



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:26 am BST

PDB ID : 6C5A
Title : Human UDP-Glucose Dehydrogenase with UDP- Glc and NADH bound
Authors : Gross, P.G.; Fallah, J.; Wood, Z.A.
Deposited on : 2018-01-15
Resolution : 2.30 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

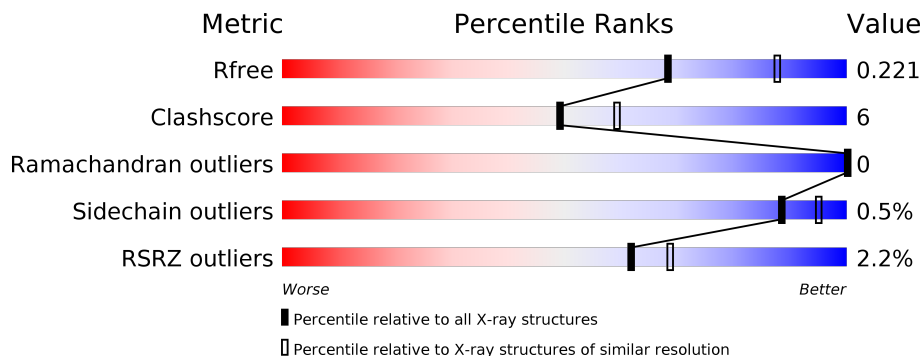
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. 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	494	 2% 83% 10% 7%
1	B	494	 % 84% 9% 7%
1	C	494	 % 83% 10% 7%
1	D	494	 2% 79% 14% 7%
1	E	494	 6% 78% 14% 8%
1	F	494	 82% 11% 7%

2 Entry composition [i](#)

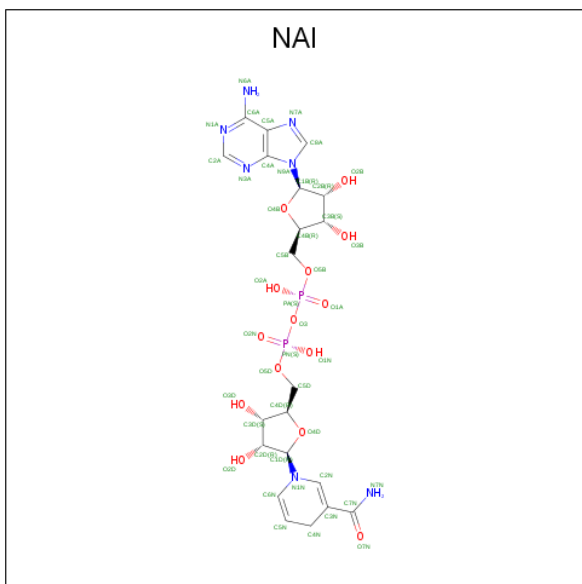
There are 5 unique types of molecules in this entry. The entry contains 22720 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-glucose 6-dehydrogenase.

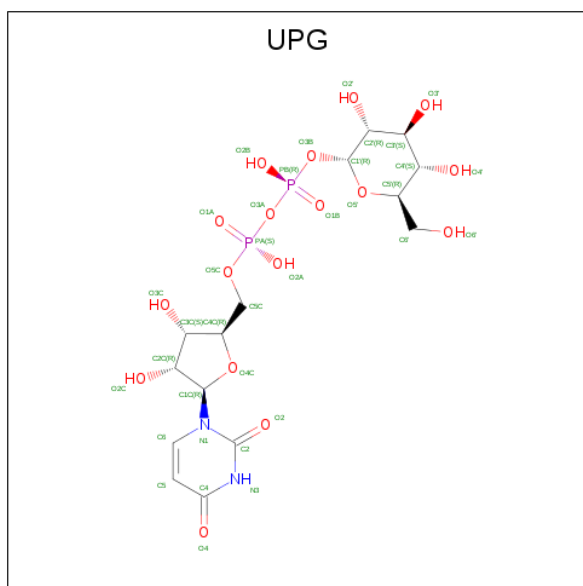
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	459	Total 3599	C 2277	N 622	O 680	S 20	0	0	0
1	B	459	Total 3599	C 2277	N 622	O 680	S 20	0	0	0
1	C	459	Total 3599	C 2277	N 622	O 680	S 20	0	0	0
1	D	459	Total 3599	C 2277	N 622	O 680	S 20	0	0	0
1	E	456	Total 3574	C 2260	N 618	O 677	S 19	0	0	0
1	F	459	Total 3598	C 2277	N 622	O 680	S 19	0	0	0

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



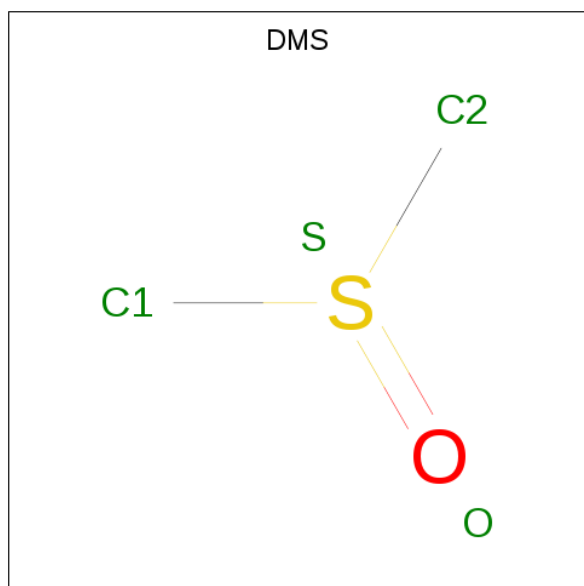
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	C	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	D	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	E	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	F	1	36	15	2	17	2	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	A	1	4	2	1	1	0	0
4	B	1	4	2	1	1	0	0
4	C	1	4	2	1	1	0	0
4	F	1	4	2	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	125	125	125	0	0
5	B	122	122	122	0	0
5	C	132	132	132	0	0
5	D	74	74	74	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	45	Total O 45 45	0	0
5	F	158	Total O 158 158	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.45Å 199.87Å 200.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.75 – 2.30 56.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (54.75-2.30) 99.8 (56.85-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.193 , 0.221 0.192 , 0.221	Depositor DCC
R_{free} test set	8516 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtrriage
Anisotropy	0.591	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.002 for -h,l,k	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22720	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UPG, NAI, DMS

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	0.59	0/3664	0.59	0/4956
1	B	0.56	0/3664	0.60	0/4956
1	C	0.52	0/3664	0.61	0/4956
1	D	0.53	0/3664	0.59	0/4956
1	E	0.50	0/3637	0.58	0/4918
1	F	0.53	0/3663	0.61	0/4956
All	All	0.54	0/21956	0.60	0/29698

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3599	0	3618	28	0
1	B	3599	0	3618	35	0
1	C	3599	0	3618	39	0
1	D	3599	0	3618	56	0
1	E	3574	0	3580	50	0
1	F	3598	0	3615	43	0
2	A	44	0	27	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	27	3	0
2	C	44	0	27	3	0
2	D	44	0	27	3	0
2	E	44	0	27	4	0
2	F	44	0	27	3	0
3	A	36	0	22	2	0
3	B	36	0	22	2	0
3	C	36	0	22	2	0
3	D	36	0	22	2	0
3	E	36	0	22	3	0
3	F	36	0	22	2	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	F	4	0	6	0	0
5	A	125	0	0	1	0
5	B	122	0	0	10	0
5	C	132	0	0	4	0
5	D	74	0	0	7	0
5	E	45	0	0	5	0
5	F	158	0	0	5	0
All	All	22720	0	21985	258	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 6.

