



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2024 – 12:56 AM EST

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

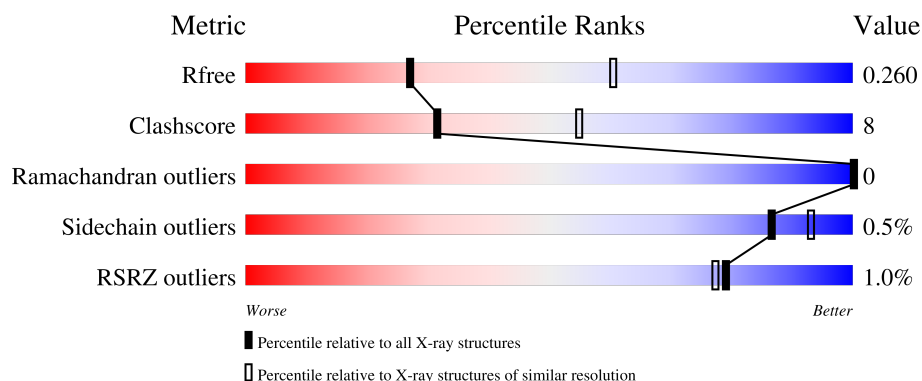
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	164625	1044 (2.98-2.94)
Clashscore	180529	1097 (2.98-2.94)
Ramachandran outliers	177936	1049 (2.98-2.94)
Sidechain outliers	177891	1049 (2.98-2.94)
RSRZ outliers	164620	1044 (2.98-2.94)

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  $\geq 3$ , 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	
1	B	494	
1	C	494	
1	D	494	
1	E	494	

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Mol	Chain	Length	Quality of chain
1	F	494	<div><div><div>%</div><div><div></div></div><div>77%</div><div>16%</div><div>7%</div></div></div>

## 2 Entry composition

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.

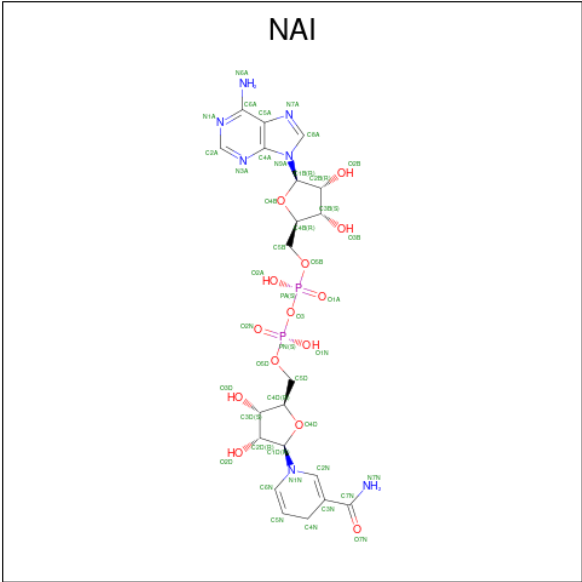
- Molecule 1 is a protein called UDP-glucose 6-dehydrogenase.

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

There are 6 discrepancies between the modelled and reference sequences:

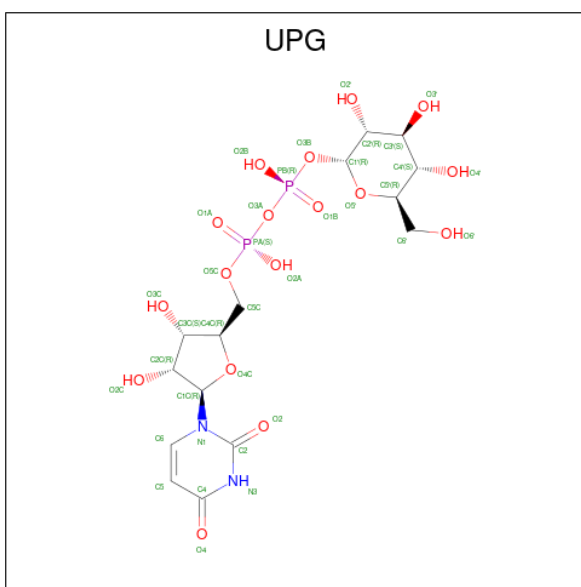
Chain	Residue	Modelled	Actual	Comment	Reference
A	225	LEU	ALA	engineered mutation	UNP O60701
B	225	LEU	ALA	engineered mutation	UNP O60701
C	225	LEU	ALA	engineered mutation	UNP O60701
D	225	LEU	ALA	engineered mutation	UNP O60701
E	225	LEU	ALA	engineered mutation	UNP O60701
F	225	LEU	ALA	engineered mutation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

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	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<sub>15</sub>H<sub>24</sub>N<sub>2</sub>O<sub>17</sub>P<sub>2</sub>).




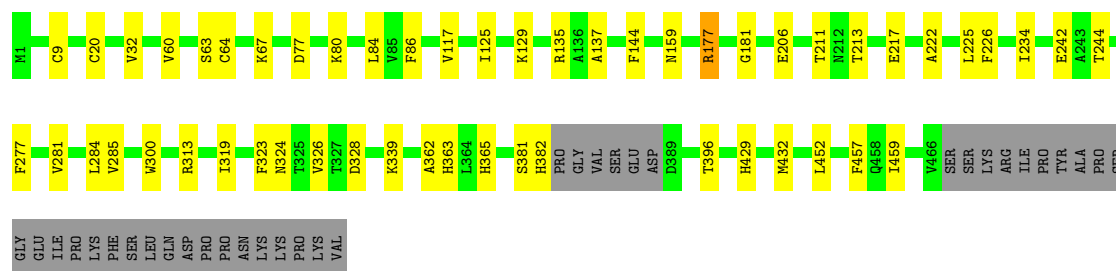
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	C	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	D	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	E	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	F	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 4 is water.

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

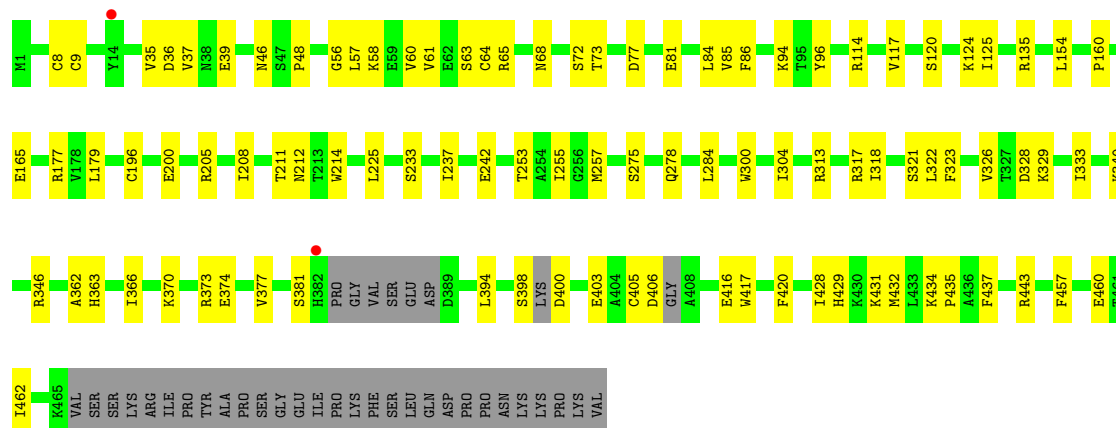


Chain C: 




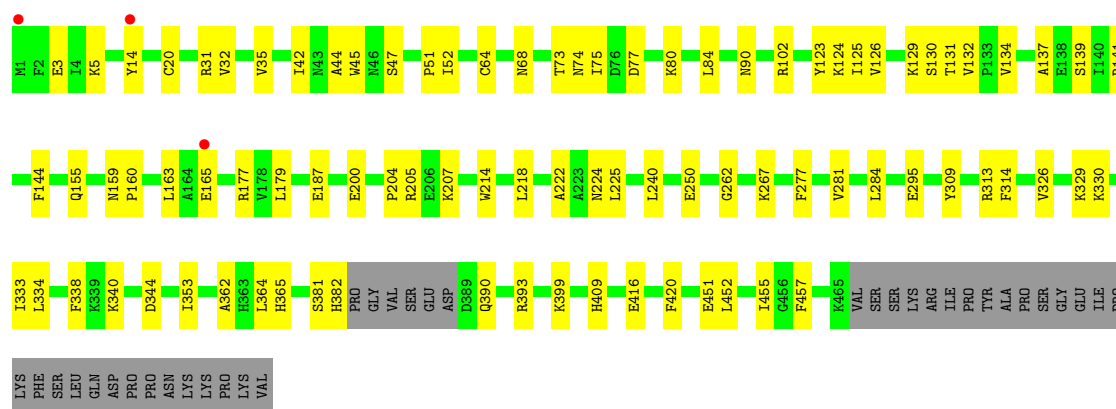
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain D: 




• Molecule 1: UDP-glucose 6-dehydrogenase

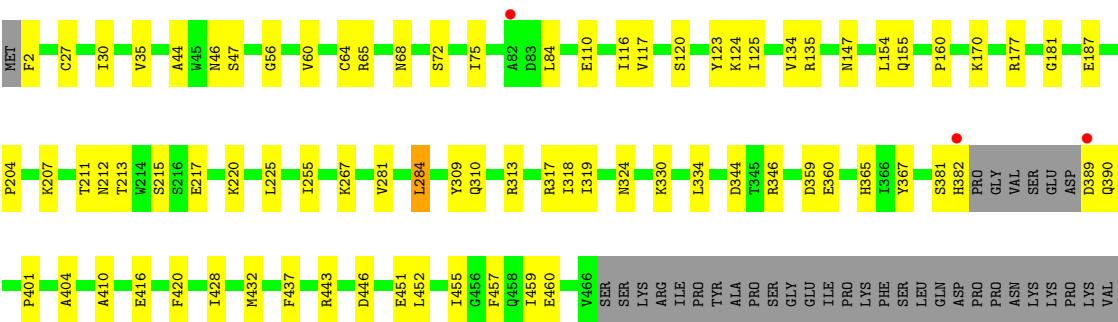
Chain E: 



