Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 08:31 PM EDT

PDB ID	:	6C5Z
Title	:	Human UDP-Glucose Dehydrogenase A225L substitutuion with UDP-glucose and NADH bound
Authors	:	Gross, P.G.; Sidlo, A.M.; Walsh, R.M.; Peeples, W.B.; Wood, Z.A.
Deposited on	:	2018-01-17
Resolution	:	2.95 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

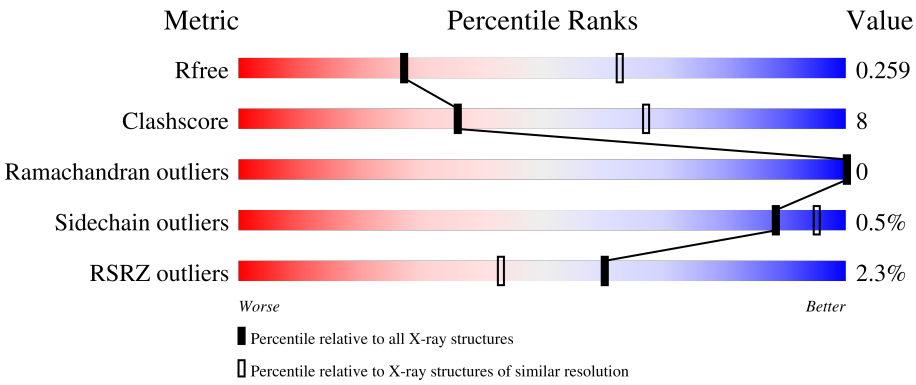
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	494	3% 79% 12% 8%
1	B	494	4% 48% 17% 35%
1	C	494	% 82% 11% 7%
1	D	494	2% 73% 19% 7%
1	E	494	2% 75% 18% 7%

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Mol	Chain	Length	Quality of chain
1	F	494	% 77% 16% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21261 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.

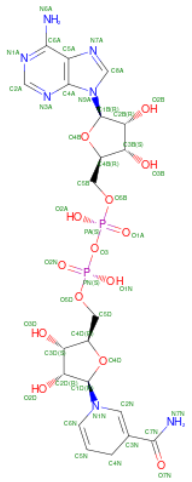
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	3562	2254	615	674	19	0	0	0
1	B	323	2568	1626	448	482	12	0	1	0
1	C	460	3609	2285	623	681	20	0	0	0
1	D	457	3589	2272	619	678	20	0	0	0
1	E	459	3602	2280	622	680	20	0	0	0
1	F	459	3601	2280	622	680	19	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	LEU	ALA	engineered mutation	UNP O60701
B	225	LEU	ALA	engineered mutation	UNP O60701
C	225	LEU	ALA	engineered mutation	UNP O60701
D	225	LEU	ALA	engineered mutation	UNP O60701
E	225	LEU	ALA	engineered mutation	UNP O60701
F	225	LEU	ALA	engineered mutation	UNP O60701

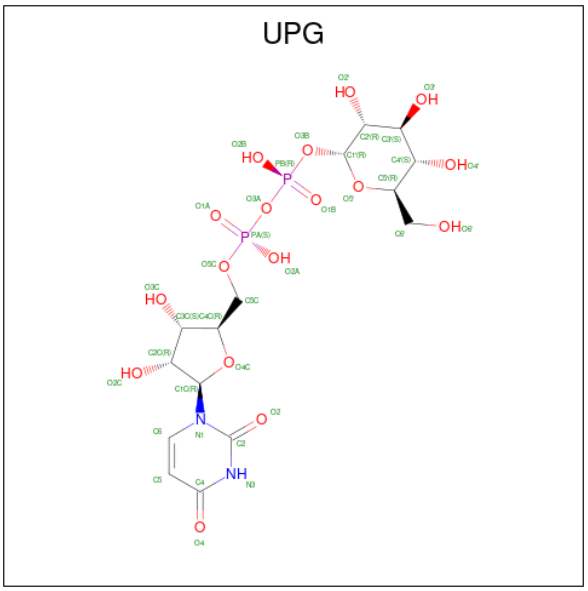
- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

NAI



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

- 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
			Total	C	N	O	P		
3	A	1	36	15	2	17	2	0	0
3	B	1	36	15	2	17	2	0	0
3	C	1	36	15	2	17	2	0	0
3	D	1	36	15	2	17	2	0	0
3	E	1	36	15	2	17	2	0	0
3	F	1	36	15	2	17	2	0	0

- Molecule 4 is water.

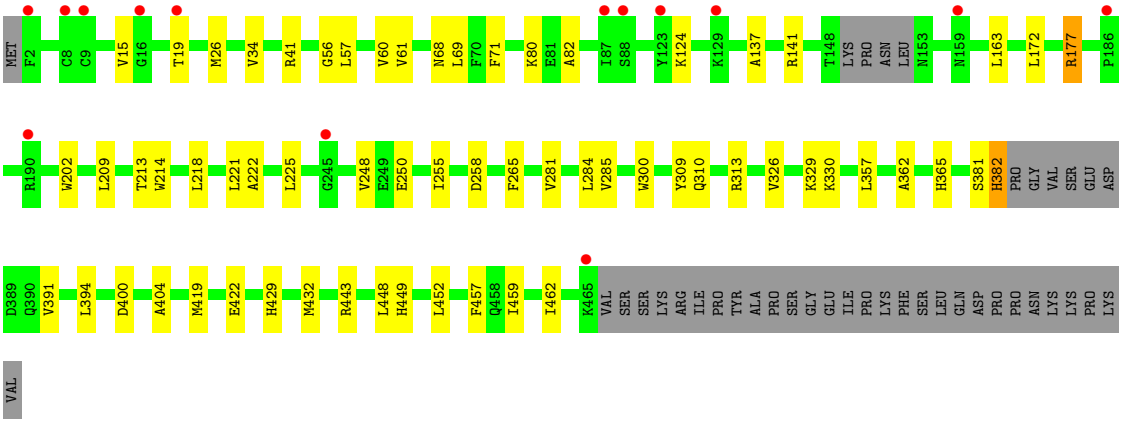
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	29	29	29	0	0
4	B	23	23	23	0	0
4	C	67	67	67	0	0
4	D	49	49	49	0	0
4	E	32	32	32	0	0
4	F	94	94	94	0	0

3 Residue-property plots (i)

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

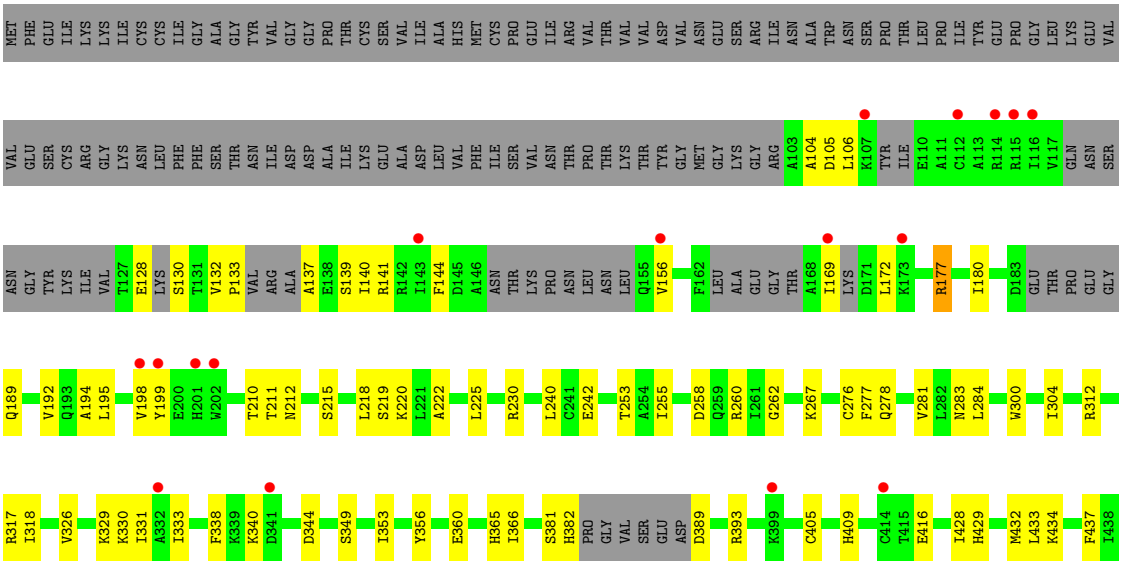
• Molecule 1: UDP-glucose 6-dehydrogenase

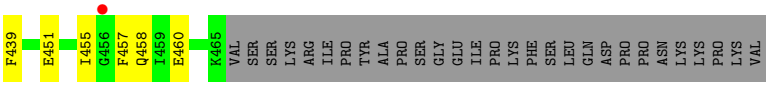
Chain A:



• Molecule 1: UDP-glucose 6-dehydrogenase

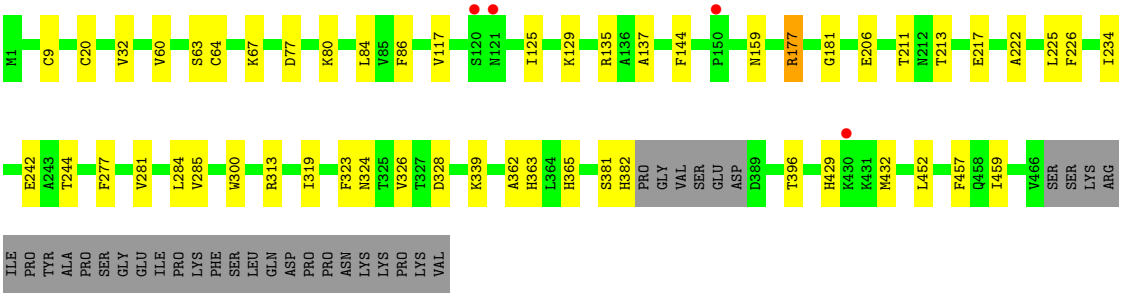
Chain B:





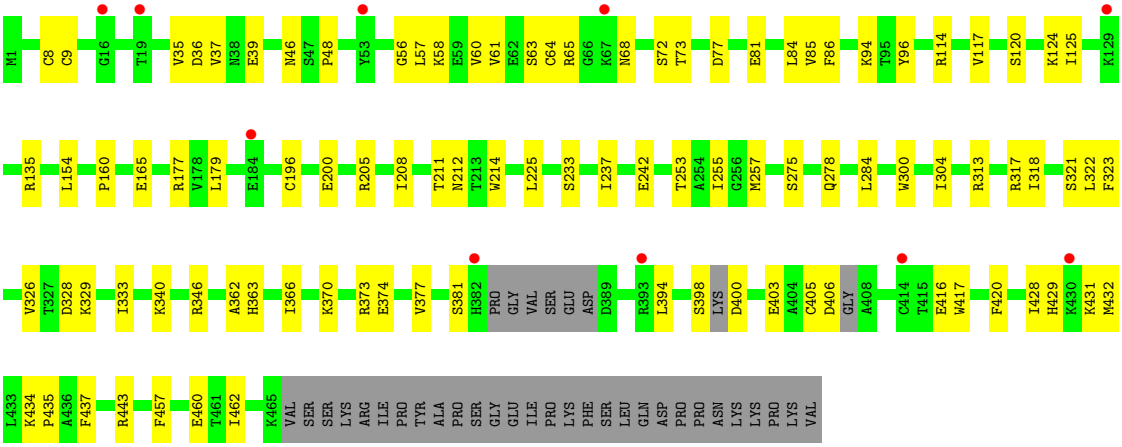
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain C:



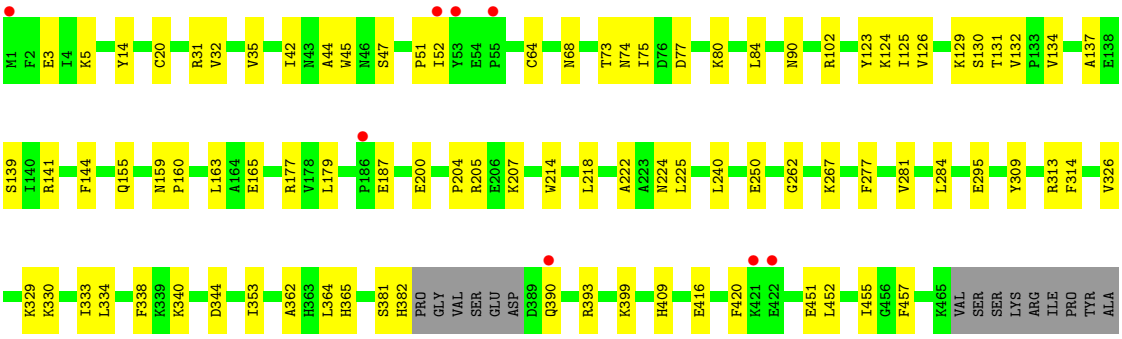
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain D:



• Molecule 1: UDP-glucose 6-dehydrogenase

Chain E:



PRO SER GLY GLU ILE PRO LYS PHE SER LEU GLN ASP PRO PRO ASN LYS LYS PRO LYS VAL

- Molecule 1: UDP-glucose 6-dehydrogenase

Chain F:

MET F2 C27 I30 V35 A44 W45 N46 S47 G56 V60 C64 R65 N68 S72 I75 L84 E110 I116 V117 S120 Y123 K124 I125 S130 V134 R135 N147 L154 Q155 N159 P160 K170 R177 G181 E187

P204 K207 T211 N212 T213 W214 S215 S216 E217 K220 L225 I255 K267 V281 L284 Y309 Q310 R313 R317 I318 I319 N324 K330 L334 D344 T345 R346 D359 E360 H365 I366 Y367 S381 H382 PRO GLY VAL SER GLU ASP D389

Q390 P401 A404 A410 E416 F420 I428 M432 F437 R443 D446 E451 L452 I455 G456 F457 Q458 I459 E460 V466 SER SER LYS ARG ILE PRO TYR ALA PRO SER GLY GLU ILE PRO LYS PHE SER LEU GLN ASP PRO PRO ASN LYS LYS PRO LYS

VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.77Å 199.80Å 200.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.06 – 2.95 30.06 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.06-2.95) 99.3 (30.06-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.203 , 0.259 0.203 , 0.259	Depositor DCC
R_{free} test set	3978 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	61.7	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21261	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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 (i)

5.1 Standard geometry (i)

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

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	0.44	0/3625	0.56	0/4902
1	B	0.41	0/2608	0.57	0/3510
1	C	0.53	0/3674	0.60	0/4970
1	D	0.48	0/3652	0.59	0/4938
1	E	0.48	0/3667	0.60	0/4960
1	F	0.56	0/3666	0.63	0/4960
All	All	0.49	0/20892	0.59	0/28240

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	3562	0	3574	57	0
1	B	2568	0	2568	65	0
1	C	3609	0	3633	38	0
1	D	3589	0	3606	66	0
1	E	3602	0	3624	70	0
1	F	3601	0	3621	55	0
2	A	44	0	27	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	44	0	27	3	0
2	D	44	0	27	0	0
2	E	44	0	27	2	0
2	F	44	0	27	2	0
3	A	36	0	22	2	0
3	B	36	0	21	4	0
3	C	36	0	22	3	0
3	D	36	0	22	0	0
3	E	36	0	22	3	0
3	F	36	0	22	2	0
4	A	29	0	0	0	0
4	B	23	0	0	0	0
4	C	67	0	0	0	0
4	D	49	0	0	1	0
4	E	32	0	0	3	0
4	F	94	0	0	1	0
All	All	21261	0	20892	335	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 8.

