



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:09 PM UTC

PDB ID : 6C5A / pdb_00006c5a
Title : Human UDP-Glucose Dehydrogenase with UDP- Glc and NADH bound
Authors : Gross, P.G.; Fallah, J.; Wood, Z.A.
Deposited on : 2018-01-15
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

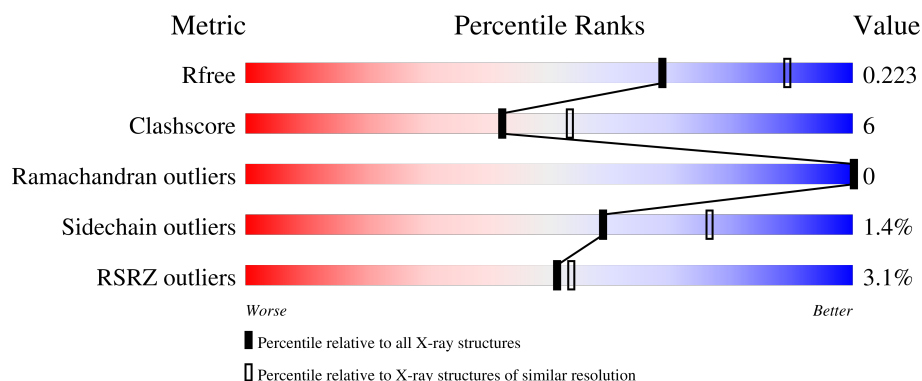
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	82% 11% 7%
1	B	494	82% 10% 7%
1	C	494	81% 11% 7%
1	D	494	78% 14% 7%
1	E	494	77% 15% 8%

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Mol	Chain	Length	Quality of chain
1	F	494	% 80%13%7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	C	503	-	-	X	-

2 Entry composition [i](#)

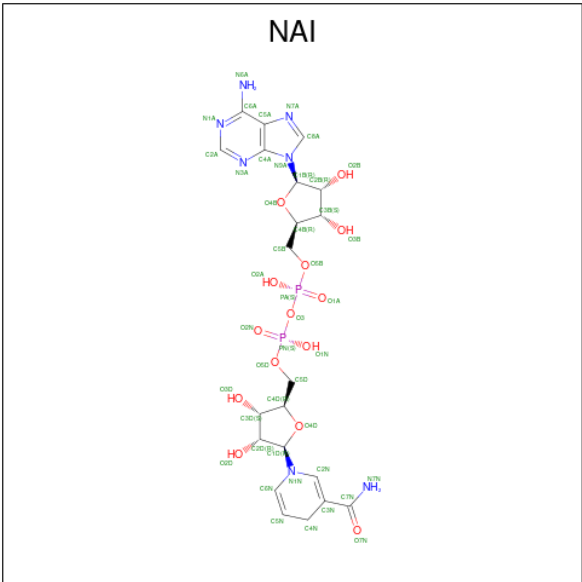
There are 5 unique types of molecules in this entry. The entry contains 22720 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

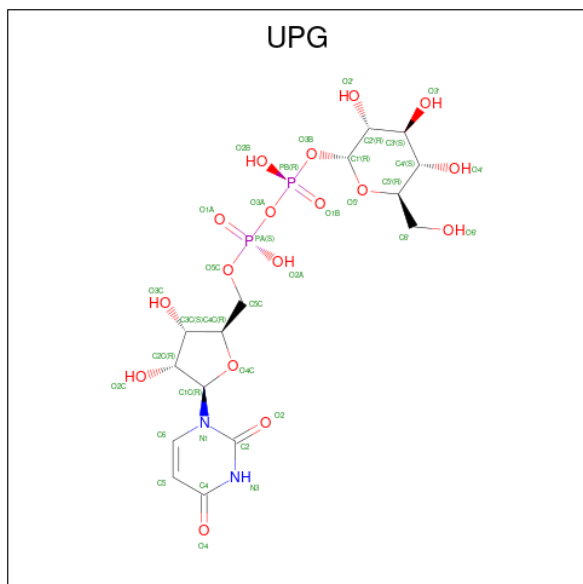
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3599	2277	622	680	20			
1	B	459	Total	C	N	O	S	0	0	0
			3599	2277	622	680	20			
1	C	459	Total	C	N	O	S	0	0	0
			3599	2277	622	680	20			
1	D	459	Total	C	N	O	S	0	0	0
			3599	2277	622	680	20			
1	E	456	Total	C	N	O	S	0	0	0
	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

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



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

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



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

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

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 5 is water.

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

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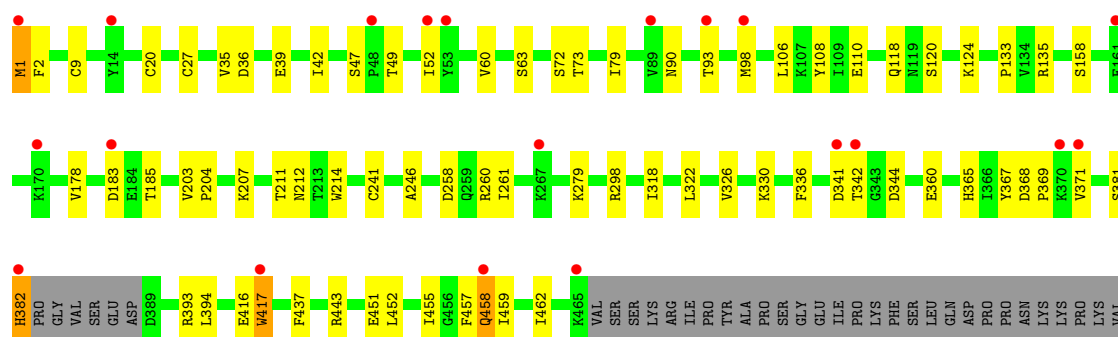
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	45	Total 45	O 45	0	0
5	F	158	Total 158	O 158	0	0

ARG
ILE
PRO
TYR
ALA
PRO
SER
GLY
ILE
PRO
LYS
PHE
SER
LEU
GLN
ASP
PRO
PRO
ASN
LYS
PRO
LYS
VAL

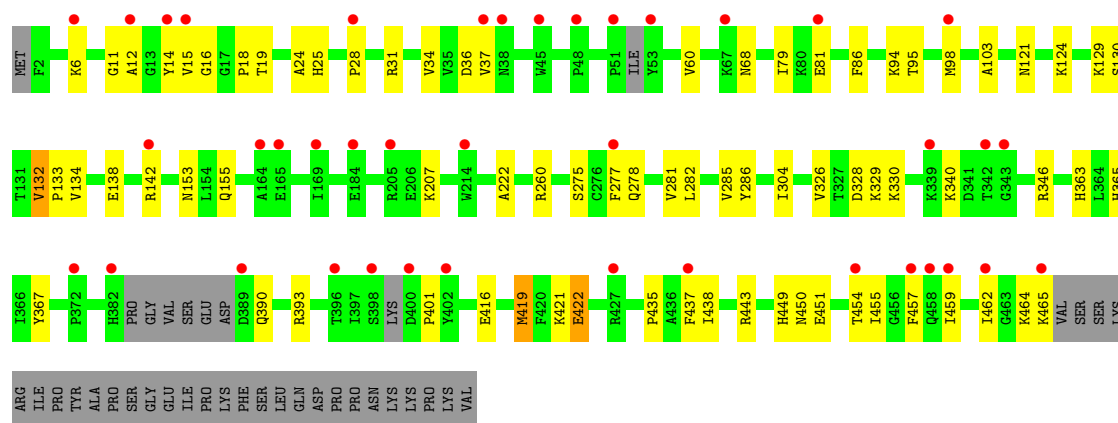
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain D: 4% 78% 14% 7%



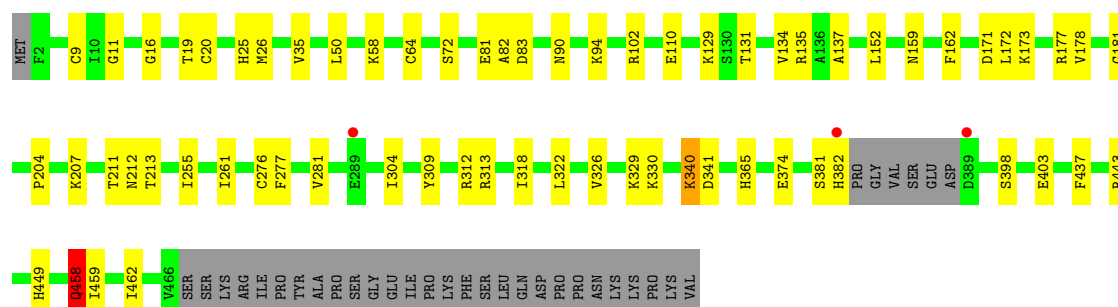
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain E: 8% 77% 15% 8%