All (258) 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)
2:E:500:NAI:H4N	3:E:501:UPG:H6'1	1.56	0.86
2:D:500:NAI:H4N	3:D:501:UPG:H6'1	1.65	0.77
1:E:275:SER:HB3	1:E:346:ARG:HD2	1.67	0.75
1:D:39:GLU:HG3	1:D:73:THR:HG21	1.72	0.69
1:B:224:ASN:ND2	1:B:280:ASP:OD2	2.27	0.68
3:E:501:UPG:H6'2	5:E:623:HOH:O	1.92	0.68
1:B:137:ALA:HB3	1:B:213:THR:CG2	2.24	0.67
1:B:137:ALA:CB	1:B:213:THR:CG2	2.73	0.66
1:B:137:ALA:CB	1:B:213:THR:HG21	2.25	0.66
1:B:409:HIS:ND1	5:B:605:HOH:O	2.29	0.65
1:E:421:LYS:HB3	1:E:422:GLU:OE2	1.96	0.65
1:D:369:PRO:HD2	1:D:417:TRP:NE1	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HG2	1:D:2:PHE:H	1.62	0.65
1:F:137:ALA:HB3	1:F:213:THR:HG21	1.77	0.65
1:B:181:GLY:HA2	1:B:211:THR:O	1.97	0.64
2:A:501:NAI:H4N	3:A:502:UPG:H6'1	1.78	0.64
2:F:501:NAI:H4N	3:F:502:UPG:H6'1	1.80	0.64
1:B:278:GLN:HB3	5:B:604:HOH:O	1.97	0.64
1:E:340:LYS:HD3	1:E:416:GLU:HG2	1.80	0.64
1:E:153:ASN:OD1	1:E:155:GLN:NE2	2.31	0.63
1:D:451:GLU:O	1:D:455:ILE:HG13	1.98	0.63
1:F:322:LEU:HD22	1:F:326:VAL:HG12	1.79	0.63
1:C:326:VAL:O	1:C:326:VAL:HG12	1.99	0.62
1:C:451:GLU:O	1:C:455:ILE:HG13	1.99	0.62
2:C:501:NAI:H4N	3:C:502:UPG:H6'1	1.80	0.62
1:A:137:ALA:HB3	1:A:213:THR:HG21	1.82	0.62
1:F:381:SER:O	1:F:382:HIS:HB2	1.99	0.61
1:C:327:THR:O	1:C:328:ASP:HB2	2.00	0.61
1:D:60:VAL:O	1:D:63:SER:OG	2.12	0.61
1:E:103:ALA:HB2	1:E:286:TYR:CD2	2.36	0.61
1:C:247:ASP:OD1	1:C:464:LYS:HG3	2.01	0.61
1:D:178:VAL:HA	5:D:610:HOH:O	2.01	0.61
1:C:330:LYS:HD2	1:C:365:HIS:CD2	2.36	0.60
1:B:3:GLU:OE2	1:B:5:LYS:HE3	2.01	0.60
1:C:204:PRO:HG2	1:C:207:LYS:HD2	1.83	0.60
1:F:322:LEU:CD2	1:F:326:VAL:HG12	2.31	0.60
1:B:275:SER:HB2	5:B:701:HOH:O	2.01	0.60
1:F:318:ILE:O	1:F:322:LEU:HD13	2.02	0.60
1:C:452:LEU:CD2	1:C:457:PHE:CD2	2.86	0.59
1:E:451:GLU:O	1:E:454:THR:HB	2.02	0.59
1:A:64:CYS:O	1:A:67:LYS:HB2	2.03	0.59
1:C:452:LEU:HD22	1:C:457:PHE:CD2	2.38	0.59
1:D:211:THR:HG23	1:D:212:ASN:O	2.02	0.58
1:E:278:GLN:HG3	1:E:304:ILE:HD12	1.84	0.58
1:E:449:HIS:HE1	5:E:609:HOH:O	1.86	0.58
1:B:137:ALA:HB3	1:B:213:THR:HG21	1.82	0.58
1:E:36:ASP:OD2	2:E:500:NAI:O3B	2.22	0.58
1:E:36:ASP:OD1	2:E:500:NAI:H1B	2.04	0.58
1:B:183:ASP:HB3	1:B:185:THR:HG23	1.85	0.58
1:C:84:LEU:HD12	1:C:125:ILE:O	2.04	0.58
1:A:381:SER:O	1:A:382:HIS:CG	2.56	0.58
1:A:451:GLU:O	1:A:455:ILE:HG13	2.03	0.57
1:B:277:PHE:HB2	5:B:620:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:ASN:O	1:C:454:THR:HG23	2.04	0.57
1:F:11:GLY:O	1:F:16:GLY:HA3	2.05	0.57
1:D:342:THR:HG22	1:D:344:ASP:H	1.69	0.56
1:C:426:GLU:HB2	5:C:630:HOH:O	2.04	0.56
1:A:165:GLU:O	1:A:339:LYS:NZ	2.27	0.56
1:A:450:ASN:O	1:A:454:THR:HG23	2.05	0.56
1:D:330:LYS:HE3	1:D:365:HIS:CD2	2.41	0.56
2:A:501:NAI:C4N	3:A:502:UPG:H6'1	2.36	0.56
1:D:452:LEU:HD22	1:D:457:PHE:CD2	2.41	0.56
2:B:501:NAI:H4N	3:B:502:UPG:H6'1	1.87	0.56
1:D:330:LYS:HE3	1:D:365:HIS:CE1	2.41	0.55
1:E:340:LYS:HB3	1:E:416:GLU:HG2	1.89	0.55
1:C:324:ASN:OD1	1:E:94:LYS:NZ	2.39	0.55
1:E:103:ALA:HB2	1:E:286:TYR:CE2	2.42	0.55
1:F:330:LYS:HE3	1:F:365:HIS:CG	2.42	0.55
1:E:25:HIS:HB2	1:E:60:VAL:HG13	1.89	0.54
2:F:501:NAI:C4N	3:F:502:UPG:H6'1	2.37	0.54
1:E:281:VAL:O	1:E:285:VAL:HG23	2.08	0.54
1:E:14:TYR:O	1:E:18:PRO:HD2	2.08	0.54
1:C:326:VAL:CG1	1:C:362:ALA:HB2	2.39	0.53
1:E:438:ILE:HG22	1:E:459:ILE:CD1	2.38	0.53
1:E:28:PRO:HA	1:E:68:ASN:ND2	2.23	0.53
1:F:255:ILE:HG23	1:F:261:ILE:HD13	1.90	0.53
1:B:137:ALA:HB3	1:B:213:THR:HG22	1.90	0.53
1:B:165:GLU:O	1:B:339:LYS:NZ	2.32	0.53
1:B:381:SER:O	1:B:382:HIS:CD2	2.62	0.53
1:F:152:LEU:HB3	5:F:605:HOH:O	2.09	0.52
1:E:449:HIS:CE1	5:E:609:HOH:O	2.60	0.52
2:C:501:NAI:C4N	3:C:502:UPG:H6'1	2.39	0.52
1:D:368:ASP:OD2	1:D:371:VAL:HG23	2.10	0.52
2:D:500:NAI:C4N	3:D:501:UPG:H6'1	2.39	0.52
1:C:438:ILE:O	1:C:459:ILE:HD12	2.11	0.51
1:F:211:THR:OG1	1:F:212:ASN:N	2.43	0.51
1:D:135:ARG:HA	1:D:214:TRP:CZ3	2.45	0.51
1:D:183:ASP:HB3	1:D:185:THR:HG23	1.92	0.51
1:D:367:TYR:C	1:D:367:TYR:CD1	2.83	0.51
1:D:36:ASP:OD2	2:D:500:NAI:O3B	2.18	0.51
1:D:106:LEU:HD21	1:D:133:PRO:HD2	1.93	0.51
1:E:275:SER:HB3	1:E:346:ARG:CD	2.39	0.51
1:E:443:ARG:HD3	1:E:462:ILE:O	2.11	0.51
1:D:416:GLU:HG2	1:D:416:GLU:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137:ALA:HB3	1:F:213:THR:CG2	2.40	0.50
1:A:137:ALA:HB3	1:A:213:THR:CG2	2.41	0.50
2:B:501:NAI:C4N	3:B:502:UPG:H6'1	2.41	0.50
1:D:326:VAL:CG2	1:D:360:GLU:CB	2.89	0.50
1:F:137:ALA:CB	1:F:213:THR:HG21	2.41	0.50
1:C:421:LYS:HB3	1:C:421:LYS:NZ	2.26	0.50
1:F:437:PHE:CD2	1:F:458:GLN:HG2	2.46	0.50
1:D:326:VAL:CG2	1:D:360:GLU:HB3	2.42	0.50
1:A:185:THR:HB	1:A:186:PRO:HD2	1.92	0.50
1:C:443:ARG:HD2	1:C:461:THR:OG1	2.12	0.50
1:D:443:ARG:HD3	1:D:462:ILE:O	2.11	0.50
1:F:322:LEU:HD22	1:F:326:VAL:CG1	2.42	0.50
1:D:369:PRO:HG2	1:D:417:TRP:CE2	2.47	0.50
1:A:330:LYS:HE3	1:A:365:HIS:CG	2.47	0.50
1:A:330:LYS:HE3	1:A:365:HIS:ND1	2.27	0.49
1:B:443:ARG:HD2	1:B:461:THR:OG1	2.12	0.49
1:F:204:PRO:HD2	1:F:207:LYS:HE3	1.93	0.49
1:F:281:VAL:HB	1:F:304:ILE:HD11	1.94	0.49
1:F:181:GLY:HA2	1:F:211:THR:O	2.13	0.49
1:B:75:ILE:N	5:B:601:HOH:O	2.45	0.49
1:B:211:THR:OG1	1:B:212:ASN:N	2.46	0.48
1:C:19:THR:O	1:C:23:ILE:HG13	2.13	0.48
1:D:369:PRO:HD2	1:D:417:TRP:CD1	2.48	0.48
1:D:298:ARG:HD2	5:D:626:HOH:O	2.12	0.48
1:A:9:CYS:HB2	1:A:20:CYS:SG	2.52	0.48
1:E:326:VAL:HA	1:E:329:LYS:HD2	1.95	0.48
1:D:110:GLU:OE2	1:F:329:LYS:HE2	2.13	0.48
1:F:35:VAL:HA	1:F:72:SER:O	2.12	0.48
1:A:184:GLU:N	1:A:184:GLU:OE1	2.46	0.48
1:A:54:GLU:OE2	1:A:166:GLY:N	2.41	0.48
1:D:9:CYS:HB2	1:D:20:CYS:SG	2.53	0.48
1:E:346:ARG:HD3	5:E:621:HOH:O	2.14	0.48
1:F:398:SER:HB3	1:F:403:GLU:HG3	1.96	0.48
1:A:309:TYR:CZ	1:A:313:ARG:HD3	2.49	0.48
1:B:365:HIS:ND1	5:B:608:HOH:O	2.35	0.48
1:C:90:ASN:N	1:C:90:ASN:OD1	2.42	0.48
1:D:108:TYR:HB2	5:D:631:HOH:O	2.12	0.48
1:D:336:PHE:N	1:D:368:ASP:OD1	2.34	0.48
1:B:329:LYS:NZ	1:F:110:GLU:OE2	2.44	0.48
1:F:309:TYR:O	1:F:313:ARG:HB2	2.14	0.48
1:F:90:ASN:OD1	1:F:90:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:LEU:HD23	1:C:457:PHE:CD2	2.48	0.47
1:F:25:HIS:HA	1:F:64:CYS:SG	2.54	0.47
1:C:380:LEU:O	1:C:391:VAL:CG2	2.62	0.47
1:E:138:GLU:O	1:E:142:ARG:HG3	2.13	0.47
1:F:178:VAL:HA	5:F:608:HOH:O	2.14	0.47
1:B:325:THR:CG2	1:F:110:GLU:OE1	2.63	0.47
1:B:381:SER:O	1:B:382:HIS:CG	2.68	0.47
1:D:204:PRO:HG2	1:D:207:LYS:HD2	1.96	0.47
1:F:9:CYS:HB2	1:F:20:CYS:SG	2.55	0.47
1:C:74:ASN:ND2	1:C:77:ASP:HB2	2.30	0.47
1:D:27:CYS:C	5:D:615:HOH:O	2.54	0.47
1:D:369:PRO:CD	1:D:417:TRP:NE1	2.78	0.47
1:E:367:TYR:CE2	1:E:401:PRO:HG3	2.50	0.47
1:B:152:LEU:HB2	5:B:666:HOH:O	2.15	0.46
1:C:250:GLU:OE1	1:D:211:THR:OG1	2.34	0.46
1:C:443:ARG:HD3	1:C:462:ILE:O	2.15	0.46
1:D:207:LYS:NZ	5:D:617:HOH:O	2.47	0.46
1:E:11:GLY:O	1:E:16:GLY:HA3	2.16	0.46
1:E:330:LYS:HE3	1:E:365:HIS:CG	2.51	0.46
1:B:438:ILE:O	1:B:459:ILE:HD12	2.15	0.46
1:C:317:ARG:NH2	1:C:460:GLU:HB3	2.30	0.46
1:B:449:HIS:O	1:B:453:GLN:HG3	2.16	0.46
2:E:500:NAI:H2D	2:E:500:NAI:H2N	1.72	0.46
1:C:326:VAL:HG11	1:C:362:ALA:HB2	1.97	0.46
1:B:443:ARG:HD3	1:B:462:ILE:O	2.16	0.46
1:E:36:ASP:OD1	1:E:37:VAL:N	2.48	0.46
1:D:330:LYS:HE3	1:D:365:HIS:NE2	2.30	0.46
1:D:158:SER:OG	5:D:601:HOH:O	2.20	0.46
1:F:134:VAL:O	1:F:135:ARG:HB2	2.16	0.46
1:D:369:PRO:CD	1:D:417:TRP:CD1	2.99	0.45
1:D:93:THR:HB	5:D:605:HOH:O	2.16	0.45
1:E:450:ASN:O	1:E:454:THR:OG1	2.24	0.45
1:E:6:LYS:HD3	1:E:81:GLU:O	2.16	0.45
1:F:102:ARG:NH2	5:F:612:HOH:O	2.41	0.45
1:C:437:PHE:CE2	1:C:458:GLN:OE1	2.70	0.45
1:D:241:CYS:HB3	1:D:246:ALA:O	2.16	0.45
1:E:435:PRO:HG2	1:E:437:PHE:HE1	1.82	0.45
1:F:443:ARG:HD3	1:F:462:ILE:O	2.17	0.45
1:A:314:PHE:CD1	1:A:462:ILE:HD11	2.52	0.45
2:A:501:NAI:H2N	2:A:501:NAI:H2D	1.77	0.45
1:E:390:GLN:HG3	1:E:393:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:THR:OG1	1:A:212:ASN:N	2.50	0.45
1:A:333:ILE:HD13	1:A:412:VAL:HB	1.99	0.45
1:F:50:LEU:HD11	1:F:58:LYS:HA	1.99	0.45
1:F:330:LYS:HE3	1:F:365:HIS:CD2	2.52	0.44
1:B:59:GLU:O	1:B:63:SER:HB3	2.16	0.44
1:C:330:LYS:HD2	1:C:365:HIS:NE2	2.32	0.44
1:D:452:LEU:CD2	1:D:457:PHE:CD2	3.01	0.44
1:C:324:ASN:HB2	5:C:706:HOH:O	2.17	0.44
1:C:380:LEU:O	1:C:391:VAL:HG22	2.18	0.44
1:C:381:SER:HA	1:C:391:VAL:HG21	1.98	0.44
1:D:90:ASN:N	1:D:90:ASN:OD1	2.43	0.44
1:C:227:LEU:HG	1:D:261:ILE:HD11	1.99	0.44
1:E:6:LYS:HE2	1:E:31:ARG:NH1	2.33	0.44
1:C:279:LYS:HE2	5:C:713:HOH:O	2.17	0.44
1:D:93:THR:OG1	1:D:279:LYS:HB2	2.18	0.44
1:F:131:THR:HA	5:F:627:HOH:O	2.18	0.44
1:E:222:ALA:HB3	1:F:255:ILE:HD11	2.00	0.43
1:E:24:ALA:HB1	1:E:68:ASN:OD1	2.18	0.43
1:C:452:LEU:CD2	1:C:457:PHE:CE2	3.01	0.43
1:B:180:ILE:O	1:B:210:THR:HA	2.19	0.43
1:D:393:ARG:HG3	1:D:394:LEU:HG	2.01	0.43
1:E:464:LYS:HG3	1:E:465:LYS:H	1.84	0.43
1:F:19:THR:HG22	1:F:172:LEU:HD21	2.01	0.43
2:C:501:NAI:H2N	2:C:501:NAI:H2D	1.81	0.43
1:E:277:PHE:CE2	3:E:501:UPG:H5C2	2.54	0.43
1:E:12:ALA:HB2	1:E:34:VAL:HG12	2.00	0.43
1:D:369:PRO:HD2	1:D:417:TRP:HE1	1.82	0.43
1:A:373:ARG:HG3	1:A:374:GLU:N	2.33	0.43
1:B:370:LYS:NZ	5:B:610:HOH:O	2.38	0.43
1:D:79:ILE:O	1:D:124:LYS:HE3	2.19	0.43
1:A:241:CYS:HB3	1:A:246:ALA:O	2.18	0.43
1:B:275:SER:CB	5:B:701:HOH:O	2.65	0.43
1:E:282:LEU:HD23	1:E:282:LEU:HA	1.89	0.43
1:C:253:THR:O	1:C:257:MET:HG3	2.19	0.42
1:F:374:GLU:CD	1:F:374:GLU:H	2.22	0.42
1:D:318:ILE:O	1:D:322:LEU:HG	2.19	0.42
1:C:11:GLY:O	1:C:16:GLY:HA3	2.20	0.42
1:D:369:PRO:CG	1:D:417:TRP:CE2	3.02	0.42
1:E:121:ASN:HA	5:E:601:HOH:O	2.19	0.42
1:A:35:VAL:HA	1:A:72:SER:O	2.19	0.42
1:E:133:PRO:O	1:E:134:VAL:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:455:ILE:O	1:E:455:ILE:HG22	2.17	0.42
1:D:437:PHE:CE2	1:D:458:GLN:OE1	2.73	0.42
1:E:328:ASP:HA	1:E:363:HIS:CD2	2.55	0.42
1:D:369:PRO:CG	1:D:417:TRP:NE1	2.83	0.42
1:E:438:ILE:HG22	1:E:459:ILE:HD12	2.01	0.42
1:D:110:GLU:OE2	1:F:329:LYS:CE	2.68	0.42
1:C:326:VAL:HG12	1:C:362:ALA:HB2	2.02	0.42
1:D:47:SER:OG	1:D:49:THR:O	2.38	0.42
1:E:86:PHE:CD1	1:E:129:LYS:HE2	2.54	0.41
1:F:129:LYS:HG3	1:F:159:ASN:O	2.20	0.41
1:E:14:TYR:O	1:E:18:PRO:HG2	2.20	0.41
1:E:435:PRO:HG2	1:E:437:PHE:CE1	2.55	0.41
1:A:309:TYR:O	1:A:313:ARG:HB2	2.20	0.41
2:B:501:NAI:H2D	2:B:501:NAI:H2N	1.84	0.41
1:C:53:TYR:HA	5:C:649:HOH:O	2.20	0.41
1:E:79:ILE:O	1:E:124:LYS:HE3	2.19	0.41
1:F:326:VAL:HA	1:F:329:LYS:HD2	2.03	0.41
1:F:102:ARG:NH2	5:F:624:HOH:O	2.53	0.41
2:F:501:NAI:H2D	2:F:501:NAI:H2N	1.86	0.41
1:A:102:ARG:HD2	5:A:638:HOH:O	2.20	0.41
1:A:93:THR:OG1	1:A:279:LYS:HB2	2.20	0.41
1:D:35:VAL:HA	1:D:72:SER:O	2.20	0.41
1:E:222:ALA:CB	1:F:255:ILE:HD11	2.51	0.41
1:A:19:THR:O	1:A:23:ILE:HG13	2.20	0.41
1:A:328:ASP:HA	1:A:363:HIS:CD2	2.56	0.41
1:D:341:ASP:N	1:D:417:TRP:CH2	2.85	0.41
1:F:340:LYS:O	1:F:341:ASP:HB2	2.21	0.41
1:E:130:SER:O	1:E:132:VAL:HG13	2.20	0.41
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.94	0.40
1:B:360:GLU:HB3	5:B:631:HOH:O	2.20	0.40
1:B:74:ASN:OD1	1:B:77:ASP:HB2	2.20	0.40
1:C:438:ILE:CG2	1:C:459:ILE:HD13	2.52	0.40
1:D:42:ILE:HD13	1:D:42:ILE:HA	1.89	0.40
1:C:421:LYS:HZ3	1:C:421:LYS:HB3	1.84	0.40
1:D:258:ASP:HB3	1:D:261:ILE:HD12	2.04	0.40
1:D:381:SER:O	1:D:382:HIS:HB2	2.21	0.40
1:B:130:SER:O	1:B:132:VAL:HG13	2.21	0.40
1:A:11:GLY:O	1:A:16:GLY:HA3	2.21	0.40
1:A:255:ILE:HD11	1:B:222:ALA:HB1	2.03	0.40
1:B:137:ALA:HB1	1:B:213:THR:HG21	2.00	0.40
1:F:9:CYS:CB	1:F:20:CYS:SG	3.09	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	455/494 (92%)	442 (97%)	13 (3%)	0	100	100
1	B	455/494 (92%)	444 (98%)	11 (2%)	0	100	100
1	C	455/494 (92%)	442 (97%)	13 (3%)	0	100	100
1	D	455/494 (92%)	446 (98%)	9 (2%)	0	100	100
1	E	448/494 (91%)	435 (97%)	13 (3%)	0	100	100
1	F	455/494 (92%)	444 (98%)	11 (2%)	0	100	100
All	All	2723/2964 (92%)	2653 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/426 (92%)	391 (99%)	3 (1%)	81	91
1	B	394/426 (92%)	393 (100%)	1 (0%)	92	97
1	C	394/426 (92%)	392 (100%)	2 (0%)	88	95
1	D	394/426 (92%)	392 (100%)	2 (0%)	88	95
1	E	391/426 (92%)	388 (99%)	3 (1%)	81	91
1	F	394/426 (92%)	393 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2361/2556 (92%)	2349 (100%)	12 (0%)	88 95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	LYS
1	A	135	ARG
1	A	177	ARG
1	B	177	ARG
1	C	177	ARG
1	C	382	HIS
1	D	1	MET
1	D	177	ARG
1	E	177	ARG
1	E	457	PHE
1	E	465	LYS
1	F	177	ARG