• Molecule 1: UDP-glucose 6-dehydrogenase

Chain F: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.1 (30.06-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.203 , 0.259 0.205 , 0.260	Depositor DCC
$R_{free}$ test set	76100 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.7	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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 ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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%)	79	88
1	B	279/427 (65%)	277 (99%)	2 (1%)	81	90
1	C	396/427 (93%)	394 (100%)	2 (0%)	86	93
1	D	394/427 (92%)	393 (100%)	1 (0%)	91	96
1	E	395/427 (92%)	394 (100%)	1 (0%)	91	96
1	F	395/427 (92%)	392 (99%)	3 (1%)	79	88
All	All	2249/2562 (88%)	2237 (100%)	12 (0%)	86	93

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 ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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
3	UPG	B	501	-	37,38,38	1.20	2 (5%)	55,58,58	1.40	6 (10%)
3	UPG	F	501	-	37,38,38	1.20	2 (5%)	55,58,58	1.35	6 (10%)
3	UPG	A	501	-	37,38,38	1.19	3 (8%)	55,58,58	1.38	5 (9%)
2	NAI	D	500	-	43,48,48	1.17	5 (11%)	50,73,73	0.98	1 (2%)
3	UPG	D	501	-	37,38,38	1.24	2 (5%)	55,58,58	1.37	5 (9%)
2	NAI	A	500	-	43,48,48	1.15	5 (11%)	50,73,73	0.99	1 (2%)
3	UPG	E	501	-	37,38,38	1.24	2 (5%)	55,58,58	1.35	5 (9%)
2	NAI	E	500	-	43,48,48	1.17	5 (11%)	50,73,73	0.99	1 (2%)
2	NAI	F	500	-	43,48,48	1.16	5 (11%)	50,73,73	0.95	1 (2%)
3	UPG	C	501	-	37,38,38	1.23	2 (5%)	55,58,58	1.36	5 (9%)
2	NAI	C	500	-	43,48,48	1.16	5 (11%)	50,73,73	0.99	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
3	UPG	B	501	-	-	4/23/59/59	0/3/3/3
3	UPG	F	501	-	-	3/23/59/59	0/3/3/3
3	UPG	A	501	-	-	5/23/59/59	0/3/3/3
2	NAI	D	500	-	-	9/25/72/72	0/5/5/5
3	UPG	D	501	-	-	3/23/59/59	0/3/3/3
2	NAI	A	500	-	-	14/25/72/72	0/5/5/5
3	UPG	E	501	-	-	0/23/59/59	0/3/3/3
2	NAI	E	500	-	-	10/25/72/72	0/5/5/5
2	NAI	F	500	-	-	5/25/72/72	0/5/5/5
3	UPG	C	501	-	-	1/23/59/59	0/3/3/3
2	NAI	C	500	-	-	11/25/72/72	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	501	UPG	PA-O3A	4.98	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	UPG	PA-O3A	4.93	1.64	1.59
3	C	501	UPG	PA-O3A	4.90	1.64	1.59
3	B	501	UPG	PA-O3A	4.83	1.64	1.59
3	F	501	UPG	PA-O3A	4.65	1.64	1.59
3	A	501	UPG	PA-O3A	4.17	1.64	1.59
2	D	500	NAI	PN-O3	3.91	1.63	1.59
2	E	500	NAI	PN-O3	3.81	1.63	1.59
2	C	500	NAI	PN-O3	3.66	1.63	1.59
2	A	500	NAI	PN-O3	3.60	1.63	1.59
2	F	500	NAI	PN-O3	3.59	1.63	1.59
2	E	500	NAI	C4N-C3N	-2.75	1.44	1.50
3	A	501	UPG	C4-N3	-2.75	1.33	1.38
2	A	500	NAI	C4N-C3N	-2.73	1.44	1.50
2	C	500	NAI	C4N-C3N	-2.72	1.44	1.50
3	D	501	UPG	C4-N3	-2.71	1.34	1.38
2	D	500	NAI	C4N-C3N	-2.70	1.44	1.50
2	F	500	NAI	C4N-C3N	-2.67	1.45	1.50
3	C	501	UPG	C4-N3	-2.66	1.34	1.38
3	B	501	UPG	C4-N3	-2.65	1.34	1.38
3	F	501	UPG	C4-N3	-2.63	1.34	1.38
3	E	501	UPG	C4-N3	-2.62	1.34	1.38
2	F	500	NAI	PA-O3	-2.41	1.56	1.59
2	F	500	NAI	C1B-N9A	-2.34	1.44	1.49
2	D	500	NAI	C1B-N9A	-2.31	1.44	1.49
2	A	500	NAI	PA-O3	-2.27	1.57	1.59
2	E	500	NAI	PA-O3	-2.26	1.57	1.59
2	C	500	NAI	C7N-C3N	2.24	1.53	1.48
2	C	500	NAI	C1B-N9A	-2.24	1.44	1.49
2	E	500	NAI	C7N-C3N	2.24	1.53	1.48
3	A	501	UPG	PB-O3A	-2.19	1.57	1.59
2	A	500	NAI	C1B-N9A	-2.18	1.44	1.49
2	E	500	NAI	C1B-N9A	-2.18	1.44	1.49
2	F	500	NAI	C7N-C3N	2.15	1.53	1.48
2	C	500	NAI	PA-O3	-2.14	1.57	1.59
2	D	500	NAI	PA-O3	-2.13	1.57	1.59
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 (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	UPG	C4-N3-C2	-5.42	119.88	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	UPG	C4-N3-C2	-5.40	119.91	126.61
3	F	501	UPG	C4-N3-C2	-5.30	120.03	126.61
3	E	501	UPG	C4-N3-C2	-5.28	120.05	126.61
3	C	501	UPG	C4-N3-C2	-5.24	120.11	126.61
3	B	501	UPG	C4-N3-C2	-5.22	120.14	126.61
3	D	501	UPG	C5-C4-N3	4.87	121.62	114.80
3	F	501	UPG	C5-C4-N3	4.86	121.61	114.80
3	C	501	UPG	C5-C4-N3	4.84	121.59	114.80
3	B	501	UPG	C5-C4-N3	4.83	121.56	114.80
3	E	501	UPG	C5-C4-N3	4.82	121.56	114.80
3	A	501	UPG	C5-C4-N3	4.69	121.37	114.80
2	D	500	NAI	C6N-N1N-C2N	3.85	123.44	119.32
2	A	500	NAI	C6N-N1N-C2N	3.83	123.42	119.32
2	C	500	NAI	C6N-N1N-C2N	3.71	123.29	119.32
2	F	500	NAI	C6N-N1N-C2N	3.62	123.20	119.32
2	E	500	NAI	C6N-N1N-C2N	3.40	122.96	119.32
3	E	501	UPG	O3A-PA-O1A	-2.74	102.47	110.70
3	A	501	UPG	N3-C2-N1	2.70	118.40	114.89
3	A	501	UPG	O3A-PA-O1A	-2.62	102.84	110.70
3	D	501	UPG	N3-C2-N1	2.60	118.28	114.89
3	B	501	UPG	O3A-PA-O1A	-2.58	102.96	110.70
3	E	501	UPG	N3-C2-N1	2.54	118.20	114.89
3	B	501	UPG	N3-C2-N1	2.49	118.13	114.89
3	F	501	UPG	N3-C2-N1	2.45	118.08	114.89
3	A	501	UPG	O4-C4-N3	-2.43	115.75	119.27
3	C	501	UPG	N3-C2-N1	2.42	118.05	114.89
3	F	501	UPG	O4-C4-N3	-2.34	115.88	119.27
3	B	501	UPG	O4-C4-N3	-2.34	115.89	119.27
3	D	501	UPG	O3A-PA-O1A	-2.33	103.69	110.70
3	C	501	UPG	O4-C4-N3	-2.32	115.91	119.27
3	E	501	UPG	O4-C4-N3	-2.30	115.94	119.27
3	D	501	UPG	O4-C4-N3	-2.29	115.95	119.27
3	B	501	UPG	O2A-PA-O3A	2.21	113.24	107.27
3	C	501	UPG	O3A-PA-O1A	-2.19	104.12	110.70
3	F	501	UPG	O3A-PA-O1A	-2.14	104.26	110.70
3	F	501	UPG	O2A-PA-O3A	2.06	112.84	107.27

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	NAI	C5B-O5B-PA-O1A

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

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Mol	Chain	Res	Type	Atoms
2	F	500	NAI	C2D-C1D-N1N-C2N
3	D	501	UPG	O5'-C5'-C6'-O6'
2	A	500	NAI	C5B-O5B-PA-O2A
2	A	500	NAI	C5B-O5B-PA-O3
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
2	E	500	NAI	C5B-O5B-PA-O3
3	A	501	UPG	C5C-O5C-PA-O1A
2	A	500	NAI	O4D-C1D-N1N-C2N
2	F	500	NAI	O4D-C1D-N1N-C6N
2	A	500	NAI	O4D-C1D-N1N-C6N
2	D	500	NAI	O4D-C1D-N1N-C6N
2	F	500	NAI	O4D-C1D-N1N-C2N
2	E	500	NAI	C4B-C5B-O5B-PA
2	D	500	NAI	O4D-C1D-N1N-C2N
2	F	500	NAI	C2N-C3N-C7N-N7N
3	F	501	UPG	C2'-C1'-O3B-PB
3	F	501	UPG	C1'-O3B-PB-O2B
2	E	500	NAI	PA-O3-PN-O1N
3	A	501	UPG	C2'-C1'-O3B-PB