All (335) 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:E:340:LYS:HB3	1:E:416:GLU:HG2	1.60	0.84
1:E:14:TYR:OH	1:E:165:GLU:HA	1.75	0.84
1:A:381:SER:HB2	1:A:391:VAL:HG21	1.64	0.79
1:A:225:LEU:HD11	1:A:284:LEU:HD13	1.68	0.74
2:C:500:NAI:H4N	3:C:501:UPG:H6'1	1.69	0.74
2:E:500:NAI:H4N	3:E:501:UPG:H6'1	1.72	0.71
1:D:225:LEU:HD11	1:D:284:LEU:HD22	1.75	0.68
2:A:500:NAI:H4N	3:A:501:UPG:H6'1	1.75	0.68
1:C:323:PHE:CD1	1:E:139:SER:OG	2.47	0.67
1:F:46:ASN:HA	1:F:65:ARG:HH11	1.58	0.67
1:A:449:HIS:CD2	1:A:459:ILE:HD13	2.30	0.67
1:F:225:LEU:HD22	1:F:281:VAL:HG22	1.77	0.67
1:D:326:VAL:HG12	1:D:326:VAL:O	1.95	0.67
1:E:42:ILE:HG21	1:E:73:THR:HG23	1.77	0.67
1:D:94:LYS:NZ	1:F:360:GLU:OE1	2.28	0.66
1:A:255:ILE:HD11	1:B:222:ALA:HB1	1.77	0.65
1:F:116:ILE:O	1:F:120:SER:OG	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:HIS:HB2	1:C:457:PHE:CE2	2.32	0.65
1:A:137:ALA:HB3	1:A:213:THR:HG21	1.79	0.65
2:F:500:NAI:H4N	3:F:501:UPG:H6'1	1.79	0.65
1:F:451:GLU:O	1:F:455:ILE:HG13	1.97	0.65
1:A:381:SER:O	1:A:382:HIS:HB2	1.97	0.64
1:D:61:VAL:HG12	1:D:65:ARG:HB2	1.78	0.64
1:B:317:ARG:HH11	1:B:460:GLU:HB3	1.61	0.64
1:C:64:CYS:HA	1:C:67:LYS:HD3	1.79	0.64
1:E:14:TYR:O	1:E:14:TYR:HD1	1.81	0.63
1:F:381:SER:O	1:F:382:HIS:HB2	1.98	0.63
1:A:419:MET:HA	1:A:422:GLU:HG2	1.80	0.63
1:B:317:ARG:NH1	1:B:460:GLU:HB3	2.14	0.63
1:D:326:VAL:HG11	1:D:362:ALA:HB2	1.80	0.63
1:B:312[B]:ARG:NH1	1:B:356:TYR:HE1	1.98	0.62
1:D:225:LEU:HD13	1:D:300:TRP:CD2	2.34	0.62
1:E:14:TYR:O	1:E:14:TYR:CD1	2.52	0.62
1:D:326:VAL:CG1	1:D:362:ALA:HB2	2.29	0.62
1:A:432:MET:SD	1:A:457:PHE:HE1	2.23	0.61
1:D:340:LYS:HB3	1:D:416:GLU:HG2	1.81	0.61
1:C:323:PHE:HD1	1:E:139:SER:HG	1.46	0.61
1:E:204:PRO:HG2	1:E:207:LYS:HE2	1.82	0.61
1:C:129:LYS:HG2	1:C:159:ASN:O	2.01	0.61
1:B:278:GLN:HG3	1:B:304:ILE:HD12	1.83	0.60
1:D:278:GLN:HG3	1:D:304:ILE:HD12	1.83	0.60
1:D:84:LEU:HD12	1:D:125:ILE:O	2.02	0.60
1:F:330:LYS:HE3	1:F:365:HIS:CG	2.37	0.60
1:D:205:ARG:NH1	1:D:208:ILE:O	2.35	0.60
1:A:222:ALA:HB1	1:B:255:ILE:HD11	1.82	0.60
1:C:177:ARG:HB3	1:D:257:MET:HE2	1.83	0.60
1:E:134:VAL:HG21	1:E:218:LEU:HD13	1.85	0.59
1:A:326:VAL:HA	1:A:329:LYS:HD2	1.85	0.58
1:F:416:GLU:HG2	1:F:416:GLU:O	2.02	0.58
1:F:134:VAL:O	1:F:135:ARG:HB2	2.02	0.58
1:C:339:LYS:NZ	3:C:501:UPG:O1A	2.26	0.58
1:A:309:TYR:CZ	1:A:313:ARG:HD3	2.39	0.58
1:D:160:PRO:HG2	1:D:179:LEU:HD23	1.86	0.58
1:A:281:VAL:O	1:A:285:VAL:HG23	2.04	0.58
1:B:429:HIS:HB2	1:B:457:PHE:CE2	2.39	0.57
1:D:317:ARG:NH2	1:D:460:GLU:HB3	2.18	0.57
1:A:221:LEU:O	1:A:225:LEU:HG	2.04	0.57
1:C:326:VAL:CG1	1:C:362:ALA:HB2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:451:GLU:O	1:E:455:ILE:HG13	2.04	0.57
1:B:215:SER:O	1:B:219:SER:OG	2.15	0.57
1:F:84:LEU:HD12	1:F:125:ILE:HB	1.86	0.56
1:E:381:SER:O	1:E:382:HIS:CB	2.53	0.56
1:A:82:ALA:O	1:A:124:LYS:NZ	2.38	0.56
1:B:242:GLU:OE1	1:B:317:ARG:NH2	2.39	0.55
1:E:340:LYS:CB	1:E:416:GLU:HG2	2.35	0.55
1:A:330:LYS:HE3	1:A:365:HIS:CG	2.41	0.55
1:B:330:LYS:HE3	1:B:365:HIS:CG	2.42	0.55
1:F:124:LYS:HB2	1:F:154:LEU:HD23	1.88	0.55
1:B:381:SER:O	1:B:382:HIS:HB2	2.07	0.55
1:C:244:THR:O	1:D:135:ARG:NH1	2.37	0.55
1:A:459:ILE:HG23	1:A:459:ILE:O	2.07	0.55
1:A:255:ILE:HD11	1:B:222:ALA:CB	2.37	0.54
1:C:242:GLU:CD	1:C:313:ARG:HH12	2.11	0.54
1:C:281:VAL:O	1:C:285:VAL:HG23	2.07	0.54
1:E:137:ALA:O	1:E:141:ARG:HG3	2.08	0.54
1:B:169:ILE:HD13	1:B:172:LEU:HD12	1.90	0.53
1:A:137:ALA:CB	1:A:213:THR:HG21	2.38	0.53
1:D:48:PRO:O	1:D:58:LYS:NZ	2.38	0.53
1:B:326:VAL:HG23	1:B:331:ILE:HD11	1.90	0.53
1:F:310:GLN:OE1	1:F:313:ARG:NH2	2.35	0.53
1:E:390:GLN:HG3	1:E:393:ARG:HH21	1.74	0.53
1:B:141:ARG:NH2	1:B:156:VAL:O	2.42	0.53
1:B:225:LEU:HD11	1:B:284:LEU:HD13	1.89	0.52
1:C:84:LEU:HD12	1:C:125:ILE:HB	1.92	0.52
2:A:500:NAI:C4N	3:A:501:UPG:H6'1	2.40	0.52
1:E:74:ASN:OD1	1:E:77:ASP:HB2	2.09	0.52
1:B:312[B]:ARG:NH1	1:B:356:TYR:CE1	2.78	0.52
1:D:326:VAL:O	1:D:326:VAL:CG1	2.57	0.52
1:B:437:PHE:CD2	1:B:458:GLN:HG2	2.44	0.52
1:F:317:ARG:NH2	1:F:460:GLU:HB3	2.25	0.52
3:B:501:UPG:H6	3:B:501:UPG:H5C2	1.92	0.52
1:E:416:GLU:HG2	1:E:416:GLU:O	2.09	0.52
1:B:326:VAL:HG13	1:B:360:GLU:HB2	1.92	0.52
1:C:181:GLY:HA2	1:C:211:THR:O	2.09	0.52
1:B:326:VAL:CG2	1:B:331:ILE:HD11	2.40	0.52
1:F:211:THR:OG1	1:F:215:SER:HB2	2.10	0.52
1:C:381:SER:O	1:C:382:HIS:HB2	2.10	0.51
1:A:400:ASP:OD1	1:A:400:ASP:C	2.49	0.51
1:D:225:LEU:HB3	1:D:300:TRP:CZ3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:SER:HB3	1:D:437:PHE:CE2	2.46	0.51
1:E:129:LYS:HE3	1:E:159:ASN:O	2.11	0.51
1:E:225:LEU:HD22	1:E:281:VAL:HG22	1.92	0.51
1:B:128:GLU:O	1:B:130:SER:N	2.44	0.51
1:B:180:ILE:O	1:B:210:THR:HA	2.10	0.51
1:D:46:ASN:HA	1:D:65:ARG:HD2	1.92	0.50
1:D:405:CYS:HB3	1:D:428:ILE:HG23	1.93	0.50
1:A:250:GLU:OE1	1:B:211:THR:OG1	2.29	0.50
1:E:224:ASN:ND2	3:E:501:UPG:O6'	2.32	0.50
1:B:276:CYS:CB	3:B:501:UPG:H6'2	2.42	0.50
1:D:253:THR:O	1:D:257:MET:HG3	2.11	0.50
1:D:275:SER:HB3	1:D:346:ARG:HD2	1.94	0.50
1:A:137:ALA:HB3	1:A:213:THR:CG2	2.40	0.50
1:B:106:LEU:HD11	1:B:133:PRO:HG3	1.93	0.50
1:E:3:GLU:HG2	1:E:5:LYS:HE3	1.94	0.50
1:A:362:ALA:O	1:A:394:LEU:HD22	2.13	0.49
1:D:443:ARG:HD3	1:D:462:ILE:O	2.12	0.49
1:F:44:ALA:O	1:F:47:SER:OG	2.23	0.49
1:A:452:LEU:HD12	1:A:459:ILE:HD12	1.93	0.49
1:B:220:LYS:NZ	3:B:501:UPG:H6'1	2.27	0.49
1:C:326:VAL:HG11	1:C:362:ALA:HB2	1.94	0.49
1:A:326:VAL:HG12	1:A:362:ALA:HB2	1.94	0.49
1:B:432:MET:O	1:B:434:LYS:NZ	2.30	0.49
1:F:64:CYS:HB2	1:F:68:ASN:OD1	2.12	0.49
2:C:500:NAI:C4N	3:C:501:UPG:H6'1	2.42	0.49
1:D:417:TRP:HB2	1:D:420:PHE:CE2	2.48	0.49
1:B:277:PHE:O	1:B:281:VAL:HG23	2.13	0.48
1:B:329:LYS:HB3	1:B:409:HIS:CD2	2.48	0.48
1:E:262:GLY:HA2	4:E:620:HOH:O	2.13	0.48
1:D:56:GLY:O	1:D:60:VAL:HG23	2.13	0.48
1:A:432:MET:SD	1:A:457:PHE:CE1	3.05	0.48
1:E:381:SER:O	1:E:382:HIS:HB2	2.12	0.48
1:A:449:HIS:NE2	1:A:459:ILE:HD13	2.29	0.48
1:E:330:LYS:HE3	1:E:365:HIS:CD2	2.49	0.48
1:B:128:GLU:CD	1:B:132:VAL:HG11	2.34	0.48
1:E:329:LYS:HD3	1:E:409:HIS:ND1	2.29	0.48
1:B:326:VAL:CG1	1:B:360:GLU:CB	2.92	0.48
1:C:225:LEU:HD11	1:C:284:LEU:HD13	1.94	0.48
1:E:52:ILE:O	1:E:52:ILE:HG13	2.13	0.48
1:B:139:SER:HG	1:D:323:PHE:HD1	1.58	0.47
1:E:329:LYS:HD3	1:E:409:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:ILE:HD13	1:F:360:GLU:HG3	1.96	0.47
2:F:500:NAI:C4N	3:F:501:UPG:H6'1	2.42	0.47
1:A:381:SER:OG	1:A:382:HIS:N	2.48	0.47
2:A:500:NAI:H2D	2:A:500:NAI:H2N	1.72	0.47
1:D:362:ALA:O	1:D:394:LEU:HB3	2.15	0.47
1:E:84:LEU:HD12	1:E:125:ILE:HG22	1.97	0.47
1:E:160:PRO:HG2	1:E:179:LEU:HD23	1.96	0.47
1:F:367:TYR:CE2	1:F:401:PRO:HG3	2.50	0.47
1:F:443:ARG:HE	1:F:446:ASP:CG	2.18	0.47
1:A:163:LEU:HD23	1:A:172:LEU:HD21	1.96	0.47
1:C:429:HIS:HB2	1:C:457:PHE:CZ	2.50	0.47
1:A:443:ARG:HD3	1:A:462:ILE:O	2.15	0.46
1:C:326:VAL:HG12	1:C:326:VAL:O	2.15	0.46
1:E:102:ARG:O	4:E:601:HOH:O	2.21	0.46
1:F:160:PRO:HB3	1:F:220:LYS:HB2	1.96	0.46
1:B:104:ALA:HB2	1:B:283:ASN:OD1	2.15	0.46
1:F:56:GLY:O	1:F:60:VAL:HG23	2.15	0.46
1:A:15:VAL:O	1:A:19:THR:OG1	2.19	0.46
1:E:44:ALA:O	1:E:47:SER:OG	2.22	0.46
1:E:222:ALA:CB	1:F:255:ILE:HD11	2.45	0.46
1:F:389:ASP:OD1	1:F:390:GLN:N	2.48	0.46
1:C:225:LEU:HD23	1:C:281:VAL:HG22	1.98	0.46
1:D:435:PRO:HG2	1:D:437:PHE:CE1	2.51	0.46
1:F:170:LYS:HA	1:F:170:LYS:HD2	1.59	0.46
1:B:211:THR:HG23	1:B:212:ASN:O	2.16	0.46
1:C:20:CYS:HB3	1:C:32:VAL:HG11	1.97	0.46
1:A:429:HIS:HB2	1:A:457:PHE:CE2	2.51	0.46
1:B:140:ILE:CG2	1:B:144:PHE:CE2	2.99	0.46
1:D:57:LEU:O	1:D:61:VAL:HG23	2.16	0.46
1:E:399:LYS:HB2	1:E:399:LYS:HE3	1.65	0.46
1:E:14:TYR:HE1	1:E:163:LEU:CD1	2.29	0.46
1:D:124:LYS:HB2	1:D:154:LEU:CD2	2.46	0.45
1:E:309:TYR:CZ	1:E:313:ARG:HD3	2.51	0.45
1:D:328:ASP:HA	1:D:363:HIS:CD2	2.51	0.45
