F	402	NAP	C5D-O5D-PN-O2N
2	G	401	NAP	C5D-O5D-PN-O1N
2	C	401	NAP	C2B-O2B-P2B-O1X
2	C	401	NAP	C2B-O2B-P2B-O3X
2	C	401	NAP	C5D-O5D-PN-O1N
2	C	401	NAP	C5D-O5D-PN-O2N
3	F	401	GDD	C5'-O5'-PA-O1A
3	F	401	GDD	C11-O1B-PB-O3A
2	E	401	NAP	C5D-O5D-PN-O1N
2	A	401	NAP	C4D-C5D-O5D-PN
3	C	402	GDD	PB-O3A-PA-O5'
2	H	401	NAP	C5D-O5D-PN-O3
2	H	401	NAP	C5D-O5D-PN-O1N
2	H	401	NAP	C5D-O5D-PN-O2N
3	D	402	GDD	PB-O3A-PA-O5'
3	G	402	GDD	O51-C11-O1B-PB
2	D	401	NAP	C2B-O2B-P2B-O1X
2	D	401	NAP	C2B-O2B-P2B-O3X
2	D	401	NAP	C5D-O5D-PN-O1N
2	B	401	NAP	C5D-O5D-PN-O2N
3	A	402	GDD	O51-C51-C61-O6A
3	G	402	GDD	O51-C51-C61-O6A
3	A	402	GDD	C41-C51-C61-O6A

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Mol	Chain	Res	Type	Atoms
2	F	402	NAP	C3B-C4B-C5B-O5B
3	G	402	GDD	C41-C51-C61-O6A
3	H	402	GDD	C11-O1B-PB-O3A
3	G	402	GDD	C21-C11-O1B-PB
4	D	404	EDO	O1-C1-C2-O2
3	G	402	GDD	O4'-C4'-C5'-O5'
3	H	402	GDD	C21-C11-O1B-PB
3	A	402	GDD	PB-O3A-PA-O1A
3	G	402	GDD	C3'-C4'-C5'-O5'
4	D	403	EDO	O1-C1-C2-O2
3	H	402	GDD	PB-O3A-PA-O5'
3	G	402	GDD	PB-O3A-PA-O5'
2	H	401	NAP	C2B-O2B-P2B-O1X
2	H	401	NAP	C4D-C5D-O5D-PN
2	G	401	NAP	C5D-O5D-PN-O3
3	F	401	GDD	C5'-O5'-PA-O3A
2	E	401	NAP	C5D-O5D-PN-O3
2	B	401	NAP	C5D-O5D-PN-O3
2	F	402	NAP	PA-O3-PN-O1N
3	F	401	GDD	C11-O1B-PB-O3B
3	A	402	GDD	PA-O3A-PB-O3B
3	A	402	GDD	C11-O1B-PB-O3A
2	E	401	NAP	C5D-O5D-PN-O2N
2	D	401	NAP	C5D-O5D-PN-O2N
2	B	401	NAP	C5B-O5B-PA-O2A
2	B	401	NAP	C5D-O5D-PN-O1N
2	B	401	NAP	O4D-C4D-C5D-O5D
3	B	402	GDD	PB-O3A-PA-O1A
3	C	402	GDD	C11-O1B-PB-O2B
3	G	402	GDD	C11-O1B-PB-O3A
2	F	402	NAP	O4D-C4D-C5D-O5D
2	G	401	NAP	O4D-C4D-C5D-O5D
2	D	401	NAP	O4D-C4D-C5D-O5D
2	C	401	NAP	PN-O3-PA-O1A
2	D	401	NAP	PN-O3-PA-O1A
3	B	402	GDD	PB-O3A-PA-O5'
3	D	402	GDD	C21-C11-O1B-PB
2	G	401	NAP	C3D-C4D-C5D-O5D
2	E	401	NAP	C2B-O2B-P2B-O1X
2	E	401	NAP	O4B-C4B-C5B-O5B
2	A	401	NAP	O4B-C4B-C5B-O5B
2	D	401	NAP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	B	401	NAP	C3D-C4D-C5D-O5D
2	F	402	NAP	C5B-O5B-PA-O3
2	F	402	NAP	C5D-O5D-PN-O3
2	G	401	NAP	C2B-O2B-P2B-O2X
2	C	401	NAP	C5D-O5D-PN-O3
2	E	401	NAP	C2B-O2B-P2B-O2X
2	A	401	NAP	C2B-O2B-P2B-O3X
2	D	401	NAP	C5D-O5D-PN-O3
2	B	401	NAP	C2B-O2B-P2B-O3X
2	C	401	NAP	O4B-C4B-C5B-O5B
2	C	401	NAP	O4D-C4D-C5D-O5D
2	H	401	NAP	O4B-C4B-C5B-O5B
2	B	401	NAP	O4B-C4B-C5B-O5B
2	F	402	NAP	PA-O3-PN-O2N
2	G	401	NAP	PA-O3-PN-O1N
2	C	401	NAP	PN-O3-PA-O2A
3	F	401	GDD	PA-O3A-PB-O2B
2	E	401	NAP	PN-O3-PA-O2A
3	A	402	GDD	PB-O3A-PA-O2A
2	H	401	NAP	PN-O3-PA-O2A
3	D	402	GDD	PB-O3A-PA-O1A
2	D	401	NAP	PN-O3-PA-O2A
3	C	402	GDD	C11-O1B-PB-O3A
3	A	402	GDD	C21-C11-O1B-PB
3	B	402	GDD	C21-C11-O1B-PB
2	G	401	NAP	C5D-O5D-PN-O2N
3	A	402	GDD	C5'-O5'-PA-O1A
2	G	401	NAP	O4B-C4B-C5B-O5B
2	E	401	NAP	O4D-C4D-C5D-O5D

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	402	GDD	1	0
2	F	402	NAP	1	0
3	H	402	GDD	5	0
3	F	401	GDD	1	0
3	A	402	GDD	2	0
2	A	401	NAP	2	0
3	C	402	GDD	2	0
2	H	401	NAP	3	0

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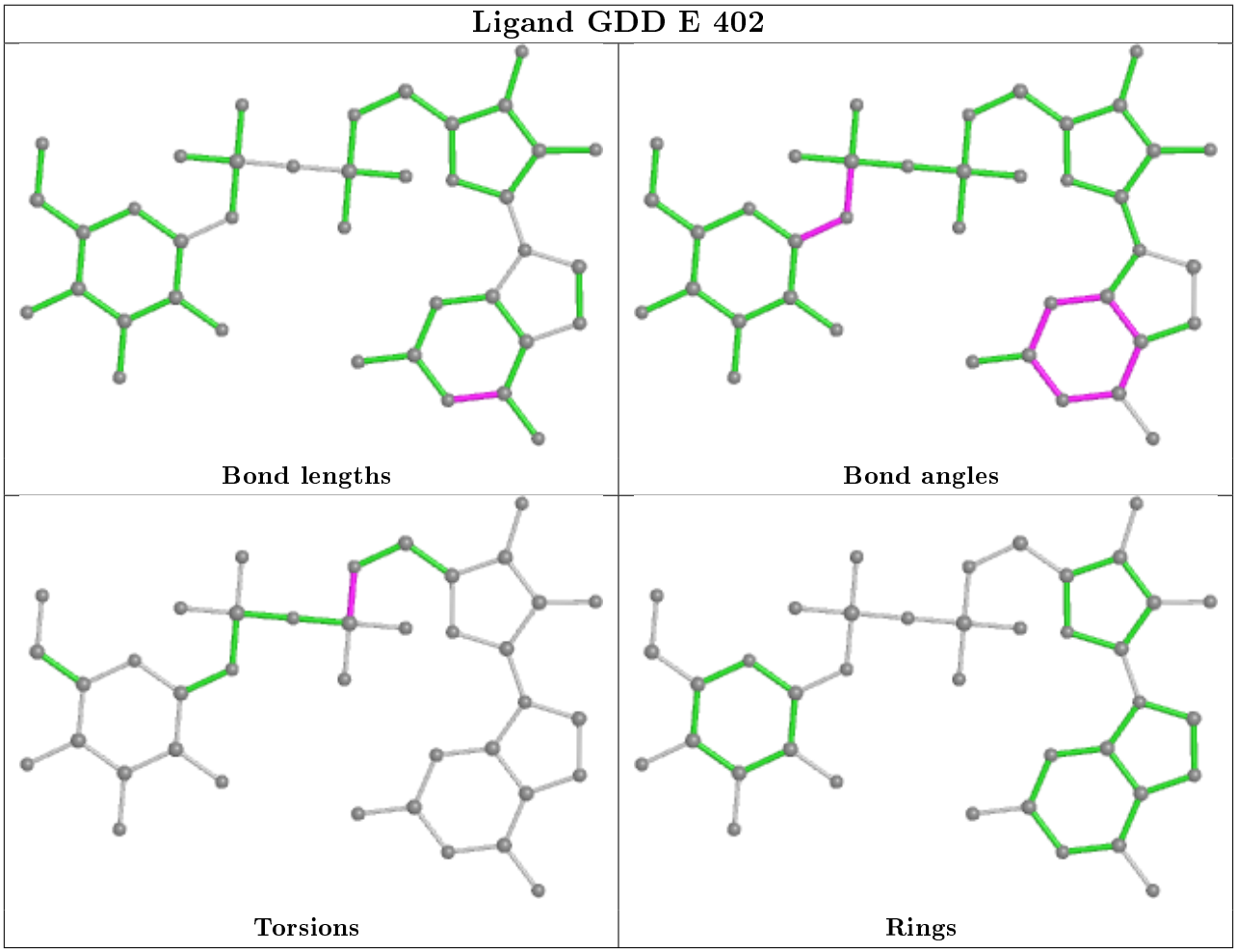
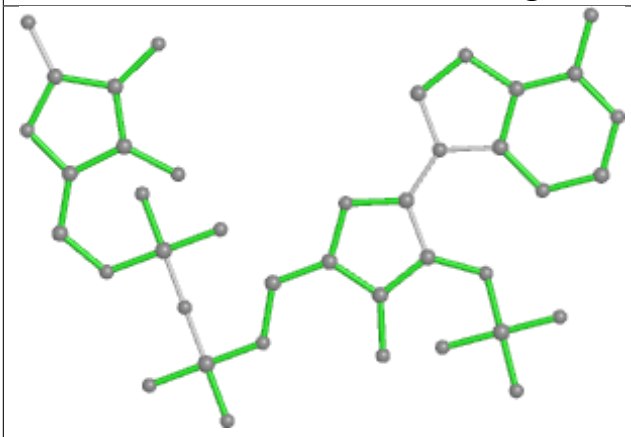
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	402	GDD	2	0
2	D	401	NAP	1	0

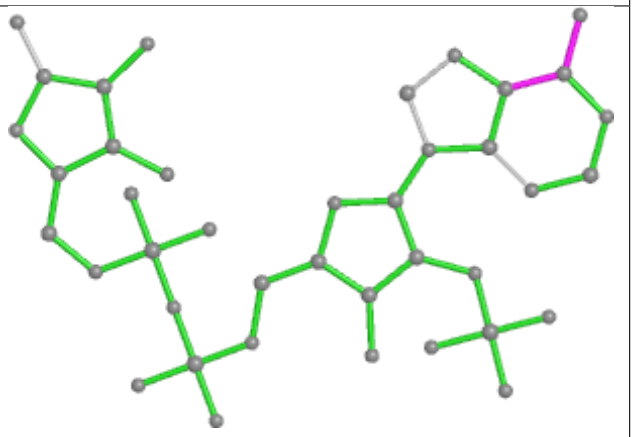
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