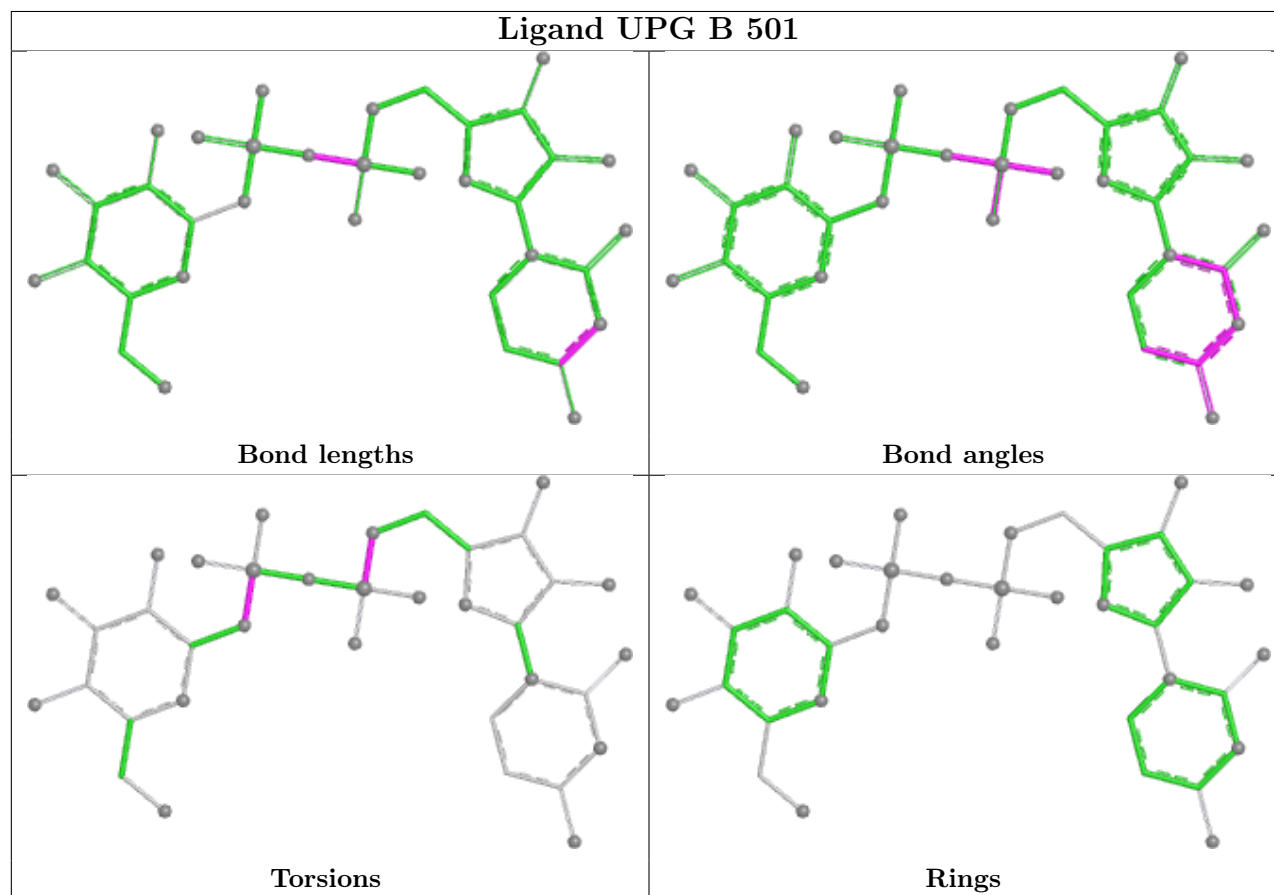
There are no ring outliers.

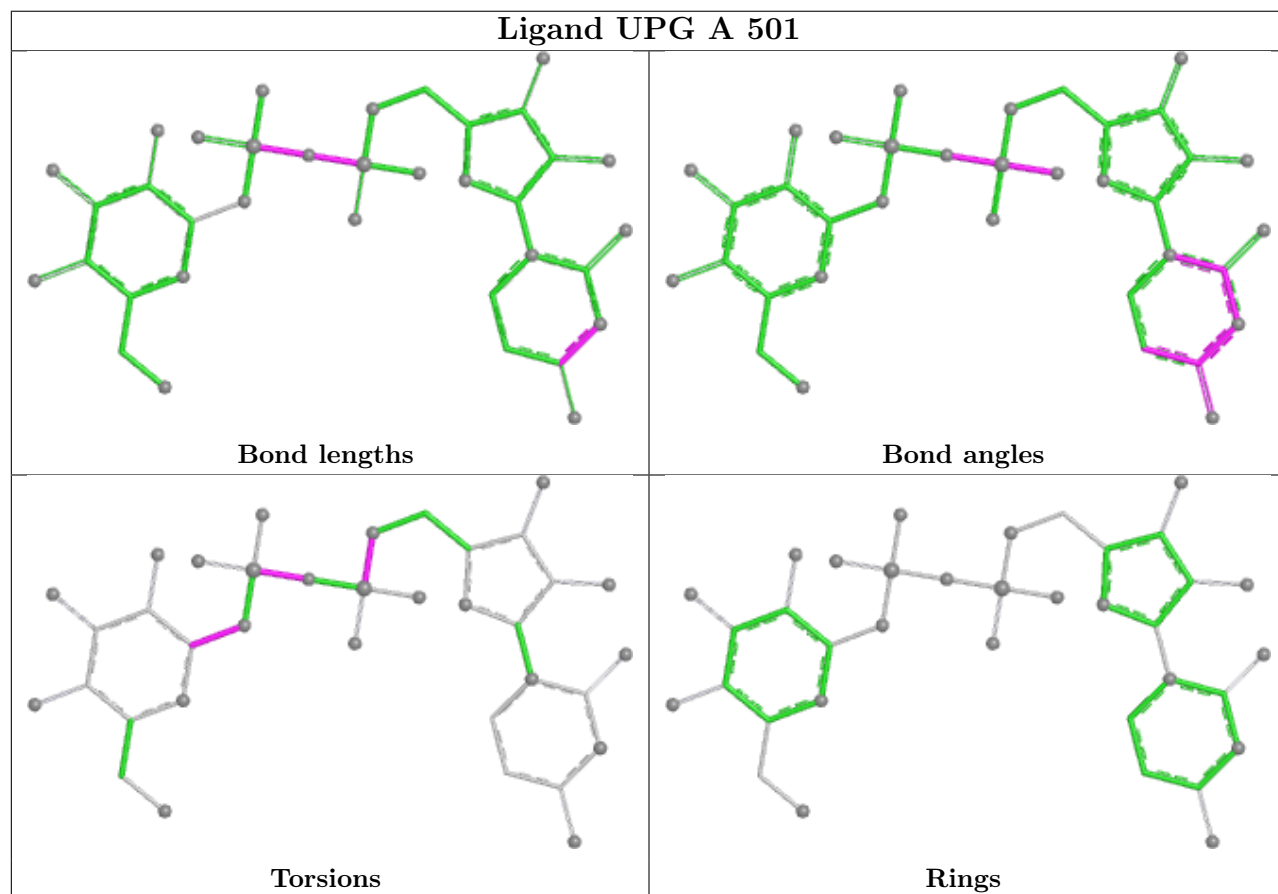
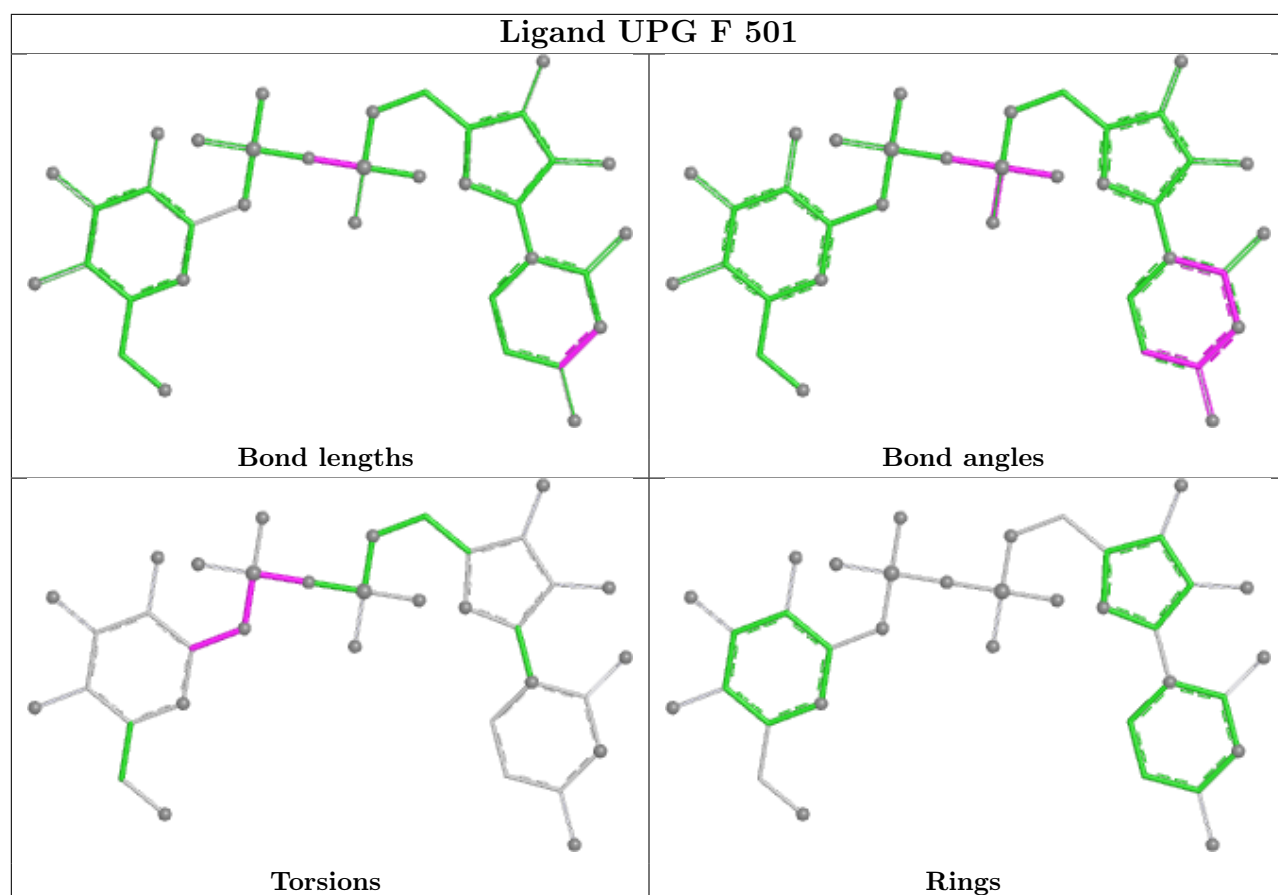
9 monomers are involved in 17 short contacts:

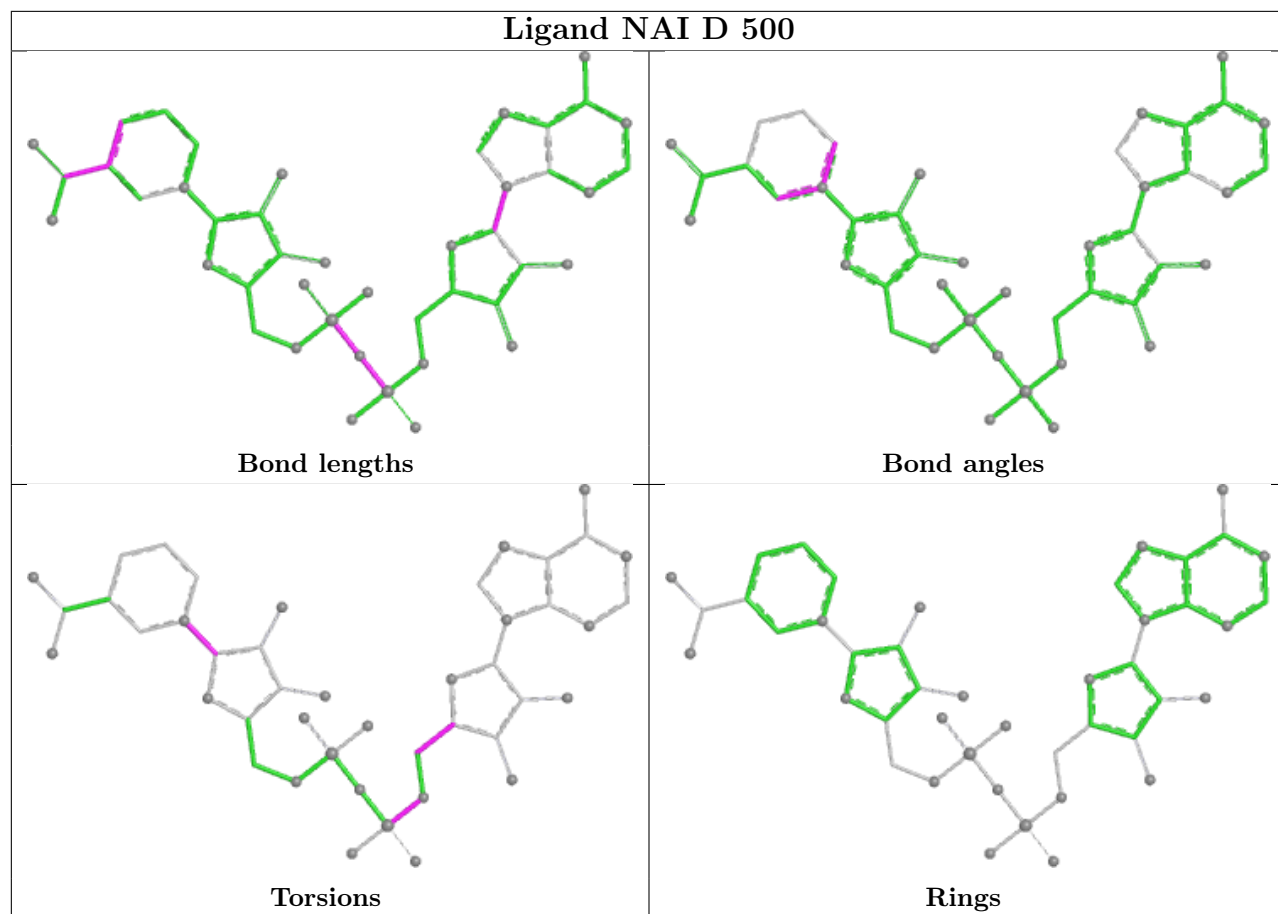
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	UPG	4	0
3	F	501	UPG	2	0
3	A	501	UPG	2	0
2	A	500	NAI	3	0
3	E	501	UPG	3	0
2	E	500	NAI	2	0
2	F	500	NAI	2	0
3	C	501	UPG	3	0
2	C	500	NAI	3	0

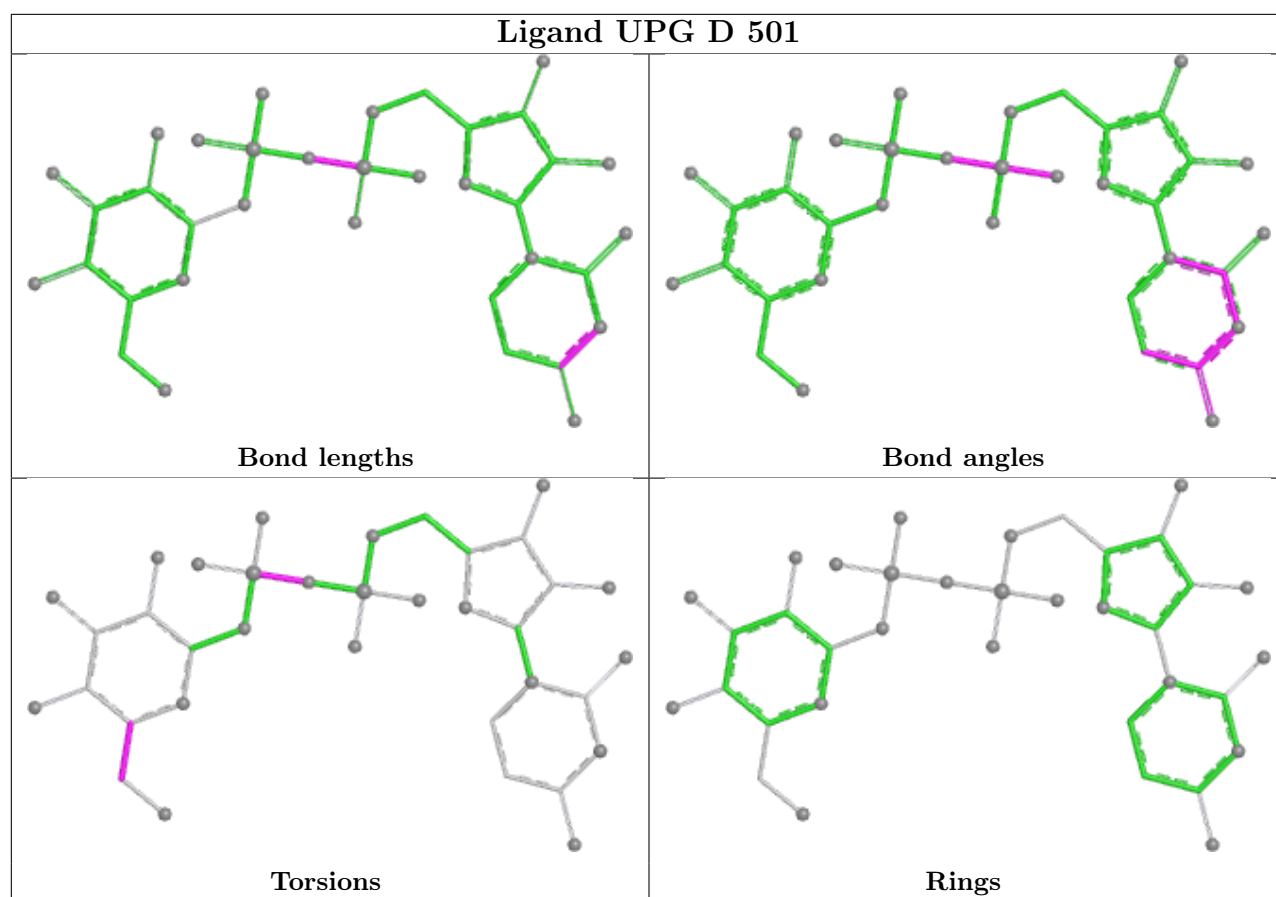
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

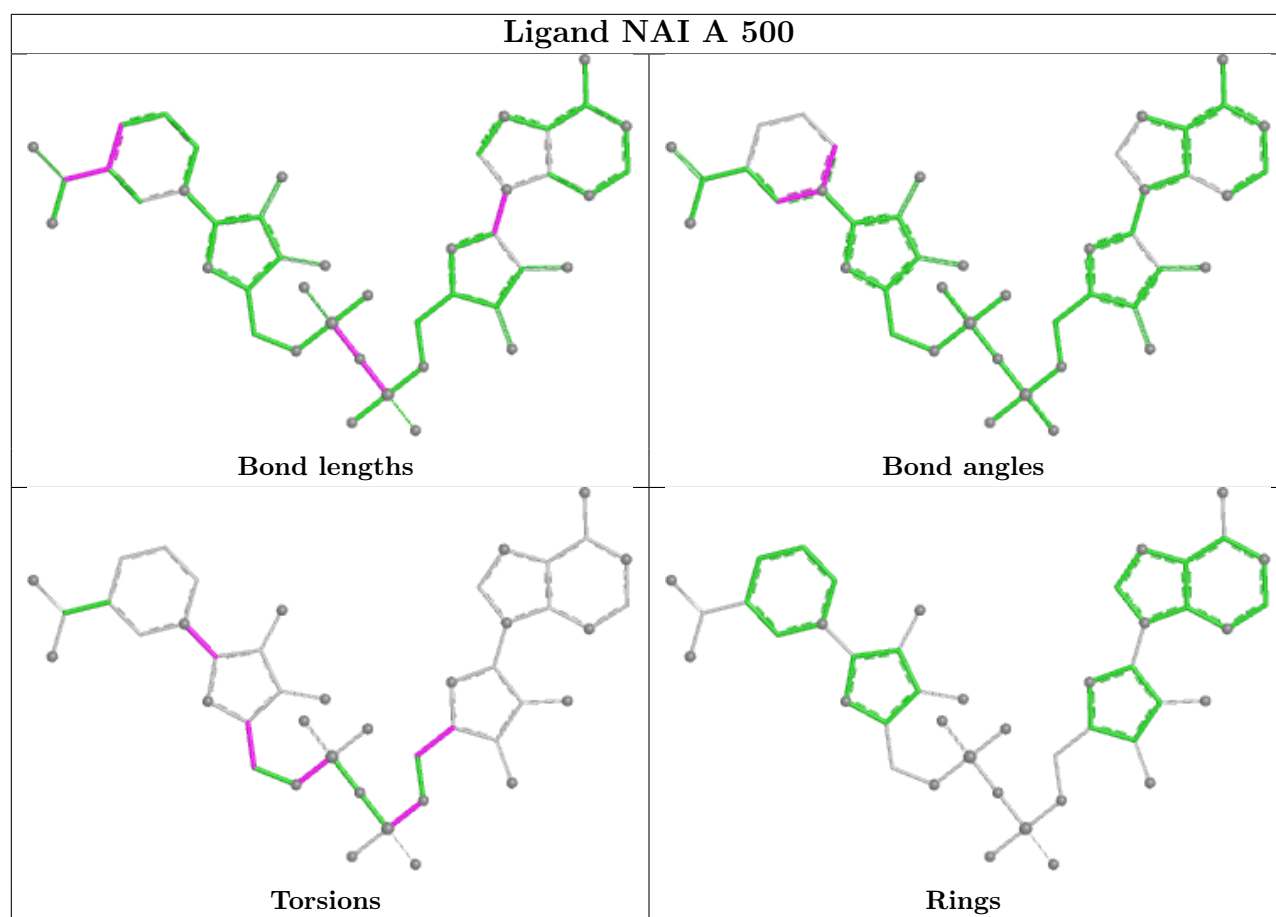
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