• Molecule 1: UDP-glucose 6-dehydrogenase

Chain F: % 80% 13% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.45Å 199.87Å 200.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.75 – 2.30 54.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (54.75-2.30) 99.9 (54.75-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.193 , 0.221 0.195 , 0.223	Depositor DCC
R_{free} test set	8516 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22720	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.70	2/3664 (0.1%)	0.64	3/4956 (0.1%)
1	B	0.68	0/3664	0.66	6/4956 (0.1%)
1	C	0.55	0/3664	0.66	6/4956 (0.1%)
1	D	0.61	1/3664 (0.0%)	0.67	4/4956 (0.1%)
1	E	0.59	3/3637 (0.1%)	0.63	0/4918
1	F	0.56	1/3663 (0.0%)	0.64	5/4956 (0.1%)
All	All	0.62	7/21956 (0.0%)	0.65	24/29698 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	ARG	C-O	-6.04	1.17	1.24
1	E	132	VAL	C-O	-5.83	1.18	1.24
1	E	132	VAL	CA-C	-5.77	1.47	1.52
1	E	132	VAL	N-CA	-5.63	1.41	1.46
1	D	203	VAL	C-O	-5.61	1.18	1.23
1	F	277	PHE	C-O	-5.22	1.18	1.24
1	A	314	PHE	C-O	-5.17	1.18	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	CYS	N-CA-C	10.84	123.18	111.36
1	C	82	ALA	N-CA-C	9.35	123.98	109.96
1	A	276	CYS	N-CA-C	8.44	123.71	113.41
1	B	394	LEU	N-CA-C	7.87	123.95	113.72
1	F	82	ALA	N-CA-C	7.84	121.56	110.50
1	F	276	CYS	N-CA-C	7.68	123.81	113.97
1	C	458	GLN	N-CA-C	-6.69	97.82	108.73
1	B	395	VAL	N-CA-C	6.59	117.39	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	81	GLU	N-CA-C	6.59	118.54	111.36
1	D	120	SER	N-CA-C	6.58	120.19	109.59
1	C	449	HIS	N-CA-C	6.51	118.04	111.07
1	A	458	GLN	N-CA-C	-6.38	98.12	108.52
1	B	458	GLN	N-CA-C	-6.37	98.34	108.73
1	D	417	TRP	N-CA-C	-5.86	101.61	110.28
1	C	81	GLU	N-CA-C	5.78	117.66	111.36
1	B	277	PHE	N-CA-C	5.67	117.14	111.07
1	B	459	ILE	N-CA-C	5.66	116.09	108.17
1	C	459	ILE	N-CA-C	5.65	116.02	108.11
1	F	458	GLN	N-CA-C	-5.54	98.74	108.20
1	C	456	GLY	N-CA-C	5.48	123.64	115.64
1	D	458	GLN	N-CA-C	-5.37	98.48	107.99
1	A	366	ILE	N-CA-C	5.20	115.45	108.17
1	D	203	VAL	N-CA-C	5.16	113.74	107.61
1	F	83	ASP	N-CA-C	-5.05	106.29	112.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3599	0	3618	32	0
1	B	3599	0	3618	35	0
1	C	3599	0	3618	42	0
1	D	3599	0	3618	60	0
1	E	3574	0	3580	56	0
1	F	3598	0	3615	49	0
2	A	44	0	27	3	0
2	B	44	0	27	3	0
2	C	44	0	27	3	0
2	D	44	0	27	3	0
2	E	44	0	27	4	0
2	F	44	0	27	3	0
3	A	36	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	36	0	22	2	0
3	C	36	0	22	2	0
3	D	36	0	22	2	0
3	E	36	0	22	3	0
3	F	36	0	22	2	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	4	0
4	F	4	0	6	3	0
5	A	125	0	0	2	0
5	B	122	0	0	9	0
5	C	132	0	0	4	0
5	D	74	0	0	7	0
5	E	45	0	0	5	0
5	F	158	0	0	6	0
All	All	22720	0	21985	278	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (278) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:500:NAI:H4N	3:E:501:UPG:H6'1	1.56	0.86
2:D:500:NAI:H4N	3:D:501:UPG:H6'1	1.65	0.77
1:E:275:SER:HB3	1:E:346:ARG:HD2	1.67	0.75
1:D:39:GLU:HG3	1:D:73:THR:HG21	1.72	0.69
1:B:224:ASN:ND2	1:B:280:ASP:OD2	2.27	0.68
3:E:501:UPG:H6'2	5:E:623:HOH:O	1.92	0.68
1:B:137:ALA:HB3	1:B:213:THR:CG2	2.24	0.67
1:B:137:ALA:CB	1:B:213:THR:CG2	2.73	0.66
1:B:137:ALA:CB	1:B:213:THR:HG21	2.25	0.66
1:B:409:HIS:ND1	5:B:605:HOH:O	2.29	0.65
1:E:421:LYS:HB3	1:E:422:GLU:OE2	1.96	0.65
1:D:369:PRO:HD2	1:D:417:TRP:NE1	2.12	0.65
1:D:1:MET:HG2	1:D:2:PHE:H	1.62	0.65
1:F:137:ALA:HB3	1:F:213:THR:HG21	1.77	0.65
1:B:181:GLY:HA2	1:B:211:THR:O	1.97	0.64
2:A:501:NAI:H4N	3:A:502:UPG:H6'1	1.78	0.64
2:F:501:NAI:H4N	3:F:502:UPG:H6'1	1.80	0.64
1:B:278:GLN:HB3	5:B:604:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:LYS:HD3	1:E:416:GLU:HG2	1.80	0.64
1:E:153:ASN:OD1	1:E:155:GLN:NE2	2.31	0.63
1:D:451:GLU:O	1:D:455:ILE:HG13	1.98	0.63
1:F:322:LEU:HD22	1:F:326:VAL:HG12	1.79	0.63
1:C:451:GLU:O	1:C:455:ILE:HG13	1.99	0.62
2:C:501:NAI:H4N	3:C:502:UPG:H6'1	1.80	0.62
1:A:137:ALA:HB3	1:A:213:THR:HG21	1.82	0.62
1:F:381:SER:O	1:F:382:HIS:HB2	1.99	0.61
1:F:26:MET:HE3	1:F:173:LYS:HG2	1.81	0.61
1:C:327:THR:O	1:C:328:ASP:HB2	2.00	0.61
1:D:60:VAL:O	1:D:63:SER:OG	2.12	0.61
1:E:103:ALA:HB2	1:E:286:TYR:CD2	2.36	0.61
1:C:247:ASP:OD1	1:C:464:LYS:HG3	2.01	0.61
1:D:178:VAL:HA	5:D:610:HOH:O	2.01	0.61
1:C:330:LYS:HD2	1:C:365:HIS:CD2	2.36	0.60
1:B:3:GLU:OE2	1:B:5:LYS:HE3	2.01	0.60
1:C:204:PRO:HG2	1:C:207:LYS:HD2	1.83	0.60
1:F:322:LEU:CD2	1:F:326:VAL:HG12	2.31	0.60
1:B:275:SER:HB2	5:B:701:HOH:O	2.01	0.60
1:C:326:VAL:HG12	1:C:326:VAL:O	1.99	0.60
1:F:318:ILE:O	1:F:322:LEU:HD13	2.02	0.60
1:C:452:LEU:CD2	1:C:457:PHE:CD2	2.86	0.59
1:E:451:GLU:O	1:E:454:THR:HB	2.02	0.59
1:C:162:PHE:O	4:C:503:DMS:H12	2.02	0.59
1:A:64:CYS:O	1:A:67:LYS:HB2	2.03	0.59
1:C:452:LEU:HD22	1:C:457:PHE:CD2	2.38	0.59
1:D:211:THR:HG23	1:D:212:ASN:O	2.02	0.58
1:E:278:GLN:HG3	1:E:304:ILE:HD12	1.84	0.58
1:E:449:HIS:HE1	5:E:609:HOH:O	1.86	0.58
1:B:137:ALA:HB3	1:B:213:THR:HG21	1.82	0.58
1:E:36:ASP:OD2	2:E:500:NAI:O3B	2.22	0.58
1:E:36:ASP:OD1	2:E:500:NAI:H1B	2.04	0.58
1:B:183:ASP:HB3	1:B:185:THR:HG23	1.85	0.58
1:C:84:LEU:HD12	1:C:125:ILE:O	2.04	0.58
1:A:381:SER:O	1:A:382:HIS:CG	2.56	0.58
1:A:451:GLU:O	1:A:455:ILE:HG13	2.03	0.57