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

Mol	Chain	Res	Type
1	A	259	GLN
1	A	363	HIS
1	A	382	HIS
1	B	363	HIS
1	B	382	HIS
1	D	449	HIS
1	E	409	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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	NAI	E	500	-	42,48,48	0.93	2 (4%)	47,73,73	0.93	2 (4%)
2	NAI	C	501	-	42,48,48	0.93	1 (2%)	47,73,73	0.97	1 (2%)
3	UPG	C	502	-	31,38,38	0.79	0	41,58,58	0.70	0
3	UPG	A	502	-	31,38,38	0.78	0	41,58,58	0.64	0
3	UPG	B	502	-	31,38,38	0.76	0	41,58,58	0.61	0
3	UPG	D	501	-	31,38,38	0.78	0	41,58,58	0.75	0
3	UPG	F	502	-	31,38,38	0.77	0	41,58,58	0.68	1 (2%)
2	NAI	A	501	-	42,48,48	0.95	2 (4%)	47,73,73	0.91	1 (2%)
4	DMS	F	503	-	3,3,3	0.72	0	3,3,3	0.82	0
4	DMS	C	503	-	3,3,3	0.54	0	3,3,3	0.51	0
4	DMS	B	503	-	3,3,3	0.66	0	3,3,3	0.50	0
2	NAI	F	501	-	42,48,48	0.91	1 (2%)	47,73,73	0.94	1 (2%)
4	DMS	A	503	-	3,3,3	0.66	0	3,3,3	0.50	0
3	UPG	E	501	-	31,38,38	0.79	0	41,58,58	0.76	1 (2%)
2	NAI	B	501	-	42,48,48	0.92	2 (4%)	47,73,73	0.92	1 (2%)
2	NAI	D	500	-	42,48,48	0.96	2 (4%)	47,73,73	0.85	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
2	NAI	E	500	-	-	5/25/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	C	501	-	-	5/25/72/72	0/5/5/5
3	UPG	C	502	-	-	6/21/59/59	0/3/3/3
3	UPG	A	502	-	-	5/21/59/59	0/3/3/3
3	UPG	B	502	-	-	5/21/59/59	0/3/3/3
3	UPG	D	501	-	-	4/21/59/59	0/3/3/3
3	UPG	F	502	-	-	6/21/59/59	0/3/3/3
2	NAI	A	501	-	-	5/25/72/72	0/5/5/5
2	NAI	F	501	-	-	5/25/72/72	0/5/5/5
3	UPG	E	501	-	-	9/21/59/59	0/3/3/3
2	NAI	B	501	-	-	5/25/72/72	0/5/5/5
2	NAI	D	500	-	-	9/25/72/72	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAI	C4N-C3N	-2.55	1.44	1.49
2	E	500	NAI	C4N-C3N	-2.53	1.45	1.49
2	A	501	NAI	C4N-C3N	-2.48	1.45	1.49
2	D	500	NAI	C4N-C3N	-2.42	1.45	1.49
2	F	501	NAI	C4N-C3N	-2.42	1.45	1.49
2	B	501	NAI	C7N-C3N	2.34	1.53	1.48
2	A	501	NAI	C7N-C3N	2.32	1.53	1.48
2	C	501	NAI	C4N-C3N	-2.27	1.45	1.49
2	D	500	NAI	C7N-C3N	2.26	1.53	1.48
2	E	500	NAI	C7N-C3N	2.21	1.53	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAI	O4B-C1B-C2B	-3.83	101.34	106.93
2	E	500	NAI	O4B-C1B-C2B	-3.41	101.94	106.93
2	A	501	NAI	O4B-C1B-C2B	-3.33	102.06	106.93
2	B	501	NAI	O4B-C1B-C2B	-3.00	102.54	106.93
2	F	501	NAI	O4B-C1B-C2B	-2.94	102.62	106.93
3	F	502	UPG	C3'-C4'-C5'	-2.22	106.28	110.24
3	E	501	UPG	O3A-PB-O3B	2.17	106.87	102.48
2	E	500	NAI	C4A-C5A-N7A	2.01	111.49	109.40

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502	UPG	O4C-C1C-N1-C6
3	A	502	UPG	C2C-C1C-N1-C6
3	A	502	UPG	O4C-C1C-N1-C6
3	B	502	UPG	C2C-C1C-N1-C6
3	B	502	UPG	O4C-C1C-N1-C6
3	F	502	UPG	PA-O3A-PB-O3B
3	E	501	UPG	C2C-C1C-N1-C6
3	E	501	UPG	O4C-C1C-N1-C6
2	D	500	NAI	C5B-O5B-PA-O1A
2	D	500	NAI	O4B-C4B-C5B-O5B
2	D	500	NAI	C3B-C4B-C5B-O5B
2	E	500	NAI	C2D-C1D-N1N-C6N
2	E	500	NAI	C2D-C1D-N1N-C2N
3	E	501	UPG	O4C-C4C-C5C-O5C
2	F	501	NAI	C2D-C1D-N1N-C6N
3	F	502	UPG	C4'-C5'-C6'-O6'
3	C	502	UPG	C1'-O3B-PB-O3A
3	A	502	UPG	C1'-O3B-PB-O3A
3	B	502	UPG	C1'-O3B-PB-O3A
3	D	501	UPG	C1'-O3B-PB-O3A
3	F	502	UPG	C1'-O3B-PB-O3A
3	B	502	UPG	PB-O3A-PA-O1A
3	F	502	UPG	PB-O3A-PA-O1A
2	C	501	NAI	C2D-C1D-N1N-C6N
2	E	500	NAI	O4D-C1D-N1N-C6N
2	A	501	NAI	C2D-C1D-N1N-C6N
2	B	501	NAI	C2D-C1D-N1N-C6N
3	E	501	UPG	C4'-C5'-C6'-O6'
3	C	502	UPG	PA-O3A-PB-O3B
3	B	502	UPG	PA-O3A-PB-O3B
3	D	501	UPG	PA-O3A-PB-O3B
3	E	501	UPG	PA-O3A-PB-O3B
2	F	501	NAI	C2D-C1D-N1N-C2N
2	D	500	NAI	C5B-O5B-PA-O3
3	D	501	UPG	PB-O3A-PA-O2A
2	C	501	NAI	O4D-C1D-N1N-C6N
2	F	501	NAI	O4D-C1D-N1N-C6N
2	D	500	NAI	C5B-O5B-PA-O2A
3	A	502	UPG	C4'-C5'-C6'-O6'
2	E	500	NAI	O4D-C1D-N1N-C2N
2	B	501	NAI	O4D-C1D-N1N-C6N
2	C	501	NAI	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	A	501	NAI	C2D-C1D-N1N-C2N
2	B	501	NAI	C2D-C1D-N1N-C2N
3	F	502	UPG	O5'-C5'-C6'-O6'
2	F	501	NAI	O4D-C1D-N1N-C2N
2	D	500	NAI	O4D-C1D-N1N-C6N
3	E	501	UPG	C3C-C4C-C5C-O5C
2	D	500	NAI	C2D-C1D-N1N-C6N
2	A	501	NAI	O4D-C1D-N1N-C6N
3	C	502	UPG	PB-O3A-PA-O1A
3	C	502	UPG	PB-O3A-PA-O2A
3	E	501	UPG	O5'-C5'-C6'-O6'
3	C	502	UPG	C4'-C5'-C6'-O6'
2	C	501	NAI	O4D-C1D-N1N-C2N
2	B	501	NAI	O4D-C1D-N1N-C2N
2	D	500	NAI	C2D-C1D-N1N-C2N
3	A	502	UPG	PB-O3A-PA-O1A
3	F	502	UPG	PB-O3A-PA-O2A
2	A	501	NAI	O4D-C1D-N1N-C2N
3	E	501	UPG	C1'-O3B-PB-O3A
2	D	500	NAI	O4D-C1D-N1N-C2N
2	C	501	NAI	O4B-C4B-C5B-O5B
2	E	500	NAI	O4B-C4B-C5B-O5B
2	A	501	NAI	O4B-C4B-C5B-O5B
2	F	501	NAI	O4B-C4B-C5B-O5B
2	B	501	NAI	O4B-C4B-C5B-O5B
3	D	501	UPG	PB-O3A-PA-O1A
3	E	501	UPG	PA-O3A-PB-O1B

There are no ring outliers.

12 monomers are involved in 21 short contacts:

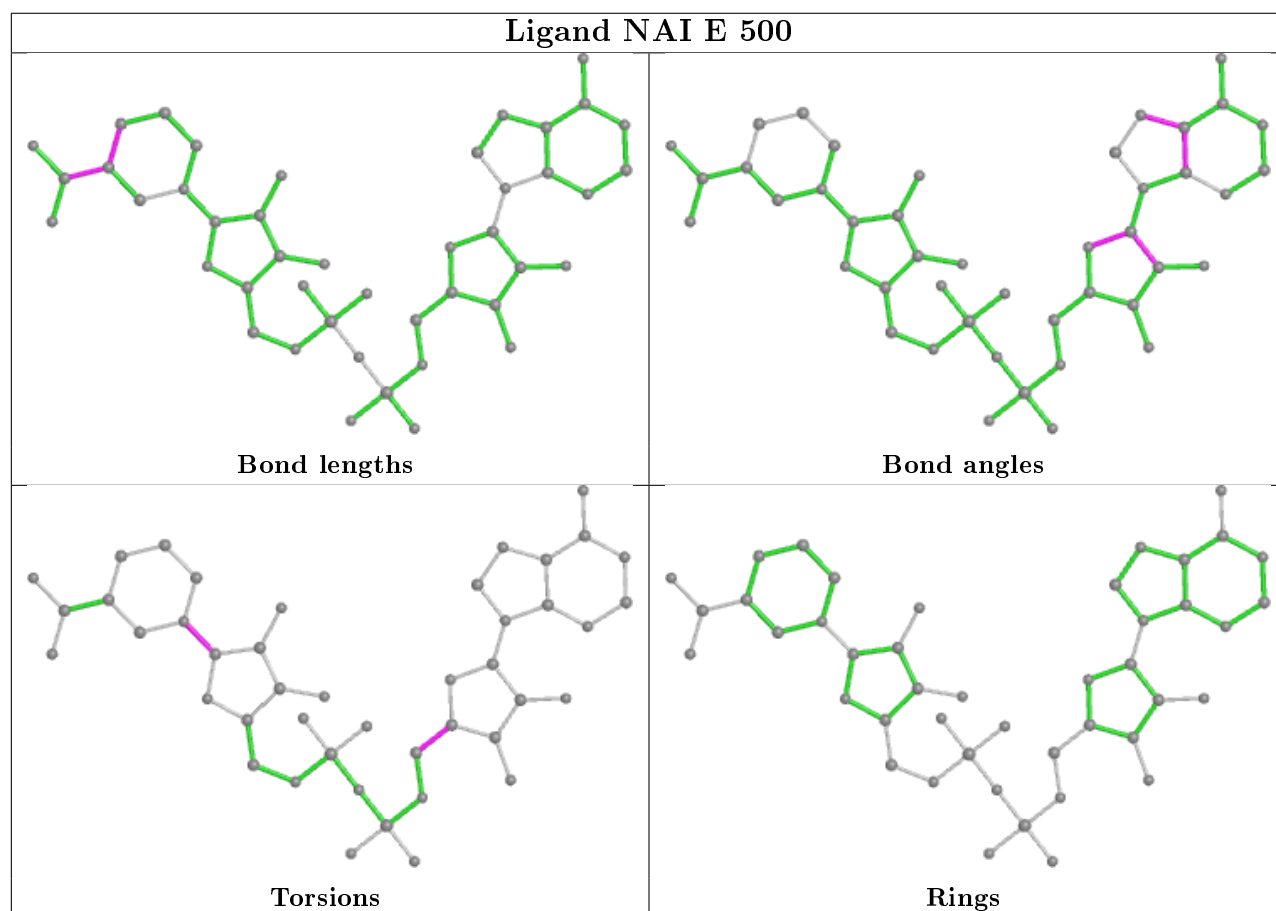
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	500	NAI	4	0
2	C	501	NAI	3	0
3	C	502	UPG	2	0
3	A	502	UPG	2	0
3	B	502	UPG	2	0
3	D	501	UPG	2	0
3	F	502	UPG	2	0
2	A	501	NAI	3	0
2	F	501	NAI	3	0
3	E	501	UPG	3	0