1:E:326:VAL:HG12	1:E:326:VAL:O	2.15	0.45
1:F:204:PRO:HD2	1:F:207:LYS:HD3	1.98	0.45
1:F:267:LYS:HA	1:F:267:LYS:HD3	1.78	0.45
1:B:439:PHE:HE1	1:B:460:GLU:OE1	2.00	0.45
1:D:326:VAL:HA	1:D:329:LYS:HD2	1.98	0.45
1:A:218:LEU:HD12	1:A:218:LEU:O	2.17	0.45
1:E:250:GLU:OE1	1:F:211:THR:OG1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:THR:OG1	1:F:212:ASN:N	2.50	0.45
1:B:451:GLU:O	1:B:455:ILE:HG13	2.16	0.45
1:A:448:LEU:O	1:A:452:LEU:HG	2.16	0.45
1:E:240:LEU:HD21	1:F:284:LEU:HD11	1.98	0.45
1:C:365:HIS:CD2	1:C:396:THR:HB	2.51	0.45
1:E:90:ASN:OD1	1:E:90:ASN:N	2.47	0.45
1:E:390:GLN:HG3	1:E:393:ARG:NH2	2.32	0.45
1:F:155:GLN:NE2	1:F:187:GLU:HB3	2.31	0.45
1:A:313:ARG:HH11	1:A:313:ARG:HG2	1.81	0.45
1:B:389:ASP:O	1:B:393:ARG:HG3	2.17	0.45
1:D:96:TYR:CD1	1:F:359:ASP:O	2.70	0.45
1:D:242:GLU:CD	1:D:313:ARG:HH12	2.20	0.45
1:B:194:ALA:O	1:B:198:VAL:HG23	2.16	0.45
1:D:35:VAL:HA	1:D:72:SER:O	2.17	0.45
1:D:64:CYS:HB2	1:D:68:ASN:OD1	2.17	0.45
1:E:42:ILE:CG2	1:E:73:THR:HG23	2.47	0.45
1:E:452:LEU:O	1:E:457:PHE:HB2	2.17	0.45
1:C:225:LEU:HB3	1:C:300:TRP:CZ3	2.51	0.44
1:D:8:CYS:O	1:D:85:VAL:HA	2.18	0.44
1:B:137:ALA:O	1:B:141:ARG:HG3	2.17	0.44
1:B:405:CYS:HB3	1:B:428:ILE:HG23	1.98	0.44
1:C:432:MET:SD	1:C:457:PHE:HE1	2.40	0.44
1:D:114:ARG:HA	1:D:117:VAL:HG12	2.00	0.44
1:C:9:CYS:HA	1:C:86:PHE:HB2	1.99	0.44
1:A:26:MET:HG3	1:A:202:TRP:CG	2.52	0.44
1:A:34:VAL:O	1:A:71:PHE:HA	2.18	0.44
1:B:409:HIS:NE2	1:B:433:LEU:HD12	2.33	0.44
1:C:117:VAL:HB	1:C:144:PHE:CE1	2.52	0.44
1:E:20:CYS:HB3	1:E:32:VAL:CG1	2.48	0.44
1:E:45:TRP:CE2	1:E:51:PRO:HG2	2.53	0.44
1:F:124:LYS:HB2	1:F:154:LEU:CD2	2.47	0.44
1:A:258:ASP:HB2	1:B:177:ARG:CZ	2.48	0.44
1:A:357:LEU:HA	1:A:357:LEU:HD23	1.76	0.44
1:B:230:ARG:NH2	1:B:262:GLY:O	2.51	0.44
1:B:318:ILE:HA	1:B:439:PHE:CZ	2.53	0.43
1:C:225:LEU:HD13	1:C:300:TRP:CE2	2.52	0.43
1:D:60:VAL:O	1:D:63:SER:HB3	2.17	0.43
1:D:9:CYS:HA	1:D:86:PHE:HB2	2.01	0.43
1:E:225:LEU:HD11	1:E:284:LEU:HD13	1.99	0.43
1:A:222:ALA:CB	1:B:255:ILE:HD11	2.48	0.43
1:D:39:GLU:HG3	1:D:73:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:452:LEU:CD1	1:F:459:ILE:HD12	2.48	0.43
1:B:225:LEU:HD13	1:B:300:TRP:CD2	2.54	0.43
1:D:135:ARG:HA	1:D:214:TRP:CZ3	2.53	0.43
1:E:84:LEU:HD12	1:E:125:ILE:CG2	2.49	0.43
1:E:130:SER:O	1:E:132:VAL:HG13	2.17	0.43
1:A:56:GLY:O	1:A:60:VAL:HG23	2.18	0.43
1:A:68:ASN:OD1	1:A:68:ASN:N	2.52	0.43
1:A:284:LEU:HD11	1:B:240:LEU:HD21	2.00	0.43
1:B:189:GLN:O	1:B:192:VAL:HG22	2.19	0.43
1:B:349:SER:O	1:B:353:ILE:HG12	2.17	0.43
1:C:326:VAL:HG12	1:C:362:ALA:HB2	1.99	0.43
1:E:129:LYS:HG2	1:E:159:ASN:O	2.19	0.43
1:F:330:LYS:HE2	1:F:404:ALA:O	2.18	0.43
1:A:330:LYS:HE2	1:A:404:ALA:O	2.18	0.43
2:C:500:NAI:H2N	2:C:500:NAI:H2D	1.68	0.43
1:D:36:ASP:OD1	1:D:37:VAL:N	2.51	0.43
1:F:319:ILE:HG22	1:F:324:ASN:HA	2.01	0.43
1:A:141:ARG:NH1	1:A:214:TRP:CH2	2.87	0.43
1:C:222:ALA:HB1	1:D:255:ILE:HD11	2.01	0.43
1:D:211:THR:HG23	1:D:212:ASN:O	2.18	0.43
1:A:265:PHE:CE1	1:B:260:ARG:HD2	2.54	0.43
1:D:377:VAL:O	1:D:381:SER:OG	2.34	0.43
1:E:330:LYS:HE3	1:E:365:HIS:NE2	2.34	0.43
1:C:277:PHE:HD1	1:C:277:PHE:HA	1.69	0.43
1:E:123:TYR:O	1:E:124:LYS:HG3	2.19	0.42
1:A:177:ARG:NH2	1:B:258:ASP:HB2	2.34	0.42
1:C:137:ALA:CB	1:C:213:THR:HG21	2.49	0.42
1:F:344:ASP:OD1	1:F:346:ARG:HG3	2.19	0.42
1:B:340:LYS:HB3	1:B:416:GLU:HG2	2.01	0.42
1:A:313:ARG:HG2	1:A:313:ARG:NH1	2.34	0.42
1:C:60:VAL:O	1:C:63:SER:HB3	2.18	0.42
1:D:318:ILE:O	1:D:322:LEU:HG	2.19	0.42
1:E:31:ARG:HG2	4:E:611:HOH:O	2.20	0.42
1:D:406:ASP:OD1	1:D:431:LYS:HD3	2.19	0.42
1:B:338:PHE:CE2	1:B:344:ASP:HB3	2.55	0.42
1:E:77:ASP:HA	1:E:80:LYS:HG2	2.02	0.42
1:B:218:LEU:HD12	1:B:218:LEU:HA	1.91	0.42
1:D:165:GLU:HB3	4:D:612:HOH:O	2.19	0.42
1:E:14:TYR:CZ	1:E:165:GLU:HG2	2.55	0.42
1:F:334:LEU:HB3	1:F:420:PHE:CZ	2.55	0.42
1:C:135:ARG:N	1:C:217:GLU:OE1	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2:PHE:CE1	1:F:123:TYR:CE2	3.08	0.42
1:F:432:MET:SD	1:F:457:PHE:HE1	2.42	0.42
1:C:77:ASP:HA	1:C:80:LYS:HG2	2.02	0.42
1:D:429:HIS:HB2	1:D:457:PHE:CZ	2.55	0.42
1:F:410:ALA:HA	1:F:437:PHE:O	2.20	0.42
1:A:69:LEU:HD12	1:A:69:LEU:HA	1.86	0.41
1:D:326:VAL:HG12	1:D:362:ALA:HB2	2.02	0.41
1:F:181:GLY:HA2	1:F:211:THR:O	2.20	0.41
1:C:452:LEU:HD13	1:C:459:ILE:HD13	2.01	0.41
1:F:160:PRO:CB	1:F:220:LYS:HB2	2.50	0.41
1:F:213:THR:O	1:F:217:GLU:HG3	2.20	0.41
1:A:214:TRP:CD2	1:A:214:TRP:N	2.88	0.41
1:B:338:PHE:HE2	1:B:344:ASP:HB3	1.85	0.41
1:D:432:MET:O	1:D:434:LYS:NZ	2.52	0.41
1:E:277:PHE:CE2	3:E:501:UPG:H5C2	2.56	0.41
1:E:314:PHE:HD2	1:E:353:ILE:HD12	1.85	0.41
1:D:77:ASP:O	1:D:81:GLU:HB2	2.21	0.41
1:D:196:CYS:O	1:D:200:GLU:HG3	2.20	0.41
1:D:225:LEU:HD13	1:D:300:TRP:CE3	2.56	0.41
1:D:373:ARG:HG3	1:D:374:GLU:N	2.35	0.41
1:E:14:TYR:HA	1:E:52:ILE:HD13	2.02	0.41
1:F:267:LYS:HE2	4:F:615:HOH:O	2.20	0.41
1:F:428:ILE:O	1:F:432:MET:HG3	2.19	0.41
1:F:443:ARG:NE	1:F:446:ASP:OD1	2.53	0.41
1:A:225:LEU:HB3	1:A:300:TRP:CZ3	2.56	0.41
1:B:195:LEU:HD11	1:B:199:TYR:HE2	1.85	0.41
1:C:328:ASP:HA	1:C:363:HIS:CD2	2.56	0.41
1:E:5:LYS:HD3	1:E:5:LYS:HA	1.84	0.41
1:E:295:GLU:HG2	1:F:309:TYR:CD1	2.55	0.41
1:A:248:VAL:HG12	1:A:443:ARG:NH1	2.36	0.41
1:D:313:ARG:O	1:D:317:ARG:HG3	2.21	0.41
1:F:35:VAL:HB	1:F:75:ILE:HG12	2.03	0.41
1:A:258:ASP:HB2	1:B:177:ARG:NH2	2.36	0.41
1:A:310:GLN:OE1	1:A:313:ARG:NH2	2.52	0.41
1:B:220:LYS:HZ3	3:B:501:UPG:H6'1	1.86	0.41
1:B:267:LYS:HD3	1:B:267:LYS:HA	1.89	0.41
1:B:326:VAL:CG1	1:B:360:GLU:HB2	2.51	0.41
1:B:333:ILE:HB	1:B:366:ILE:HG12	2.03	0.41
1:C:226:PHE:CZ	1:D:233:SER:HB3	2.56	0.41
1:D:120:SER:HB2	1:D:124:LYS:HE2	2.02	0.41
1:D:333:ILE:HB	1:D:366:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:SER:O	1:D:400:ASP:N	2.54	0.41
1:E:64:CYS:HB2	1:E:68:ASN:OD1	2.21	0.41
1:E:126:VAL:HG21	1:E:144:PHE:CE2	2.56	0.41
1:F:46:ASN:HA	1:F:65:ARG:NH1	2.30	0.41
1:F:317:ARG:HH21	1:F:460:GLU:HB3	1.85	0.41
1:D:237:ILE:HD13	1:D:237:ILE:HA	1.84	0.41
1:E:155:GLN:OE1	1:E:187:GLU:HB3	2.20	0.41
1:F:117:VAL:HG21	1:F:147:ASN:HB2	2.03	0.41
1:A:209:LEU:HD21	1:B:253:THR:HG22	2.03	0.40
1:A:284:LEU:HD11	1:B:240:LEU:CD2	2.51	0.40
1:C:234:ILE:HD12	1:C:234:ILE:HA	1.89	0.40
1:D:370:LYS:HA	1:D:370:LYS:HD3	1.95	0.40
1:E:131:THR:N	2:E:500:NAI:O2D	2.53	0.40
1:F:35:VAL:HA	1:F:72:SER:O	2.20	0.40
1:F:318:ILE:H	1:F:318:ILE:HG13	1.75	0.40
1:A:80:LYS:O	1:A:124:LYS:NZ	2.52	0.40
1:D:200:GLU:OE2	1:D:205:ARG:HD3	2.21	0.40
1:E:333:ILE:HG13	1:E:364:LEU:HD13	2.01	0.40
1:F:27:CYS:HB3	1:F:30:ILE:HD12	2.03	0.40
1:E:141:ARG:NH1	1:E:214:TRP:CH2	2.90	0.40
1:E:222:ALA:HB3	1:F:255:ILE:HD11	2.02	0.40
1:C:319:ILE:HG22	1:C:324:ASN:HA	2.04	0.40
1:D:400:ASP:O	1:D:403:GLU:HG2	2.20	0.40
1:E:35:VAL:HB	1:E:75:ILE:HG12	2.04	0.40
1:E:326:VAL:HG12	1:E:362:ALA:HB2	2.03	0.40
1:E:338:PHE:HE1	1:E:344:ASP:HB3	1.85	0.40
1:A:57:LEU:O	1:A:61:VAL:HG23	2.22	0.40
1:E:200:GLU:CD	1:E:205:ARG:HD3	2.42	0.40
1:E:267:LYS:HA	1:E:267:LYS:HD3	1.92	0.40
1:E:334:LEU:HB3	1:E:420:PHE:CZ	2.57	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	448/494 (91%)	429 (96%)	19 (4%)	0	100	100
1	B	304/494 (62%)	294 (97%)	10 (3%)	0	100	100
1	C	456/494 (92%)	436 (96%)	20 (4%)	0	100	100
1	D	449/494 (91%)	427 (95%)	22 (5%)	0	100	100
1	E	455/494 (92%)	433 (95%)	22 (5%)	0	100	100
1	F	455/494 (92%)	442 (97%)	13 (3%)	0	100	100
All	All	2567/2964 (87%)	2461 (96%)	106 (4%)	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	390/427 (91%)	387 (99%)	3 (1%)	81	92
1	B	279/427 (65%)	277 (99%)	2 (1%)	84	93
1	C	396/427 (93%)	394 (100%)	2 (0%)	88	95
1	D	394/427 (92%)	393 (100%)	1 (0%)	92	97
1	E	395/427 (92%)	394 (100%)	1 (0%)	92	97
1	F	395/427 (92%)	392 (99%)	3 (1%)	81	92
All	All	2249/2562 (88%)	2237 (100%)	12 (0%)	88	95