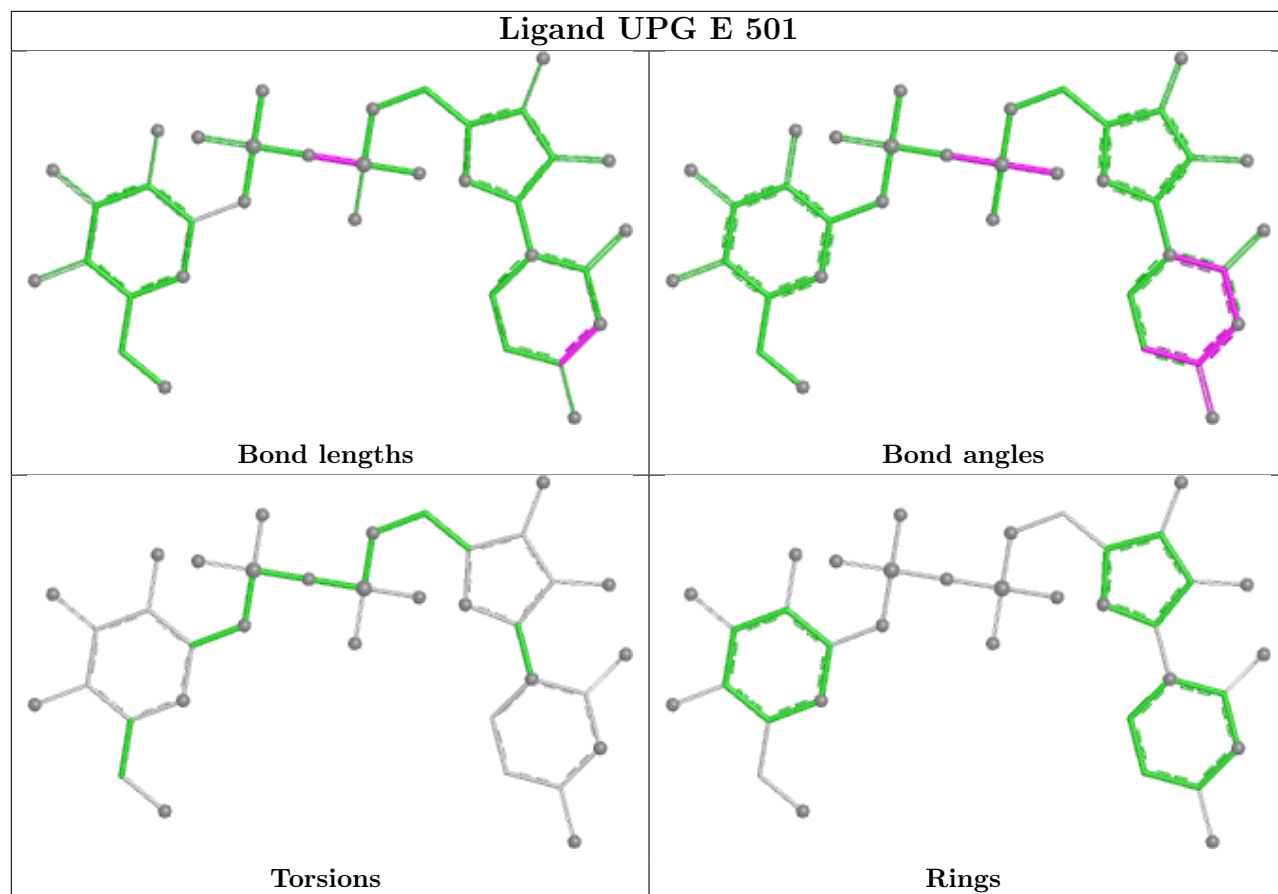


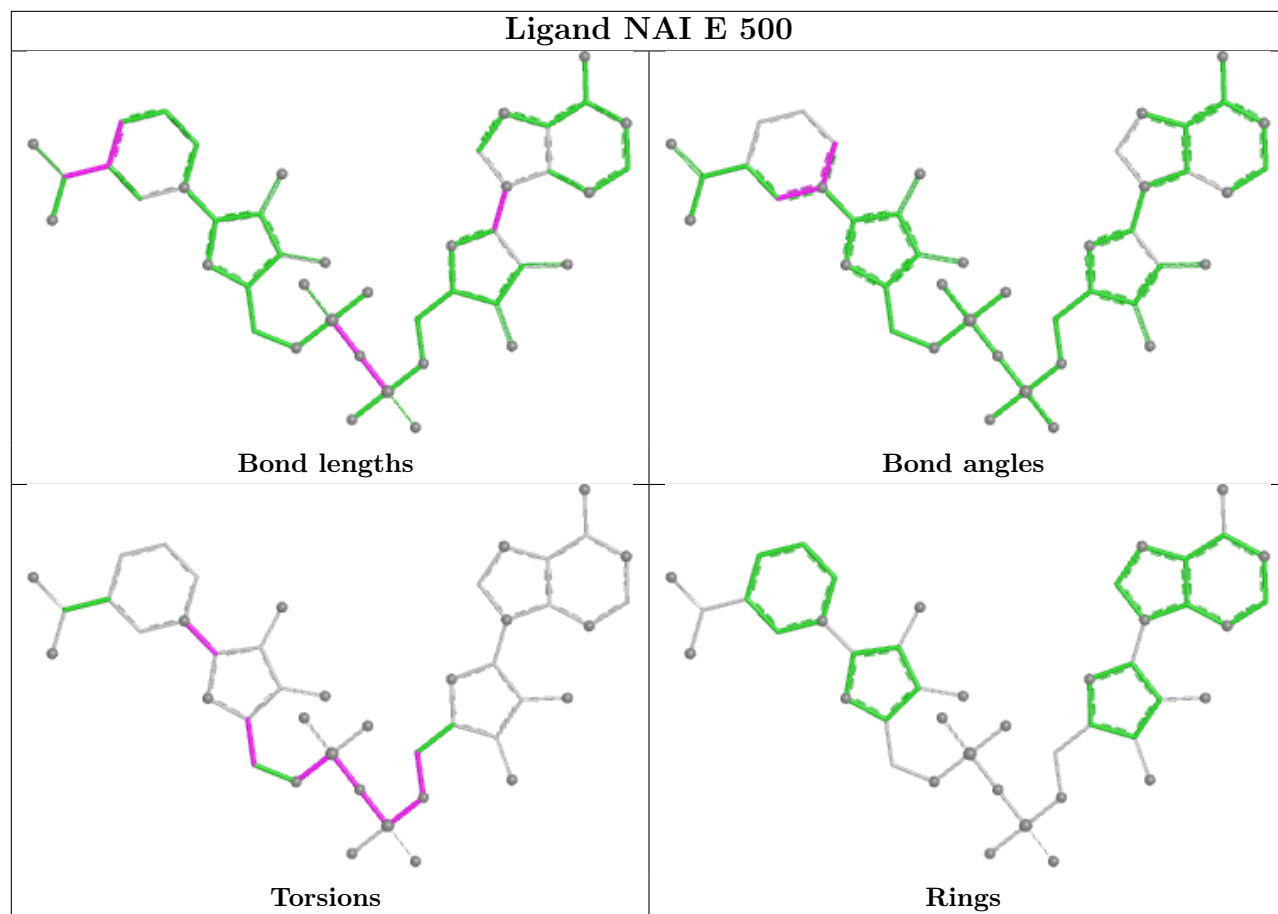


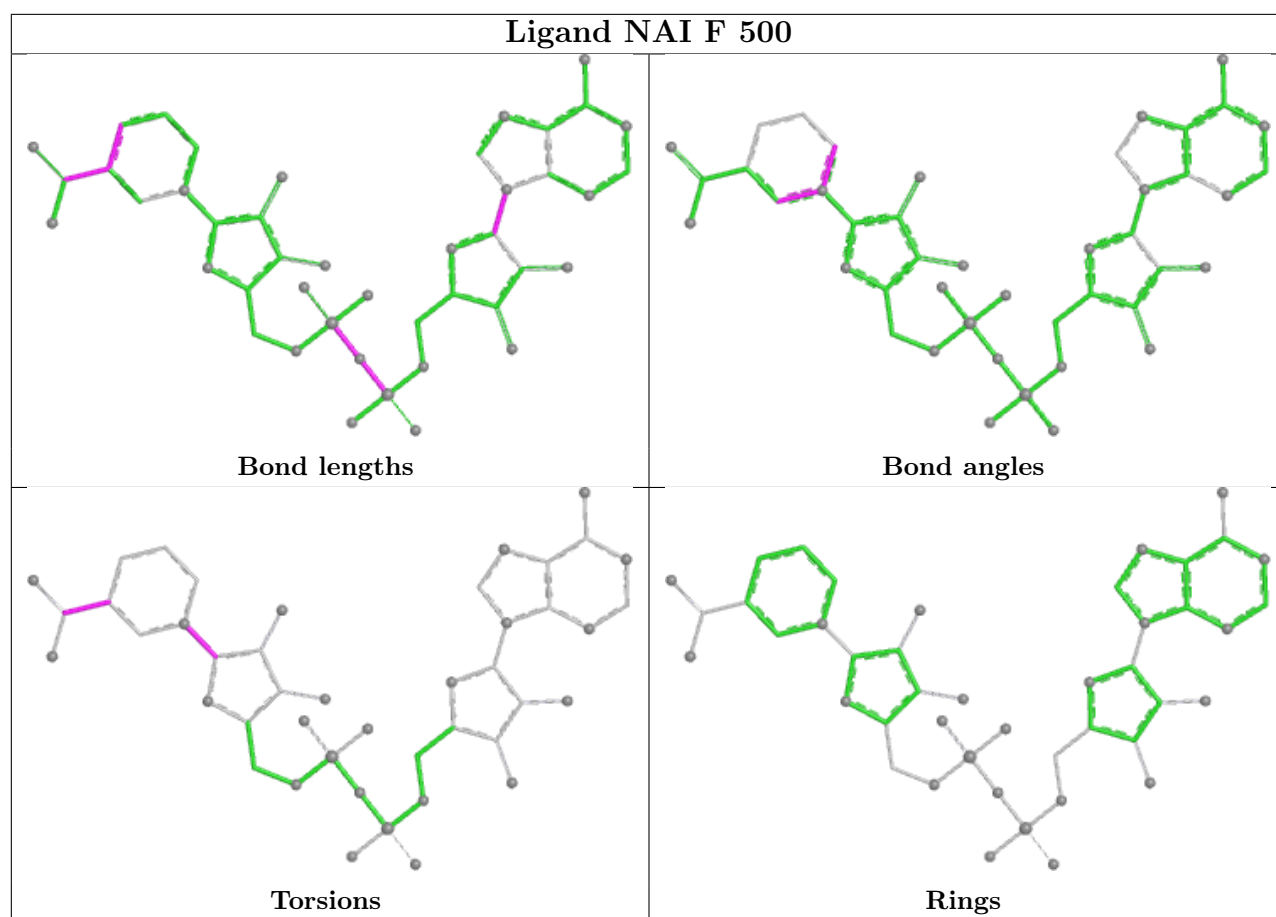


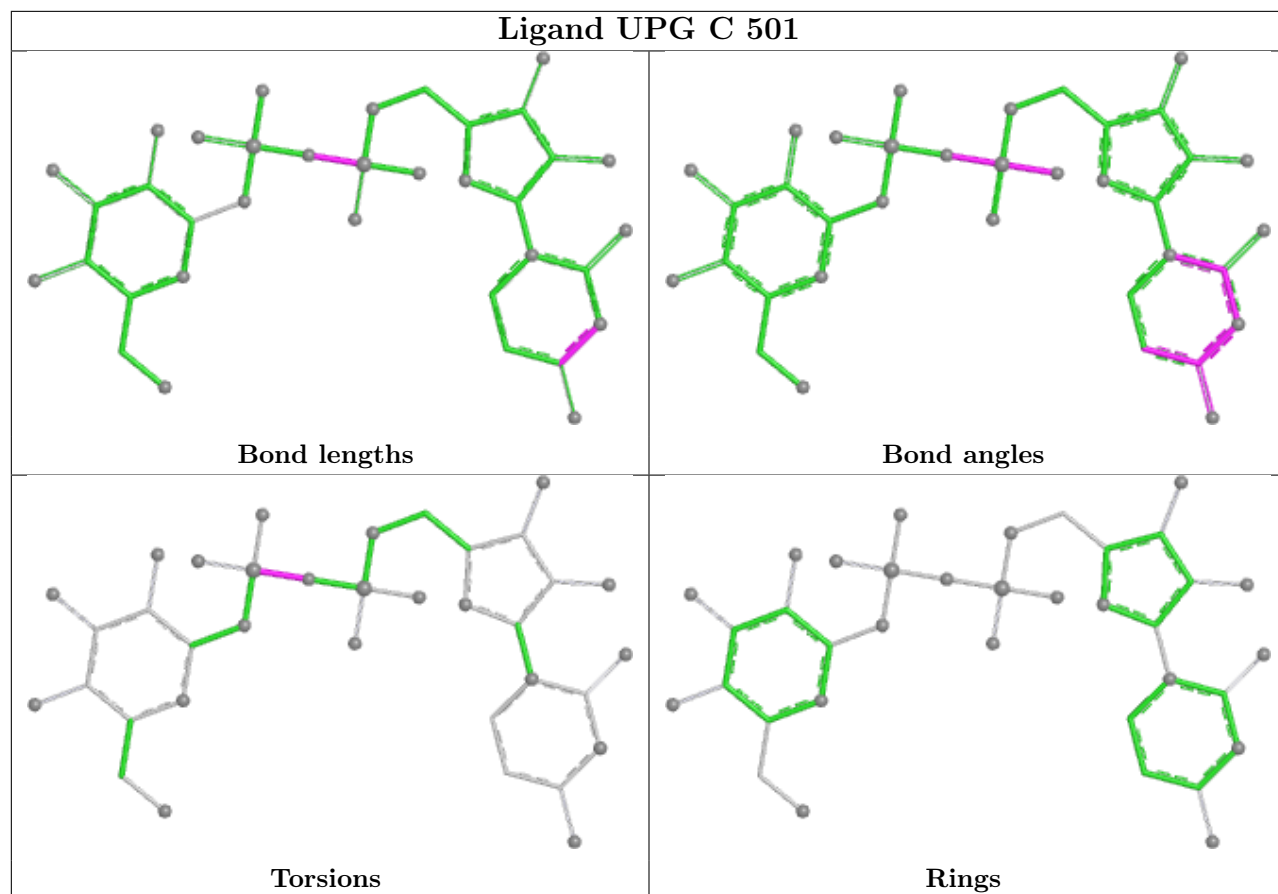


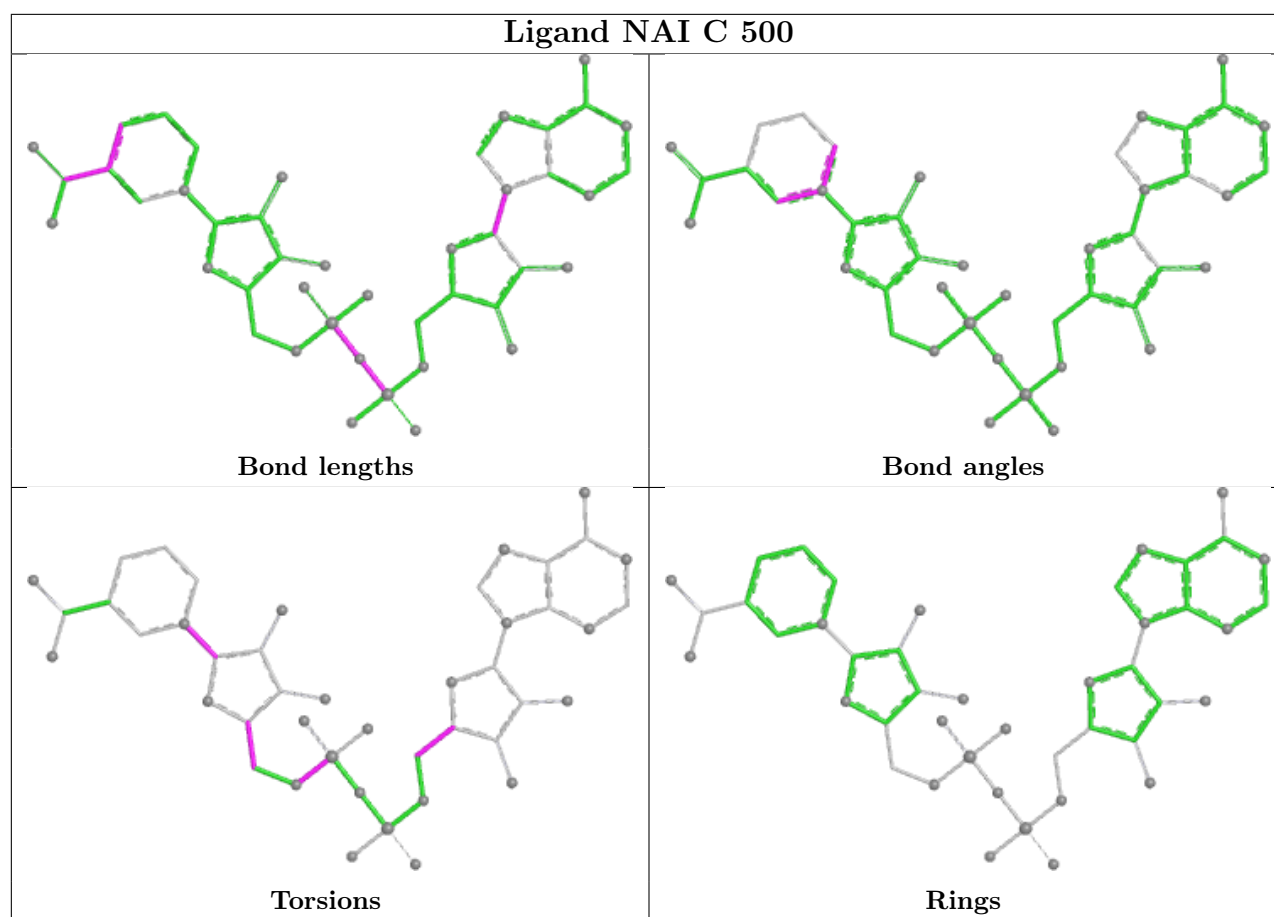












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	454/494 (91%)	-0.24	2 (0%) 89 89	33, 72, 105, 135	0
1	B	323/494 (65%)	0.00	15 (4%) 38 35	24, 66, 125, 166	1 (0%)
1	C	460/494 (93%)	-0.52	0 100 100	29, 54, 91, 135	0
1	D	457/494 (92%)	-0.39	2 (0%) 89 89	31, 63, 106, 142	0
1	E	459/494 (92%)	-0.34	3 (0%) 84 82	27, 66, 104, 129	0
1	F	459/494 (92%)	-0.72	3 (0%) 84 82	23, 43, 67, 104	0
All	All	2612/2964 (88%)	-0.39	25 (0%) 79 77	23, 60, 104, 166	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	VAL	4.5
1	B	116	ILE	3.6
1	B	113	ALA	3.4
1	B	114	ARG	3.4
1	B	189	GLN	3.3
1	B	133	PRO	3.0
1	F	382	HIS	3.0
1	B	198	VAL	2.8
1	B	206	GLU	2.6
1	D	382	HIS	2.6
1	B	112	CYS	2.6
1	B	110	GLU	2.5
1	E	165	GLU	2.5
1	A	73	THR	2.5
1	B	127	THR	2.5
1	B	146	ALA	2.5
1	E	1	MET	2.4
1	D	14	TYR	2.3
1	E	14	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	130	SER	2.3
1	F	389	ASP	2.2
1	B	137	ALA	2.2
1	A	382	HIS	2.1
1	B	111	ALA	2.0
1	F	82	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