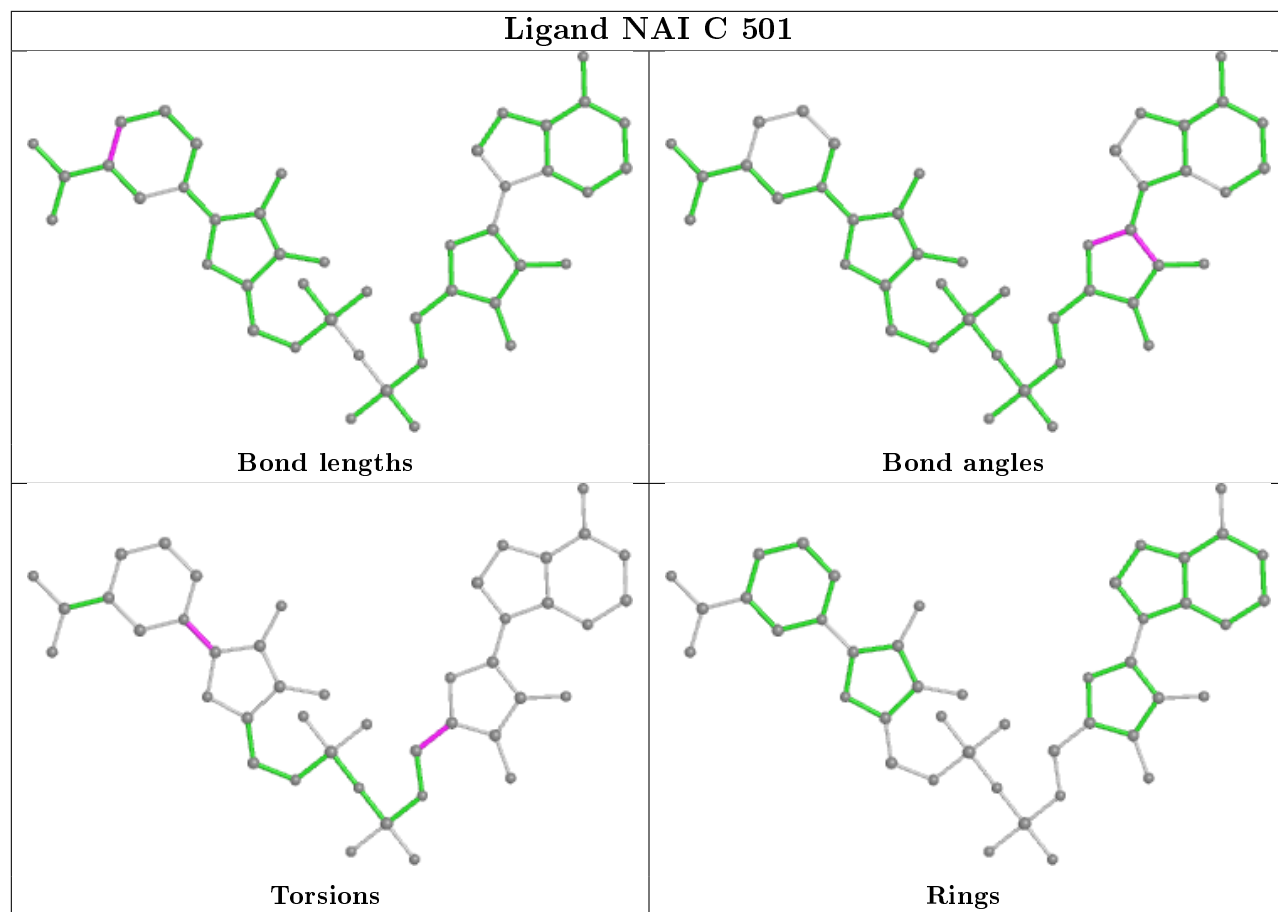
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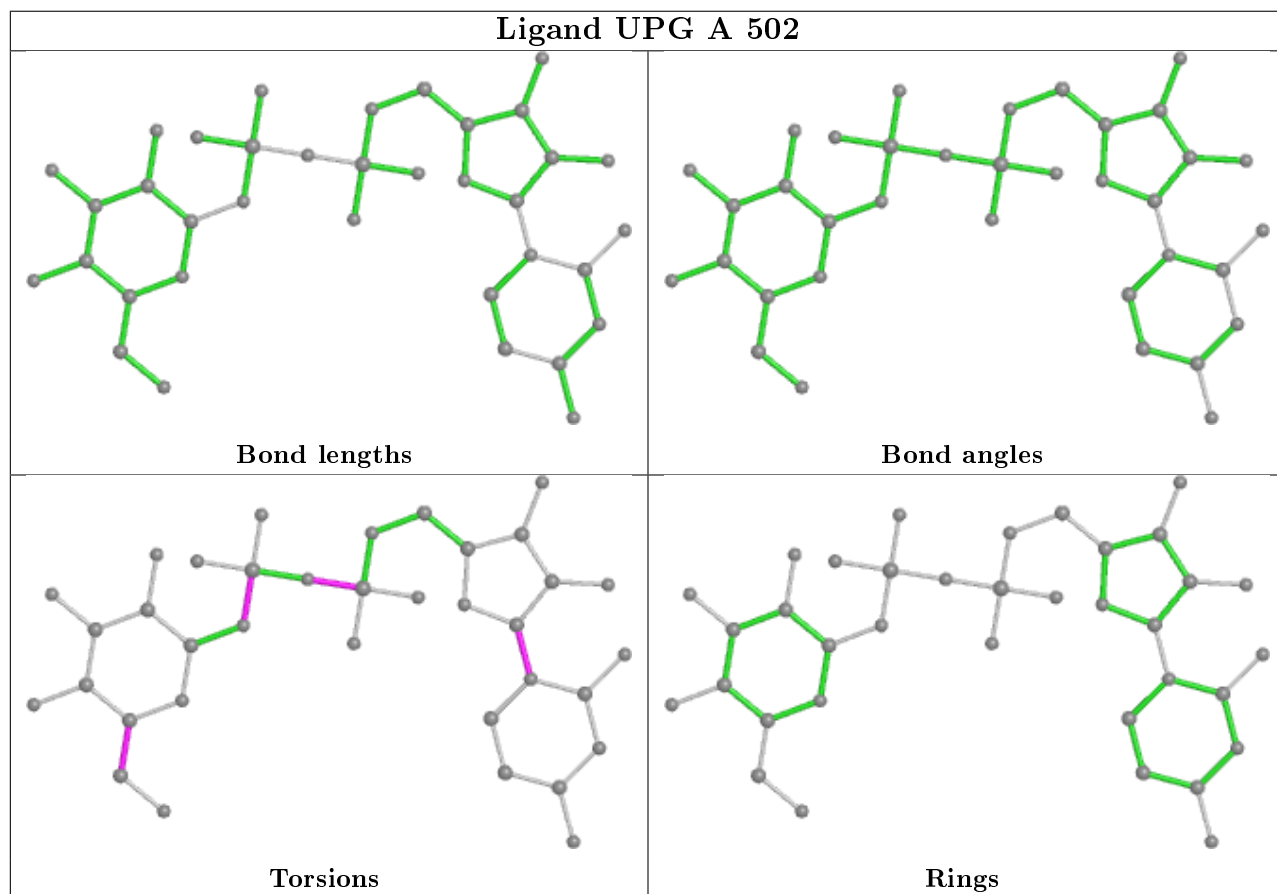
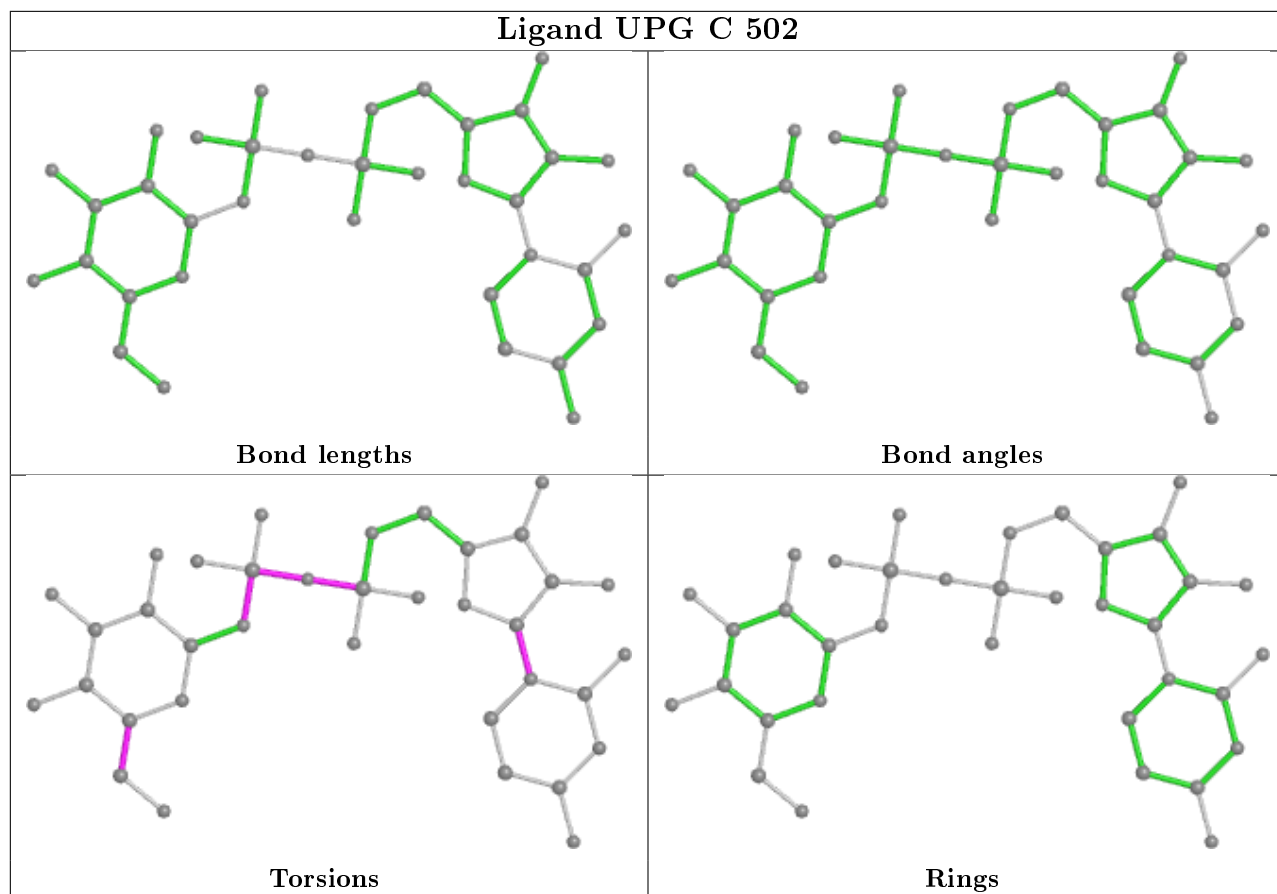
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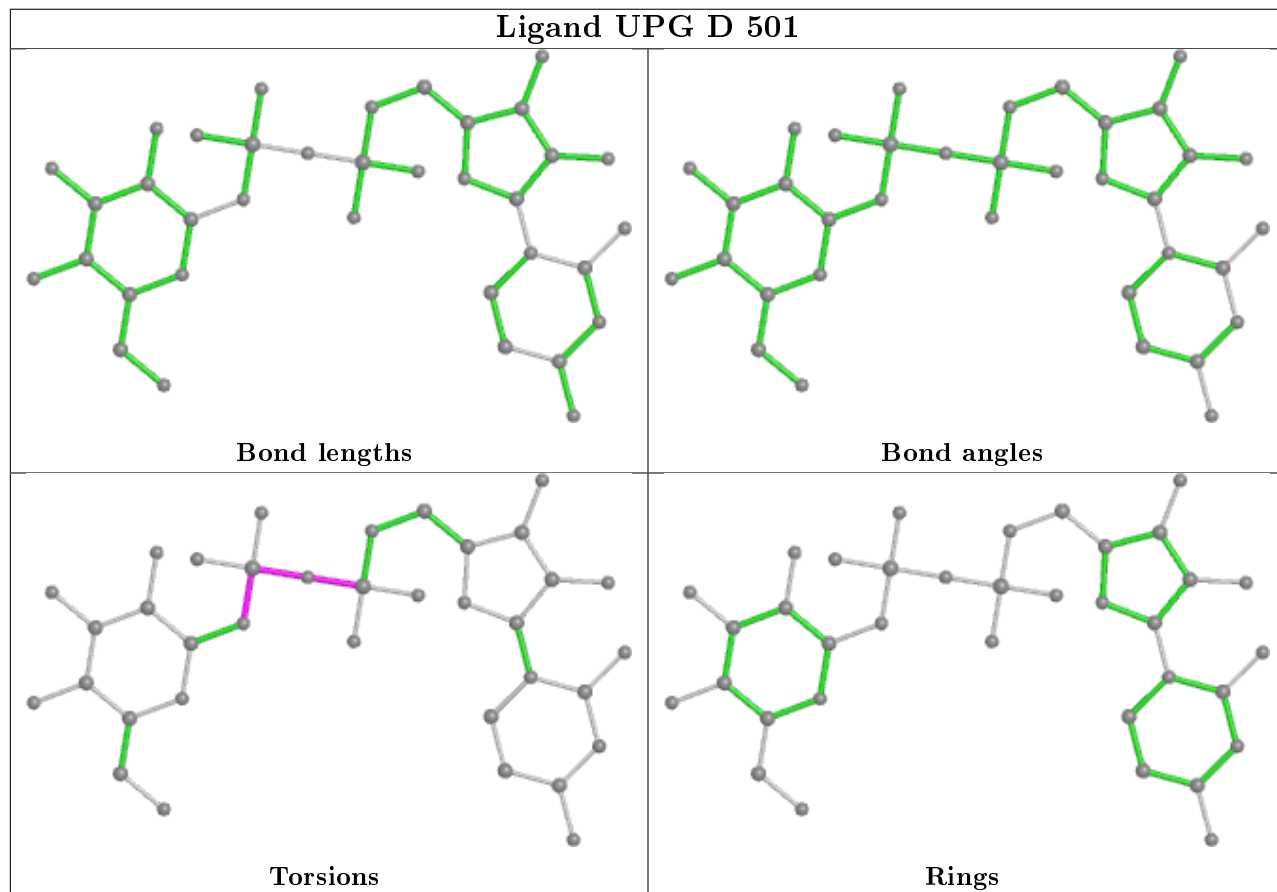
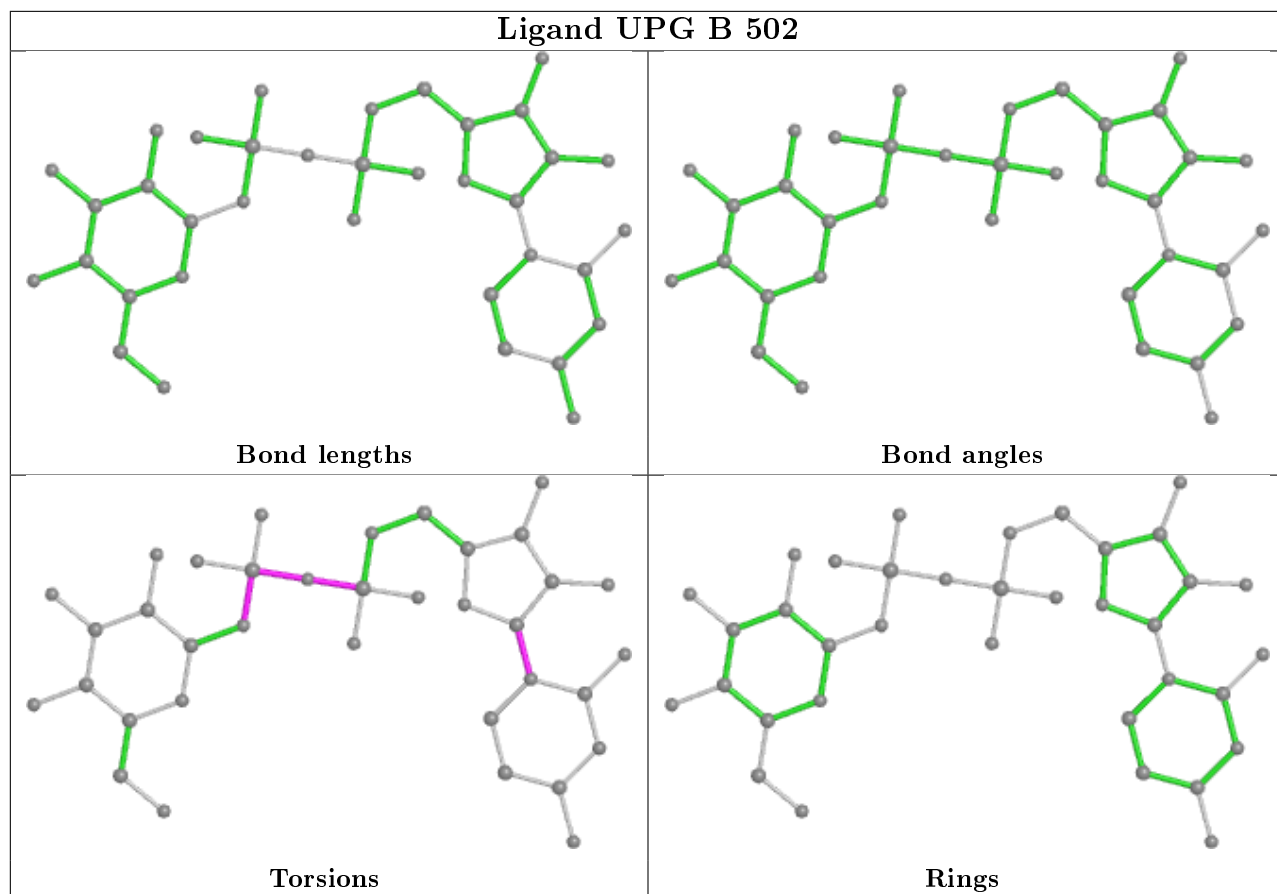
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NAI	3	0
2	D	500	NAI	3	0