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

Mol	Chain	Res	Type
1	A	41	ARG
1	A	177	ARG
1	A	382	HIS
1	B	105	ASP

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Mol	Chain	Res	Type
1	B	177	ARG
1	C	177	ARG
1	C	206	GLU
1	D	177	ARG
1	E	177	ARG
1	F	110	GLU
1	F	177	ARG
1	F	284	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	193	GLN
1	A	449	HIS
1	C	365	HIS
1	C	449	HIS
1	C	450	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 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	D	500	-	42,48,48	0.92	2 (4%)	47,73,73	0.90	1 (2%)
3	UPG	C	501	-	35,38,38	0.89	1 (2%)	53,58,58	1.26	4 (7%)
3	UPG	B	501	1	35,38,38	0.88	1 (2%)	53,58,58	1.29	4 (7%)
3	UPG	A	501	-	35,38,38	0.90	1 (2%)	53,58,58	1.28	4 (7%)
3	UPG	D	501	-	35,38,38	0.91	1 (2%)	53,58,58	1.27	4 (7%)
2	NAI	A	500	-	42,48,48	0.92	2 (4%)	47,73,73	0.86	1 (2%)
2	NAI	C	500	-	42,48,48	0.93	2 (4%)	47,73,73	0.89	1 (2%)
3	UPG	E	501	-	35,38,38	0.91	1 (2%)	53,58,58	1.23	4 (7%)
3	UPG	F	501	-	35,38,38	0.89	1 (2%)	53,58,58	1.26	4 (7%)
2	NAI	E	500	-	42,48,48	0.92	2 (4%)	47,73,73	0.95	1 (2%)
2	NAI	F	500	-	42,48,48	0.92	2 (4%)	47,73,73	0.90	1 (2%)

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	D	500	-	-	9/25/72/72	0/5/5/5
3	UPG	C	501	-	-	1/23/59/59	0/3/3/3
3	UPG	B	501	1	-	5/23/59/59	0/3/3/3
3	UPG	A	501	-	-	4/23/59/59	0/3/3/3
3	UPG	D	501	-	-	3/23/59/59	0/3/3/3
2	NAI	A	500	-	-	14/25/72/72	0/5/5/5
2	NAI	C	500	-	-	11/25/72/72	0/5/5/5
3	UPG	E	501	-	-	0/23/59/59	0/3/3/3
3	UPG	F	501	-	-	3/23/59/59	0/3/3/3
2	NAI	E	500	-	-	13/25/72/72	0/5/5/5
2	NAI	F	500	-	-	6/25/72/72	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	NAI	C4N-C3N	-2.61	1.44	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	UPG	C4-N3	-2.60	1.33	1.38
2	A	500	NAI	C4N-C3N	-2.59	1.44	1.49
2	C	500	NAI	C4N-C3N	-2.58	1.44	1.49
2	D	500	NAI	C4N-C3N	-2.56	1.44	1.49
3	D	501	UPG	C4-N3	-2.56	1.34	1.38
2	F	500	NAI	C4N-C3N	-2.53	1.45	1.49
3	C	501	UPG	C4-N3	-2.51	1.34	1.38
3	B	501	UPG	C4-N3	-2.50	1.34	1.38
3	F	501	UPG	C4-N3	-2.49	1.34	1.38
3	E	501	UPG	C4-N3	-2.47	1.34	1.38
2	C	500	NAI	C7N-C3N	2.24	1.53	1.48
2	E	500	NAI	C7N-C3N	2.24	1.53	1.48
2	F	500	NAI	C7N-C3N	2.15	1.53	1.48
2	A	500	NAI	C7N-C3N	2.13	1.53	1.48
2	D	500	NAI	C7N-C3N	2.10	1.53	1.48

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	501	UPG	C4-N3-C2	-5.08	119.88	126.58
3	A	501	UPG	C4-N3-C2	-5.06	119.91	126.58
3	F	501	UPG	C4-N3-C2	-4.96	120.03	126.58
3	E	501	UPG	C4-N3-C2	-4.95	120.05	126.58
3	C	501	UPG	C4-N3-C2	-4.90	120.11	126.58
3	B	501	UPG	C4-N3-C2	-4.88	120.14	126.58
3	D	501	UPG	C5-C4-N3	4.53	121.62	114.84
3	F	501	UPG	C5-C4-N3	4.53	121.61	114.84
3	C	501	UPG	C5-C4-N3	4.51	121.59	114.84
3	B	501	UPG	C5-C4-N3	4.49	121.56	114.84
3	E	501	UPG	C5-C4-N3	4.49	121.56	114.84
3	A	501	UPG	C5-C4-N3	4.37	121.37	114.84
2	E	500	NAI	O4B-C1B-C2B	-2.96	102.59	106.93
2	F	500	NAI	O4B-C1B-C2B	-2.86	102.75	106.93
2	D	500	NAI	O4B-C1B-C2B	-2.71	102.96	106.93
3	A	501	UPG	N3-C2-N1	2.65	118.40	114.89
2	C	500	NAI	O4B-C1B-C2B	-2.61	103.11	106.93
3	D	501	UPG	N3-C2-N1	2.55	118.28	114.89
3	E	501	UPG	N3-C2-N1	2.49	118.20	114.89
3	B	501	UPG	N3-C2-N1	2.44	118.13	114.89
3	A	501	UPG	O4-C4-N3	-2.42	115.75	119.31
3	F	501	UPG	N3-C2-N1	2.40	118.08	114.89
3	C	501	UPG	N3-C2-N1	2.38	118.05	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	501	UPG	O4-C4-N3	-2.33	115.88	119.31
3	B	501	UPG	O4-C4-N3	-2.33	115.89	119.31
2	A	500	NAI	O4B-C1B-C2B	-2.32	103.53	106.93
3	C	501	UPG	O4-C4-N3	-2.31	115.91	119.31
3	E	501	UPG	O4-C4-N3	-2.29	115.94	119.31
3	D	501	UPG	O4-C4-N3	-2.29	115.95	119.31

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	NAI	C5B-O5B-PA-O1A
2	A	500	NAI	O4B-C4B-C5B-O5B
2	A	500	NAI	C5D-O5D-PN-O2N
2	C	500	NAI	C5D-O5D-PN-O2N
2	D	500	NAI	C5B-O5B-PA-O1A
2	E	500	NAI	C5B-O5B-PA-O1A
2	E	500	NAI	C5D-O5D-PN-O3
2	E	500	NAI	O4D-C4D-C5D-O5D
2	E	500	NAI	C3D-C4D-C5D-O5D
3	A	501	UPG	C5C-O5C-PA-O3A
3	A	501	UPG	PA-O3A-PB-O3B
3	B	501	UPG	C5C-O5C-PA-O1A
3	B	501	UPG	C5C-O5C-PA-O2A
3	B	501	UPG	C5C-O5C-PA-O3A
3	B	501	UPG	C1'-O3B-PB-O3A
3	C	501	UPG	PA-O3A-PB-O3B
3	D	501	UPG	PA-O3A-PB-O3B
3	F	501	UPG	PA-O3A-PB-O3B
2	A	500	NAI	C3B-C4B-C5B-O5B
2	C	500	NAI	O4B-C4B-C5B-O5B
2	C	500	NAI	C3B-C4B-C5B-O5B
2	D	500	NAI	O4B-C4B-C5B-O5B
2	D	500	NAI	C3B-C4B-C5B-O5B
2	E	500	NAI	O4D-C1D-N1N-C6N
2	C	500	NAI	C2D-C1D-N1N-C6N
2	C	500	NAI	C2D-C1D-N1N-C2N
2	A	500	NAI	O4D-C4D-C5D-O5D
2	C	500	NAI	O4D-C4D-C5D-O5D
2	A	500	NAI	C2D-C1D-N1N-C2N
2	A	500	NAI	C2D-C1D-N1N-C6N
3	D	501	UPG	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
2	D	500	NAI	C2D-C1D-N1N-C6N
2	F	500	NAI	C2D-C1D-N1N-C6N
2	E	500	NAI	PN-O3-PA-O5B
2	C	500	NAI	O4D-C1D-N1N-C6N
2	A	500	NAI	C3D-C4D-C5D-O5D
2	C	500	NAI	O4D-C1D-N1N-C2N
2	F	500	NAI	O4D-C1D-N1N-C6N
2	A	500	NAI	C5B-O5B-PA-O3
2	A	500	NAI	C5D-O5D-PN-O3
2	C	500	NAI	C5D-O5D-PN-O3
2	D	500	NAI	C5B-O5B-PA-O3
2	E	500	NAI	C5B-O5B-PA-O3
2	A	500	NAI	O4D-C1D-N1N-C6N
2	A	500	NAI	C5B-O5B-PA-O2A
2	A	500	NAI	C5D-O5D-PN-O1N
2	C	500	NAI	C5D-O5D-PN-O1N
2	D	500	NAI	C5B-O5B-PA-O2A
2	E	500	NAI	C5B-O5B-PA-O2A
3	A	501	UPG	C5C-O5C-PA-O1A
3	A	501	UPG	C5C-O5C-PA-O2A
2	C	500	NAI	C3D-C4D-C5D-O5D
2	D	500	NAI	O4D-C1D-N1N-C6N
2	D	500	NAI	C2D-C1D-N1N-C2N
2	F	500	NAI	C2D-C1D-N1N-C2N
3	D	501	UPG	O5'-C5'-C6'-O6'
2	A	500	NAI	O4D-C1D-N1N-C2N
2	E	500	NAI	C4B-C5B-O5B-PA
2	F	500	NAI	O4D-C1D-N1N-C2N
2	D	500	NAI	O4D-C1D-N1N-C2N
2	F	500	NAI	O4B-C4B-C5B-O5B
2	E	500	NAI	PA-O3-PN-O1N
3	F	501	UPG	C1'-O3B-PB-O3A
3	F	501	UPG	C2'-C1'-O3B-PB
2	E	500	NAI	C5D-O5D-PN-O1N
2	E	500	NAI	C5D-O5D-PN-O2N
2	F	500	NAI	C2N-C3N-C7N-N7N
2	E	500	NAI	O4B-C4B-C5B-O5B
3	B	501	UPG	O4C-C4C-C5C-O5C

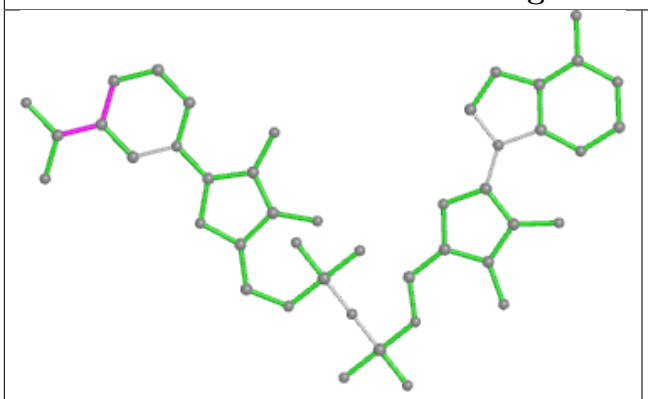
There are no ring outliers.

9 monomers are involved in 17 short contacts:

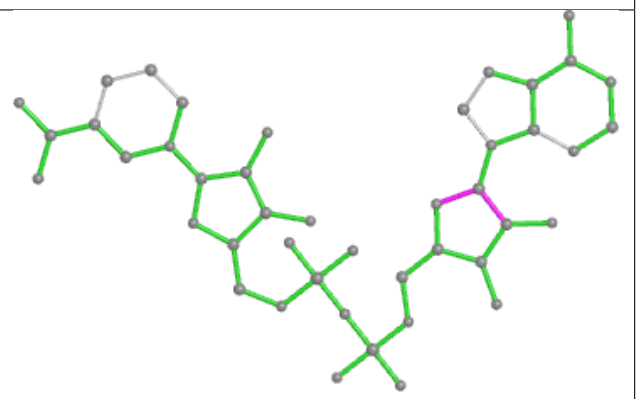
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	UPG	3	0
3	B	501	UPG	4	0
3	A	501	UPG	2	0
2	A	500	NAI	3	0
2	C	500	NAI	3	0
3	E	501	UPG	3	0
3	F	501	UPG	2	0
2	E	500	NAI	2	0
2	F	500	NAI	2	0

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.