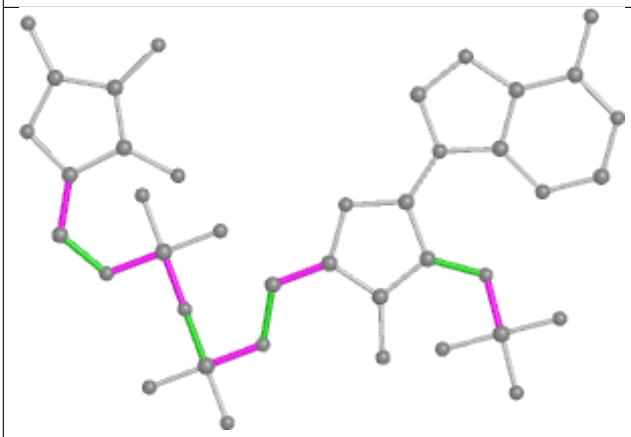
Ligand NAP F 402



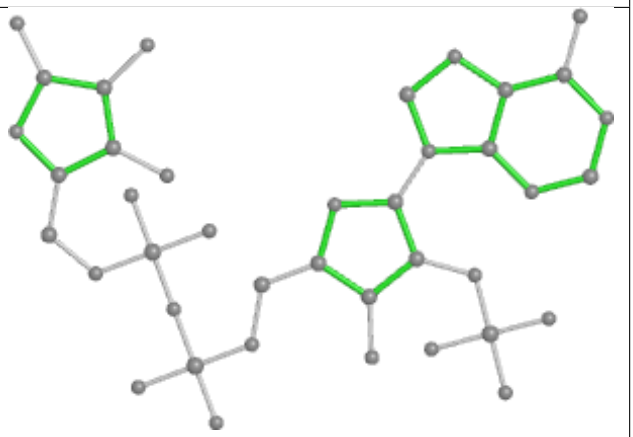
Bond lengths



Bond angles

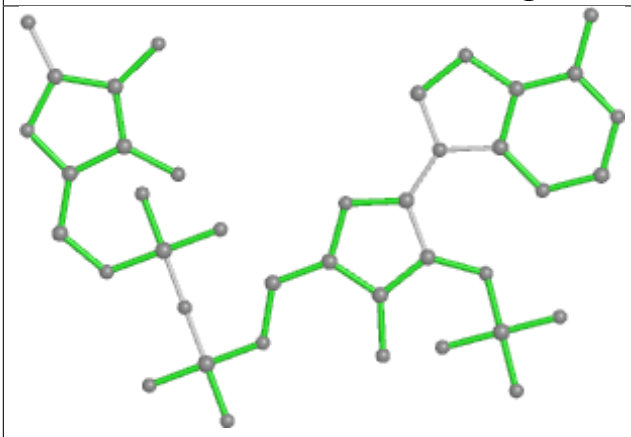


Torsions

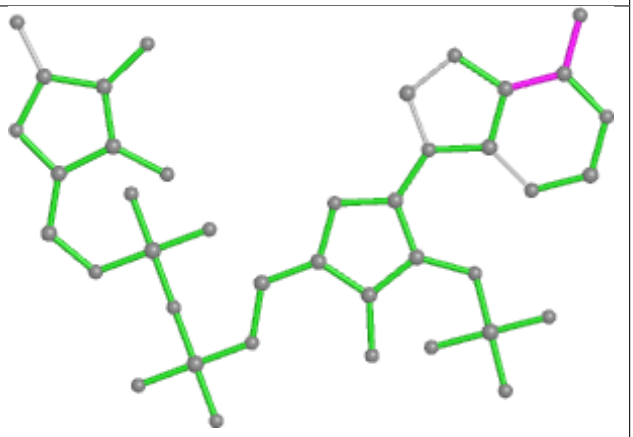


Rings

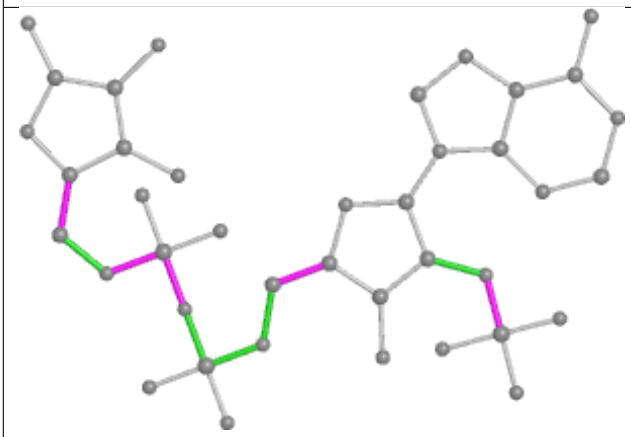
Ligand NAP G 401



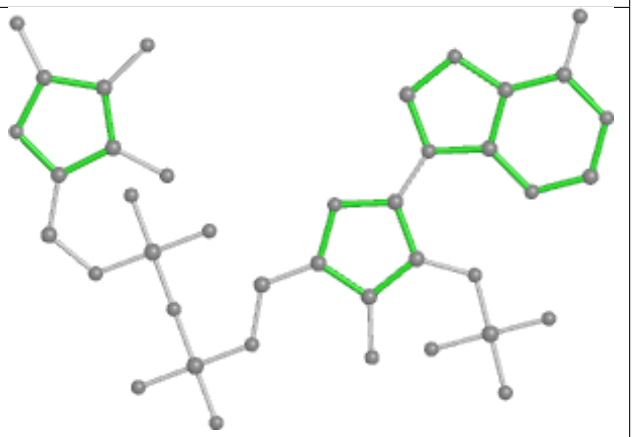
Bond lengths



Bond angles

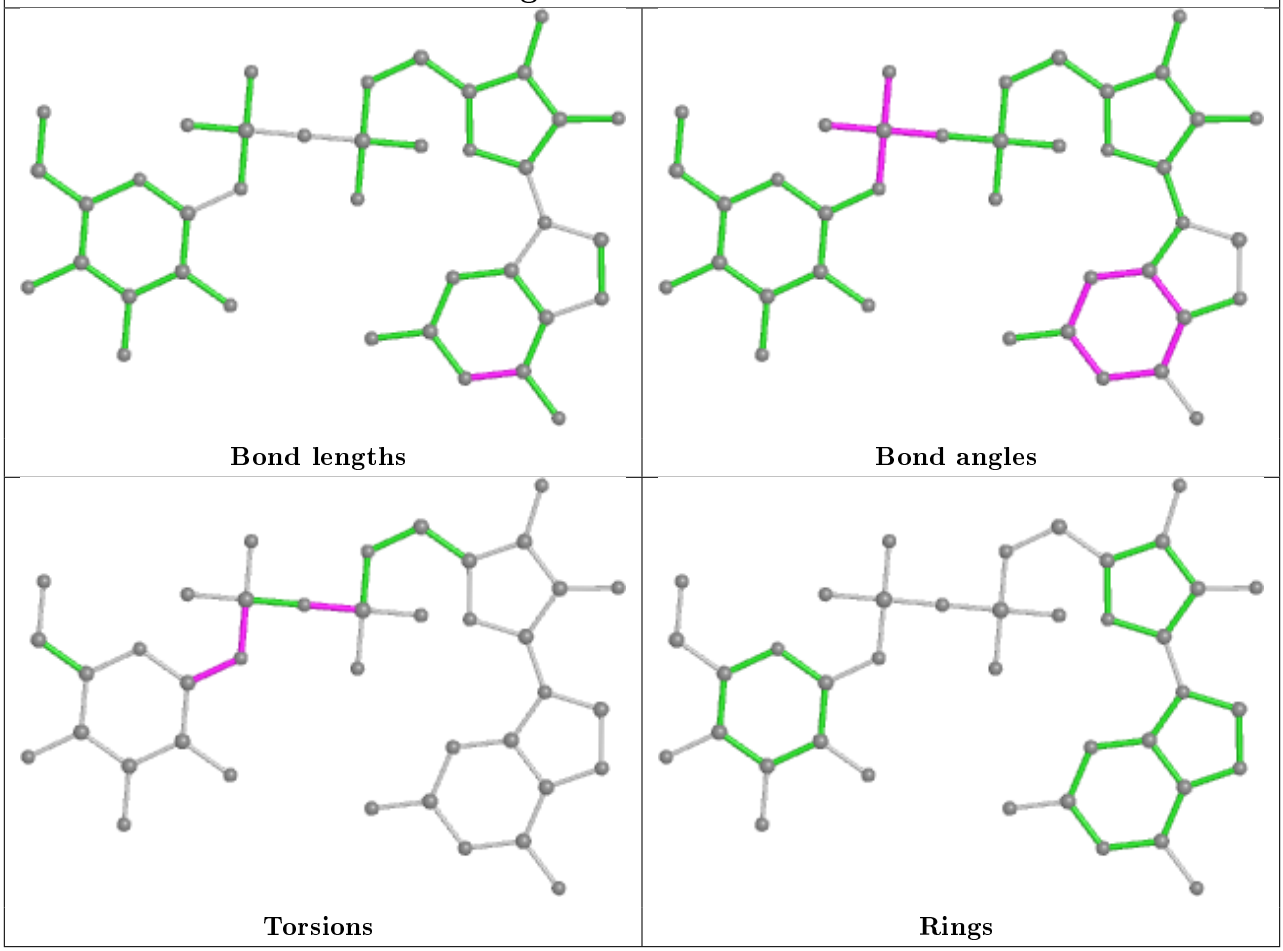


Torsions

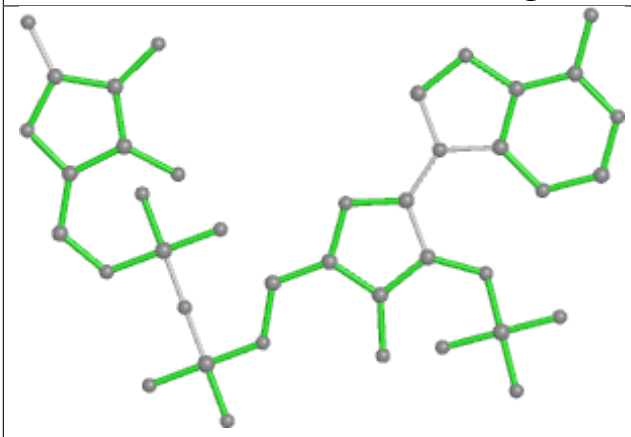


Rings

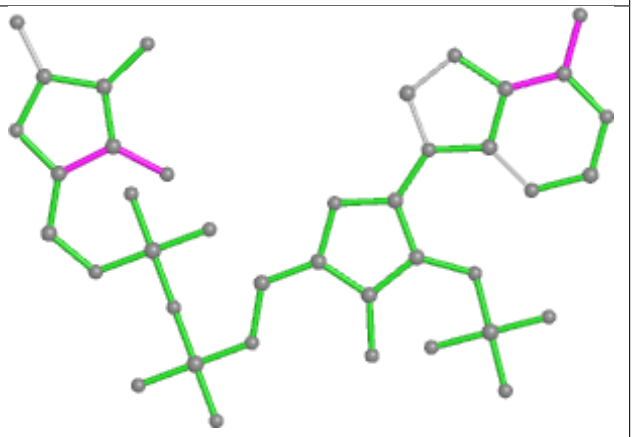
Ligand GDD H 402



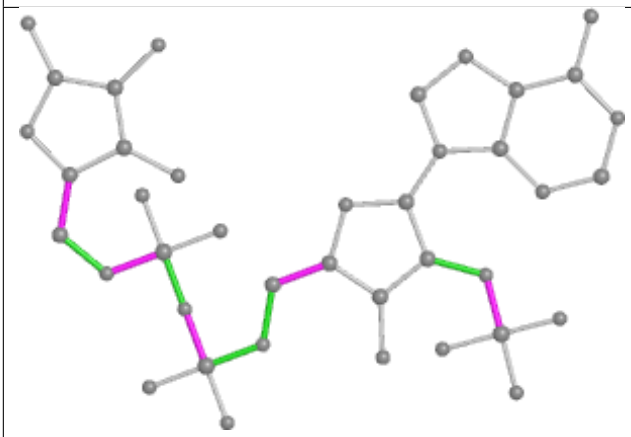
Ligand NAP C 401



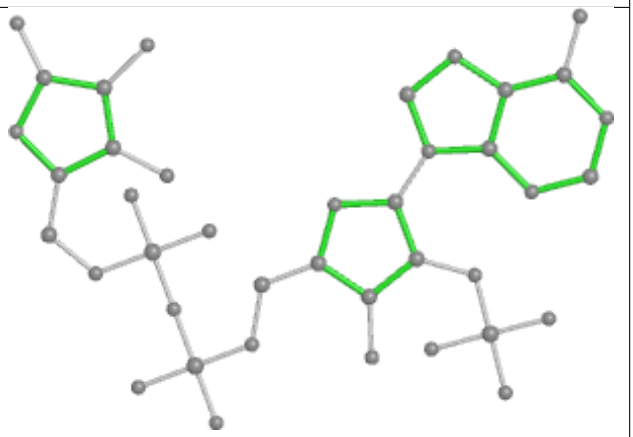
Bond lengths



Bond angles

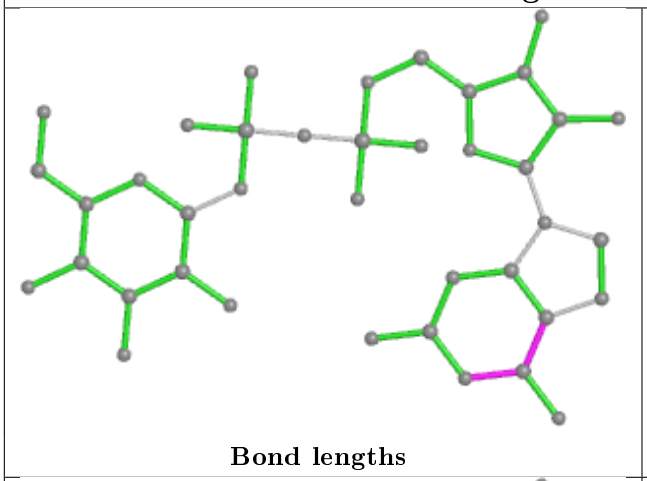


Torsions

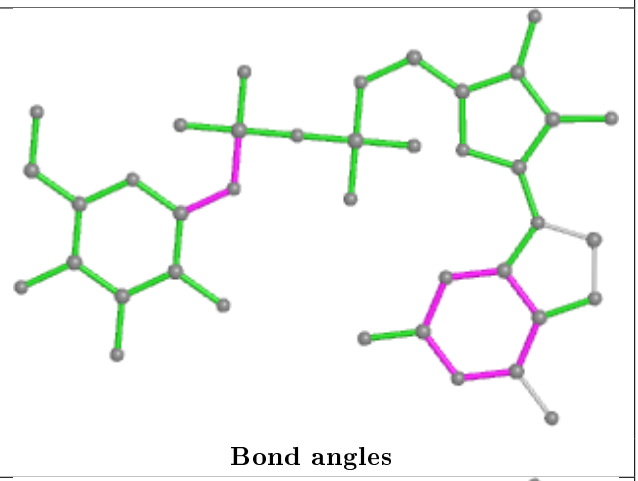


Rings