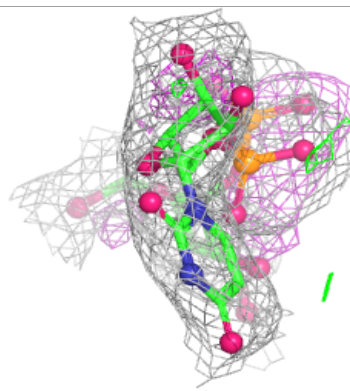
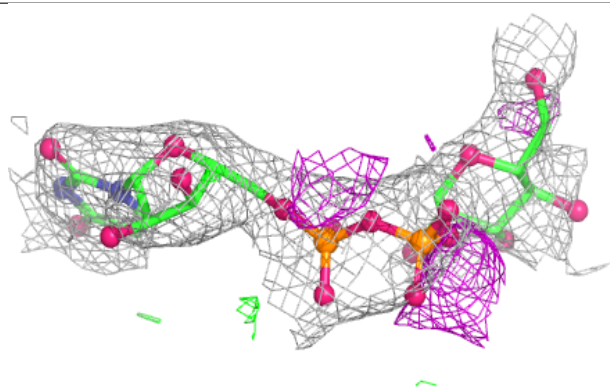
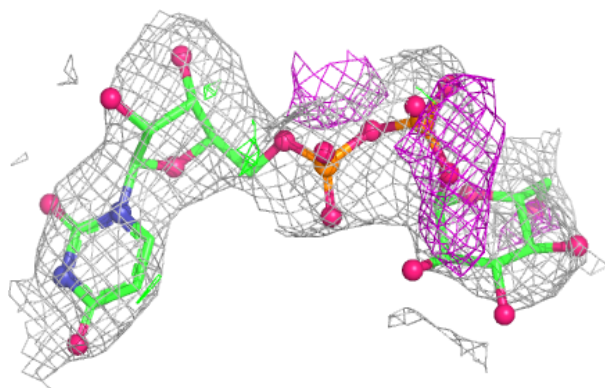
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	UPG	B	501	36/36	0.76	0.14	75,95,117,119	0
2	NAI	E	500	44/44	0.82	0.15	93,115,129,131	0
3	UPG	E	501	36/36	0.83	0.16	94,115,129,131	0
2	NAI	D	500	44/44	0.88	0.11	67,86,97,98	0
3	UPG	D	501	36/36	0.90	0.09	48,59,71,76	0
2	NAI	A	500	44/44	0.93	0.09	53,61,77,80	0
3	UPG	A	501	36/36	0.94	0.08	41,52,60,61	0
2	NAI	C	500	44/44	0.94	0.07	50,59,76,79	0
3	UPG	C	501	36/36	0.95	0.09	36,45,51,56	0
2	NAI	F	500	44/44	0.97	0.06	25,41,49,51	0
3	UPG	F	501	36/36	0.97	0.06	21,34,39,41	0

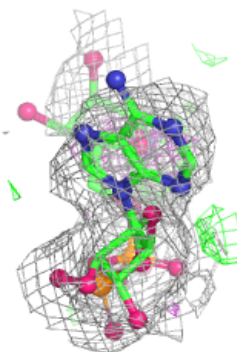
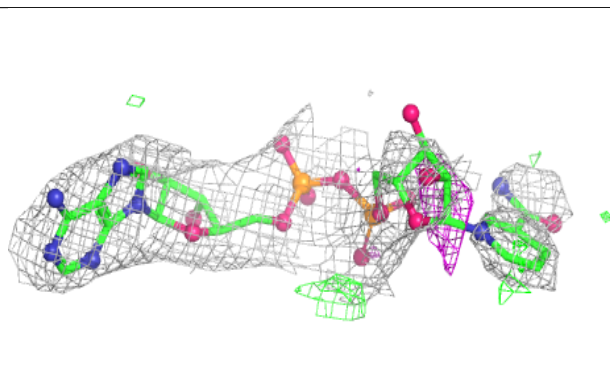
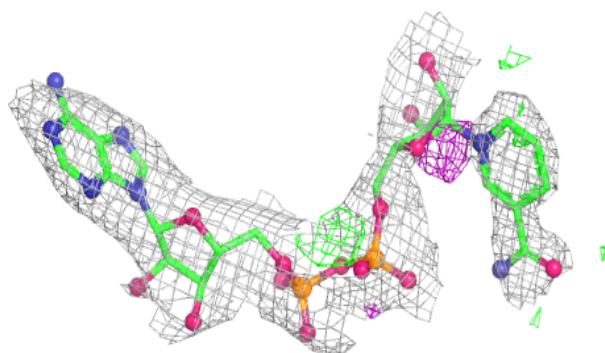
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 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 E 500:**

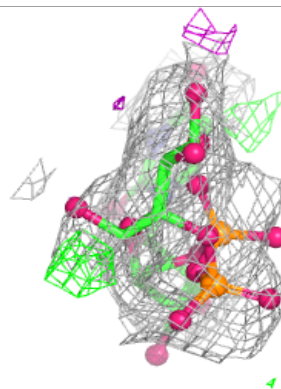
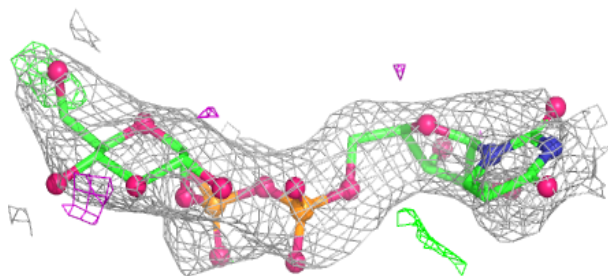
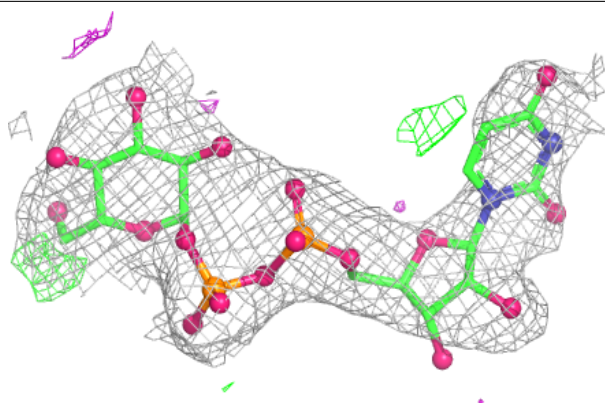
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



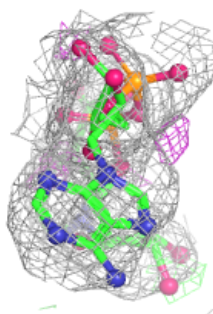
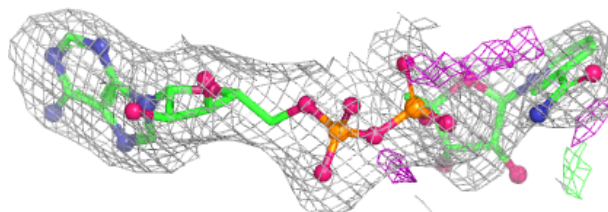
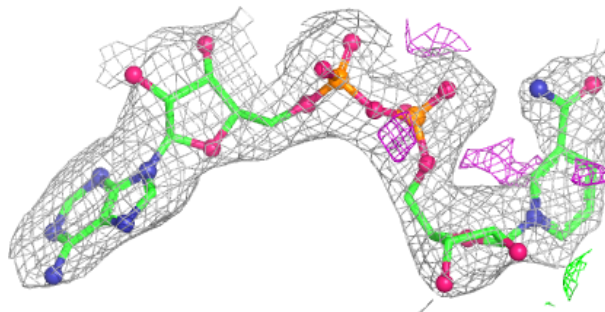


**Electron density around UPG E 501:**

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

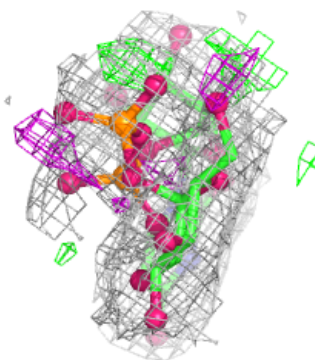
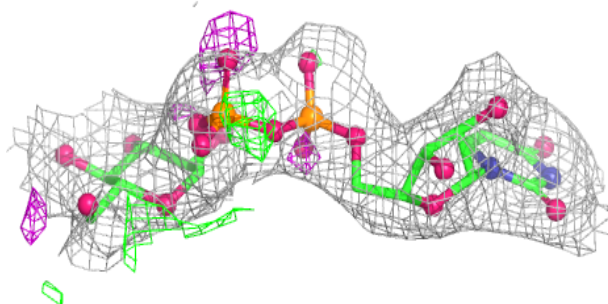
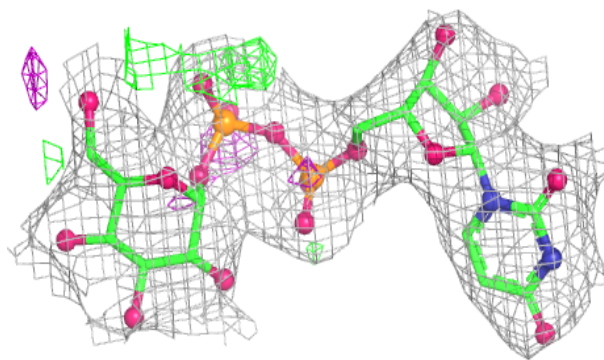
**Electron density around NAI D 500:**

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

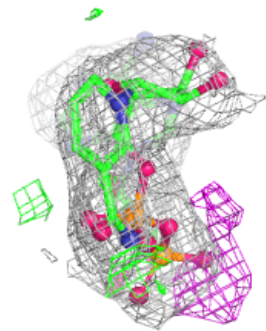
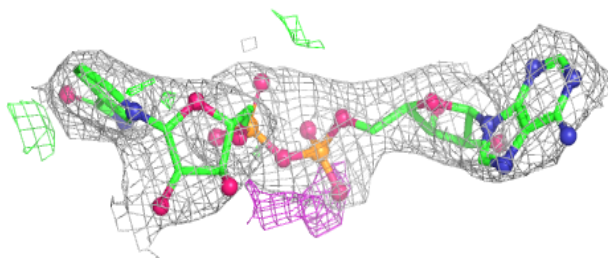
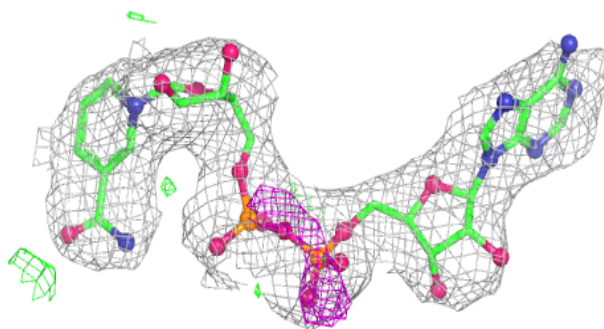