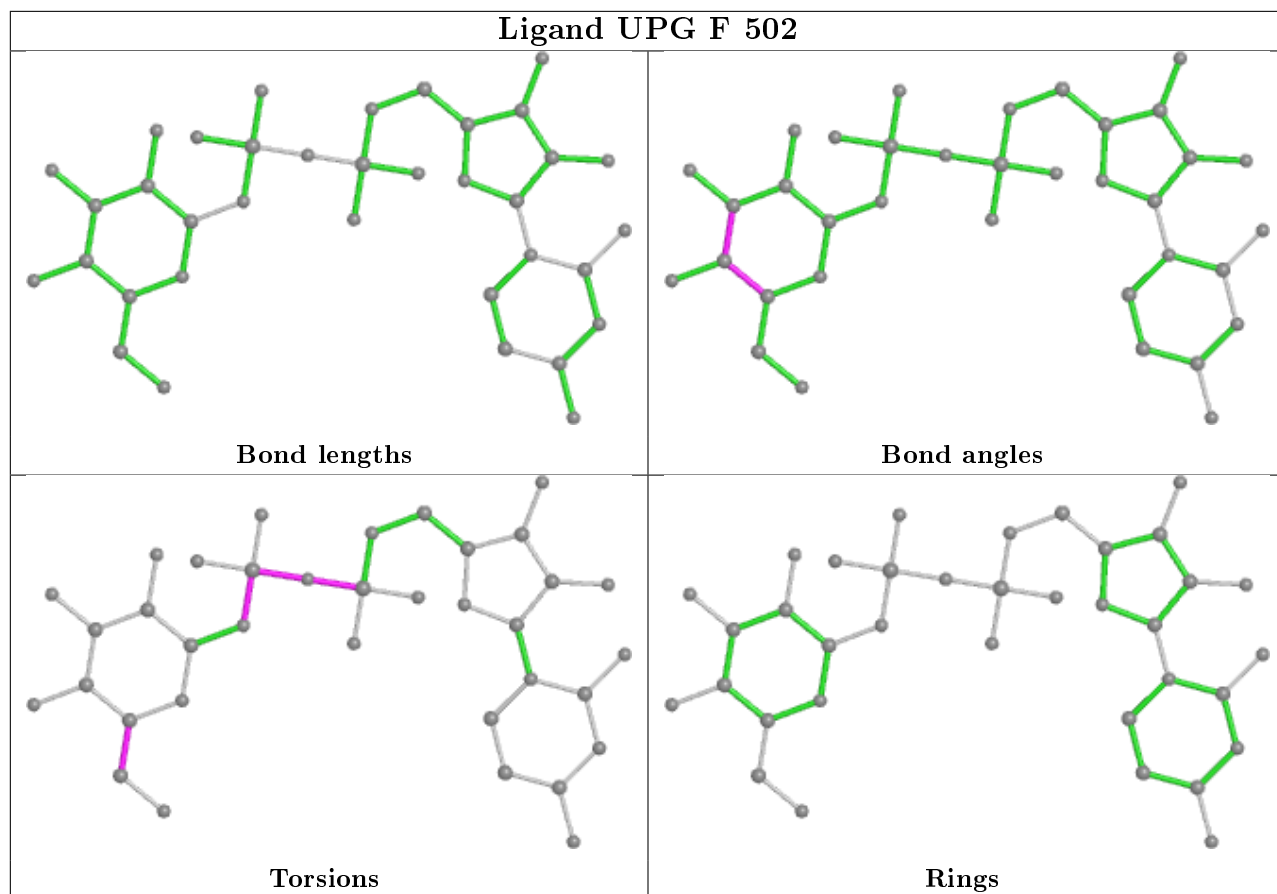
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