1:A:165:GLU:O	1:A:339:LYS:NZ	2.27	0.57
1:B:277:PHE:HB2	5:B:620:HOH:O	2.04	0.57
1:C:450:ASN:O	1:C:454:THR:HG23	2.04	0.57
1:F:11:GLY:O	1:F:16:GLY:HA3	2.05	0.57
1:D:342:THR:HG22	1:D:344:ASP:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:GLU:HB2	5:C:630:HOH:O	2.04	0.56
1:A:450:ASN:O	1:A:454:THR:HG23	2.05	0.56
1:D:330:LYS:HE3	1:D:365:HIS:CD2	2.41	0.56
2:A:501:NAI:C4N	3:A:502:UPG:H6'1	2.36	0.56
1:D:367:TYR:CD1	1:D:367:TYR:C	2.83	0.56
1:D:452:LEU:HD22	1:D:457:PHE:CD2	2.41	0.56
2:B:501:NAI:H4N	3:B:502:UPG:H6'1	1.87	0.56
1:D:330:LYS:HE3	1:D:365:HIS:CE1	2.41	0.55
1:E:340:LYS:HB3	1:E:416:GLU:HG2	1.89	0.55
1:B:370:LYS:NZ	5:B:610:HOH:O	2.38	0.55
1:C:324:ASN:OD1	1:E:94:LYS:NZ	2.39	0.55
1:E:103:ALA:HB2	1:E:286:TYR:CE2	2.42	0.55
1:F:330:LYS:HE3	1:F:365:HIS:CG	2.42	0.55
1:E:25:HIS:HB2	1:E:60:VAL:HG13	1.89	0.54
2:F:501:NAI:C4N	3:F:502:UPG:H6'1	2.37	0.54
1:E:281:VAL:O	1:E:285:VAL:HG23	2.08	0.54
1:C:26:MET:HE3	1:C:173:LYS:HG2	1.90	0.54
1:E:14:TYR:O	1:E:18:PRO:HD2	2.08	0.54
1:C:326:VAL:CG1	1:C:362:ALA:HB2	2.39	0.53
1:E:28:PRO:HA	1:E:68:ASN:ND2	2.23	0.53
1:E:438:ILE:HG22	1:E:459:ILE:CD1	2.38	0.53
1:F:255:ILE:HG23	1:F:261:ILE:HD13	1.90	0.53
1:B:137:ALA:HB3	1:B:213:THR:HG22	1.90	0.53
1:B:381:SER:O	1:B:382:HIS:CD2	2.62	0.53
1:E:260:ARG:NH2	4:F:503:DMS:H21	2.24	0.53
1:F:152:LEU:HB3	5:F:605:HOH:O	2.09	0.52
1:E:449:HIS:CE1	5:E:609:HOH:O	2.60	0.52
2:C:501:NAI:C4N	3:C:502:UPG:H6'1	2.39	0.52
1:D:368:ASP:OD2	1:D:371:VAL:HG23	2.10	0.52
2:D:500:NAI:C4N	3:D:501:UPG:H6'1	2.39	0.52
1:C:438:ILE:O	1:C:459:ILE:HD12	2.11	0.51
1:D:27:CYS:C	5:D:615:HOH:O	2.54	0.51
1:F:211:THR:OG1	1:F:212:ASN:N	2.43	0.51
1:D:135:ARG:HA	1:D:214:TRP:CZ3	2.45	0.51
1:D:36:ASP:OD2	2:D:500:NAI:O3B	2.18	0.51
1:D:183:ASP:HB3	1:D:185:THR:HG23	1.92	0.51
1:F:162:PHE:O	4:F:503:DMS:H12	2.10	0.51
1:D:106:LEU:HD21	1:D:133:PRO:HD2	1.93	0.51
4:C:503:DMS:H21	1:D:260:ARG:NH2	2.26	0.51
1:E:275:SER:HB3	1:E:346:ARG:CD	2.39	0.51
1:E:443:ARG:HD3	1:E:462:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:GLU:O	1:D:416:GLU:HG2	2.10	0.50
1:F:137:ALA:HB3	1:F:213:THR:CG2	2.40	0.50
1:A:137:ALA:HB3	1:A:213:THR:CG2	2.41	0.50
2:B:501:NAI:C4N	3:B:502:UPG:H6'1	2.41	0.50
1:D:326:VAL:CG2	1:D:360:GLU:CB	2.89	0.50
1:F:137:ALA:CB	1:F:213:THR:HG21	2.41	0.50
1:C:421:LYS:NZ	1:C:421:LYS:HB3	2.26	0.50
1:F:437:PHE:CD2	1:F:458:GLN:HG2	2.46	0.50
1:D:326:VAL:CG2	1:D:360:GLU:HB3	2.42	0.50
1:A:185:THR:HB	1:A:186:PRO:HD2	1.92	0.50
1:C:443:ARG:HD2	1:C:461:THR:OG1	2.12	0.50
1:D:443:ARG:HD3	1:D:462:ILE:O	2.11	0.50
1:F:322:LEU:HD22	1:F:326:VAL:CG1	2.42	0.50
1:D:98:MET:HE1	1:F:312:ARG:HG3	1.93	0.50
1:D:369:PRO:HG2	1:D:417:TRP:CE2	2.47	0.50
1:A:330:LYS:HE3	1:A:365:HIS:CG	2.47	0.50
1:A:330:LYS:HE3	1:A:365:HIS:ND1	2.27	0.49
1:B:443:ARG:HD2	1:B:461:THR:OG1	2.12	0.49
1:F:204:PRO:HD2	1:F:207:LYS:HE3	1.93	0.49
1:F:281:VAL:HB	1:F:304:ILE:HD11	1.94	0.49
1:F:181:GLY:HA2	1:F:211:THR:O	2.13	0.49
1:B:75:ILE:N	5:B:601:HOH:O	2.45	0.49
1:B:211:THR:OG1	1:B:212:ASN:N	2.46	0.48
1:C:19:THR:O	1:C:23:ILE:HG13	2.13	0.48
1:D:369:PRO:HD2	1:D:417:TRP:CD1	2.48	0.48
1:D:298:ARG:HD2	5:D:626:HOH:O	2.12	0.48
1:A:9:CYS:HB2	1:A:20:CYS:SG	2.52	0.48
1:E:326:VAL:HA	1:E:329:LYS:HD2	1.95	0.48
1:D:110:GLU:OE2	1:F:329:LYS:HE2	2.13	0.48
1:F:35:VAL:HA	1:F:72:SER:O	2.12	0.48
1:A:54:GLU:OE2	1:A:166:GLY:N	2.41	0.48
1:A:184:GLU:N	1:A:184:GLU:OE1	2.46	0.48
1:D:9:CYS:HB2	1:D:20:CYS:SG	2.53	0.48
1:E:346:ARG:HD3	5:E:621:HOH:O	2.14	0.48
1:F:398:SER:HB3	1:F:403:GLU:HG3	1.96	0.48
1:A:309:TYR:CZ	1:A:313:ARG:HD3	2.49	0.48
1:B:329:LYS:NZ	1:F:110:GLU:OE2	2.44	0.48
1:C:90:ASN:OD1	1:C:90:ASN:N	2.42	0.48
1:D:108:TYR:HB2	5:D:631:HOH:O	2.12	0.48
1:D:336:PHE:N	1:D:368:ASP:OD1	2.34	0.48
1:F:90:ASN:OD1	1:F:90:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:309:TYR:O	1:F:313:ARG:HB2	2.14	0.48
1:B:165:GLU:O	1:B:339:LYS:NZ	2.32	0.47
1:C:452:LEU:HD23	1:C:457:PHE:CD2	2.48	0.47
1:E:15:VAL:O	1:E:19:THR:OG1	2.27	0.47
1:F:25:HIS:HA	1:F:64:CYS:SG	2.54	0.47
1:C:380:LEU:O	1:C:391:VAL:CG2	2.62	0.47
1:F:374:GLU:CD	1:F:374:GLU:H	2.22	0.47
1:E:138:GLU:O	1:E:142:ARG:HG3	2.13	0.47
1:B:325:THR:CG2	1:F:110:GLU:OE1	2.63	0.47
1:E:133:PRO:O	1:E:134:VAL:C	2.56	0.47
1:F:178:VAL:HA	5:F:608:HOH:O	2.14	0.47
1:B:381:SER:O	1:B:382:HIS:CG	2.68	0.47
1:D:204:PRO:HG2	1:D:207:LYS:HD2	1.96	0.47
1:F:9:CYS:HB2	1:F:20:CYS:SG	2.55	0.47
1:C:74:ASN:ND2	1:C:77:ASP:HB2	2.30	0.47
1:D:369:PRO:CD	1:D:417:TRP:NE1	2.78	0.47
1:E:367:TYR:CE2	1:E:401:PRO:HG3	2.50	0.47
1:B:152:LEU:HB2	5:B:666:HOH:O	2.15	0.46
1:C:250:GLU:OE1	1:D:211:THR:OG1	2.34	0.46
1:C:443:ARG:HD3	1:C:462:ILE:O	2.15	0.46
1:D:207:LYS:NZ	5:D:617:HOH:O	2.47	0.46
1:E:11:GLY:O	1:E:16:GLY:HA3	2.16	0.46
1:E:330:LYS:HE3	1:E:365:HIS:CG	2.51	0.46
1:B:438:ILE:O	1:B:459:ILE:HD12	2.15	0.46
1:C:317:ARG:NH2	1:C:460:GLU:HB3	2.30	0.46
1:A:94:LYS:NZ	5:A:615:HOH:O	2.47	0.46
1:B:449:HIS:O	1:B:453:GLN:HG3	2.16	0.46
2:E:500:NAI:H2N	2:E:500:NAI:H2D	1.72	0.46
1:C:326:VAL:HG11	1:C:362:ALA:HB2	1.97	0.46
1:B:443:ARG:HD3	1:B:462:ILE:O	2.16	0.46
1:E:36:ASP:OD1	1:E:37:VAL:N	2.48	0.46
1:D:330:LYS:HE3	1:D:365:HIS:NE2	2.30	0.46
1:D:158:SER:OG	5:D:601:HOH:O	2.20	0.46
1:A:26:MET:HE3	1:A:202:TRP:HB2	1.98	0.46