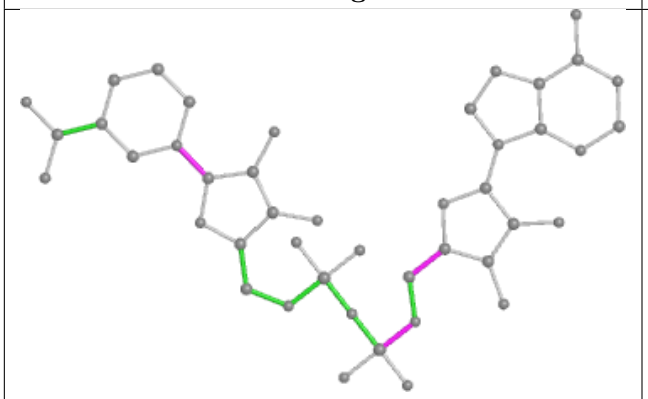
Ligand NAI D 500



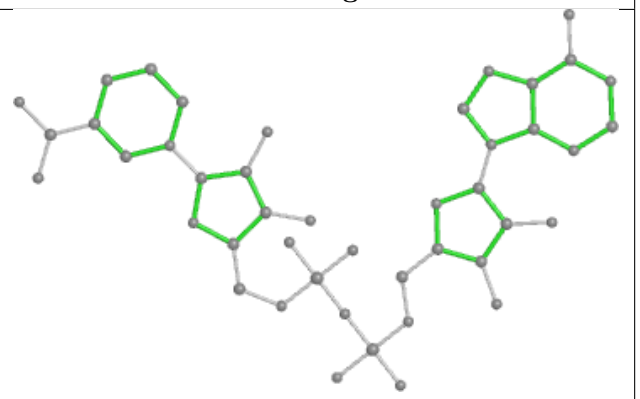
Bond lengths



Bond angles

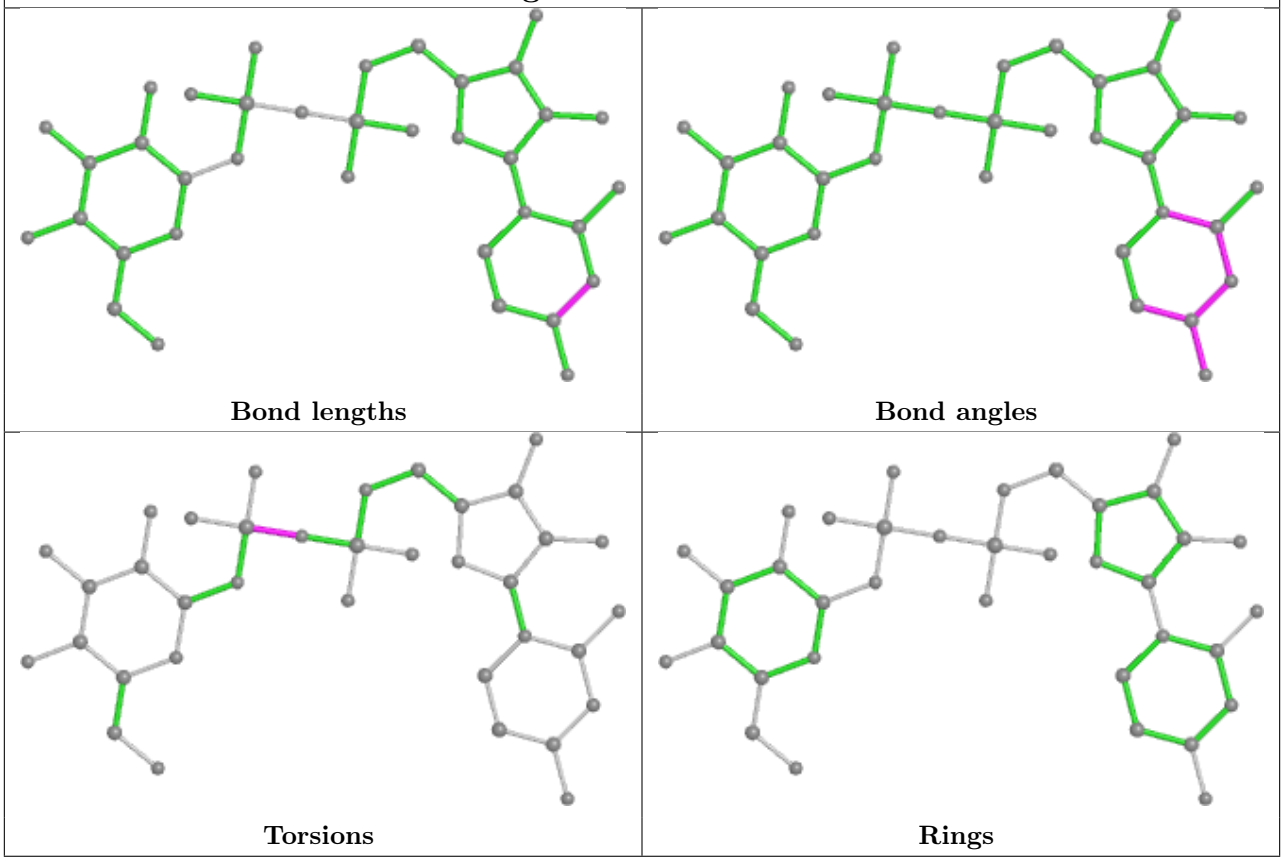


Torsions

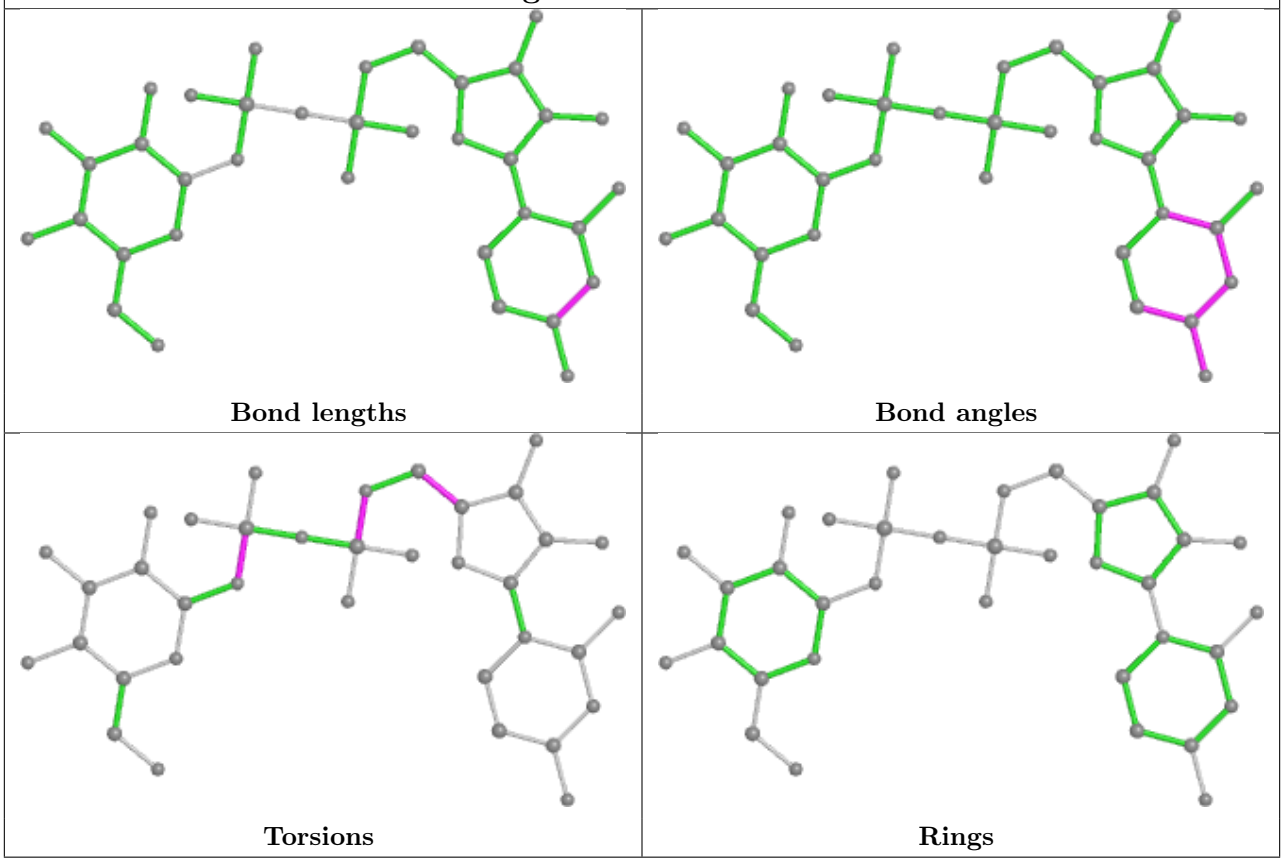


Rings

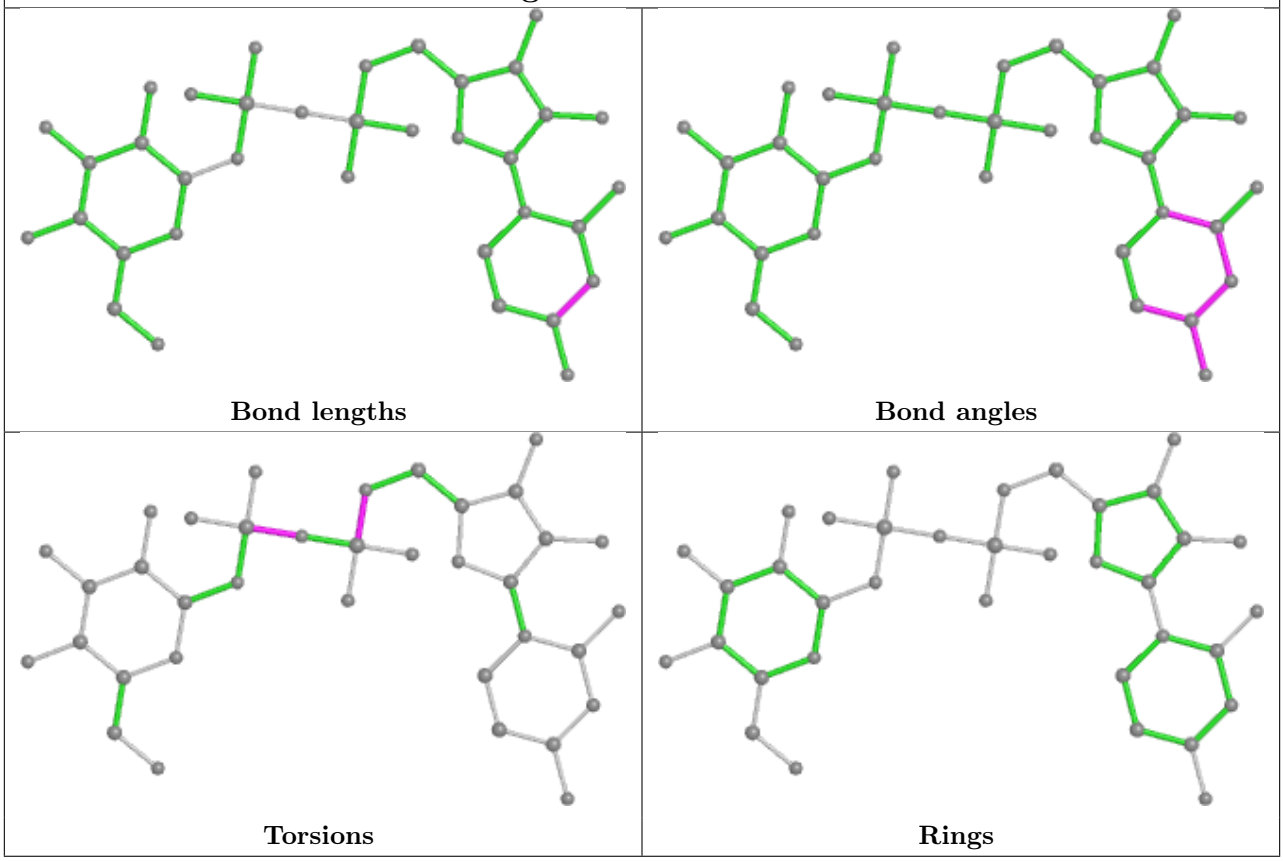
Ligand UPG C 501



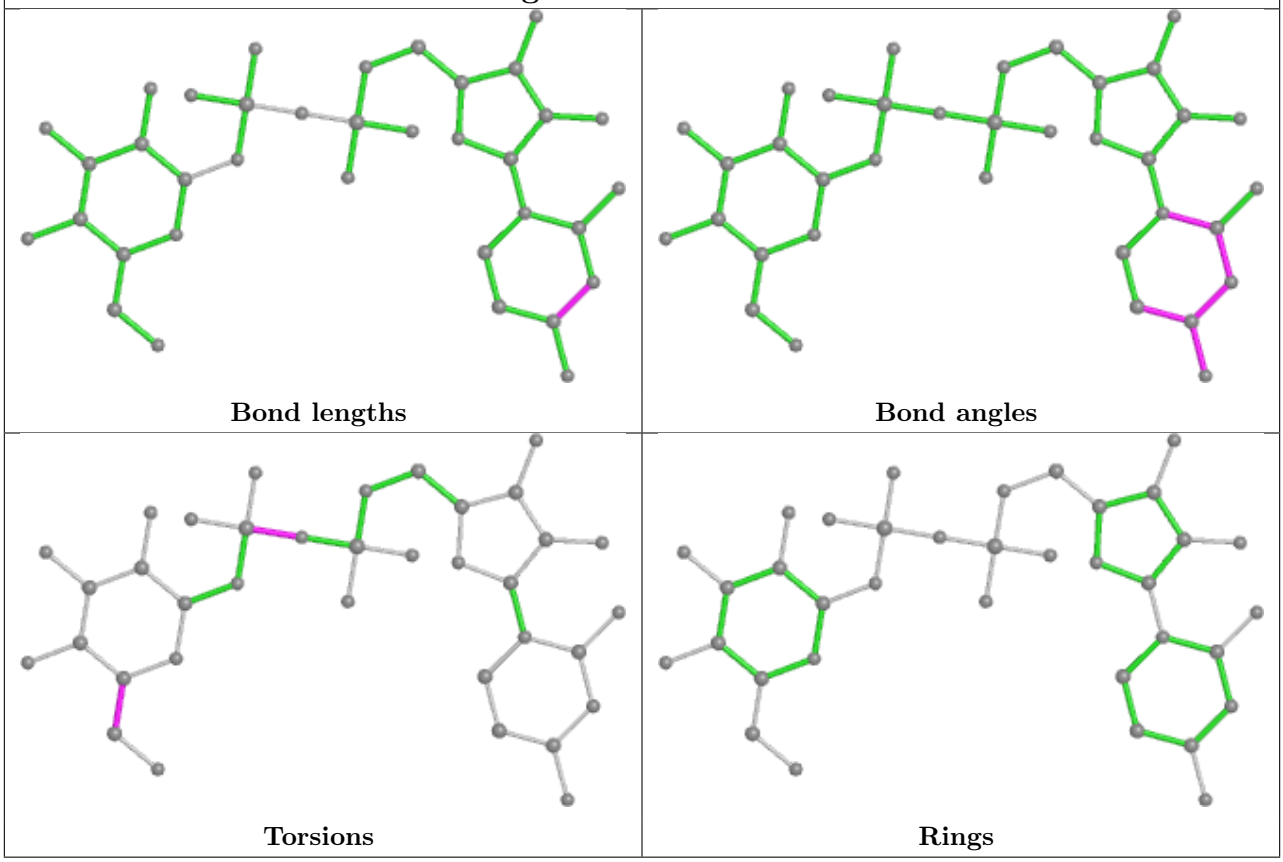
Ligand UPG B 501



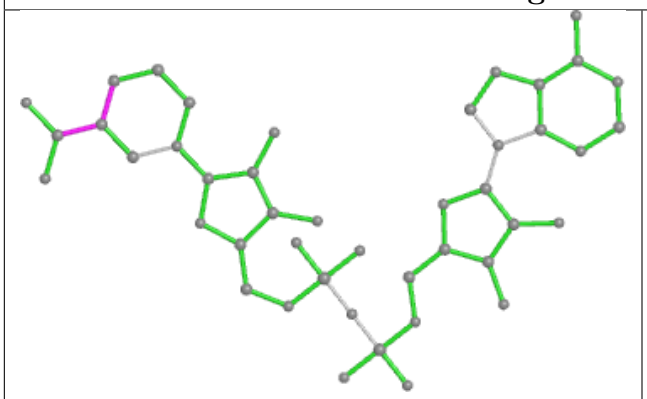
Ligand UPG A 501



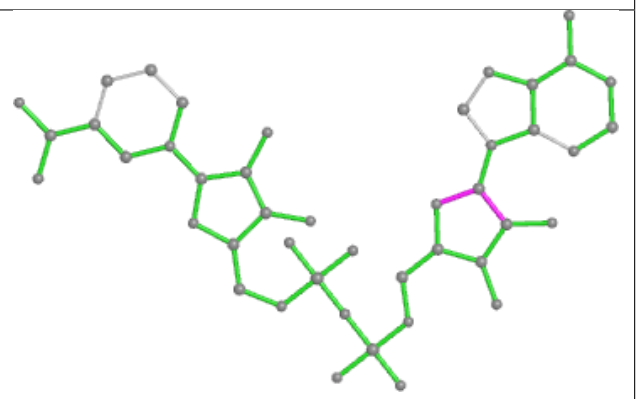
Ligand UPG D 501



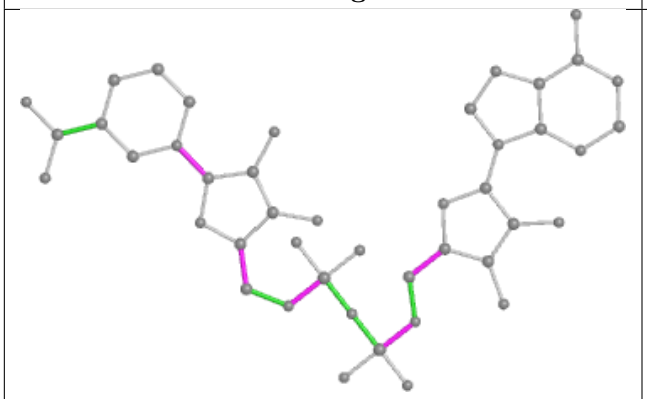
Ligand NAI A 500



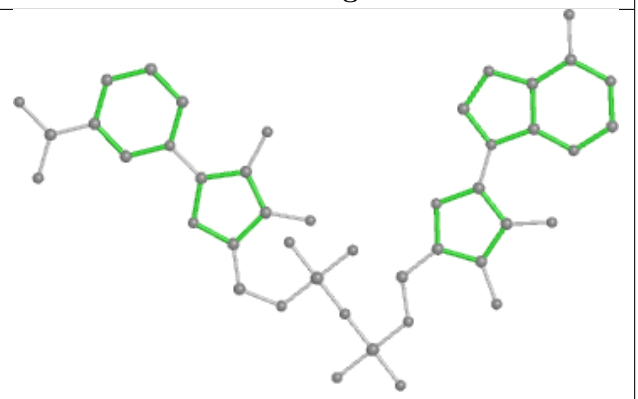
Bond lengths



Bond angles

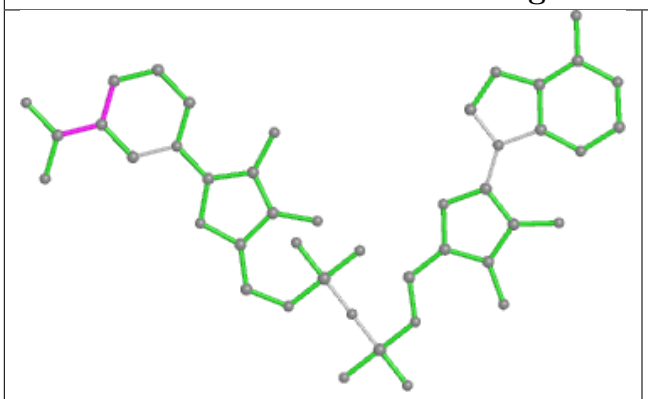


Torsions

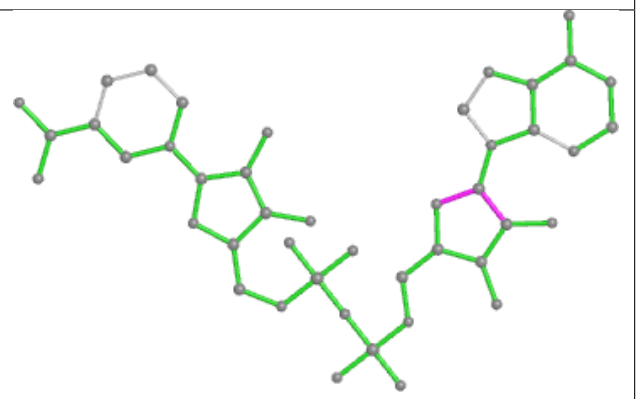


Rings

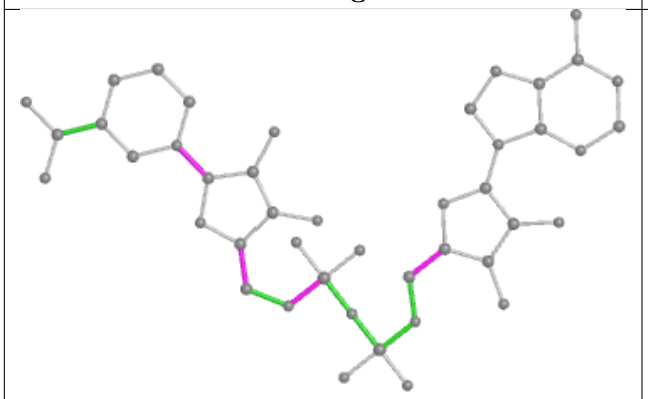
Ligand NAI C 500



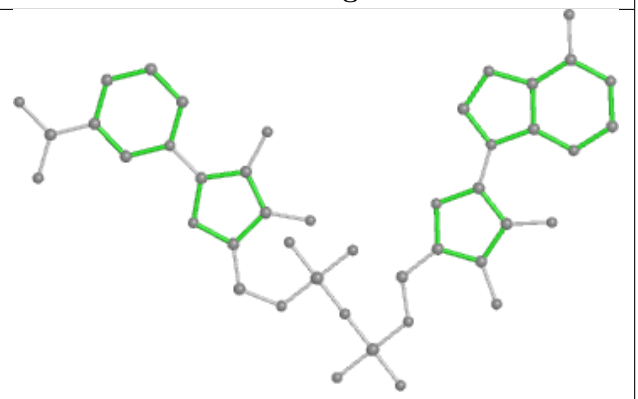
Bond lengths



Bond angles

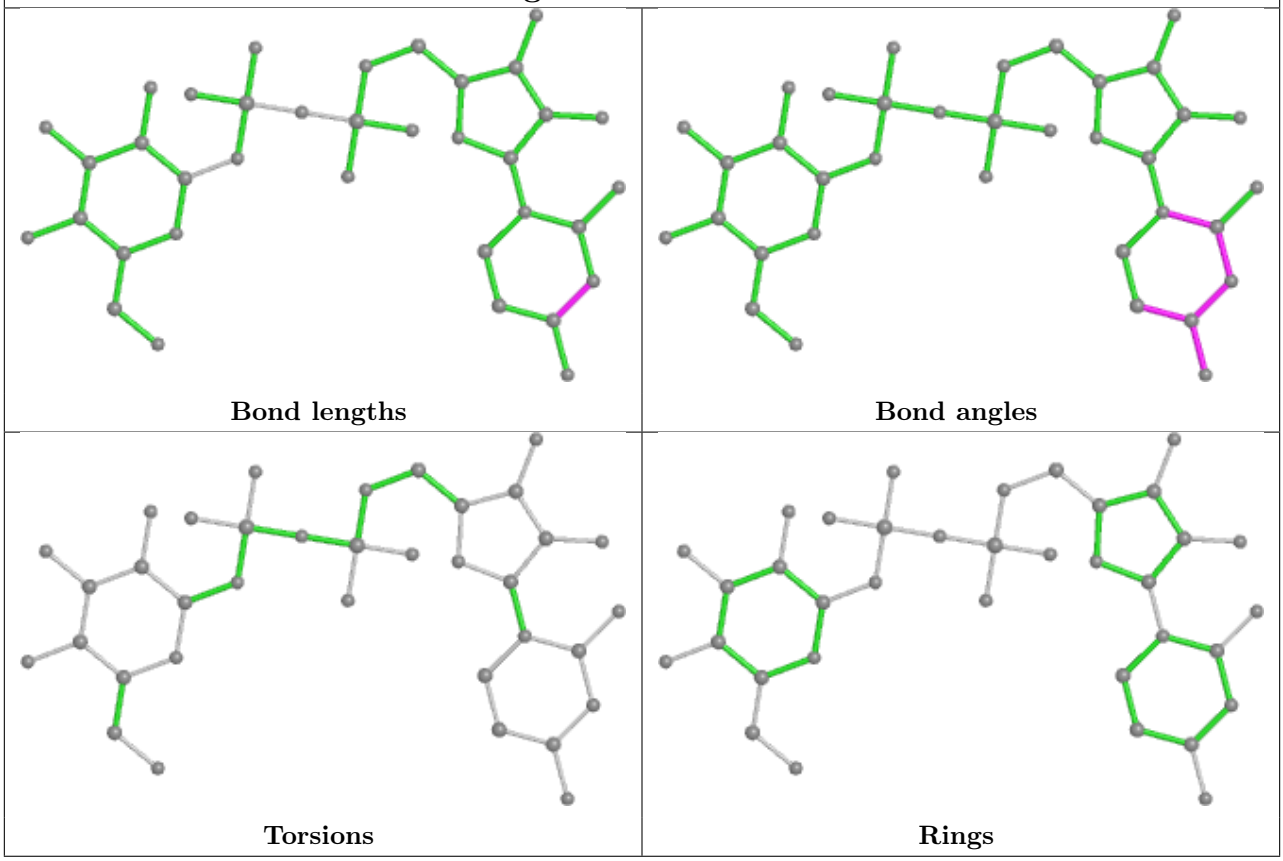


Torsions

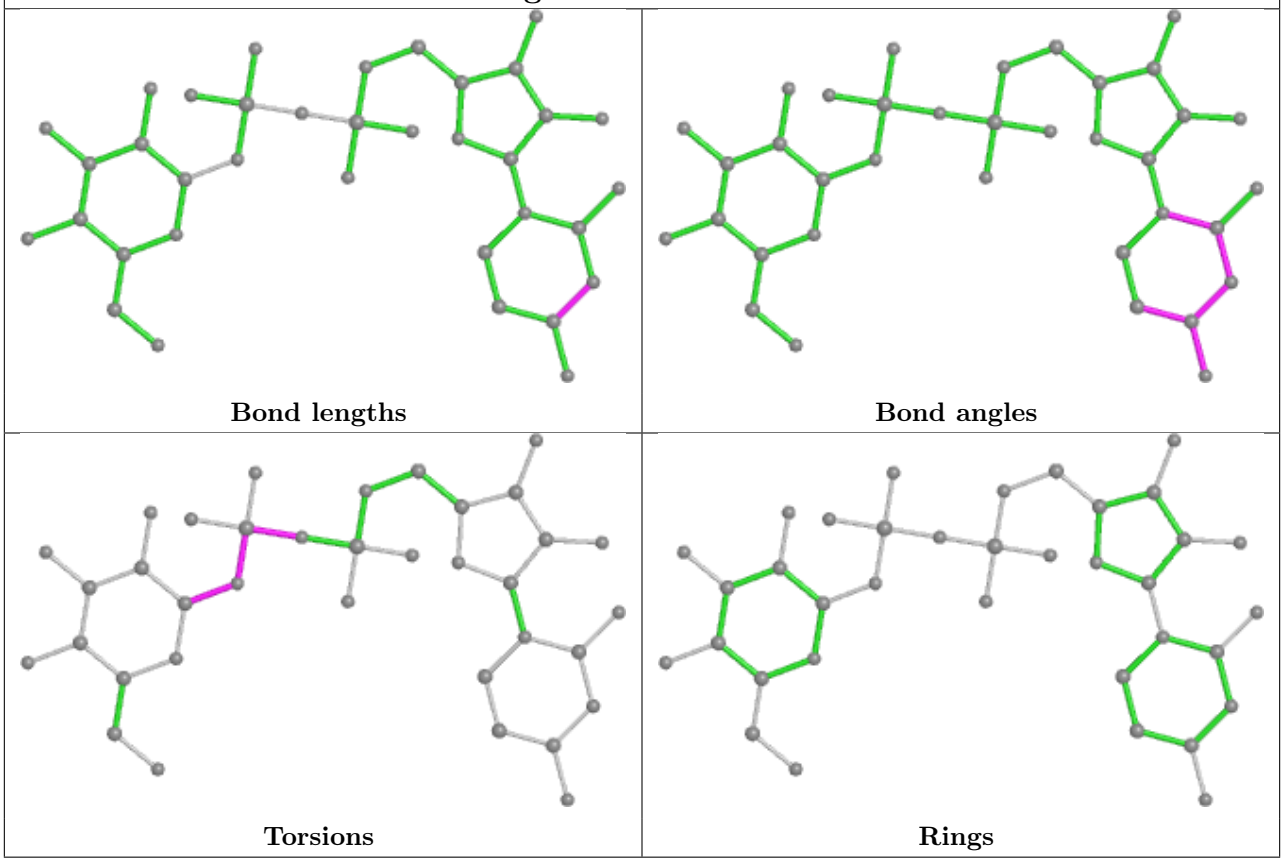


Rings

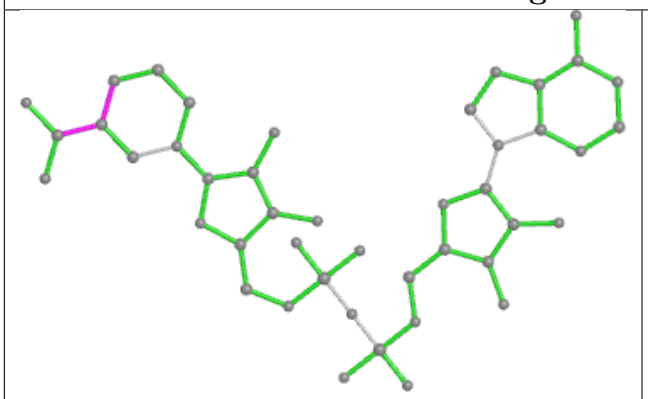
Ligand UPG E 501



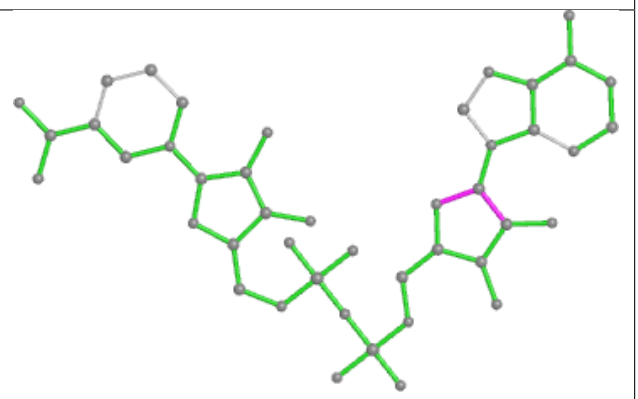
Ligand UPG F 501



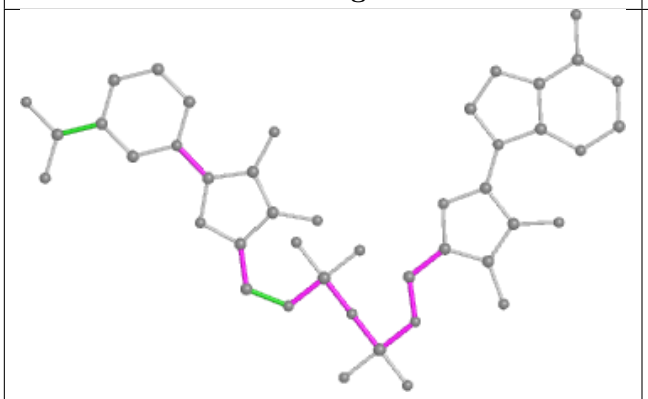
Ligand NAI E 500



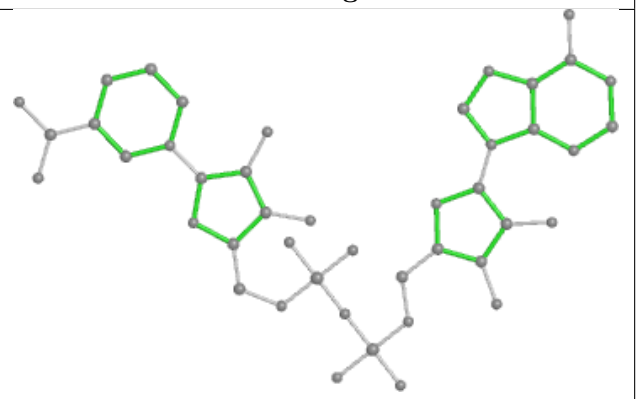
Bond lengths



Bond angles