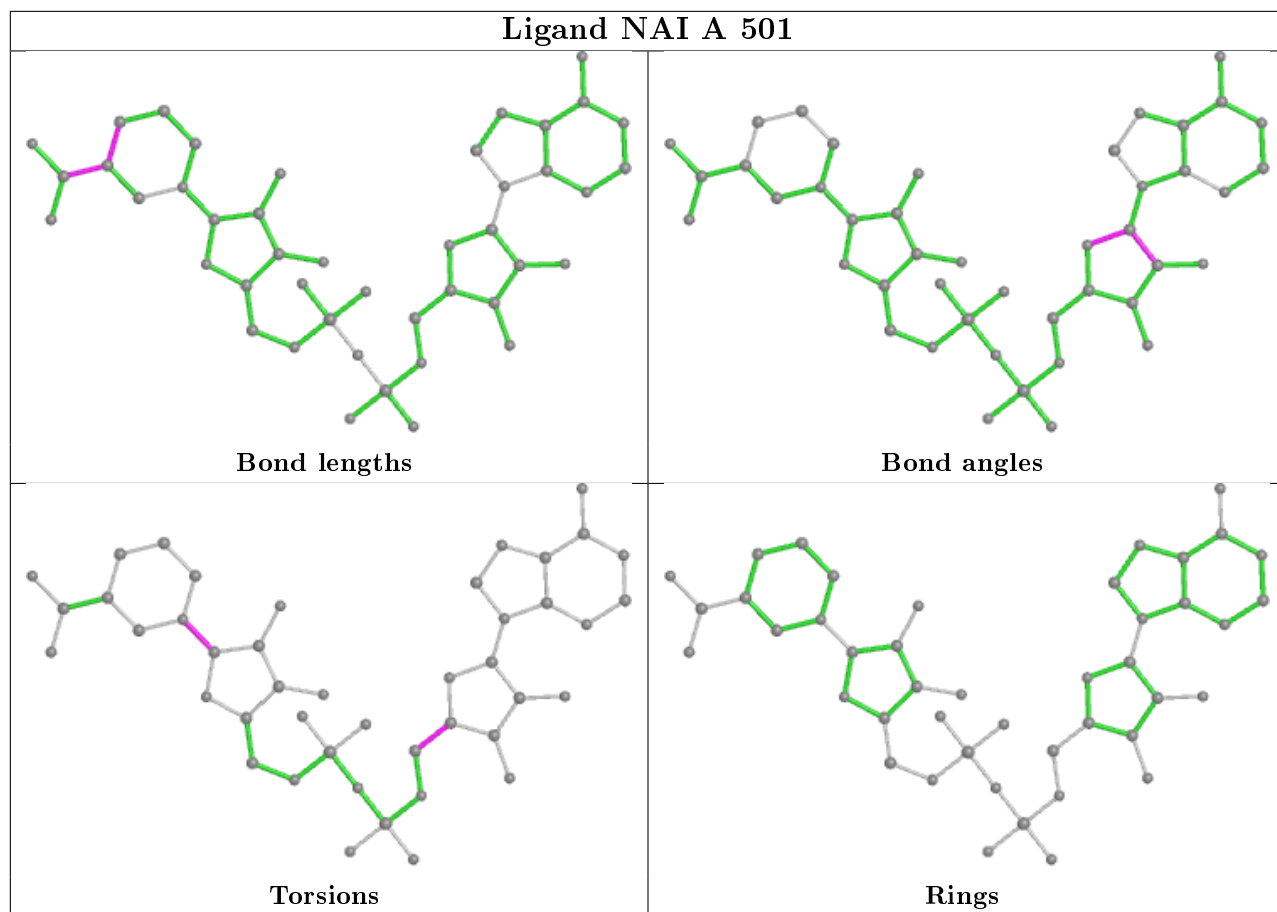


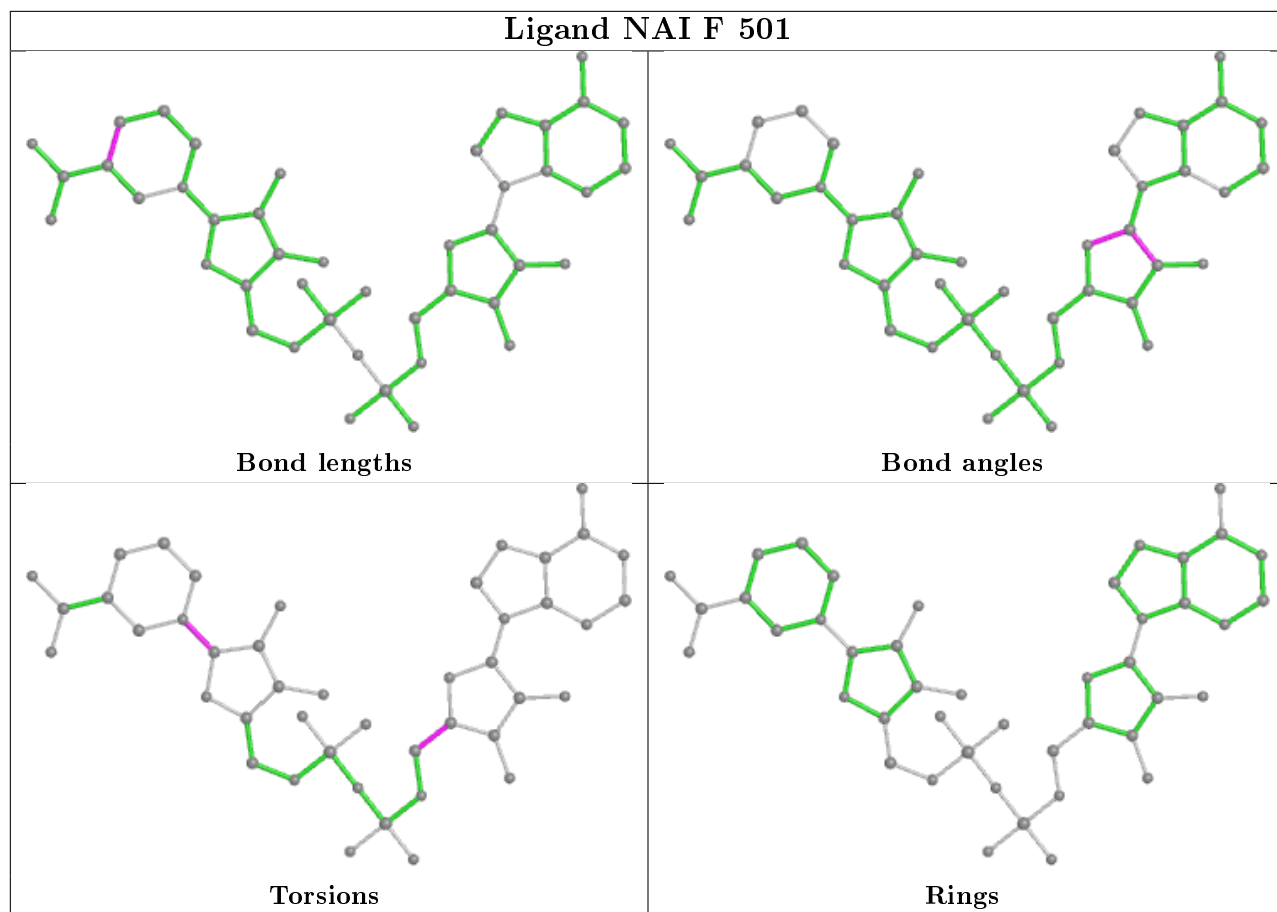


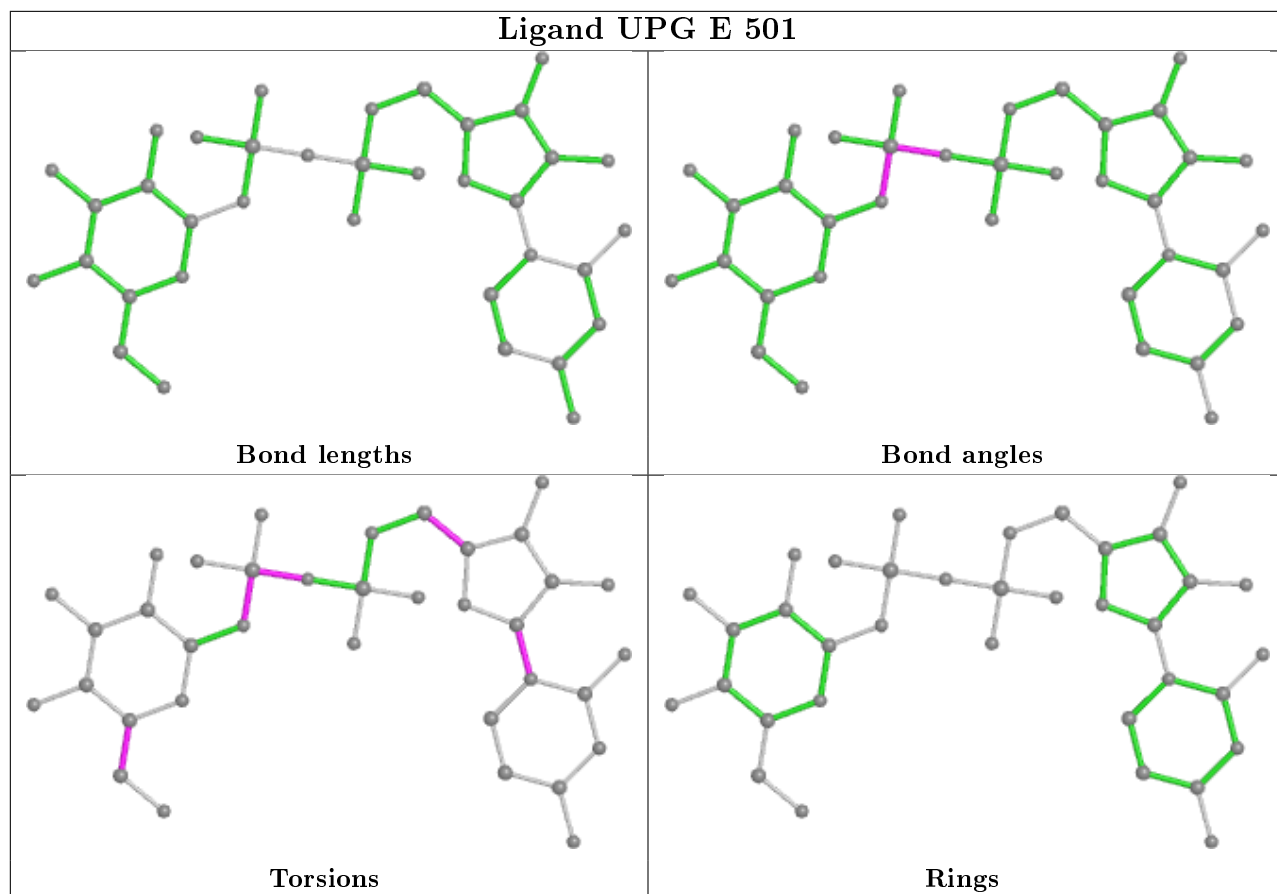


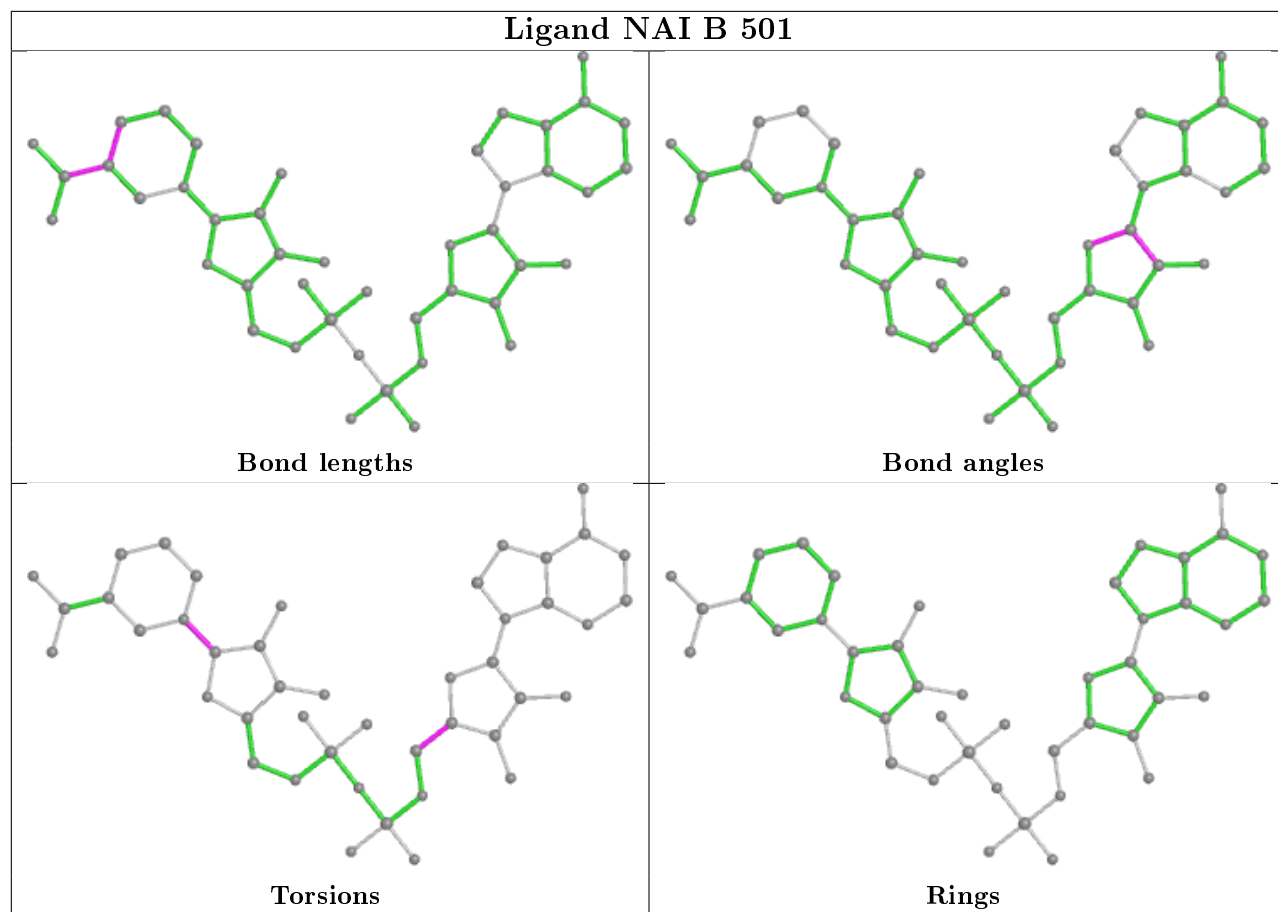


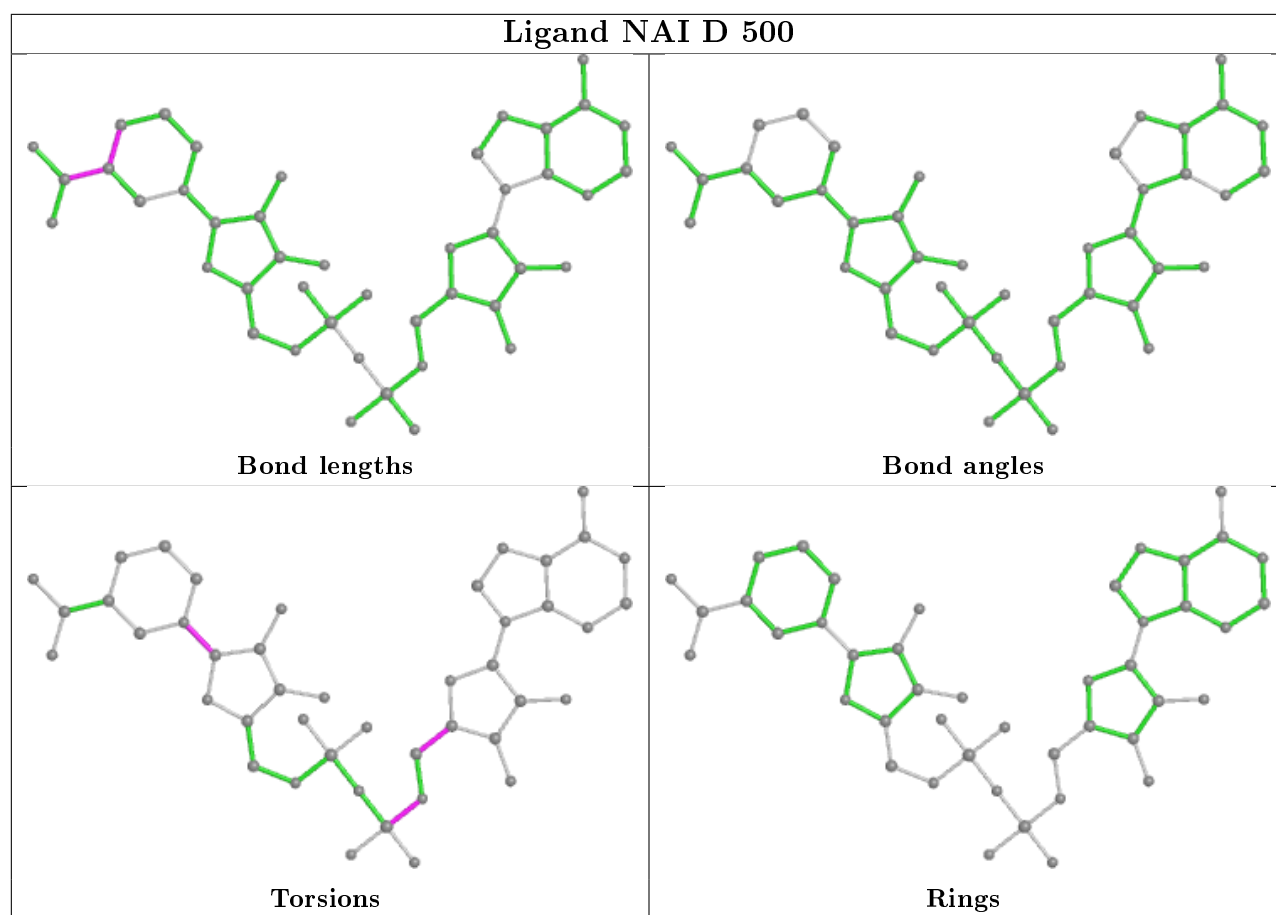












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	459/494 (92%)	0.04	10 (2%) 62 69	38, 66, 107, 141	0
1	B	459/494 (92%)	-0.17	3 (0%) 87 91	38, 63, 98, 136	0
1	C	459/494 (92%)	0.04	3 (0%) 87 91	42, 62, 96, 123	0
1	D	459/494 (92%)	0.13	11 (2%) 59 66	43, 70, 113, 138	0
1	E	456/494 (92%)	0.36	32 (7%) 16 21	49, 83, 122, 148	0
1	F	459/494 (92%)	-0.13	1 (0%) 95 96	40, 54, 79, 132	0
All	All	2751/2964 (92%)	0.04	60 (2%) 62 69	38, 65, 110, 148	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	14	TYR	4.8
1	E	367	TYR	4.4
1	E	432	MET	4.2
1	A	4	ILE	4.0
1	E	454	THR	3.8
1	E	53	TYR	3.7
1	E	407	GLY	3.6
1	E	401	PRO	3.4
1	E	430	LYS	3.4
1	E	59	GLU	3.3
1	A	183	ASP	3.3
1	D	431	LYS	3.2
1	D	184	GLU	3.2
1	D	399	LYS	3.1
1	E	438	ILE	2.9
1	E	431	LYS	2.9
1	D	400	ASP	2.8
1	D	382	HIS	2.8
1	E	458	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	152	LEU	2.8
1	D	427	ARG	2.7
1	E	403	GLU	2.7
1	E	427	ARG	2.6
1	C	184	GLU	2.6
1	E	411	VAL	2.6
1	E	456	GLY	2.5
1	E	457	PHE	2.5
1	E	436	ALA	2.5
1	E	406	ASP	2.5
1	A	190	ARG	2.5
1	E	435	PRO	2.5
1	A	123	TYR	2.4
1	C	430	LYS	2.4
1	E	184	GLU	2.4
1	A	182	GLY	2.4
1	E	12	ALA	2.4
1	A	184	GLU	2.4
1	A	187	GLU	2.3
1	E	60	VAL	2.3
1	D	402	TYR	2.3
1	D	341	ASP	2.2
1	E	402	TYR	2.2
1	E	400	ASP	2.2
1	A	156	VAL	2.2
1	E	332	ALA	2.2
1	A	140	ILE	2.2
1	D	370	LYS	2.2
1	E	67	LYS	2.2