1:F:134:VAL:O	1:F:135:ARG:HB2	2.16	0.46
1:D:369:PRO:CD	1:D:417:TRP:CD1	2.99	0.45
1:D:93:THR:HB	5:D:605:HOH:O	2.16	0.45
1:E:450:ASN:O	1:E:454:THR:OG1	2.24	0.45
1:E:6:LYS:HD3	1:E:81:GLU:O	2.16	0.45
1:F:102:ARG:NH2	5:F:612:HOH:O	2.41	0.45
1:C:437:PHE:CE2	1:C:458:GLN:OE1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:CYS:HB3	1:D:246:ALA:O	2.16	0.45
1:E:435:PRO:HG2	1:E:437:PHE:HE1	1.82	0.45
1:F:443:ARG:HD3	1:F:462:ILE:O	2.17	0.45
1:A:314:PHE:CD1	1:A:462:ILE:HD11	2.52	0.45
2:A:501:NAI:H2D	2:A:501:NAI:H2N	1.77	0.45
1:E:390:GLN:HG3	1:E:393:ARG:NH2	2.32	0.45
1:A:211:THR:OG1	1:A:212:ASN:N	2.50	0.45
1:A:333:ILE:HD13	1:A:412:VAL:HB	1.99	0.45
1:E:419:MET:HB2	1:E:419:MET:HE3	1.71	0.45
1:F:50:LEU:HD11	1:F:58:LYS:HA	1.99	0.45
1:F:330:LYS:HE3	1:F:365:HIS:CD2	2.52	0.44
1:B:59:GLU:O	1:B:63:SER:HB3	2.16	0.44
1:C:330:LYS:HD2	1:C:365:HIS:NE2	2.32	0.44
1:B:360:GLU:OE1	1:F:94:LYS:NZ	2.45	0.44
1:D:452:LEU:CD2	1:D:457:PHE:CD2	3.01	0.44
1:A:163:LEU:HD12	1:A:163:LEU:C	2.41	0.44
1:C:324:ASN:HB2	5:C:706:HOH:O	2.17	0.44
1:C:380:LEU:O	1:C:391:VAL:HG22	2.18	0.44
1:C:381:SER:HA	1:C:391:VAL:HG21	1.98	0.44
1:D:90:ASN:OD1	1:D:90:ASN:N	2.43	0.44
1:C:227:LEU:HG	1:D:261:ILE:HD11	1.99	0.44
1:E:6:LYS:HE2	1:E:31:ARG:NH1	2.33	0.44
1:C:279:LYS:HE2	5:C:713:HOH:O	2.17	0.44
1:D:93:THR:OG1	1:D:279:LYS:HB2	2.18	0.44
1:F:131:THR:HA	5:F:627:HOH:O	2.18	0.44
1:E:24:ALA:HB1	1:E:68:ASN:OD1	2.18	0.43
1:E:222:ALA:HB3	1:F:255:ILE:HD11	2.00	0.43
1:C:452:LEU:CD2	1:C:457:PHE:CE2	3.01	0.43
1:B:180:ILE:O	1:B:210:THR:HA	2.19	0.43
1:D:393:ARG:HG3	1:D:394:LEU:HG	2.01	0.43
1:E:464:LYS:HG3	1:E:465:LYS:H	1.84	0.43
1:F:19:THR:HG22	1:F:172:LEU:HD21	2.01	0.43
2:C:501:NAI:H2N	2:C:501:NAI:H2D	1.81	0.43
1:E:277:PHE:CE2	3:E:501:UPG:H5C2	2.54	0.43
1:E:12:ALA:HB2	1:E:34:VAL:HG12	2.00	0.43
1:F:449:HIS:NE2	5:F:606:HOH:O	2.36	0.43
1:D:369:PRO:HD2	1:D:417:TRP:HE1	1.82	0.43
1:A:373:ARG:HG3	1:A:374:GLU:N	2.33	0.43
1:D:79:ILE:O	1:D:124:LYS:HE3	2.19	0.43
1:A:241:CYS:HB3	1:A:246:ALA:O	2.18	0.43
1:B:275:SER:CB	5:B:701:HOH:O	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:LEU:HD23	1:E:282:LEU:HA	1.89	0.43
1:C:253:THR:O	1:C:257:MET:HG3	2.19	0.42
1:D:318:ILE:O	1:D:322:LEU:HG	2.19	0.42
1:C:11:GLY:O	1:C:16:GLY:HA3	2.20	0.42
1:D:369:PRO:CG	1:D:417:TRP:CE2	3.02	0.42
1:E:121:ASN:HA	5:E:601:HOH:O	2.19	0.42
1:E:465:LYS:HD3	1:E:465:LYS:C	2.43	0.42
1:A:35:VAL:HA	1:A:72:SER:O	2.19	0.42
1:E:455:ILE:O	1:E:455:ILE:HG22	2.17	0.42
1:D:437:PHE:CE2	1:D:458:GLN:OE1	2.73	0.42
1:E:328:ASP:HA	1:E:363:HIS:CD2	2.55	0.42
1:D:369:PRO:CG	1:D:417:TRP:NE1	2.83	0.42
1:E:438:ILE:HG22	1:E:459:ILE:HD12	2.01	0.42
1:D:110:GLU:OE2	1:F:329:LYS:CE	2.68	0.42
1:C:326:VAL:HG12	1:C:362:ALA:HB2	2.02	0.42
1:D:47:SER:OG	1:D:49:THR:O	2.38	0.42
1:C:171:ASP:CG	4:C:503:DMS:H13	2.45	0.41
1:E:86:PHE:CD1	1:E:129:LYS:HE2	2.54	0.41
1:F:129:LYS:HG3	1:F:159:ASN:O	2.20	0.41
1:C:312:ARG:HG3	1:E:98:MET:HE1	2.02	0.41
1:E:14:TYR:O	1:E:18:PRO:HG2	2.20	0.41
1:E:435:PRO:HG2	1:E:437:PHE:CE1	2.55	0.41
1:A:309:TYR:O	1:A:313:ARG:HB2	2.20	0.41
2:B:501:NAI:H2N	2:B:501:NAI:H2D	1.84	0.41
1:C:53:TYR:HA	5:C:649:HOH:O	2.20	0.41
1:E:79:ILE:O	1:E:124:LYS:HE3	2.19	0.41
1:F:326:VAL:HA	1:F:329:LYS:HD2	2.03	0.41
1:E:28:PRO:C	1:E:68:ASN:HD22	2.28	0.41
1:F:102:ARG:NH2	5:F:624:HOH:O	2.53	0.41
2:F:501:NAI:H2D	2:F:501:NAI:H2N	1.86	0.41
1:A:93:THR:OG1	1:A:279:LYS:HB2	2.20	0.41
1:A:102:ARG:HD2	5:A:638:HOH:O	2.20	0.41
4:C:503:DMS:H21	1:D:260:ARG:HH21	1.86	0.41
1:D:35:VAL:HA	1:D:72:SER:O	2.20	0.41
1:E:222:ALA:CB	1:F:255:ILE:HD11	2.51	0.41
1:A:19:THR:O	1:A:23:ILE:HG13	2.20	0.41
1:A:328:ASP:HA	1:A:363:HIS:CD2	2.56	0.41
1:D:341:ASP:N	1:D:417:TRP:CH2	2.85	0.41
1:D:437:PHE:CE2	1:D:458:GLN:CD	2.99	0.41
1:F:340:LYS:O	1:F:341:ASP:HB2	2.21	0.41
1:A:1:MET:HE3	1:A:1:MET:HB2	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:SER:O	1:E:132:VAL:HG13	2.20	0.41
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.94	0.40
1:B:74:ASN:OD1	1:B:77:ASP:HB2	2.20	0.40
1:B:360:GLU:HB3	5:B:631:HOH:O	2.20	0.40
1:C:438:ILE:CG2	1:C:459:ILE:HD13	2.52	0.40
1:D:42:ILE:HD13	1:D:42:ILE:HA	1.89	0.40
1:D:258:ASP:HB3	1:D:261:ILE:HD12	2.04	0.40
1:D:381:SER:O	1:D:382:HIS:HB2	2.21	0.40
1:B:130:SER:O	1:B:132:VAL:HG13	2.21	0.40
1:A:11:GLY:O	1:A:16:GLY:HA3	2.21	0.40
1:A:255:ILE:HD11	1:B:222:ALA:HB1	2.03	0.40
1:B:137:ALA:HB1	1:B:213:THR:HG21	2.00	0.40
1:F:9:CYS:CB	1:F:20:CYS:SG	3.09	0.40
1:F:171:ASP:CG	4:F:503:DMS:H13	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/494 (92%)	442 (97%)	13 (3%)	0	100	100
1	B	455/494 (92%)	444 (98%)	11 (2%)	0	100	100
1	C	455/494 (92%)	442 (97%)	13 (3%)	0	100	100
1	D	455/494 (92%)	446 (98%)	9 (2%)	0	100	100
1	E	448/494 (91%)	435 (97%)	13 (3%)	0	100	100
1	F	455/494 (92%)	444 (98%)	11 (2%)	0	100	100
All	All	2723/2964 (92%)	2653 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/426 (92%)	392 (100%)	2 (0%)	81	90
1	B	394/426 (92%)	386 (98%)	8 (2%)	48	67
1	C	394/426 (92%)	386 (98%)	8 (2%)	48	67
1	D	394/426 (92%)	389 (99%)	5 (1%)	61	77
1	E	391/426 (92%)	386 (99%)	5 (1%)	61	77
1	F	394/426 (92%)	390 (99%)	4 (1%)	68	82
All	All	2361/2556 (92%)	2329 (99%)	32 (1%)	59	76