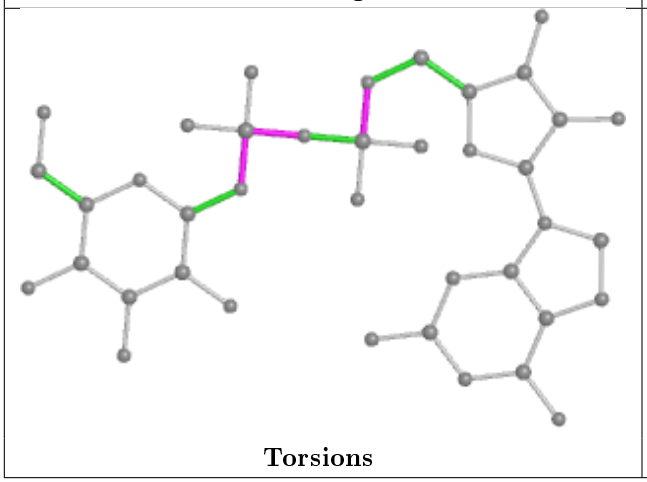
Ligand GDD F 401



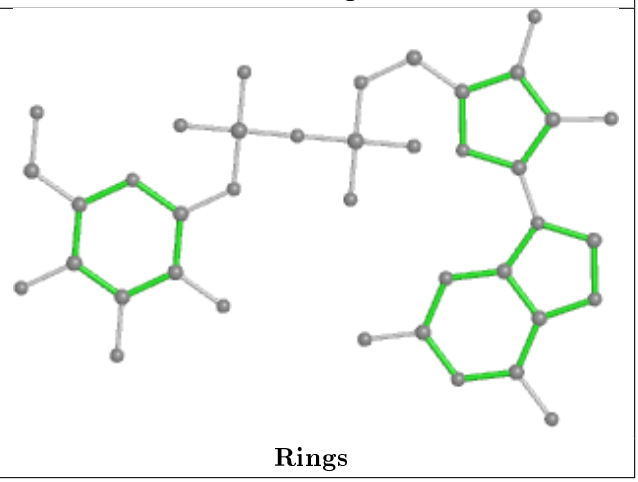
Bond lengths



Bond angles

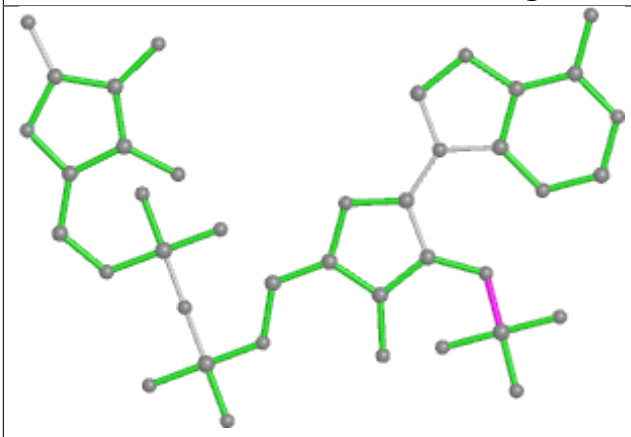


Torsions

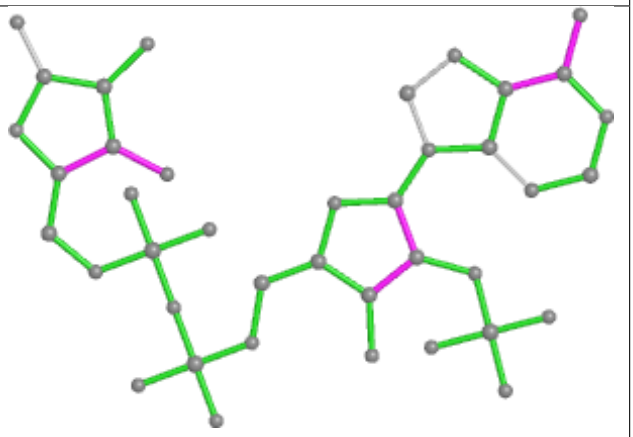


Rings

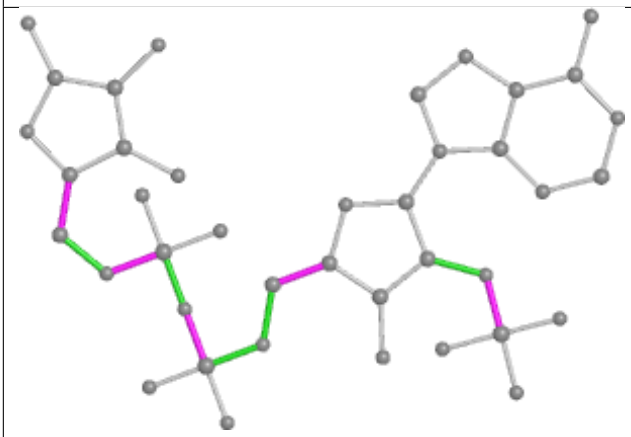
Ligand NAP E 401



Bond lengths



Bond angles



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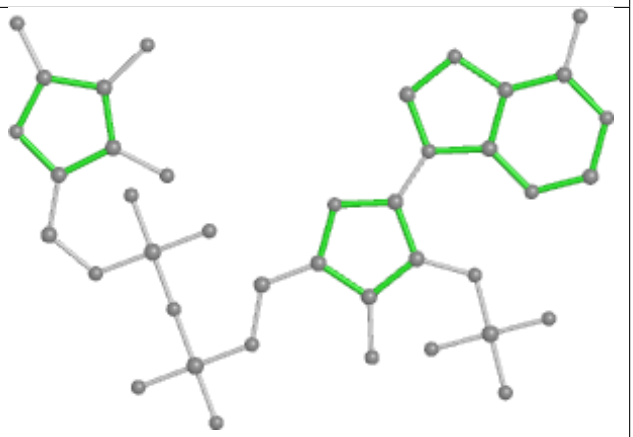
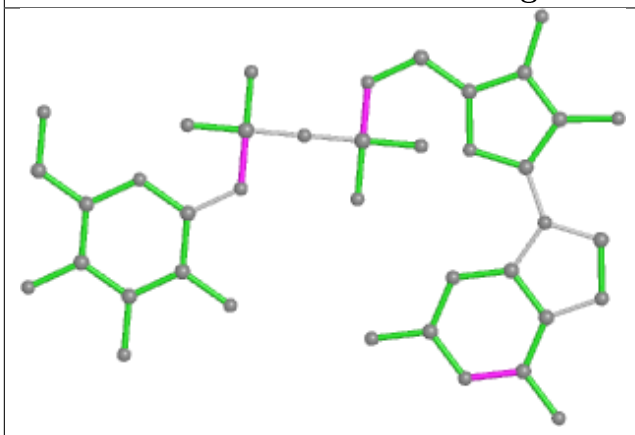


Rings

Ligand GDD A 402



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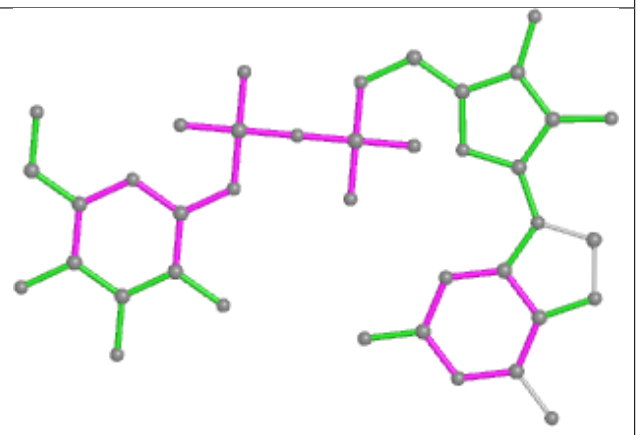

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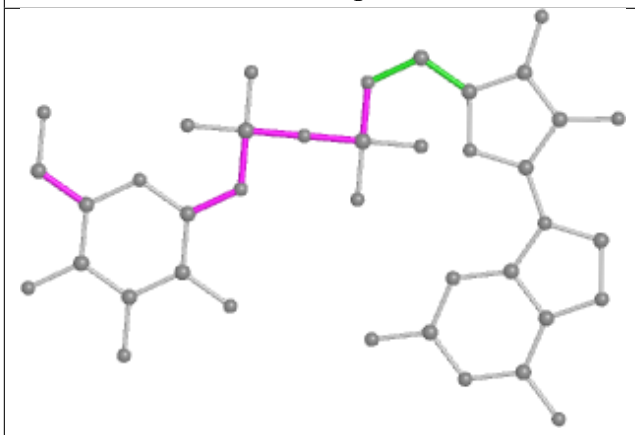
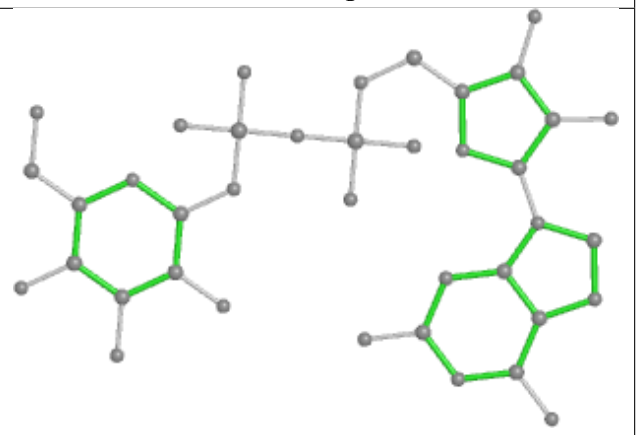
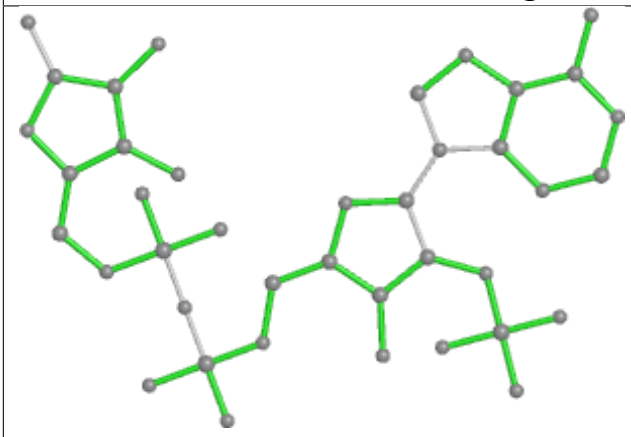