**Electron density around UPG D 501:**

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

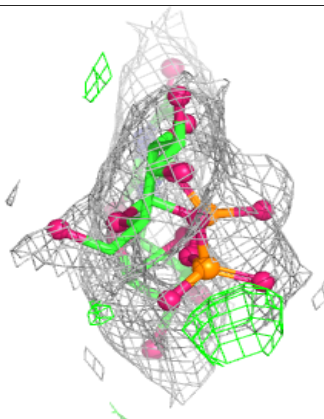
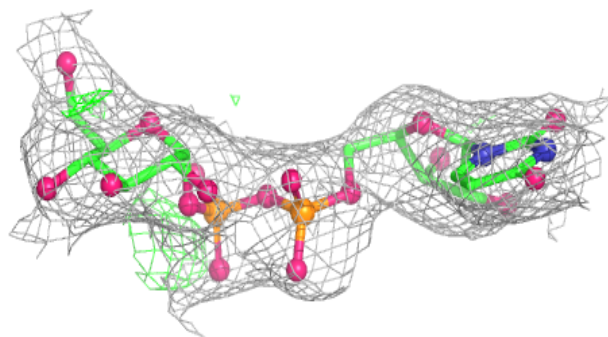
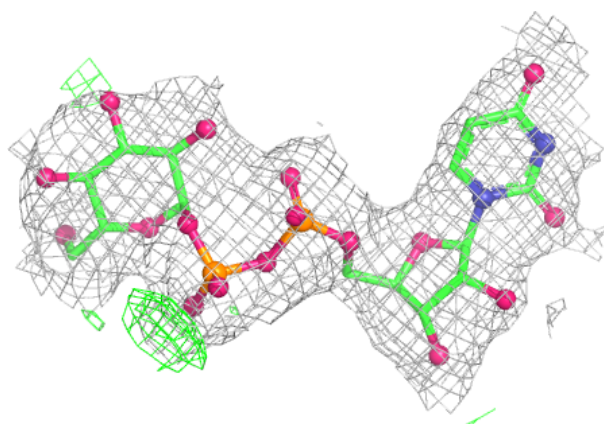
**Electron density around NAI A 500:**

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

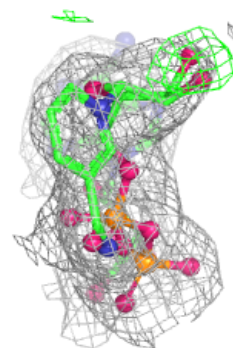
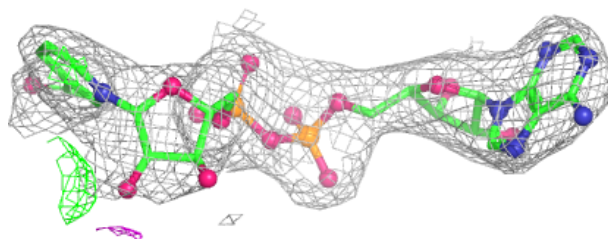


**Electron density around UPG A 501:**

$2mF_o-DF_c$  (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:**

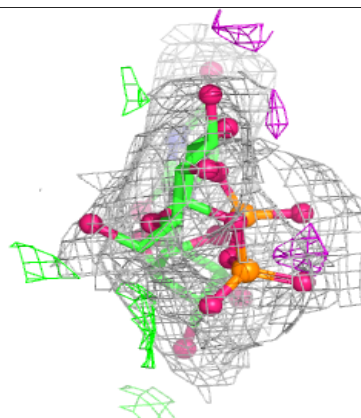
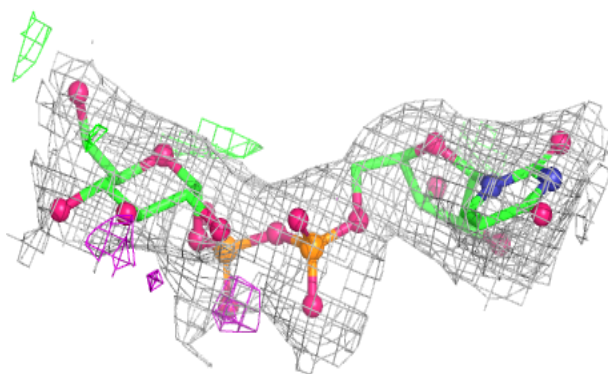
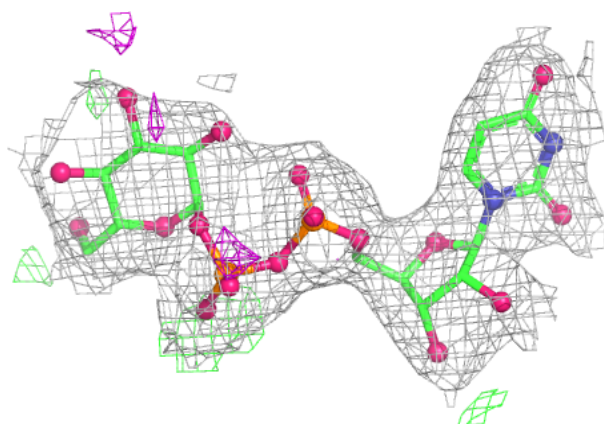
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



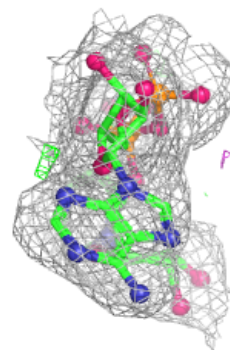
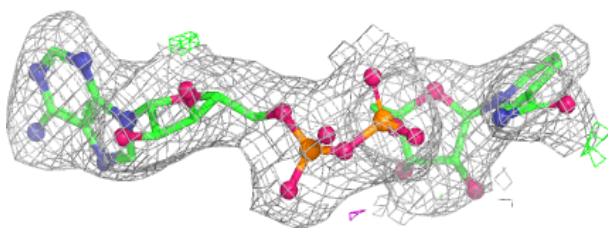
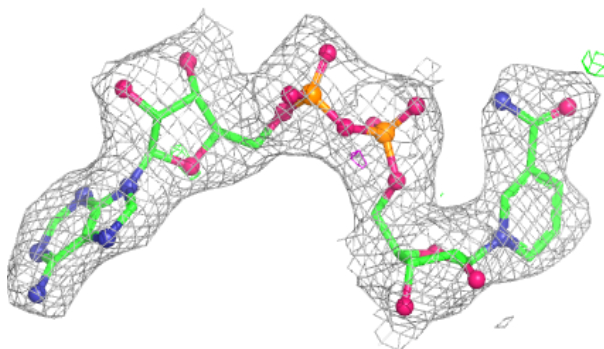


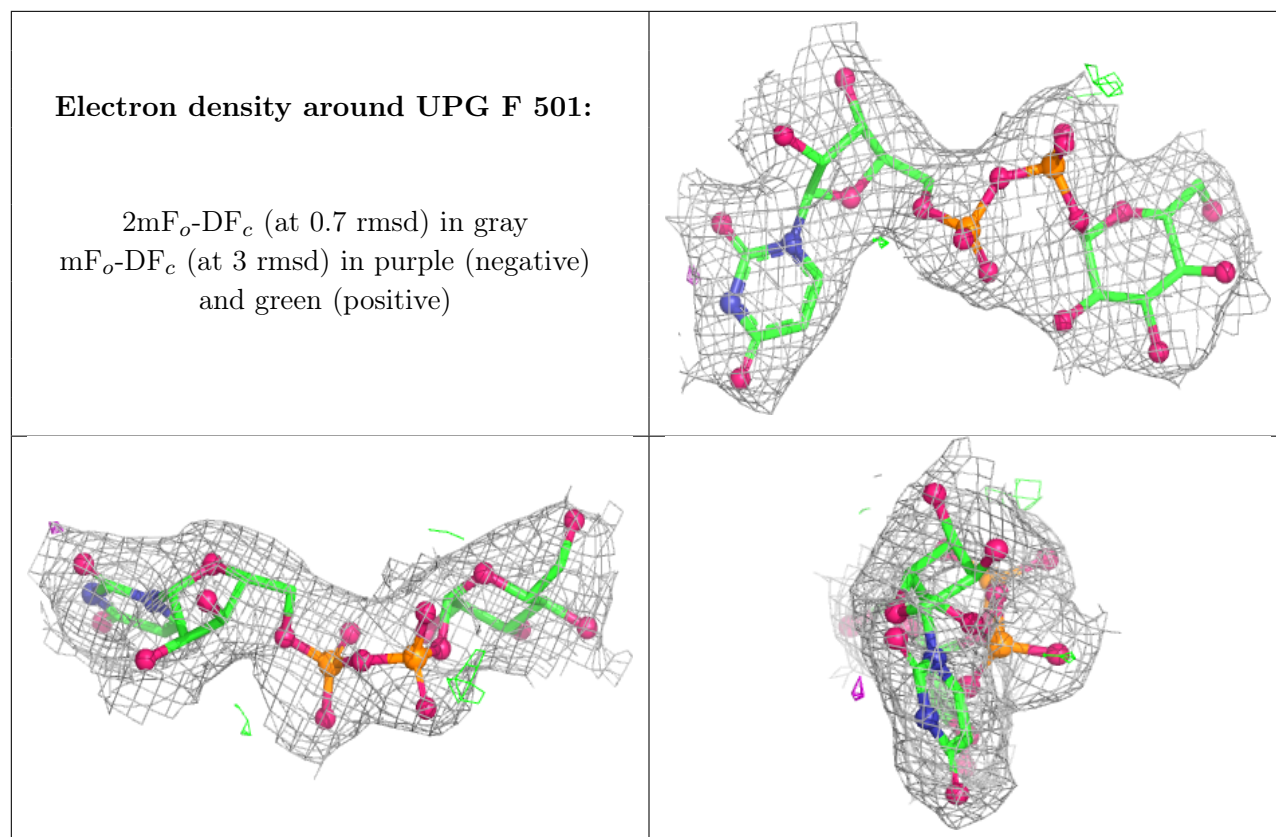
**Electron density around UPG C 501:**

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

**Electron density around NAI F 500:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.