1	B	392	SER	2.2
1	E	28	PRO	2.2
1	E	425	TYR	2.1
1	F	66	GLY	2.1
1	E	39	GLU	2.1
1	D	448	LEU	2.1
1	E	333	ILE	2.1
1	B	39	GLU	2.0
1	C	431	LYS	2.0
1	E	74	ASN	2.0
1	B	184	GLU	2.0
1	D	397	ILE	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](#)

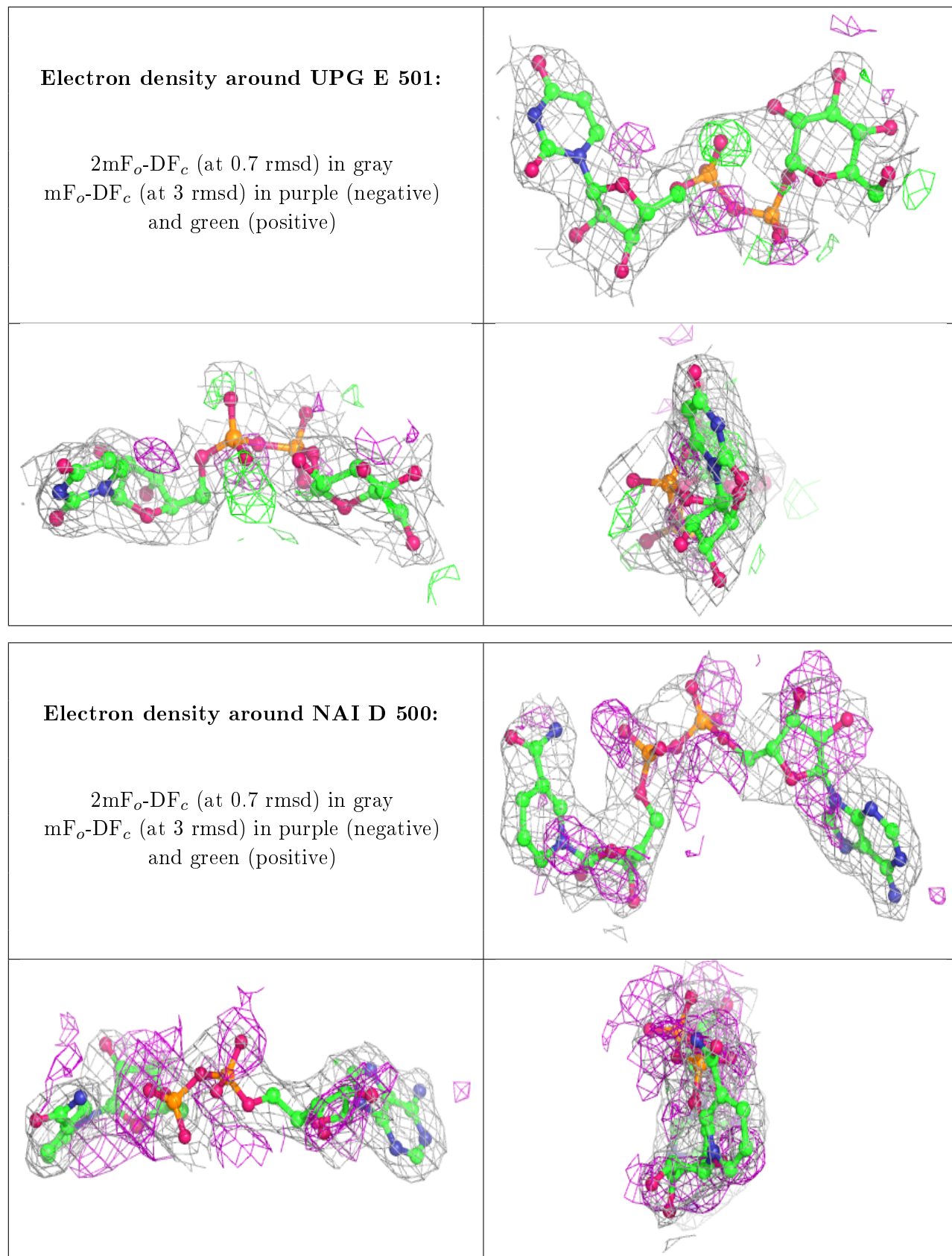
There are no carbohydrates in this entry.

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, 95th 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.

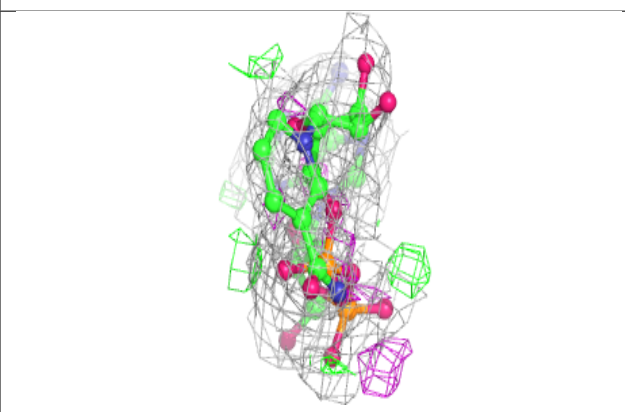
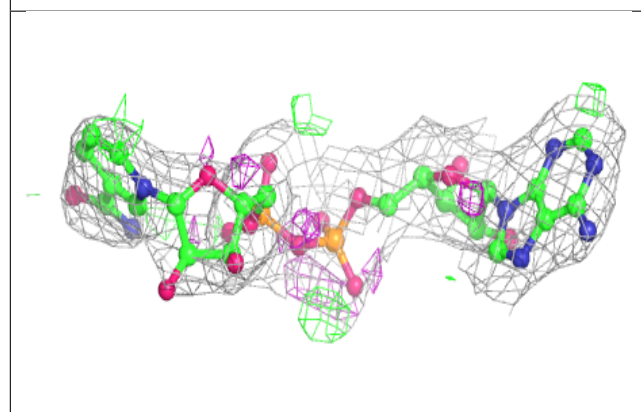
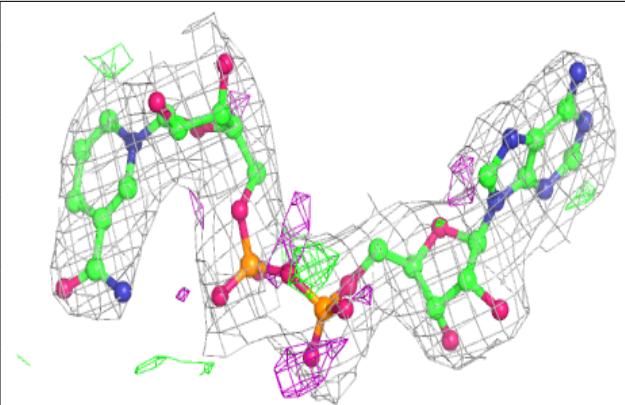
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DMS	C	503	4/4	0.88	0.30	105,107,107,109	0
3	UPG	E	501	36/36	0.90	0.15	71,84,94,95	0
2	NAI	D	500	44/44	0.90	0.19	61,67,80,85	0
2	NAI	E	500	44/44	0.91	0.13	83,90,96,100	0
4	DMS	F	503	4/4	0.93	0.20	91,94,94,95	0
3	UPG	D	501	36/36	0.94	0.14	49,59,64,67	0
4	DMS	B	503	4/4	0.94	0.17	106,106,108,108	0
4	DMS	A	503	4/4	0.95	0.13	97,98,99,100	0
2	NAI	C	501	44/44	0.96	0.13	38,49,61,63	0
2	NAI	A	501	44/44	0.96	0.16	41,56,81,82	0
2	NAI	B	501	44/44	0.97	0.12	46,57,73,75	0
3	UPG	B	502	36/36	0.97	0.13	41,46,50,54	0
3	UPG	A	502	36/36	0.98	0.15	33,44,49,52	0
3	UPG	F	502	36/36	0.98	0.13	38,43,49,50	0
3	UPG	C	502	36/36	0.98	0.13	38,44,53,55	0
2	NAI	F	501	44/44	0.98	0.14	35,40,50,51	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.

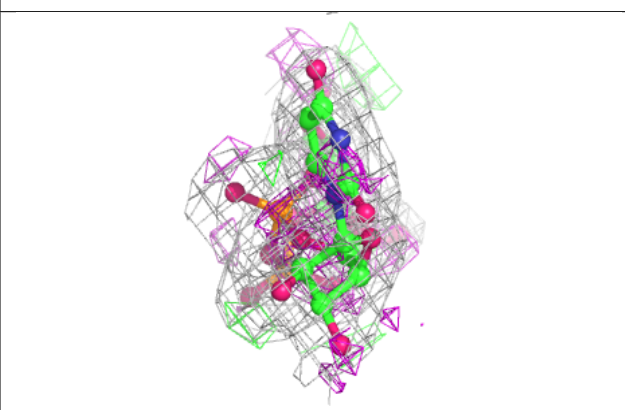
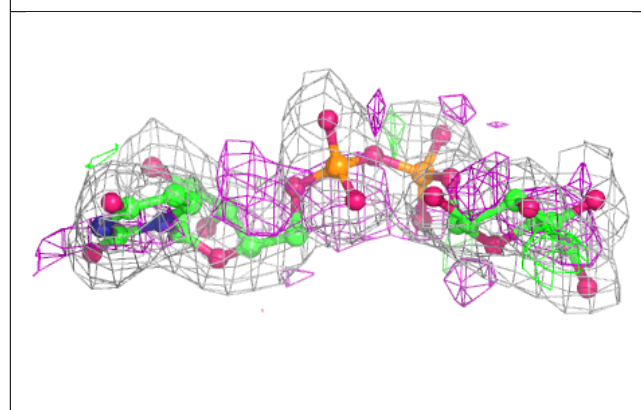
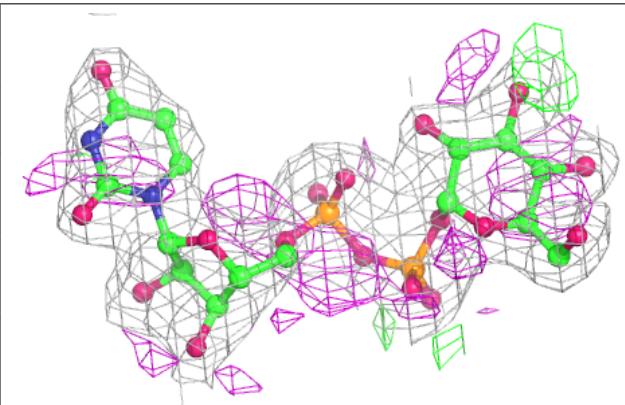


Electron density around NAI E 500:

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

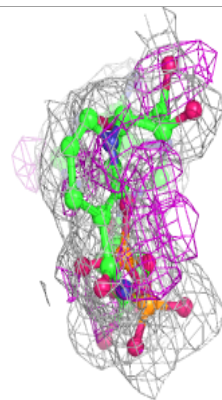
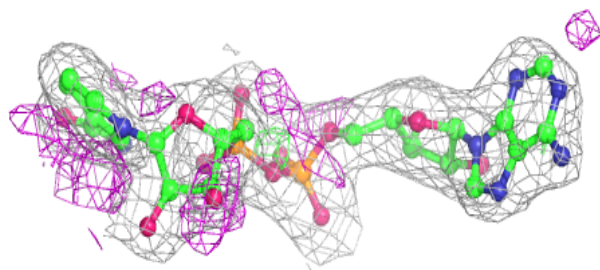
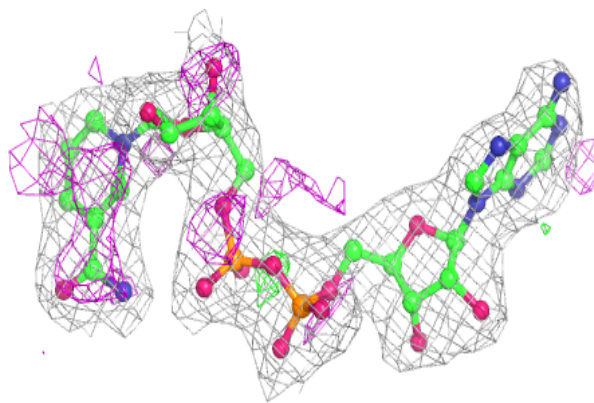
**Electron density around UPG D 501:**

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

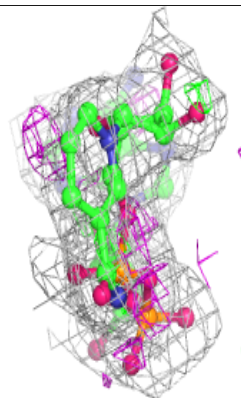
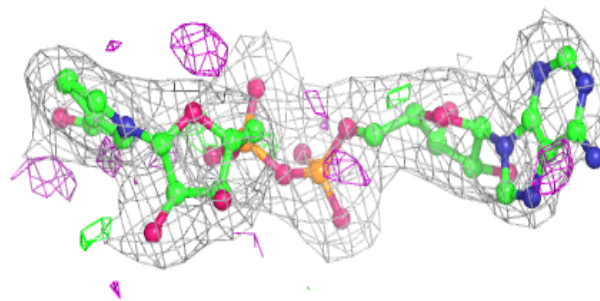
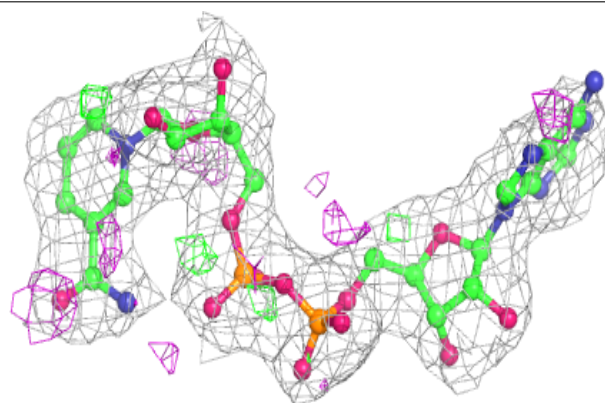


Electron density around NAI C 501:

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

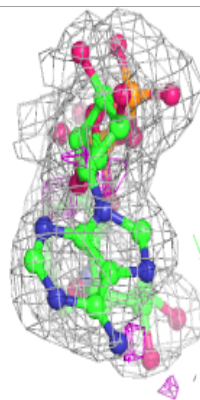
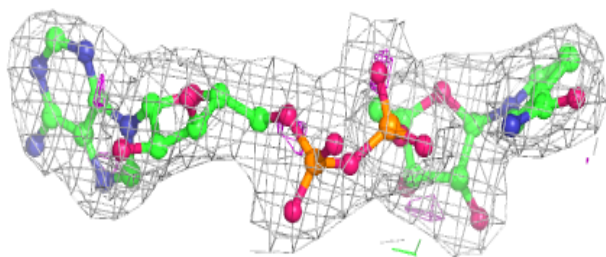
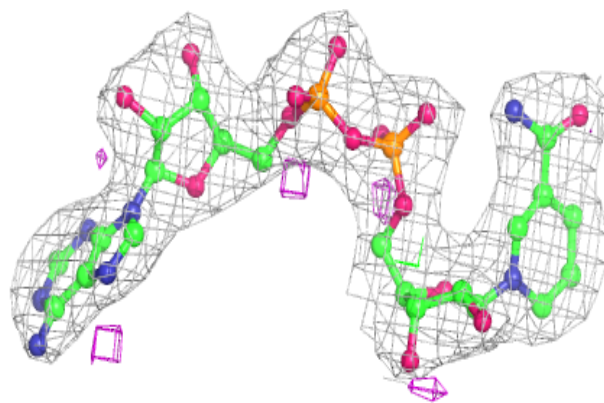
**Electron density around NAI A 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

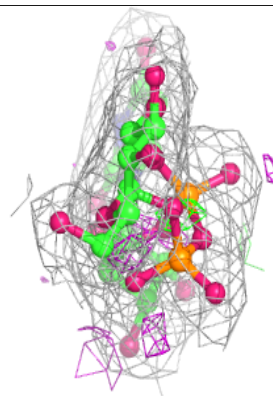
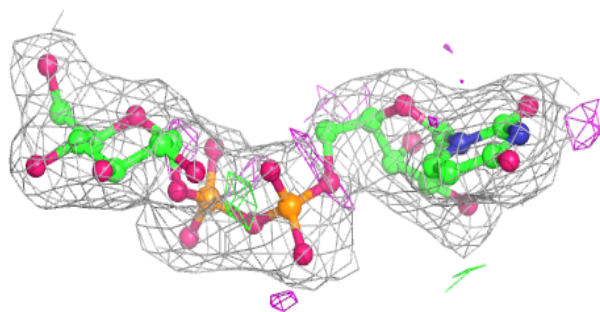
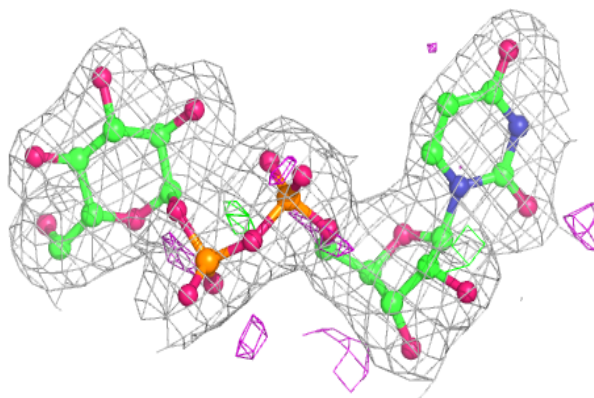


Electron density around NAI B 501:

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

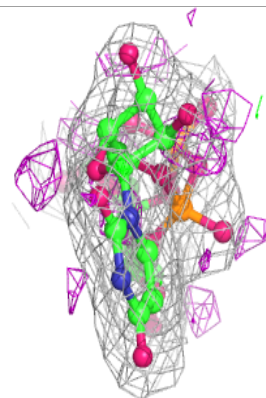
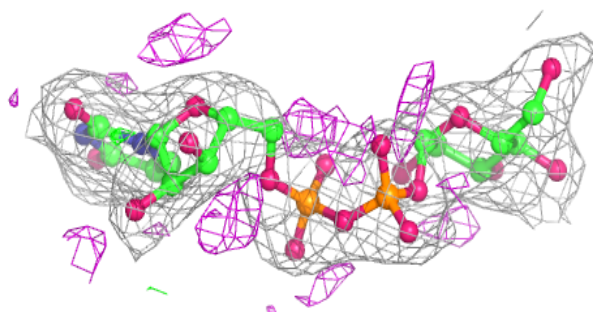
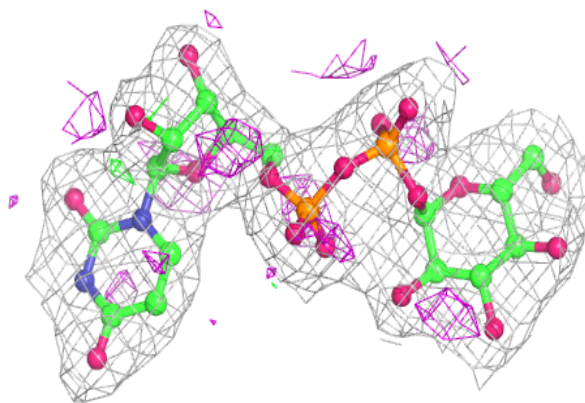
**Electron density around UPG B 502:**

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

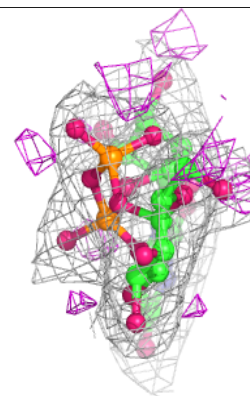
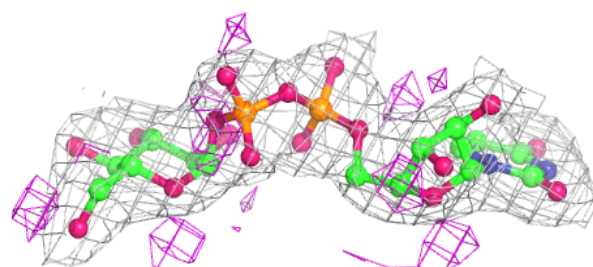
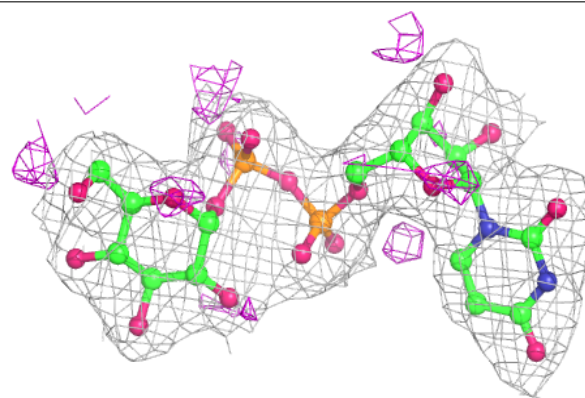


Electron density around UPG A 502:

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

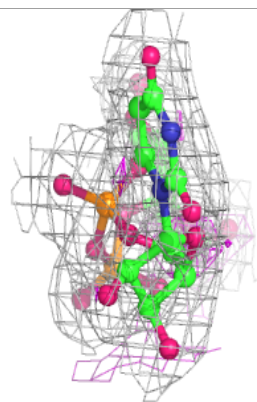
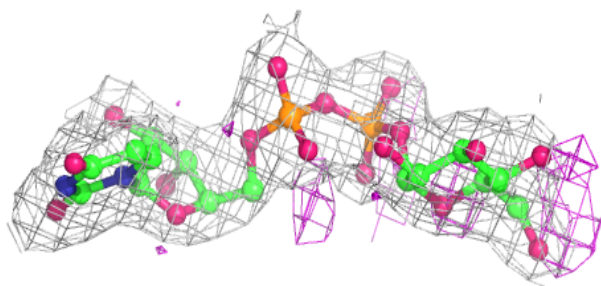
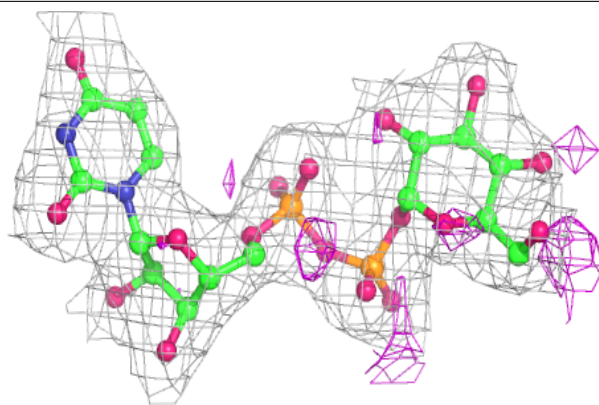
**Electron density around UPG F 502:**

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

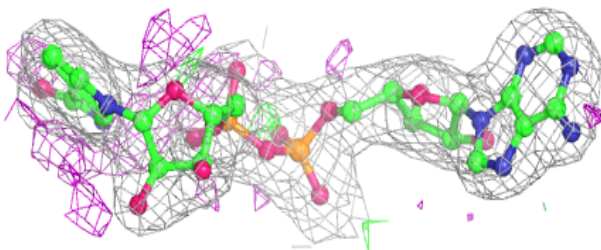
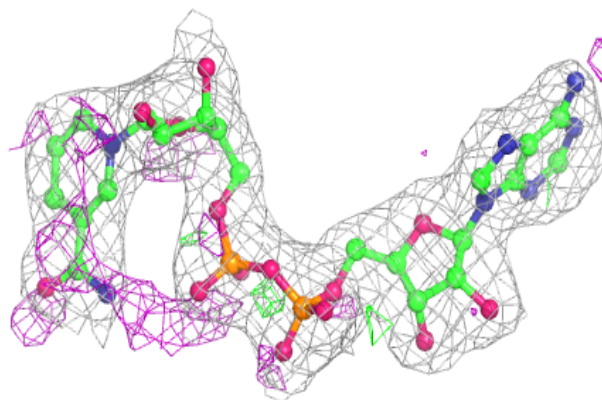


Electron density around UPG C 502:

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

**Electron density around NAI F 501:**

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



6.5 Other polymers

There are no such residues in this entry.