Torsions

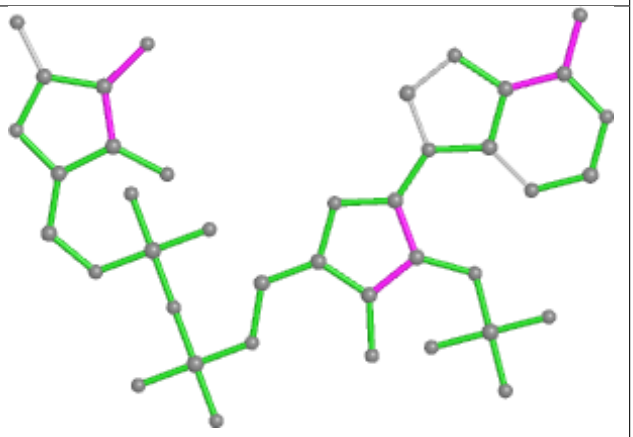


Rings

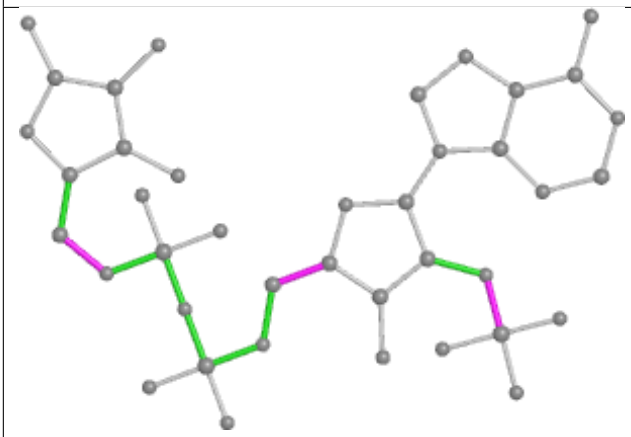
Ligand NAP A 401



Bond lengths



Bond angles



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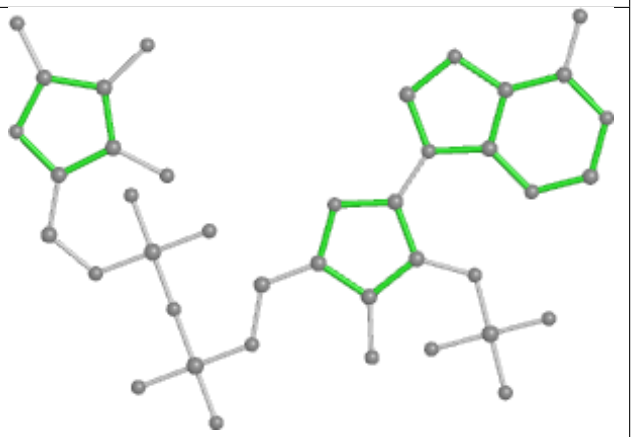
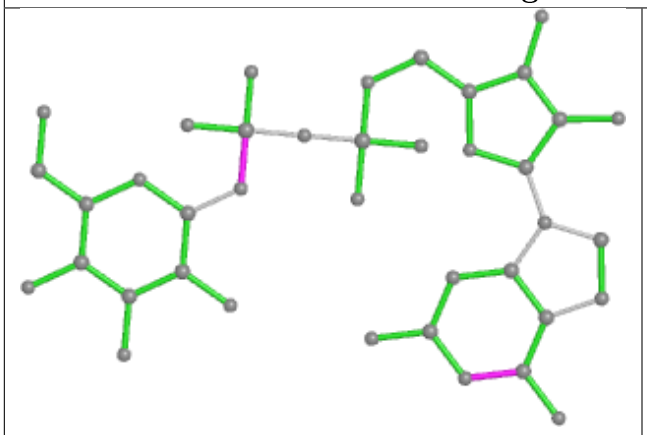
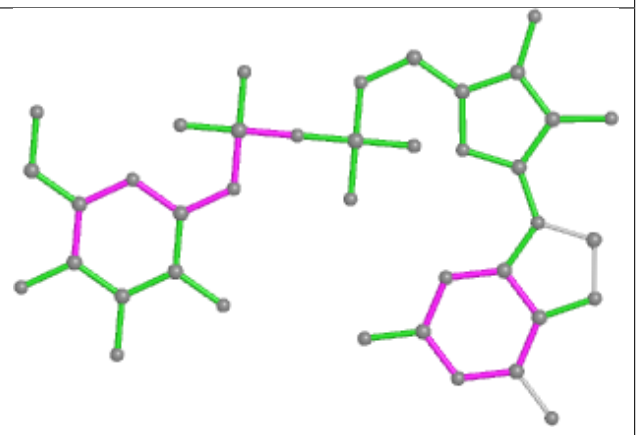