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	LYS
1	A	462	ILE
1	B	32	VAL
1	B	100	LYS
1	B	177	ARG
1	B	206	GLU
1	B	207	LYS
1	B	322	LEU
1	B	393	ARG
1	B	397	ILE
1	C	90	ASN
1	C	98	MET
1	C	177	ARG
1	C	373	ARG
1	C	382	HIS
1	C	421	LYS
1	C	459	ILE
1	C	464	LYS
1	D	1	MET
1	D	52	ILE
1	D	118	GLN
1	D	382	HIS

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Mol	Chain	Res	Type
1	D	459	ILE
1	E	95	THR
1	E	207	LYS
1	E	419	MET
1	E	422	GLU
1	E	457	PHE
1	F	177	ARG
1	F	340	LYS
1	F	458	GLN
1	F	459	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	GLN
1	A	302	GLN
1	A	324	ASN
1	A	363	HIS
1	A	382	HIS
1	B	153	ASN
1	B	155	GLN
1	B	159	ASN
1	B	324	ASN
1	B	363	HIS
1	B	382	HIS
1	B	390	GLN
1	C	302	GLN
1	C	375	GLN
1	D	25	HIS
1	D	46	ASN
1	D	159	ASN
1	D	189	GLN
1	D	259	GLN
1	D	302	GLN
1	D	324	ASN
1	D	409	HIS
1	D	429	HIS
1	E	189	GLN
1	E	301	GLN
1	E	302	GLN
1	E	390	GLN
1	E	409	HIS

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Mol	Chain	Res	Type
1	F	159	ASN
1	F	302	GLN
1	F	375	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAI	B	501	-	47,48,48	1.07	4 (8%)	64,73,73	0.80	1 (1%)
2	NAI	C	501	-	47,48,48	1.12	3 (6%)	64,73,73	0.76	2 (3%)
3	UPG	A	502	-	37,38,38	1.08	2 (5%)	55,58,58	1.39	5 (9%)
3	UPG	E	501	-	37,38,38	1.27	2 (5%)	55,58,58	1.31	5 (9%)
4	DMS	B	503	-	3,3,3	0.67	0	3,3,3	0.52	0
2	NAI	A	501	-	47,48,48	1.05	3 (6%)	64,73,73	0.81	2 (3%)
4	DMS	C	503	-	3,3,3	0.58	0	3,3,3	0.52	0
2	NAI	E	500	-	47,48,48	1.10	3 (6%)	64,73,73	0.87	2 (3%)
3	UPG	B	502	-	37,38,38	1.13	2 (5%)	55,58,58	1.36	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	F	503	-	3,3,3	0.76	0	3,3,3	0.84	0
2	NAI	F	501	-	47,48,48	1.10	4 (8%)	64,73,73	0.80	1 (1%)
3	UPG	F	502	-	37,38,38	1.19	3 (8%)	55,58,58	1.40	6 (10%)
2	NAI	D	500	-	47,48,48	1.14	5 (10%)	64,73,73	0.81	1 (1%)
3	UPG	C	502	-	37,38,38	1.25	2 (5%)	55,58,58	1.46	6 (10%)
3	UPG	D	501	-	37,38,38	1.26	2 (5%)	55,58,58	1.44	6 (10%)
4	DMS	A	503	-	3,3,3	0.66	0	3,3,3	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	B	501	-	-	4/29/72/72	0/5/5/5
2	NAI	C	501	-	-	5/29/72/72	0/5/5/5
3	UPG	A	502	-	-	3/23/59/59	0/3/3/3
3	UPG	E	501	-	-	6/23/59/59	0/3/3/3
2	NAI	A	501	-	-	5/29/72/72	0/5/5/5
2	NAI	E	500	-	-	4/29/72/72	0/5/5/5
3	UPG	B	502	-	-	3/23/59/59	0/3/3/3
2	NAI	F	501	-	-	4/29/72/72	0/5/5/5
3	UPG	F	502	-	-	5/23/59/59	0/3/3/3
2	NAI	D	500	-	-	9/29/72/72	0/5/5/5
3	UPG	C	502	-	-	4/23/59/59	0/3/3/3
3	UPG	D	501	-	-	3/23/59/59	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	501	UPG	PA-O3A	5.47	1.65	1.59
3	D	501	UPG	PA-O3A	5.23	1.65	1.59
3	C	502	UPG	PA-O3A	4.97	1.64	1.59
2	D	500	NAI	PN-O3	4.23	1.64	1.59
3	F	502	UPG	PA-O3A	4.23	1.64	1.59
2	E	500	NAI	PN-O3	4.18	1.64	1.59
3	A	502	UPG	PA-O3A	3.97	1.63	1.59
3	B	502	UPG	PA-O3A	3.84	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAI	PN-O3	3.45	1.63	1.59
2	C	501	NAI	PN-O3	3.44	1.63	1.59
2	B	501	NAI	PN-O3	3.29	1.63	1.59
2	C	501	NAI	PA-O3	-3.28	1.56	1.59
2	F	501	NAI	PA-O3	-3.21	1.56	1.59
2	F	501	NAI	PN-O3	3.10	1.62	1.59
3	C	502	UPG	C4-N3	-2.91	1.33	1.38
3	D	501	UPG	C4-N3	-2.90	1.33	1.38
3	B	502	UPG	C4-N3	-2.88	1.33	1.38
2	B	501	NAI	C4N-C3N	-2.69	1.44	1.50
2	E	500	NAI	C4N-C3N	-2.67	1.45	1.50
2	A	501	NAI	C4N-C3N	-2.62	1.45	1.50
3	F	502	UPG	C4-N3	-2.60	1.34	1.38
2	D	500	NAI	C4N-C3N	-2.56	1.45	1.50
2	F	501	NAI	C4N-C3N	-2.56	1.45	1.50
3	E	501	UPG	C4-N3	-2.50	1.34	1.38
2	B	501	NAI	PA-O3	-2.46	1.56	1.59
2	C	501	NAI	C4N-C3N	-2.40	1.45	1.50
2	B	501	NAI	C7N-C3N	2.34	1.53	1.48
3	A	502	UPG	C4-N3	-2.32	1.34	1.38
2	A	501	NAI	C7N-C3N	2.32	1.53	1.48
2	D	500	NAI	C7N-C3N	2.26	1.53	1.48
2	E	500	NAI	C7N-C3N	2.21	1.53	1.48
2	F	501	NAI	PN-O1N	-2.03	1.45	1.55
3	F	502	UPG	PB-O3A	-2.01	1.57	1.59
2	D	500	NAI	C8A-N7A	2.01	1.35	1.31
2	D	500	NAI	C6N-N1N	2.01	1.42	1.37

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	UPG	C4-N3-C2	-5.54	119.73	126.61
3	B	502	UPG	C4-N3-C2	-5.47	119.82	126.61
3	C	502	UPG	C4-N3-C2	-5.40	119.90	126.61
3	F	502	UPG	C4-N3-C2	-5.23	120.12	126.61
3	A	502	UPG	C4-N3-C2	-5.22	120.13	126.61
3	E	501	UPG	C4-N3-C2	-5.19	120.17	126.61
3	C	502	UPG	C5-C4-N3	5.14	122.00	114.80
3	D	501	UPG	C5-C4-N3	4.98	121.78	114.80
3	A	502	UPG	C5-C4-N3	4.76	121.47	114.80
3	F	502	UPG	C5-C4-N3	4.69	121.37	114.80
3	B	502	UPG	C5-C4-N3	4.63	121.28	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	UPG	C5-C4-N3	4.62	121.27	114.80
2	E	500	NAI	C6N-N1N-C2N	3.91	123.50	119.32
2	A	501	NAI	C6N-N1N-C2N	3.82	123.40	119.32
2	D	500	NAI	C6N-N1N-C2N	3.38	122.93	119.32
2	B	501	NAI	C6N-N1N-C2N	3.31	122.87	119.32
3	C	502	UPG	O4-C4-N3	-3.21	114.63	119.27
3	F	502	UPG	O2A-PA-O3A	3.00	115.37	107.27
2	C	501	NAI	C6N-N1N-C2N	2.95	122.47	119.32
3	D	501	UPG	O4-C4-N3	-2.93	115.03	119.27
3	A	502	UPG	O3A-PA-O1A	-2.88	102.04	110.70
2	F	501	NAI	C6N-N1N-C2N	2.86	122.38	119.32
3	B	502	UPG	N3-C2-N1	2.84	118.59	114.89
3	A	502	UPG	O2A-PA-O3A	2.73	114.64	107.27
3	D	501	UPG	N3-C2-N1	2.70	118.41	114.89
3	B	502	UPG	O3A-PA-O1A	-2.64	102.75	110.70
3	C	502	UPG	O2A-PA-O3A	2.63	114.37	107.27
3	F	502	UPG	O3A-PA-O1A	-2.59	102.92	110.70
3	E	501	UPG	N3-C2-N1	2.51	118.16	114.89
3	F	502	UPG	N3-C2-N1	2.49	118.13	114.89
2	C	501	NAI	O4B-C1B-C2B	-2.47	101.34	106.62
3	C	502	UPG	N3-C2-N1	2.43	118.06	114.89
3	D	501	UPG	O3A-PA-O1A	-2.41	103.44	110.70
3	B	502	UPG	O4-C4-N3	-2.39	115.82	119.27
3	E	501	UPG	O3A-PA-O1A	-2.35	103.64	110.70
3	D	501	UPG	O2A-PA-O3A	2.23	113.31	107.27
3	C	502	UPG	O3A-PA-O1A	-2.23	104.00	110.70
2	E	500	NAI	O4B-C1B-C2B	-2.18	101.94	106.62
3	A	502	UPG	N3-C2-N1	2.18	117.73	114.89
3	F	502	UPG	C3'-C4'-C5'	-2.18	106.28	110.23
2	A	501	NAI	O4B-C1B-C2B	-2.13	102.06	106.62
3	E	501	UPG	O4-C4-N3	-2.04	116.31	119.27
3	B	502	UPG	O2A-PA-O3A	2.00	112.69	107.27