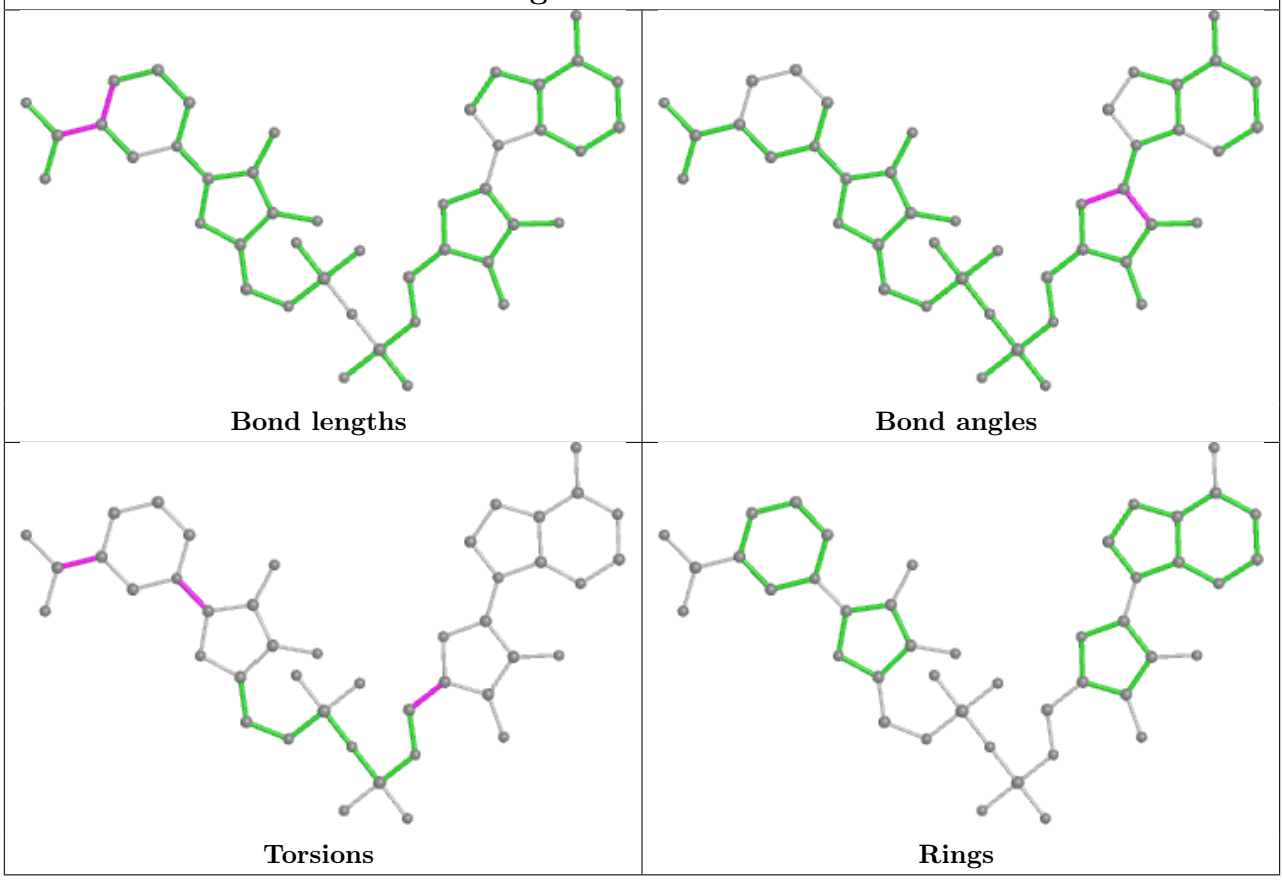


Torsions



Rings

Ligand NAI F 500



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	454/494 (91%)	0.13	14 (3%)	49	32	33, 72, 105, 135	0
1	B	323/494 (65%)	0.19	18 (5%)	24	15	38, 66, 125, 166	0
1	C	460/494 (93%)	-0.18	4 (0%)	84	71	29, 54, 91, 135	0
1	D	457/494 (92%)	-0.07	10 (2%)	62	45	31, 63, 106, 142	0
1	E	459/494 (92%)	-0.04	8 (1%)	70	53	27, 66, 104, 129	0
1	F	459/494 (92%)	-0.29	5 (1%)	80	65	23, 43, 67, 104	0
All	All	2612/2964 (88%)	-0.05	59 (2%)	60	43	23, 60, 104, 166	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	CYS	4.9
1	A	88	SER	4.3
1	B	173	LYS	3.9
1	B	116	ILE	3.8
1	D	53	TYR	3.6
1	A	2	PHE	3.5
1	B	202	TRP	3.3
1	E	421	LYS	3.3
1	B	115	ARG	3.2
1	A	16	GLY	3.1
1	B	198	VAL	3.1
1	B	201	HIS	3.0
1	E	53	TYR	3.0
1	D	382	HIS	3.0
1	A	465	LYS	2.9
1	F	159	ASN	2.9
1	A	129	LYS	2.7
1	D	67	LYS	2.7
1	A	159	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	87	ILE	2.6
1	B	341	ASP	2.6
1	B	399	LYS	2.6
1	A	190	ARG	2.5
1	C	121	ASN	2.5
1	E	1	MET	2.4
1	B	414	CYS	2.4
1	F	130	SER	2.4
1	F	382	HIS	2.3
1	B	114	ARG	2.3
1	A	8	CYS	2.3
1	D	414	CYS	2.3
1	C	120	SER	2.3
1	B	156	VAL	2.3
1	B	332	ALA	2.3
1	E	52	ILE	2.3
1	A	245	GLY	2.3
1	D	129	LYS	2.3
1	B	169	ILE	2.2