Rings

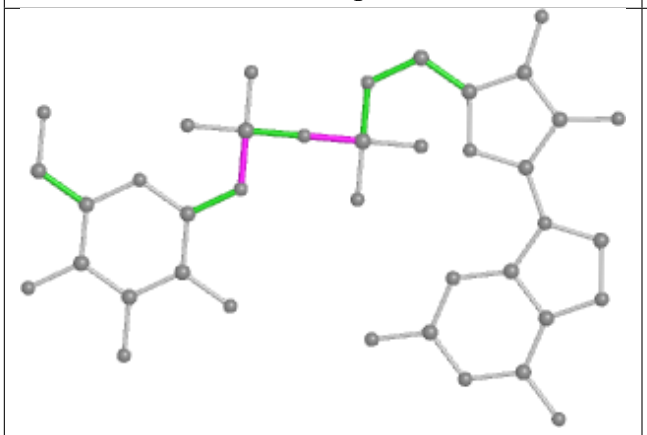
Ligand GDD C 402



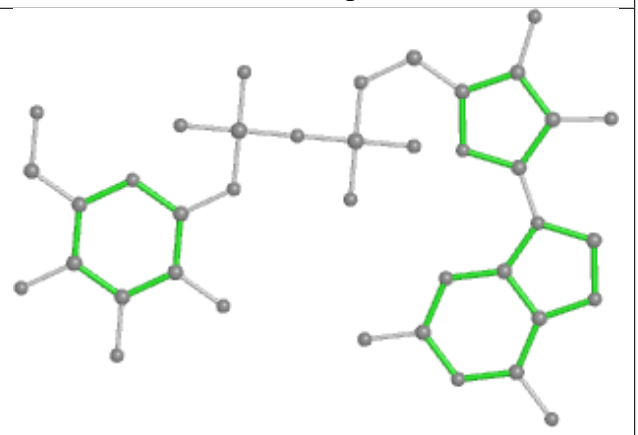
Bond lengths



Bond angles

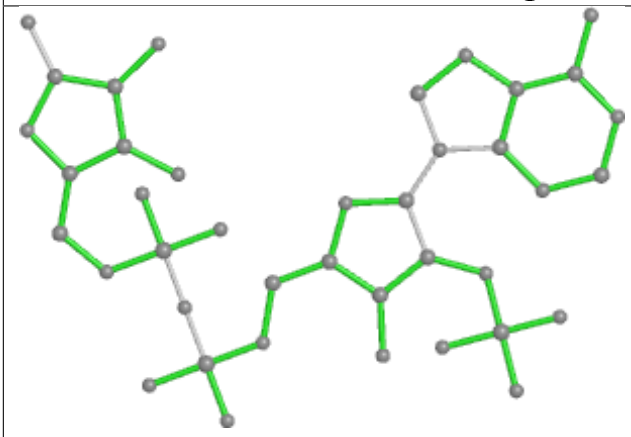


Torsions

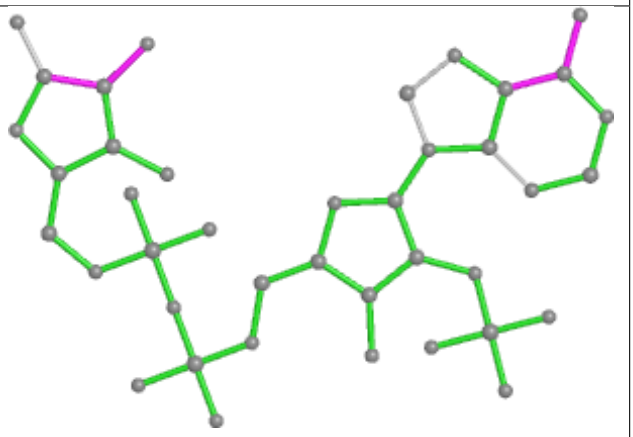


Rings

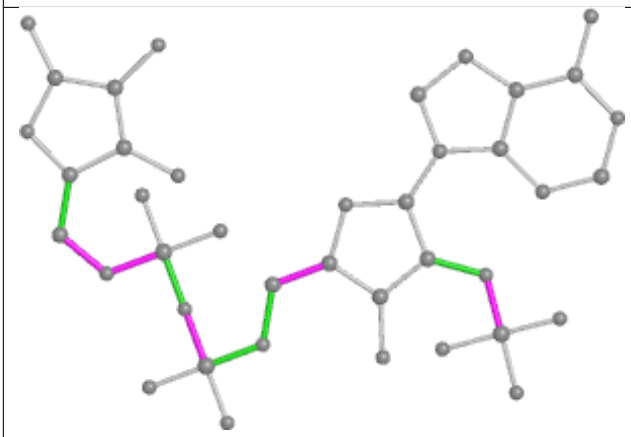
Ligand NAP H 401



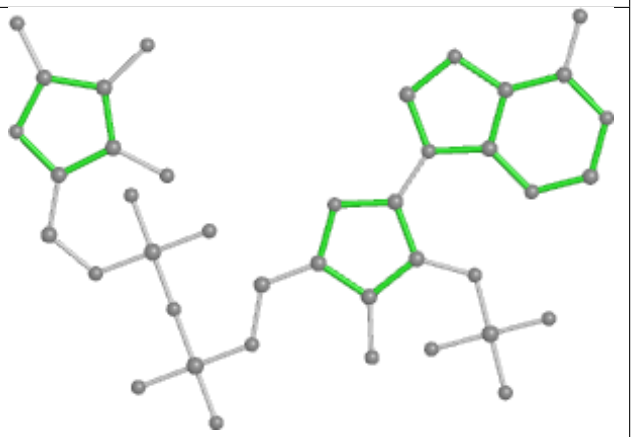
Bond lengths



Bond angles

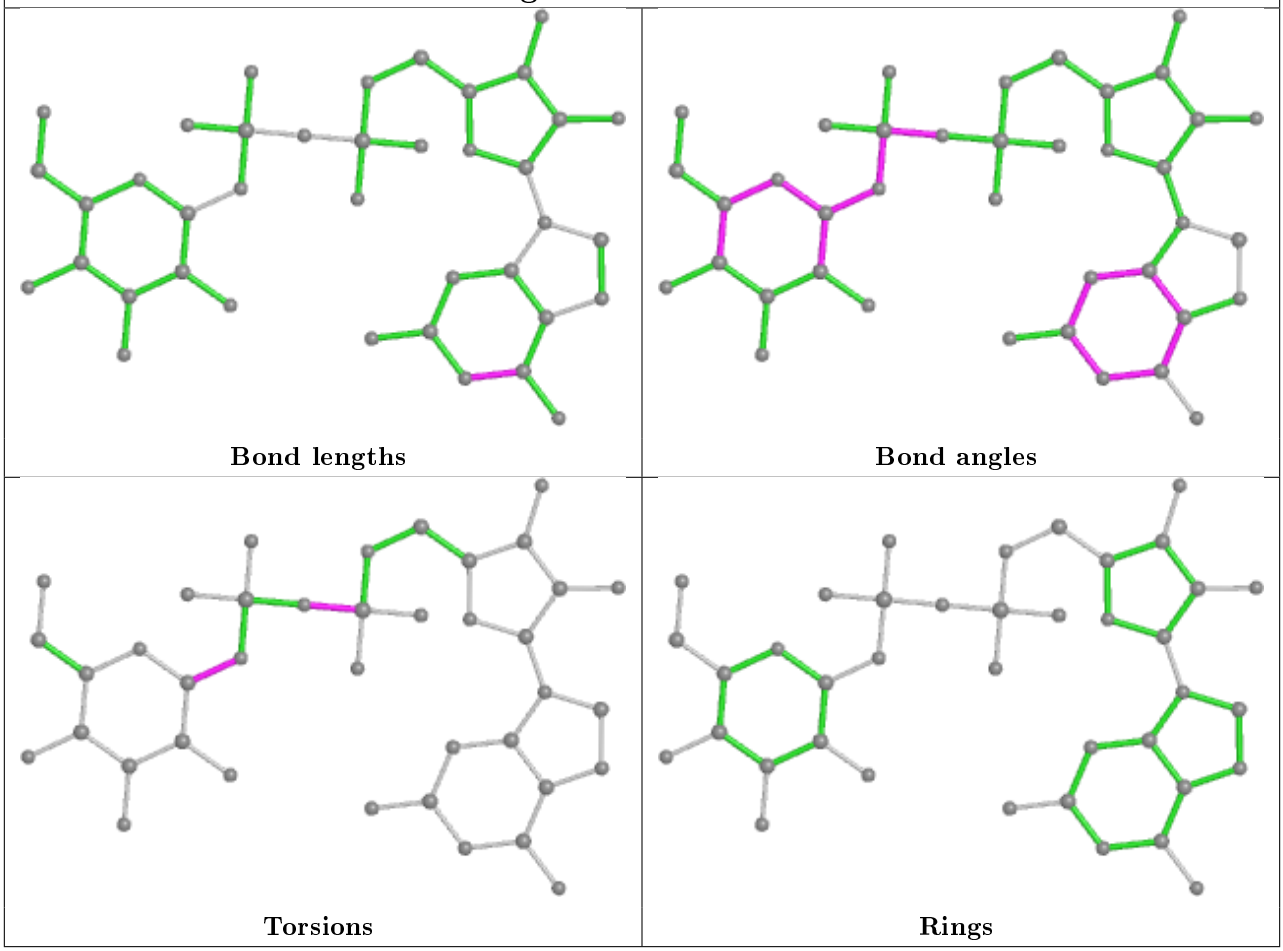


Torsions

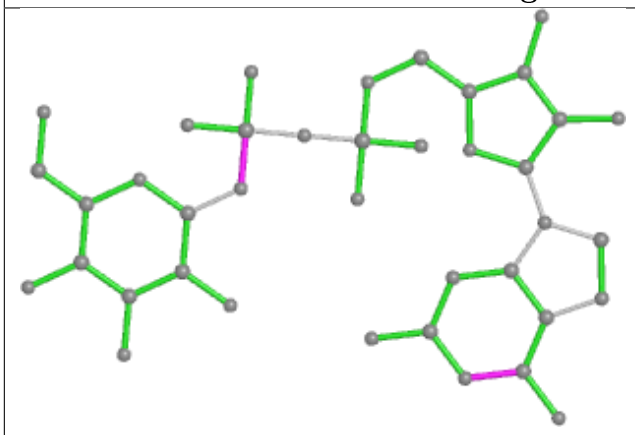


Rings

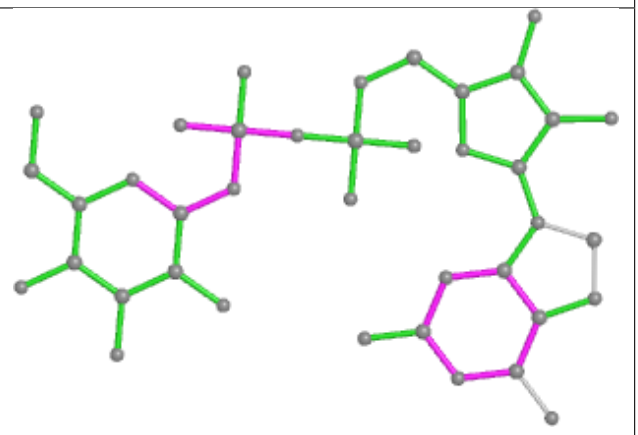
Ligand GDD D 402



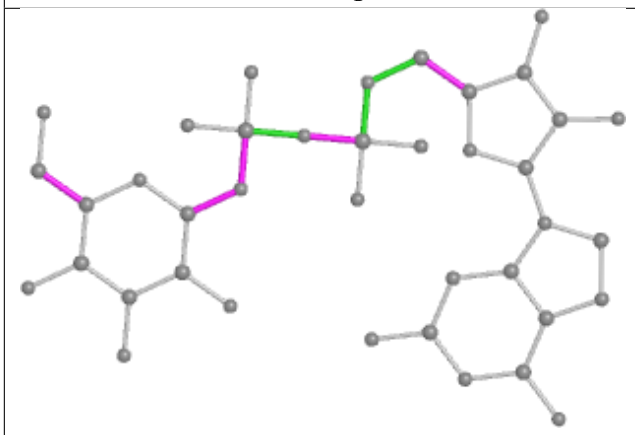
Ligand GDD G 402



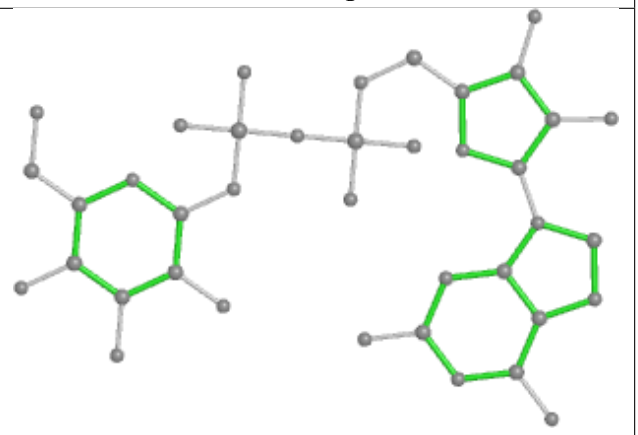
Bond lengths



Bond angles

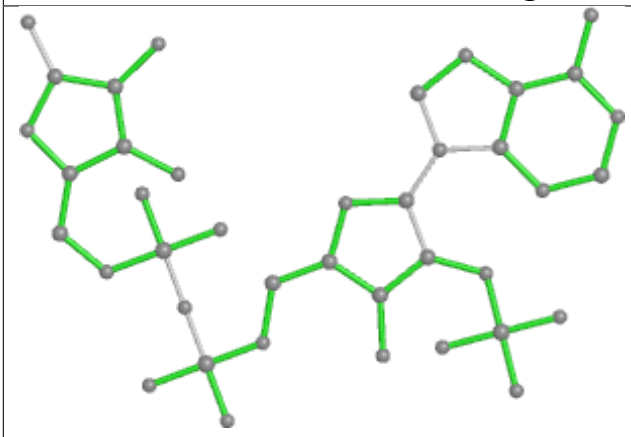


Torsions

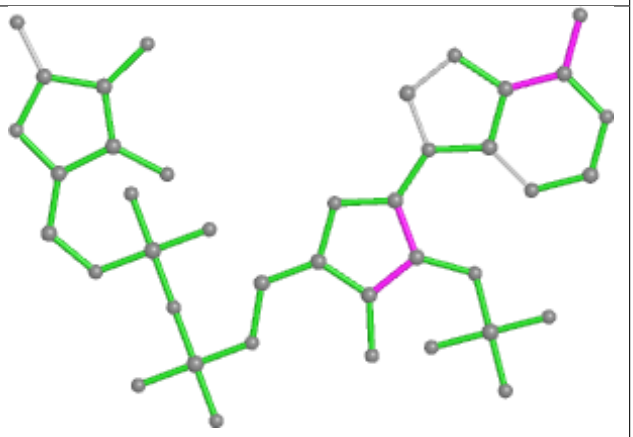


Rings

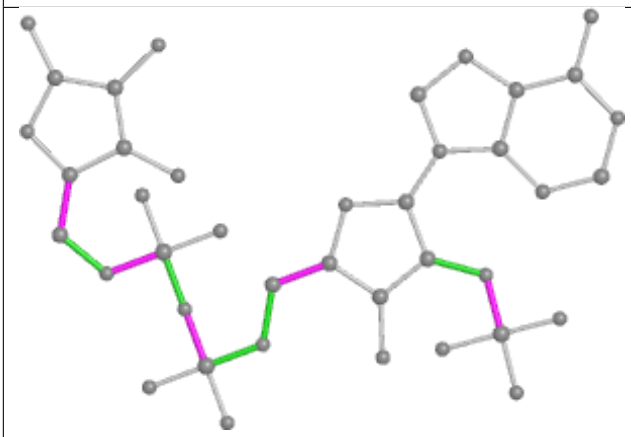
Ligand NAP D 401



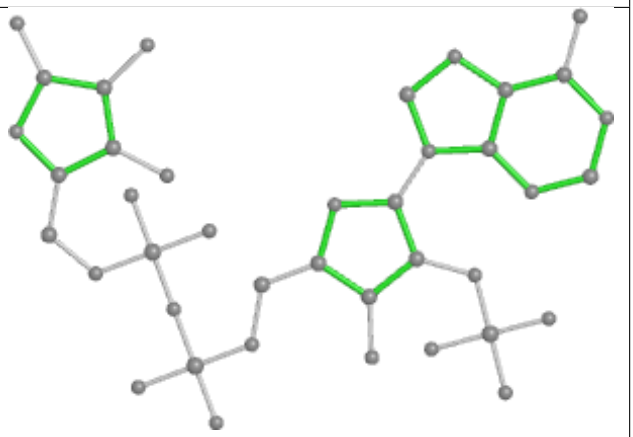
Bond lengths



Bond angles

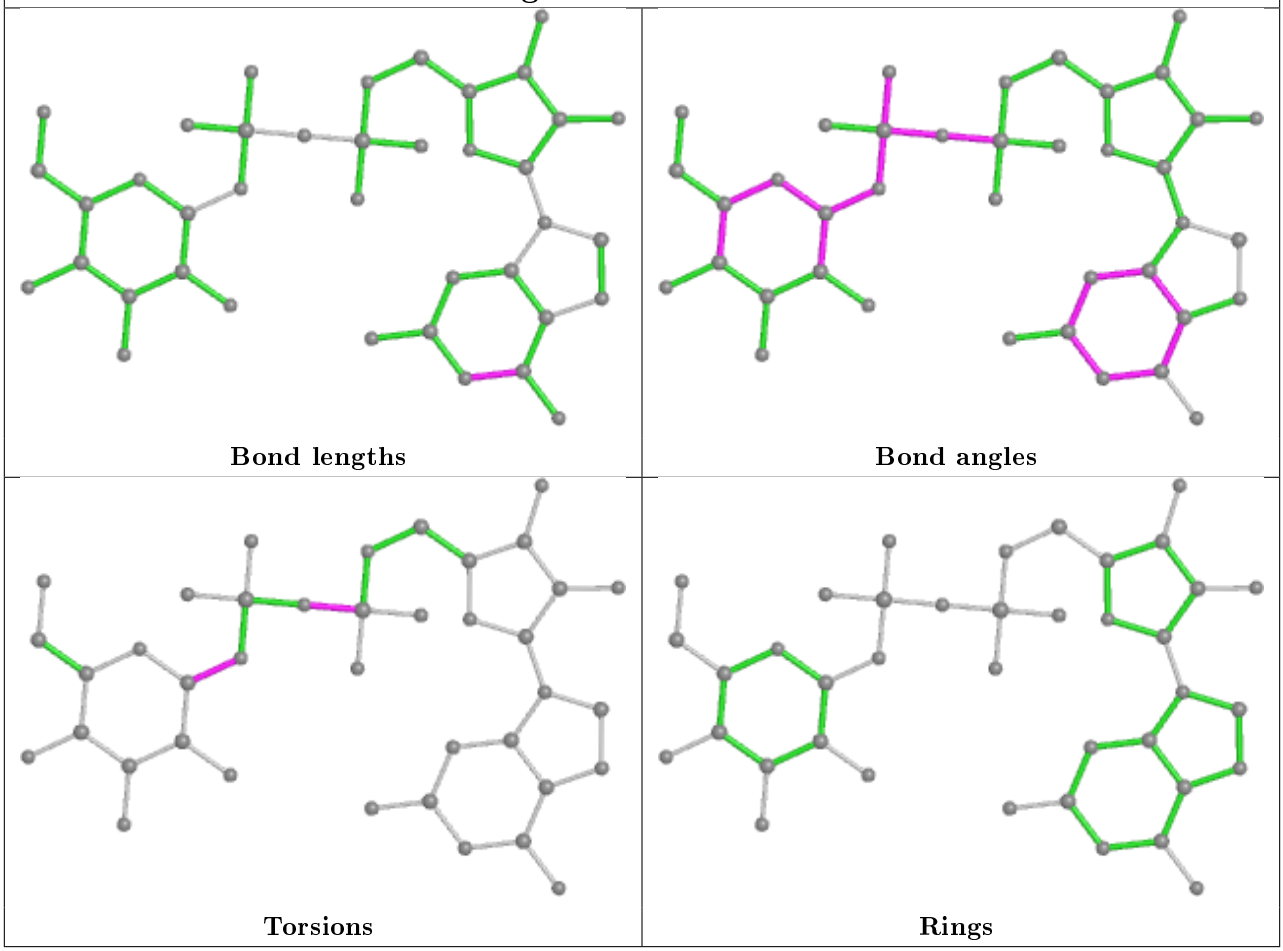


Torsions

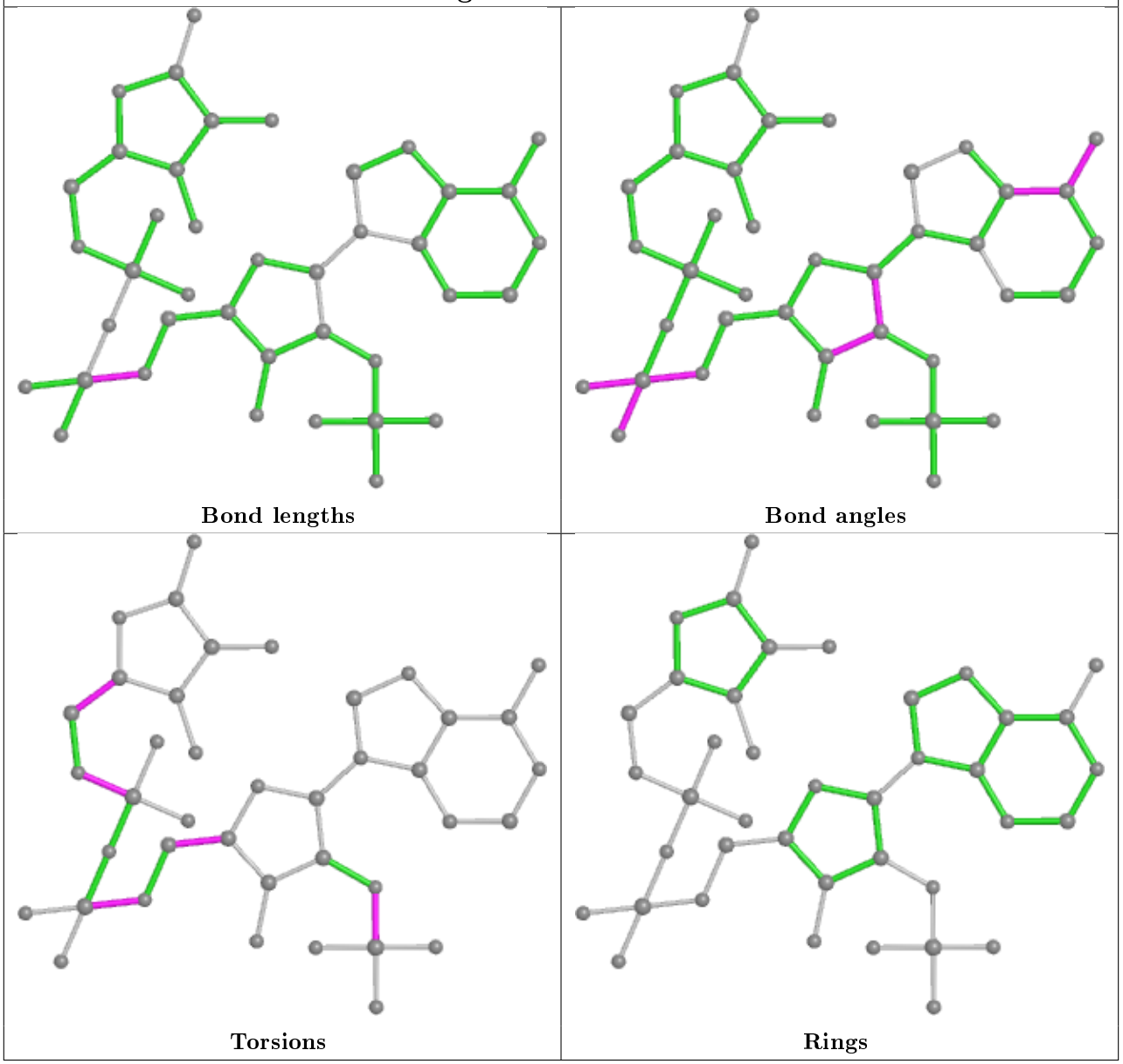


Rings

Ligand GDD B 402



Ligand NAP B 401



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	350/352 (99%)	-0.26	1 (0%) 94 93	48, 68, 103, 147	0
1	B	344/352 (97%)	-0.26	0 100 100	49, 66, 89, 140	0
1	C	348/352 (98%)	-0.19	0 100 100	52, 70, 100, 138	0
1	D	343/352 (97%)	-0.17	0 100 100	55, 78, 111, 149	0
1	E	350/352 (99%)	-0.21	1 (0%) 94 93	50, 73, 104, 173	0
1	F	350/352 (99%)	-0.12	1 (0%) 94 93	52, 81, 131, 157	0
1	G	350/352 (99%)	-0.15	1 (0%) 94 93	55, 77, 106, 154	0
1	H	341/352 (96%)	-0.24	0 100 100	68, 106, 135, 152	0