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	500	NAI	C5B-O5B-PA-O1A
3	A	502	UPG	C1'-O3B-PB-O3A
3	F	502	UPG	PA-O3A-PB-O3B
2	E	500	NAI	C2D-C1D-N1N-C6N
2	E	500	NAI	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	D	500	NAI	C3B-C4B-C5B-O5B
2	D	500	NAI	O4B-C4B-C5B-O5B
3	E	501	UPG	O4C-C4C-C5C-O5C
3	F	502	UPG	C4'-C5'-C6'-O6'
2	F	501	NAI	C2D-C1D-N1N-C6N
3	B	502	UPG	PB-O3A-PA-O1A
3	F	502	UPG	PB-O3A-PA-O1A
3	E	501	UPG	C4'-C5'-C6'-O6'
3	B	502	UPG	PA-O3A-PB-O3B
3	C	502	UPG	PA-O3A-PB-O3B
3	D	501	UPG	PA-O3A-PB-O3B
3	E	501	UPG	PA-O3A-PB-O3B
2	F	501	NAI	C2D-C1D-N1N-C2N
2	C	501	NAI	C2D-C1D-N1N-C6N
2	E	500	NAI	O4D-C1D-N1N-C6N
2	A	501	NAI	C2B-C1B-N9A-C8A
3	D	501	UPG	PB-O3A-PA-O2A
2	A	501	NAI	C2D-C1D-N1N-C2N
2	A	501	NAI	C2D-C1D-N1N-C6N
2	B	501	NAI	C2D-C1D-N1N-C6N
2	C	501	NAI	C2D-C1D-N1N-C2N
3	E	501	UPG	C3C-C4C-C5C-O5C
3	A	502	UPG	C4'-C5'-C6'-O6'
2	E	500	NAI	O4D-C1D-N1N-C2N
2	B	501	NAI	C2D-C1D-N1N-C2N
3	F	502	UPG	O5'-C5'-C6'-O6'
2	D	500	NAI	C5B-O5B-PA-O2A
2	D	500	NAI	C5B-O5B-PA-O3
2	F	501	NAI	O4D-C1D-N1N-C2N
2	F	501	NAI	O4D-C1D-N1N-C6N
3	C	502	UPG	PB-O3A-PA-O1A
3	C	502	UPG	PB-O3A-PA-O2A
2	C	501	NAI	O4D-C1D-N1N-C6N
3	E	501	UPG	O5'-C5'-C6'-O6'
2	B	501	NAI	O4D-C1D-N1N-C6N
2	D	500	NAI	C2D-C1D-N1N-C6N
2	A	501	NAI	O4D-C1D-N1N-C6N
2	D	500	NAI	O4D-C1D-N1N-C6N
3	C	502	UPG	C4'-C5'-C6'-O6'
3	A	502	UPG	PB-O3A-PA-O1A
3	F	502	UPG	PB-O3A-PA-O2A
2	C	501	NAI	O4D-C1D-N1N-C2N

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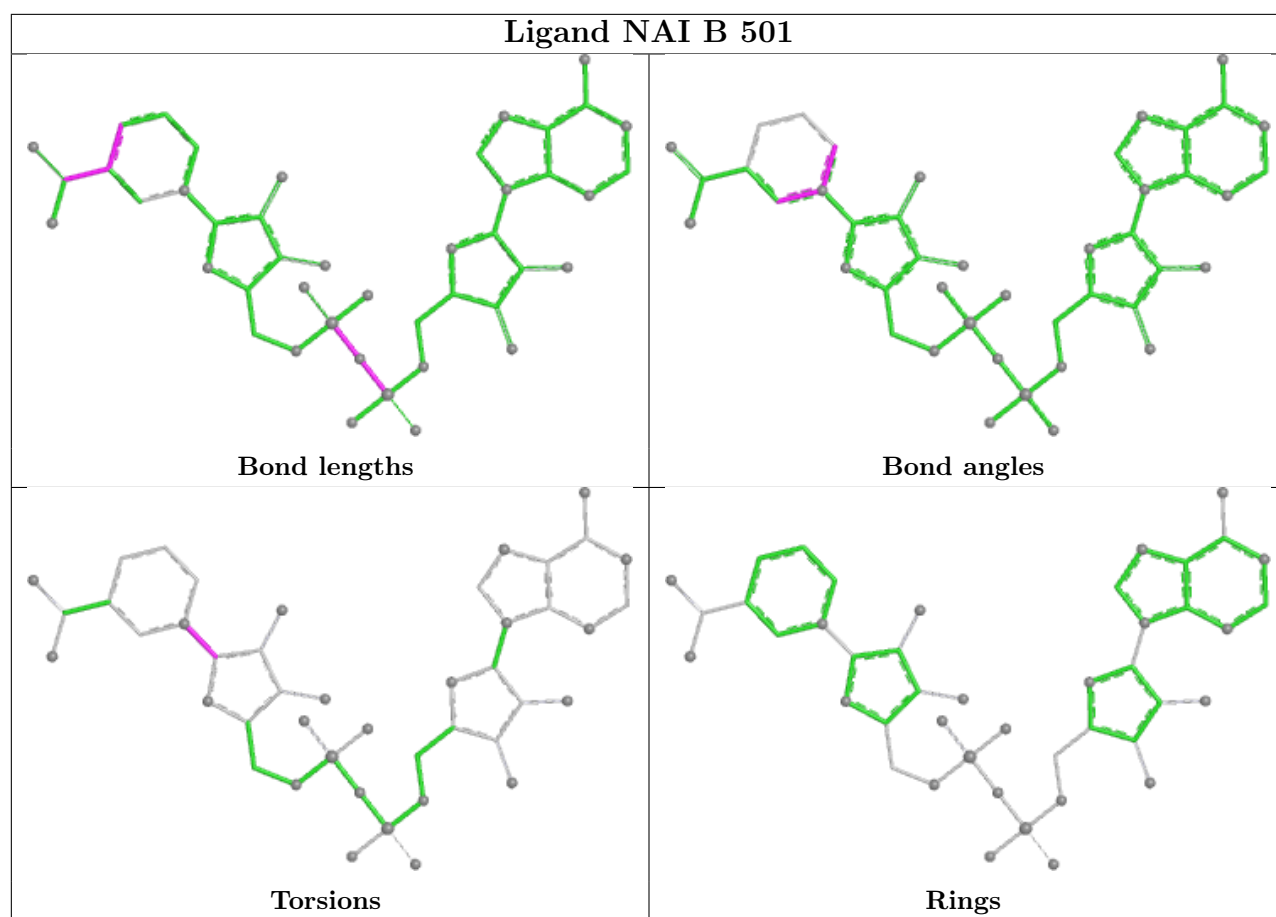
Mol	Chain	Res	Type	Atoms
2	B	501	NAI	O4D-C1D-N1N-C2N
2	A	501	NAI	O4D-C1D-N1N-C2N
3	D	501	UPG	PB-O3A-PA-O1A
3	E	501	UPG	PA-O3A-PB-O1B
2	D	500	NAI	C2D-C1D-N1N-C2N
2	D	500	NAI	O4D-C1D-N1N-C2N
3	B	502	UPG	PB-O3A-PA-O2A
2	C	501	NAI	O4B-C4B-C5B-O5B