1	B	456	GLY	2.2
1	D	184	GLU	2.2
1	F	390	GLN	2.2
1	D	19	THR	2.2
1	B	107	LYS	2.2
1	F	389	ASP	2.2
1	E	186	PRO	2.2
1	C	150	PRO	2.1
1	D	430	LYS	2.1
1	E	390	GLN	2.1
1	D	393	ARG	2.1
1	B	112	CYS	2.1
1	E	422	GLU	2.1
1	A	123	TYR	2.1
1	D	16	GLY	2.1
1	A	19	THR	2.1
1	A	186	PRO	2.1
1	E	55	PRO	2.1
1	B	199	TYR	2.0
1	B	143	ILE	2.0
1	C	430	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

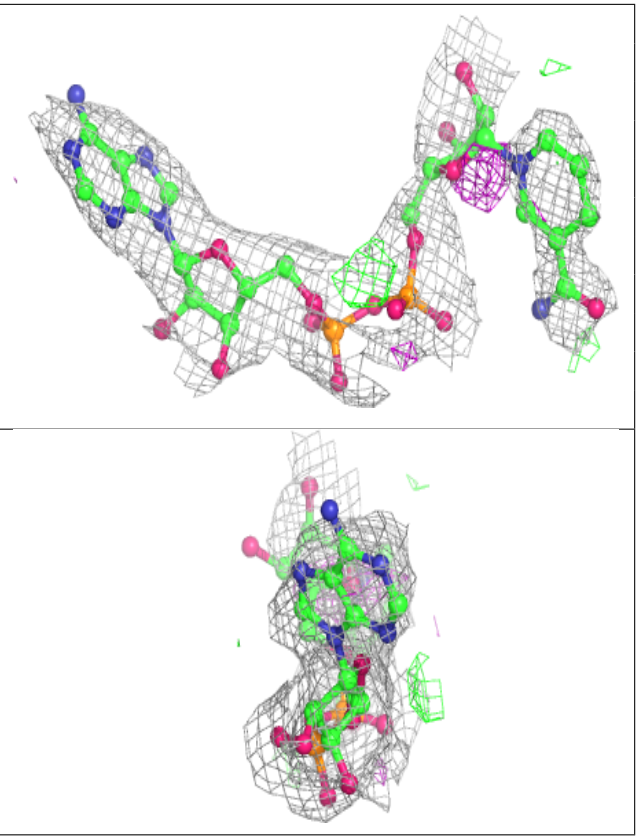
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAI	E	500	44/44	0.84	0.27	93,115,129,131	0
3	UPG	E	501	36/36	0.84	0.25	94,115,129,131	0
3	UPG	B	501	36/36	0.87	0.20	75,95,117,119	0
2	NAI	D	500	44/44	0.91	0.21	67,86,97,98	0
2	NAI	A	500	44/44	0.92	0.20	53,61,77,80	0
3	UPG	D	501	36/36	0.93	0.17	48,59,71,76	0
2	NAI	C	500	44/44	0.95	0.14	50,59,76,79	0
3	UPG	A	501	36/36	0.96	0.17	41,52,60,61	0
3	UPG	C	501	36/36	0.96	0.15	36,45,51,56	0
2	NAI	F	500	44/44	0.97	0.17	25,41,49,51	0
3	UPG	F	501	36/36	0.98	0.15	21,34,39,41	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.

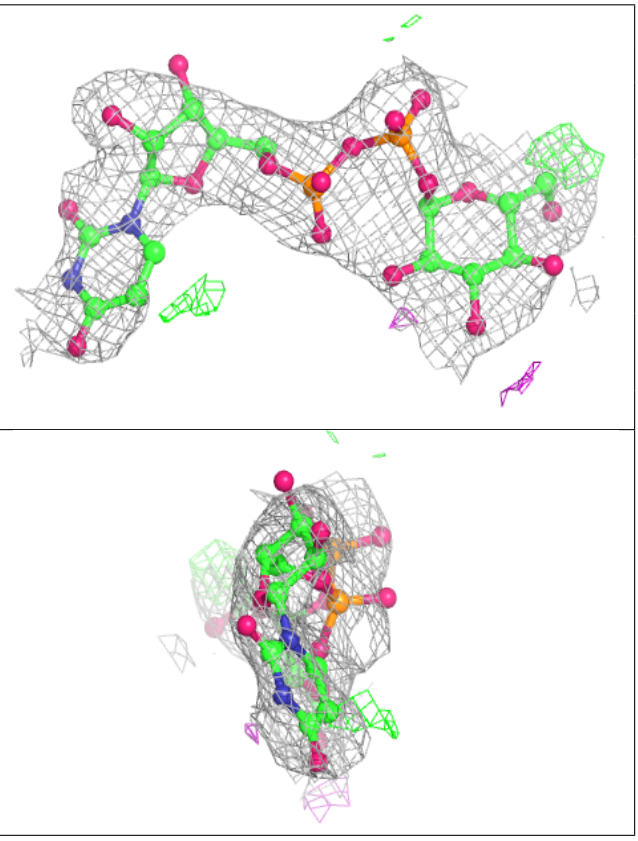
Electron density around NAI E 500:

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



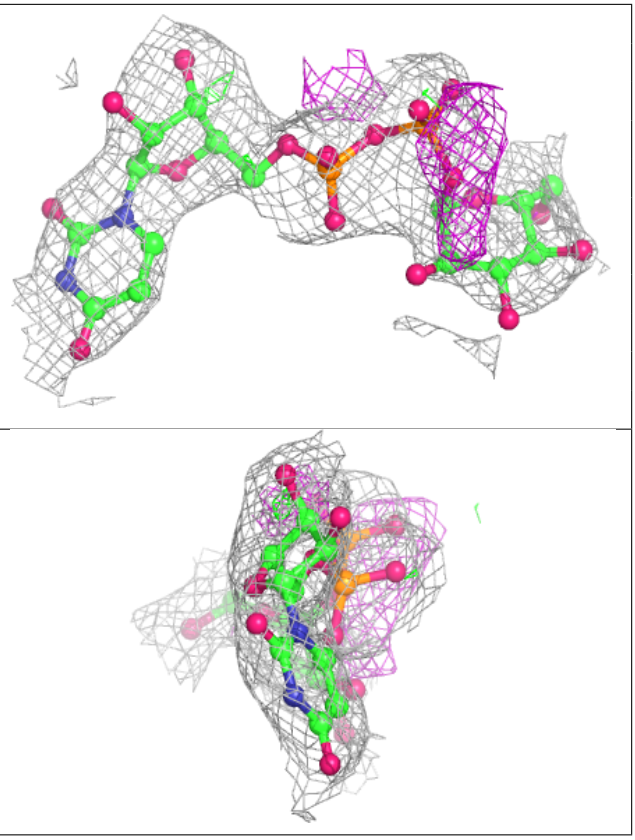
Electron density around UPG E 501:

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



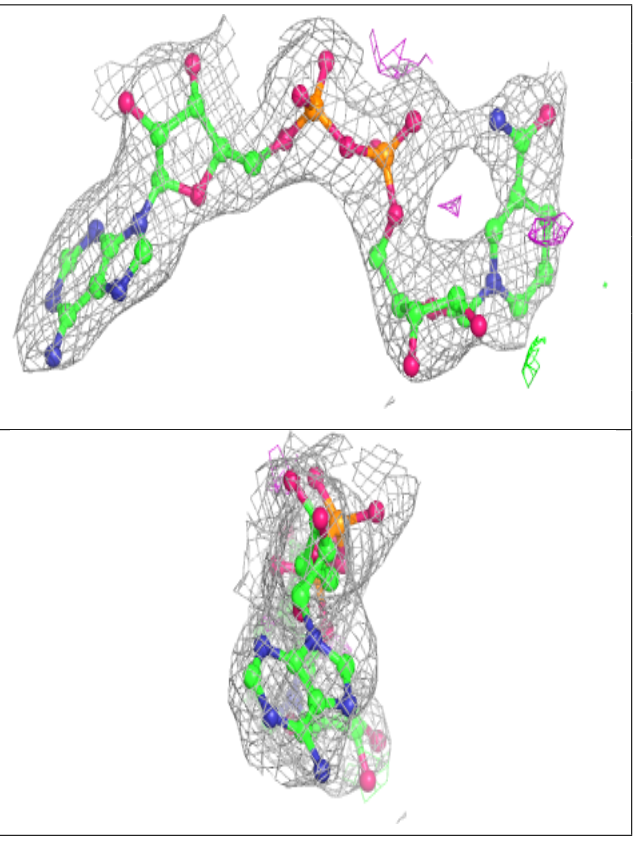
Electron density around UPG B 501:

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



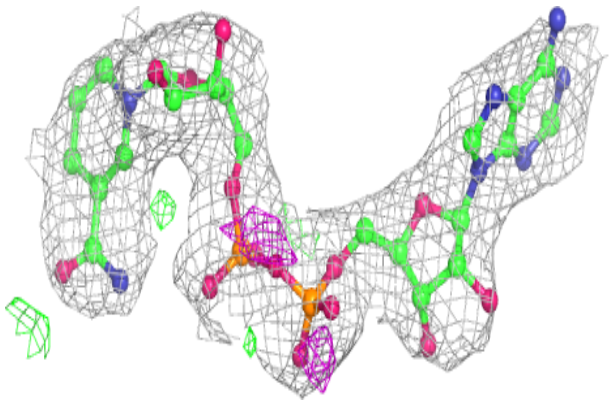
Electron density around NAI D 500:

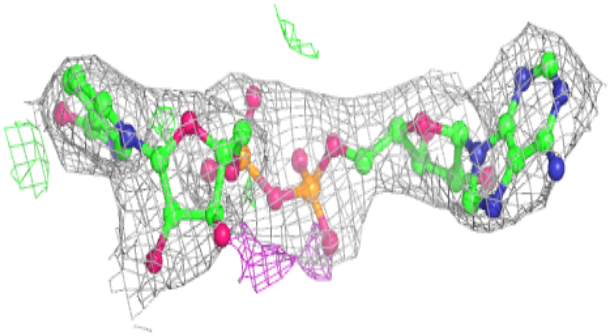
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAI A 500:

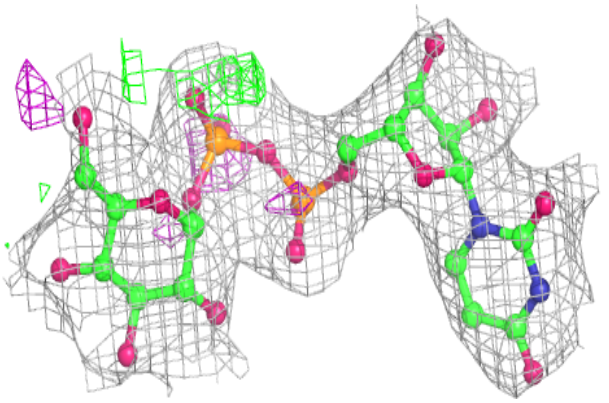
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

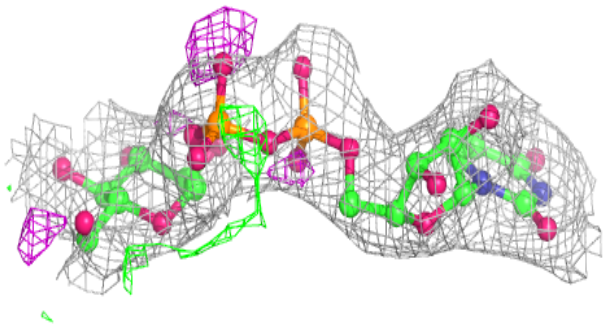


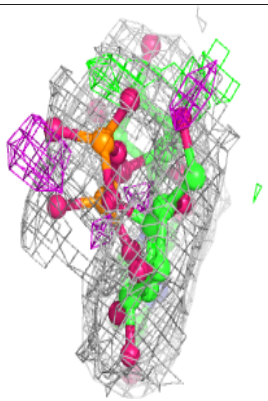


Electron density around UPG D 501:

$2mF_o$-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 500:

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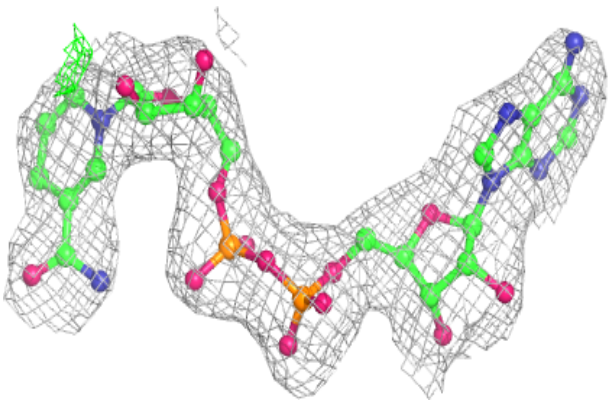
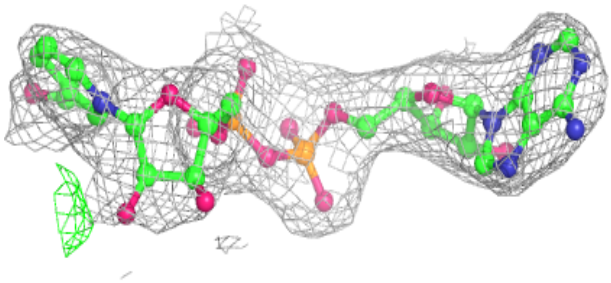
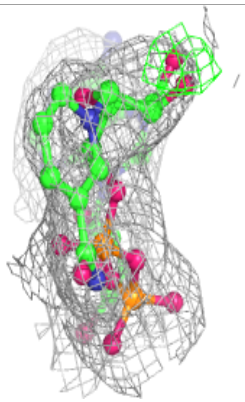
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around UPG A 501:

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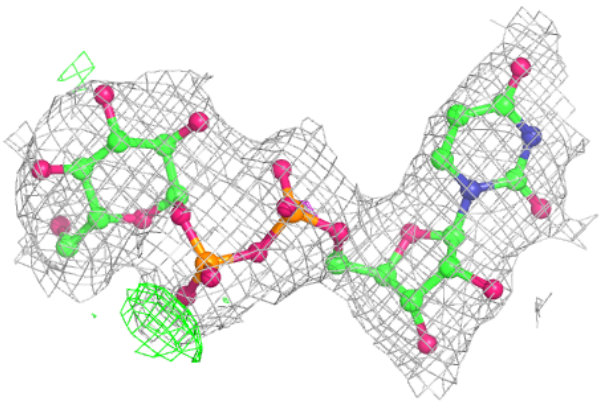
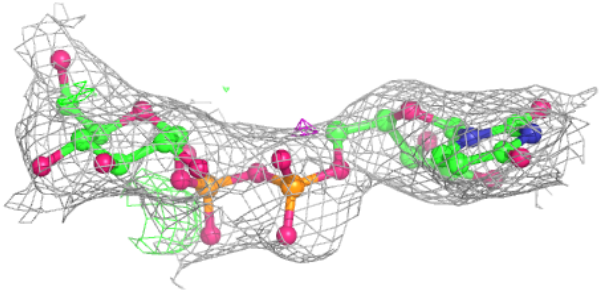
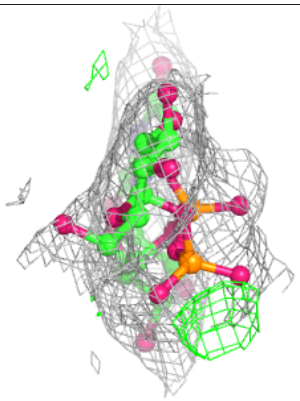
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around UPG C 501:

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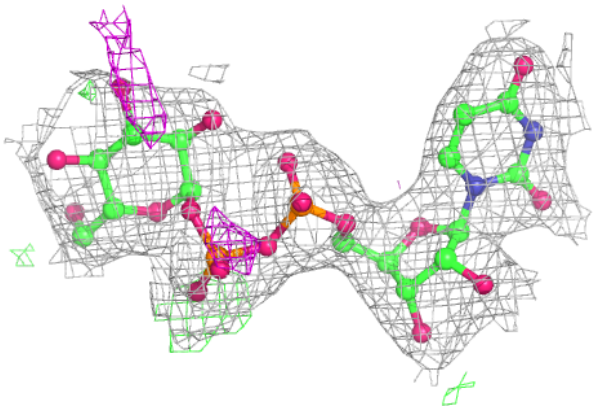
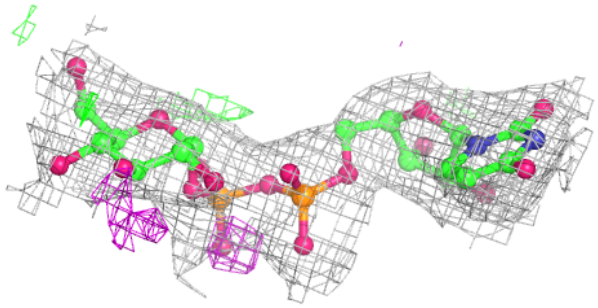
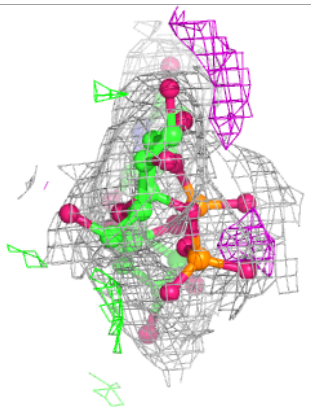
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around NAI F 500:

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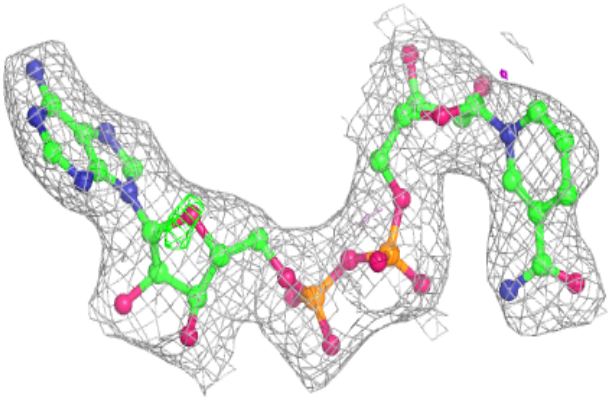
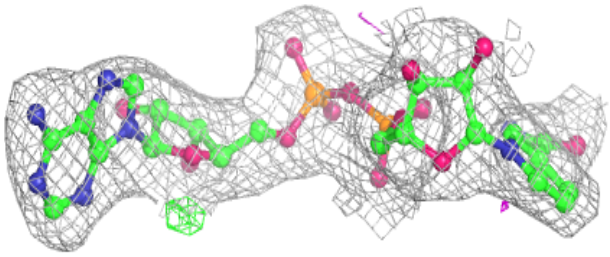
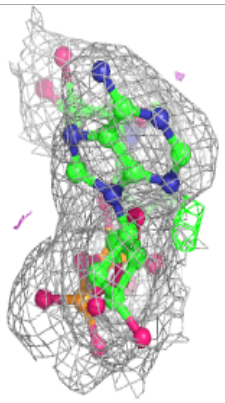
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around UPG F 501:

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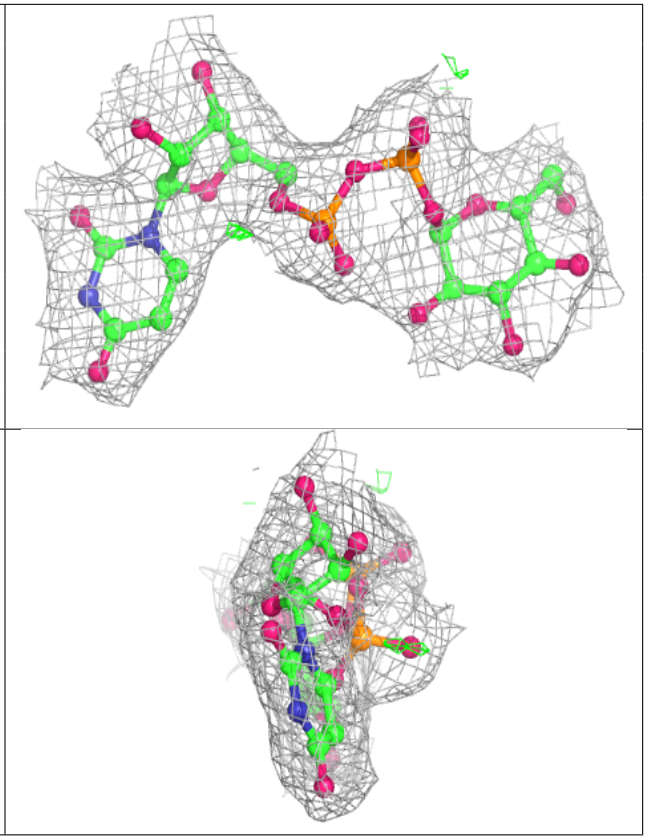
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.