All	All	2776/2816 (98%)	-0.20	4 (0%) 95 95	48, 75, 122, 173	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	348	ARG	2.5
1	E	69	TYR	2.3
1	F	331	PHE	2.3
1	A	372	ALA	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands (i)

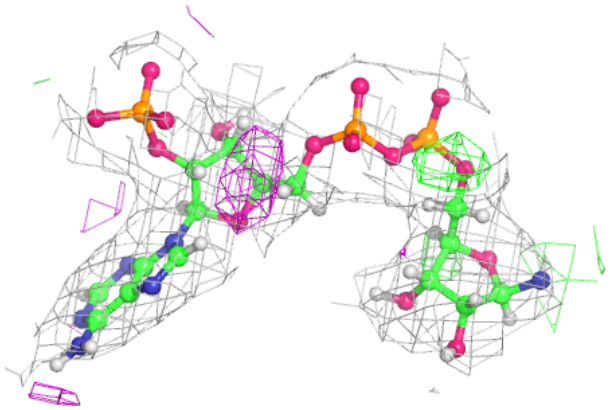
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

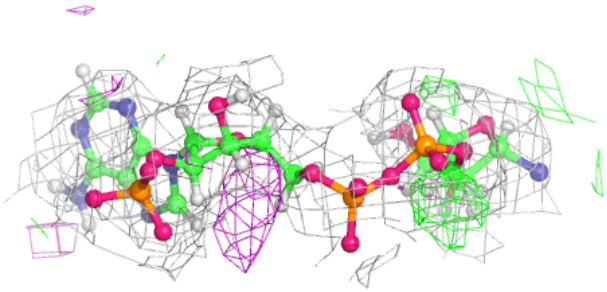
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	G	403	4/4	0.54	0.18	92,110,112,112	0
4	EDO	H	403	4/4	0.77	0.25	78,94,101,101	0
4	EDO	D	404	4/4	0.79	0.23	68,82,93,93	0
4	EDO	D	403	4/4	0.81	0.29	70,84,96,96	0
2	NAP	H	401	40/48	0.95	0.17	71,93,120,129	0
3	GDD	H	402	39/39	0.95	0.13	87,97,108,112	0
2	NAP	A	401	40/48	0.96	0.19	49,64,94,96	0
3	GDD	E	402	39/39	0.97	0.17	46,58,68,79	0
2	NAP	C	401	40/48	0.97	0.17	44,65,90,95	0
3	GDD	D	402	39/39	0.97	0.17	58,66,74,80	0
3	GDD	G	402	39/39	0.97	0.16	60,70,74,78	0
2	NAP	D	401	40/48	0.97	0.17	61,72,97,100	0
2	NAP	E	401	40/48	0.97	0.18	52,64,90,100	0
2	NAP	F	402	40/48	0.97	0.16	55,67,87,90	0
3	GDD	A	402	39/39	0.97	0.19	48,64,71,78	0
3	GDD	F	401	39/39	0.98	0.16	68,78,85,85	0
3	GDD	B	402	39/39	0.98	0.15	45,57,66,73	0
3	GDD	C	402	39/39	0.98	0.17	60,66,76,88	0
2	NAP	B	401	40/48	0.98	0.17	52,63,83,89	0
2	NAP	G	401	40/48	0.98	0.17	58,68,83,85	0

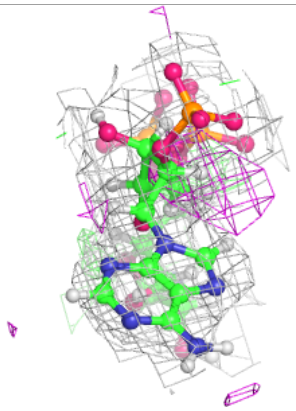
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP H 401:

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

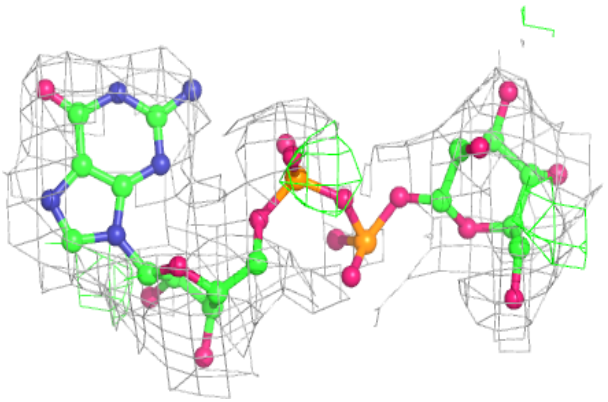


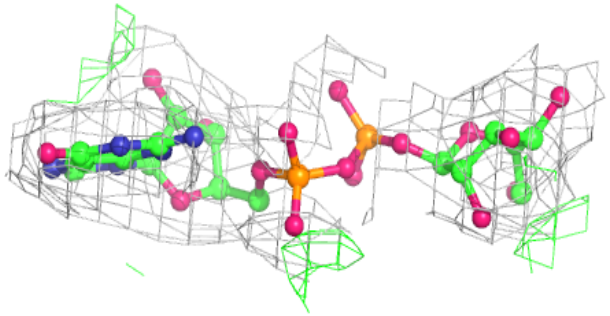


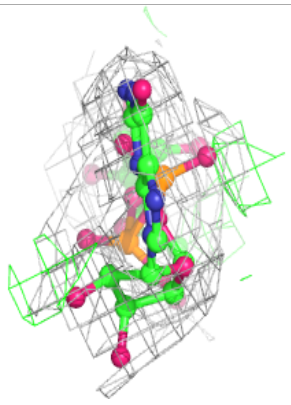


Electron density around GDD H 402:

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

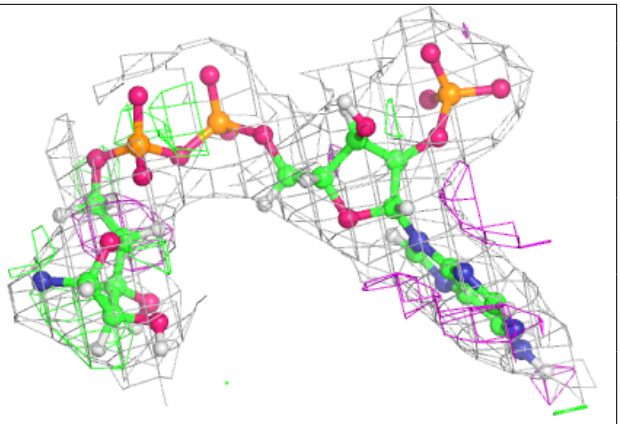


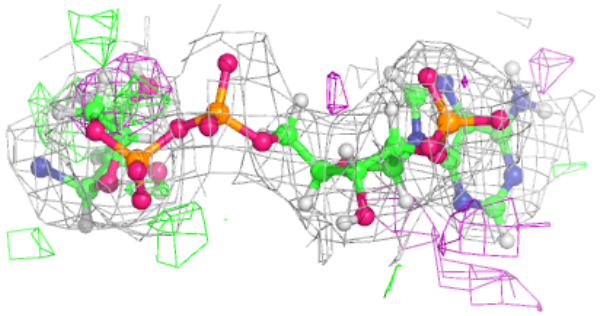




Electron density around NAP A 401:

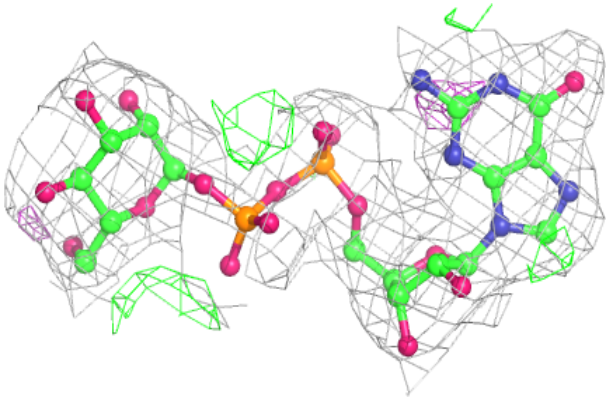
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

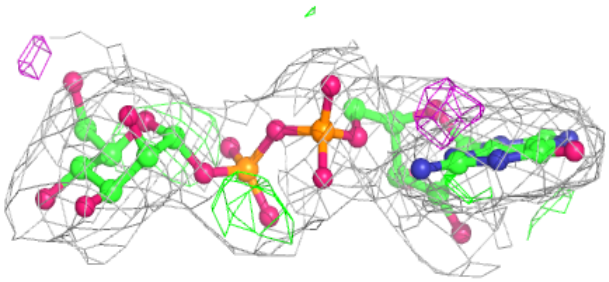


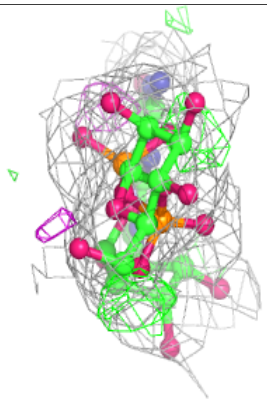


Electron density around GDD E 402:

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

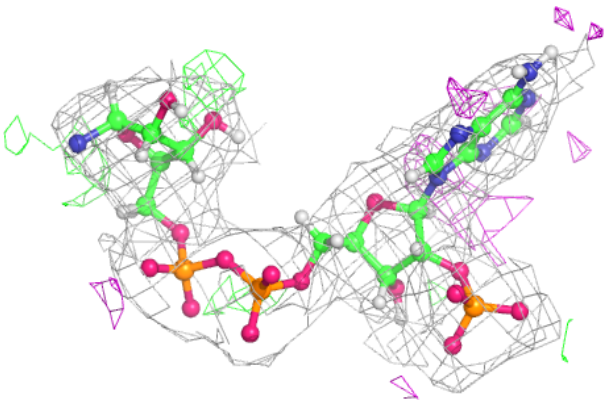


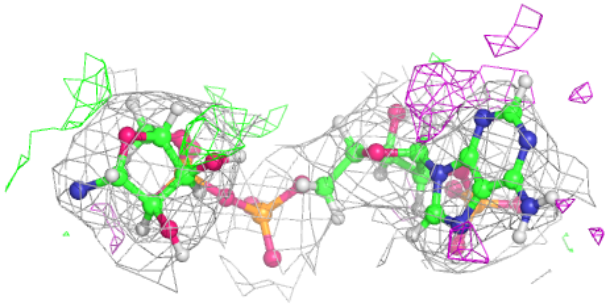


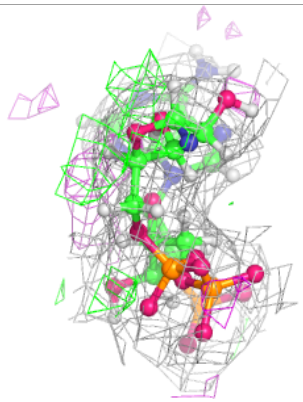


Electron density around NAP C 401:

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

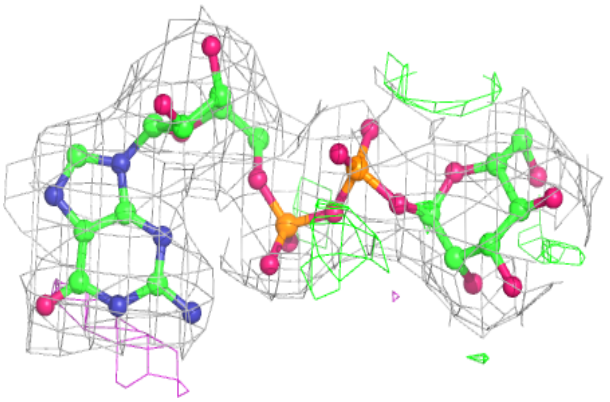


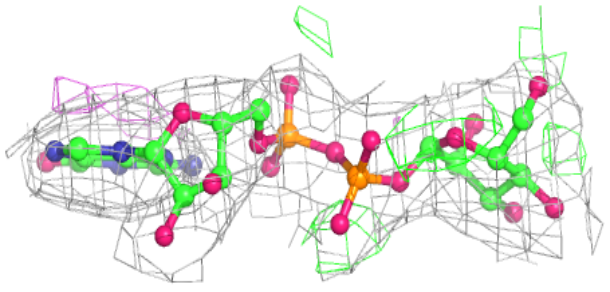


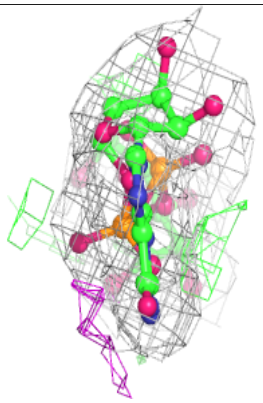


Electron density around GDD D 402:

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

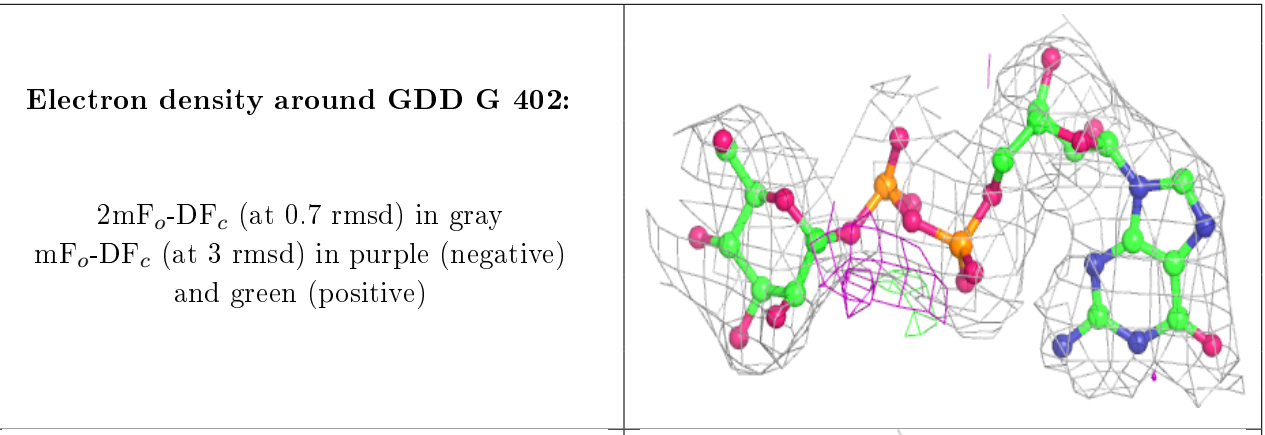






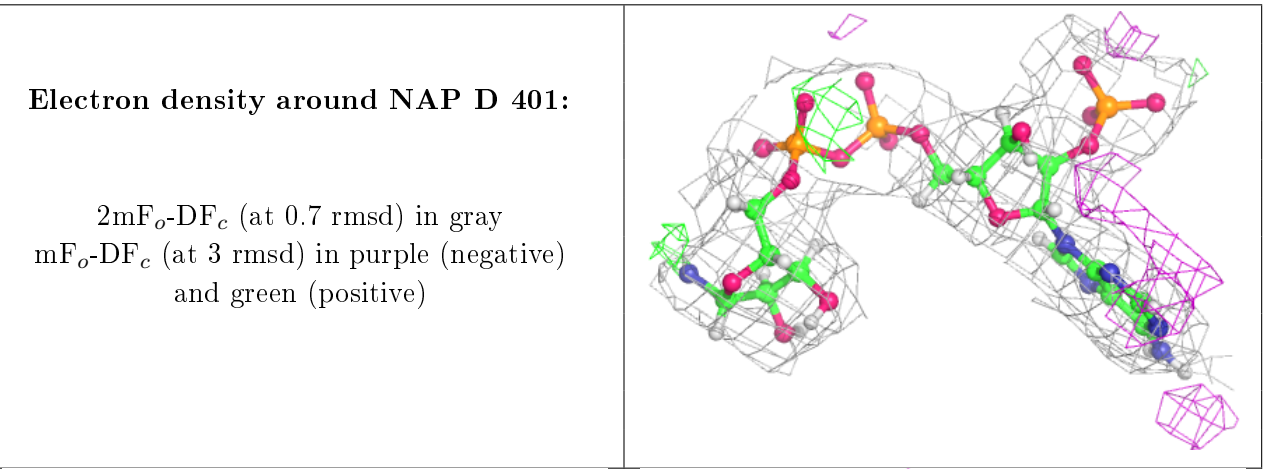
Electron density around GDD G 402:

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



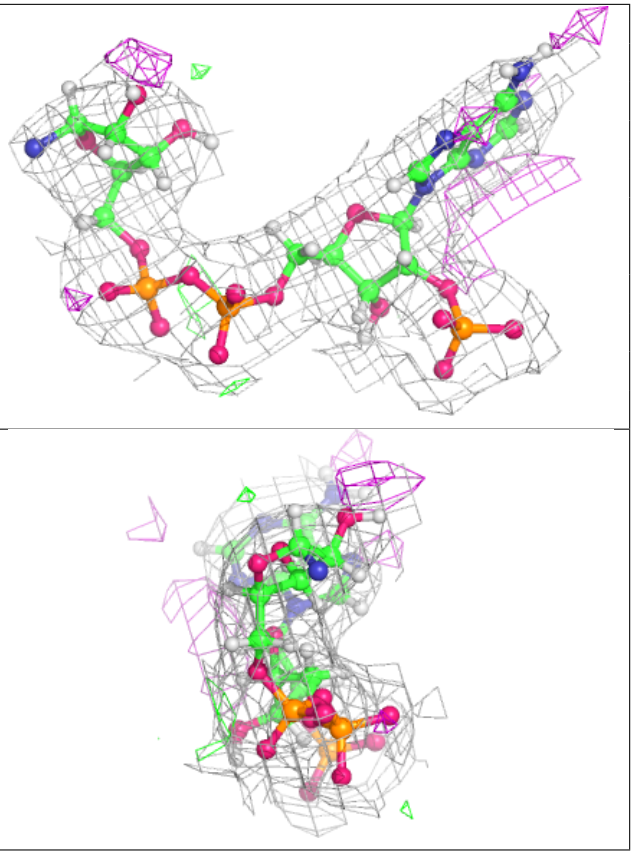
Electron density around NAP D 401:

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



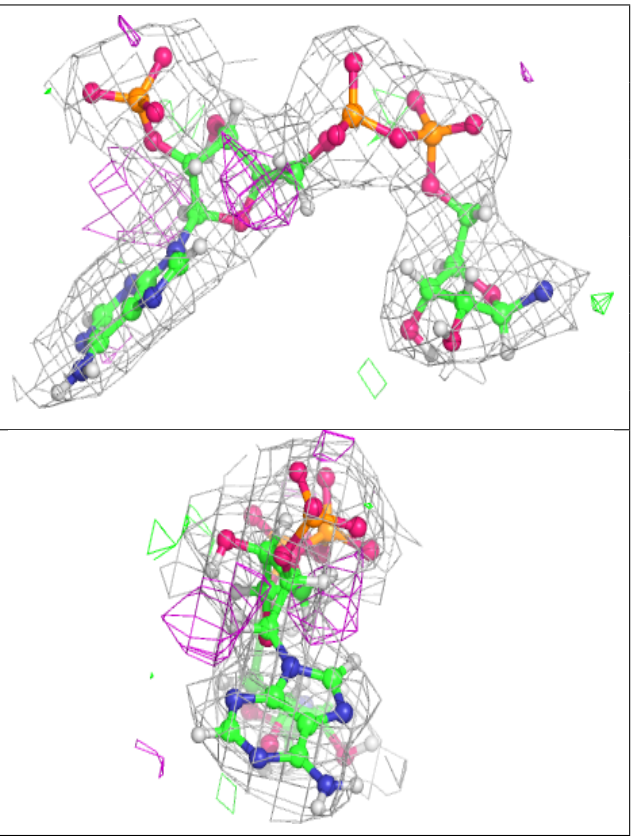
Electron density around NAP E 401:

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



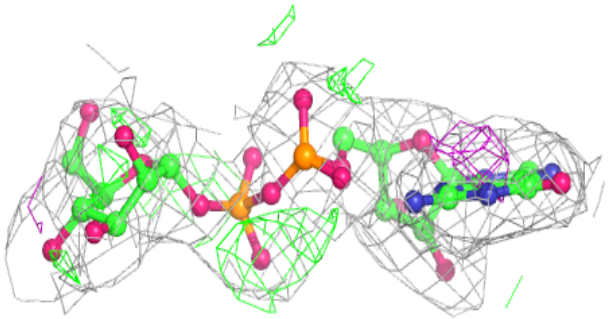
Electron density around NAP F 402:

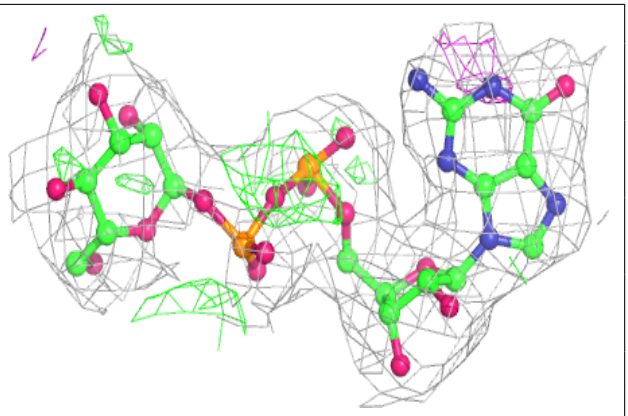
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

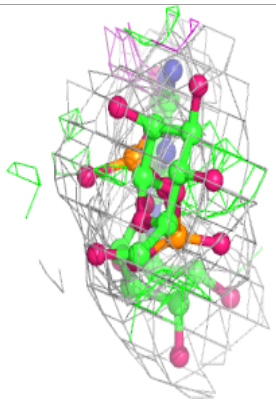


Electron density around GDD A 402:

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

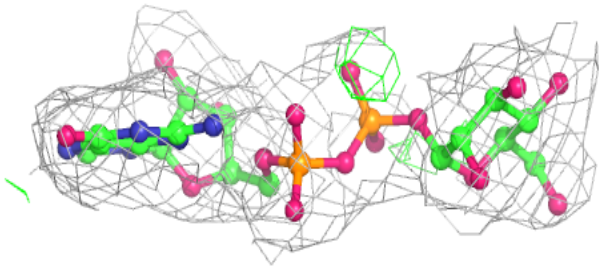


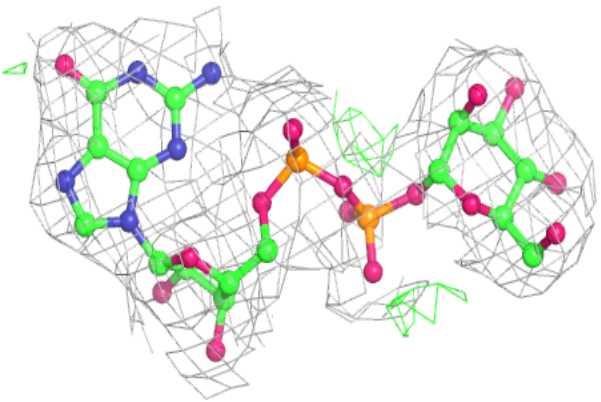




Electron density around GDD F 401:

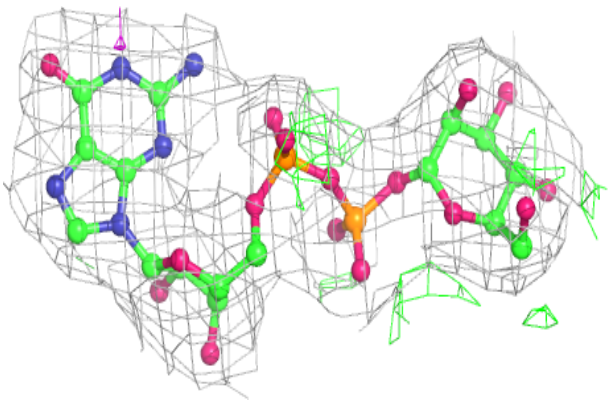
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

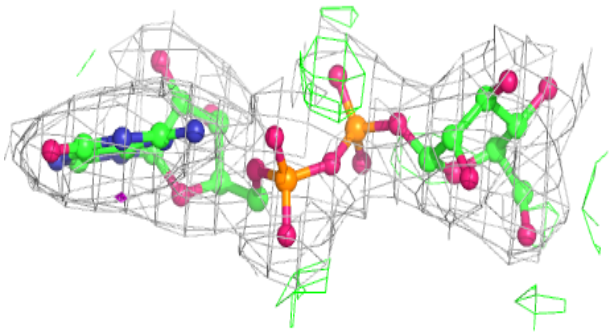


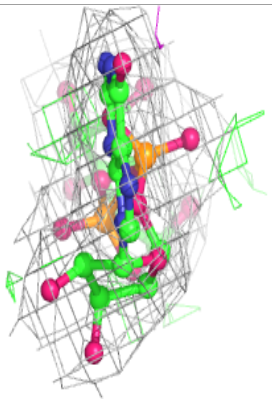


Electron density around GDD B 402:

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

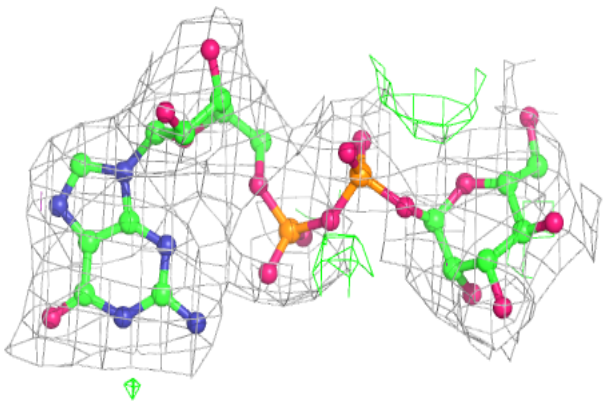


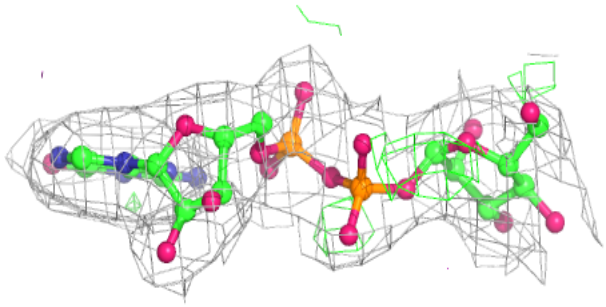


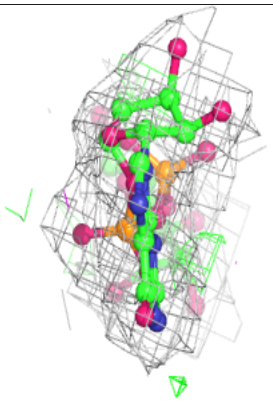


Electron density around GDD C 402:

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

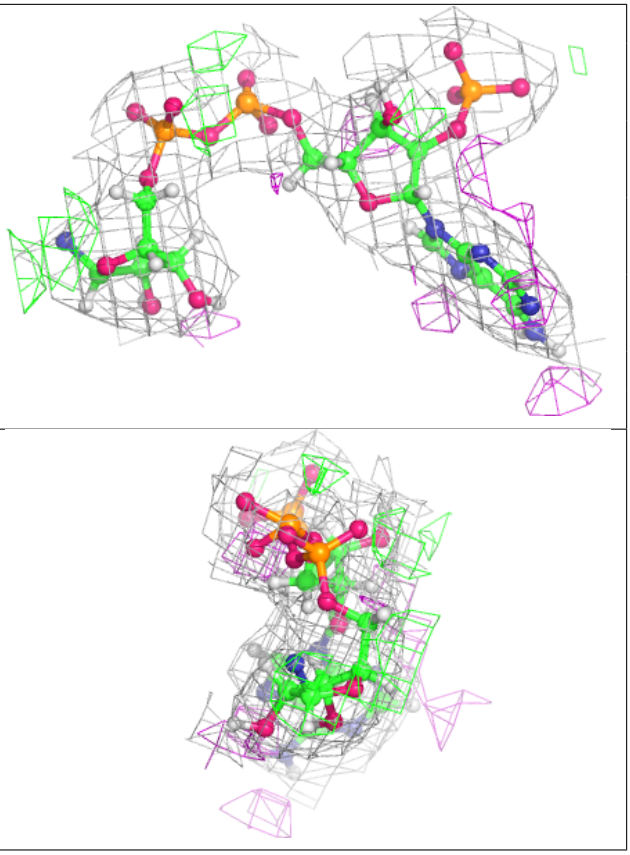






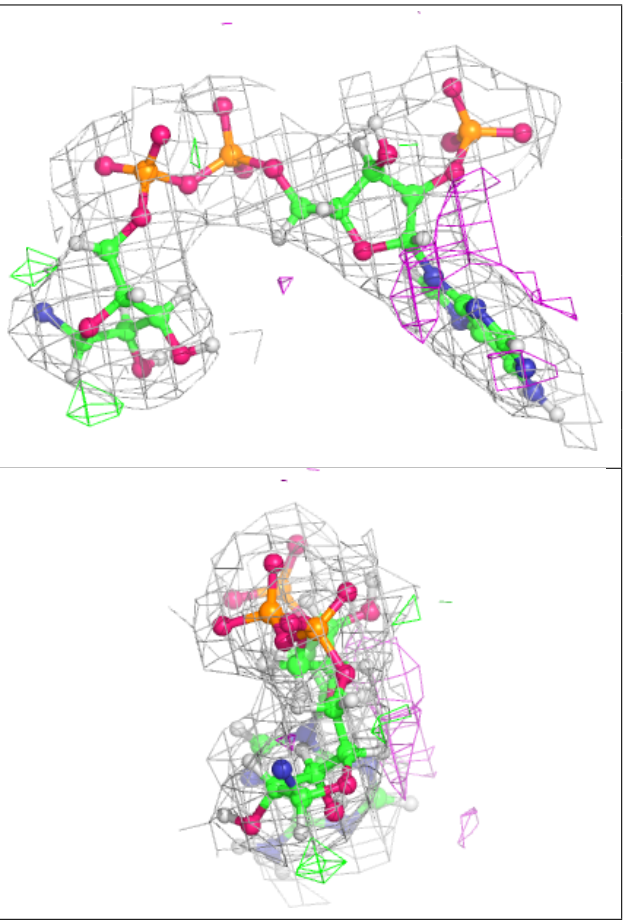
Electron density around NAP B 401:

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



Electron density around NAP G 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.