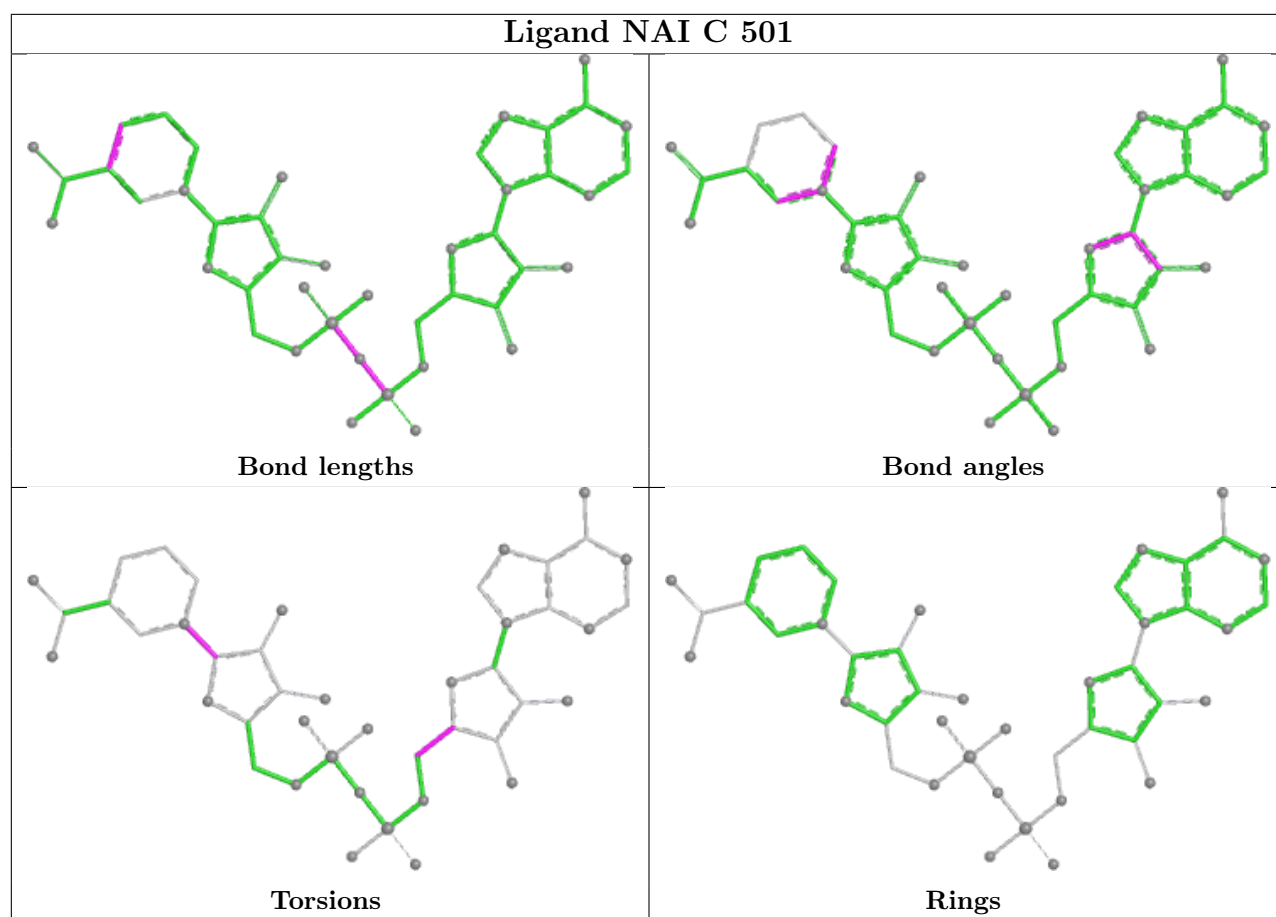
There are no ring outliers.

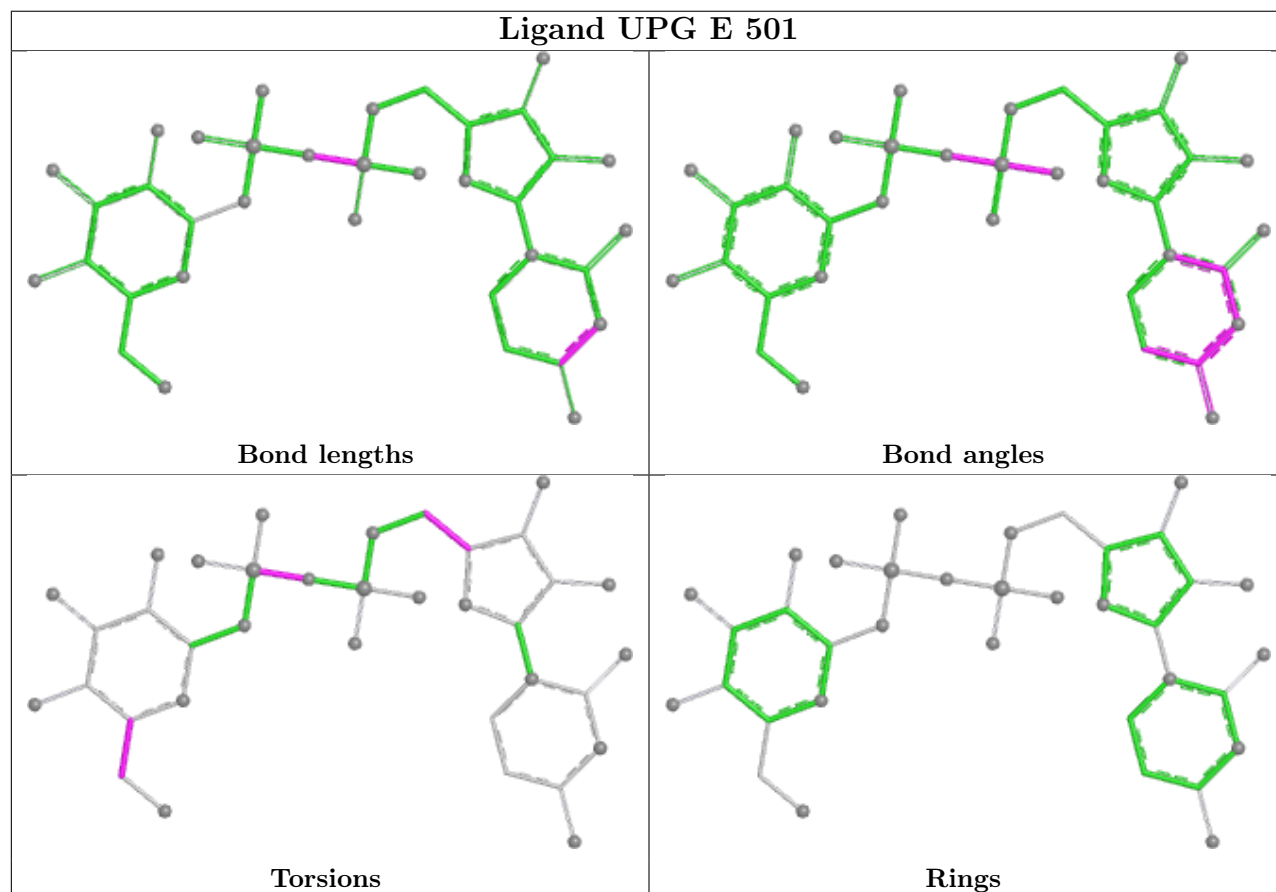
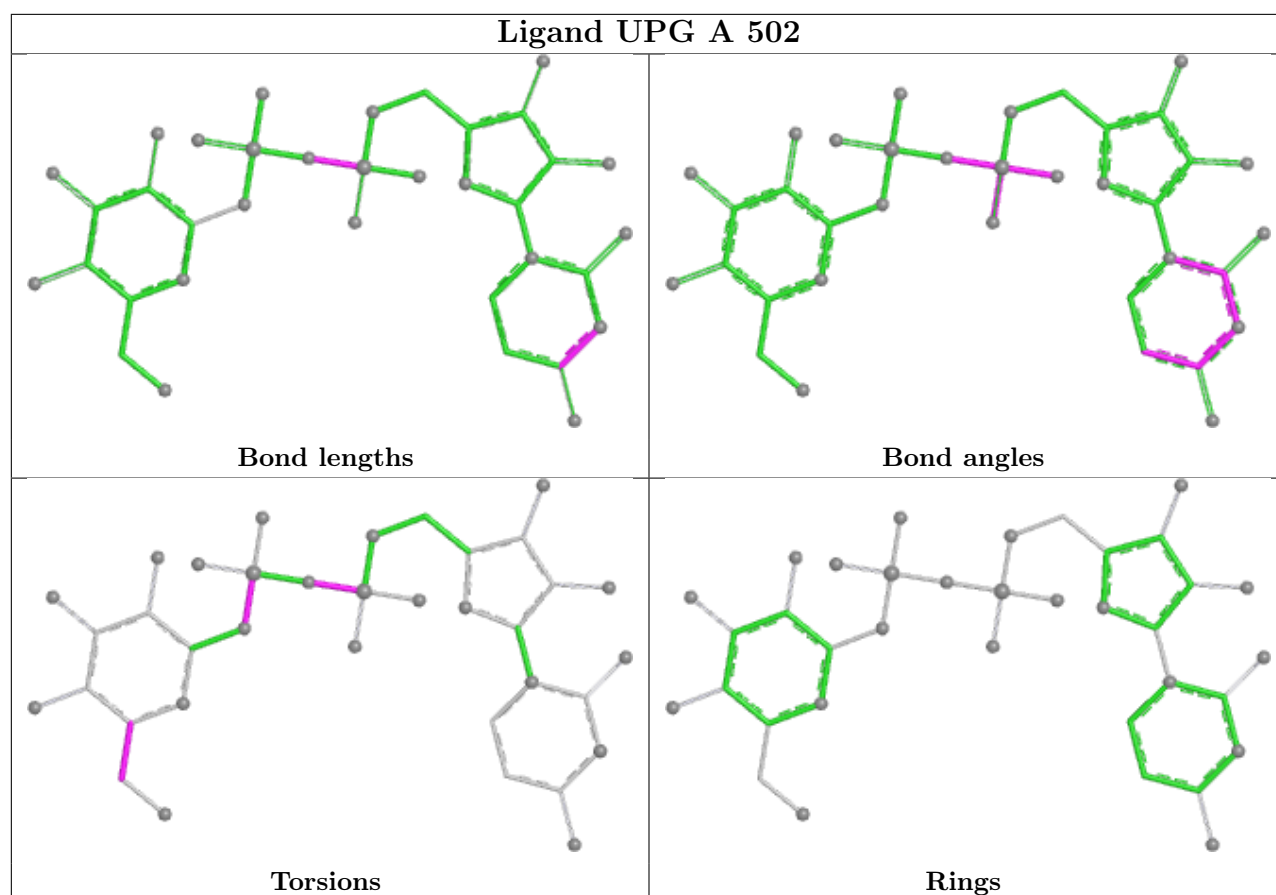
14 monomers are involved in 28 short contacts:

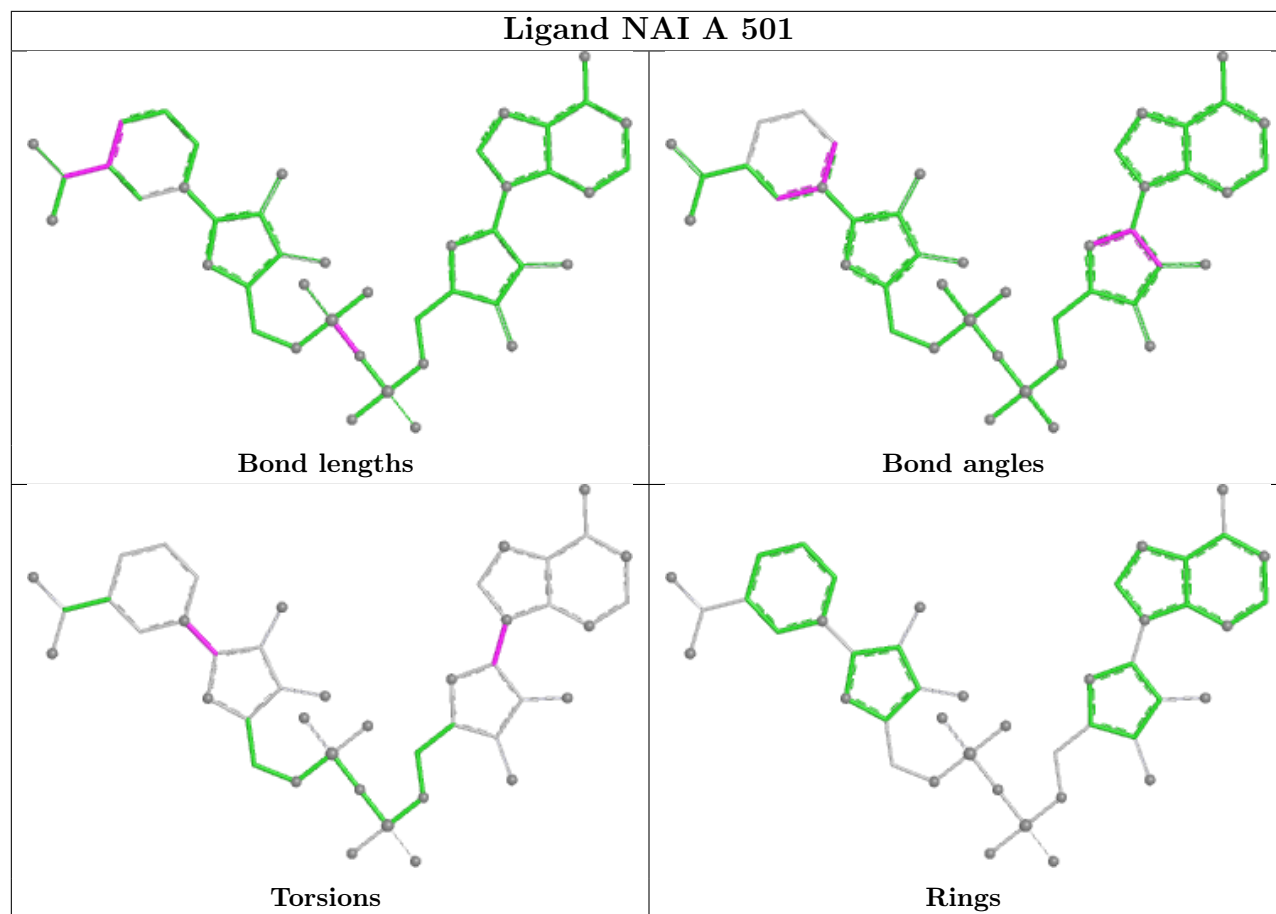
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NAI	3	0
2	C	501	NAI	3	0
3	A	502	UPG	2	0
3	E	501	UPG	3	0
2	A	501	NAI	3	0
4	C	503	DMS	4	0
2	E	500	NAI	4	0
3	B	502	UPG	2	0
4	F	503	DMS	3	0
2	F	501	NAI	3	0
3	F	502	UPG	2	0
2	D	500	NAI	3	0
3	C	502	UPG	2	0
3	D	501	UPG	2	0

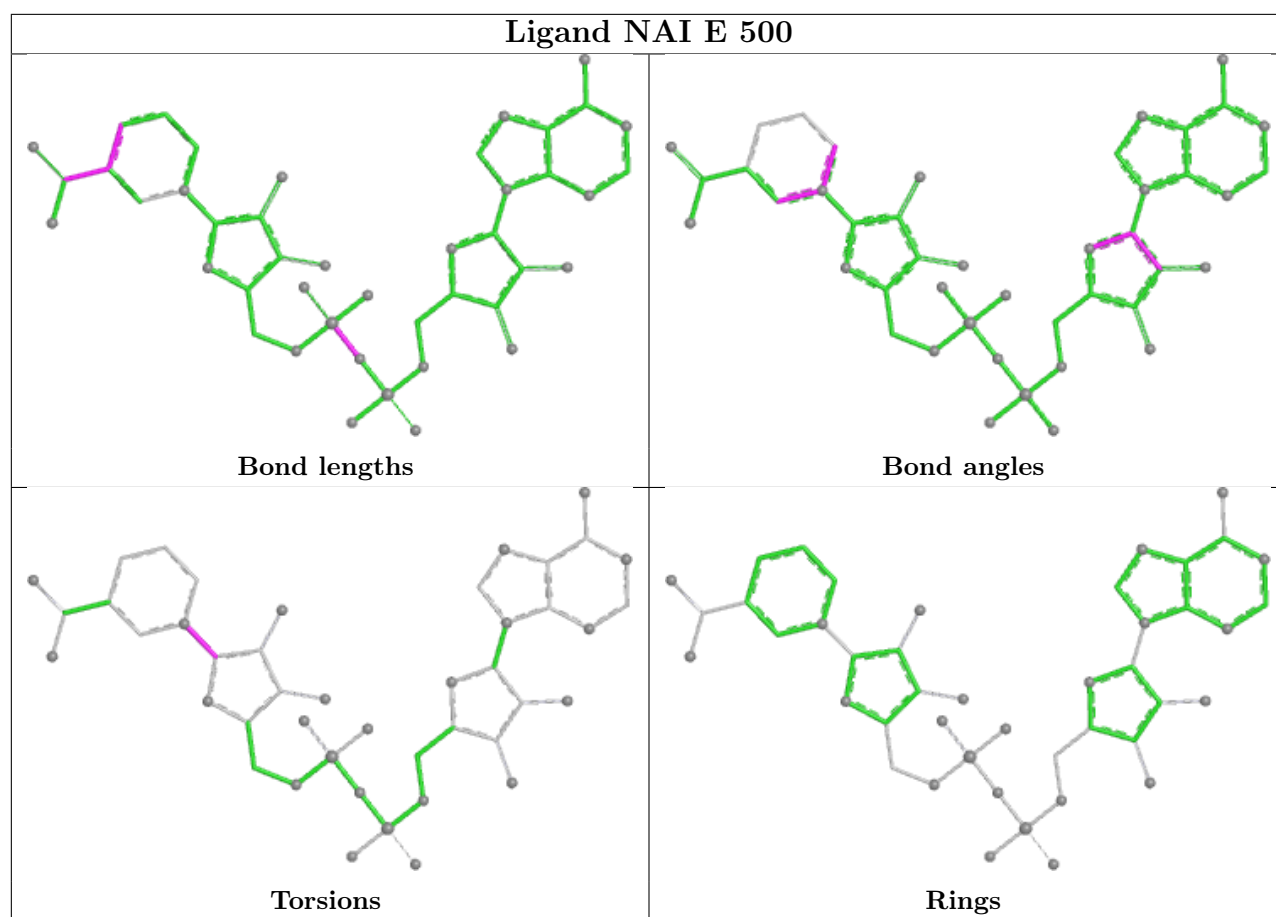
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

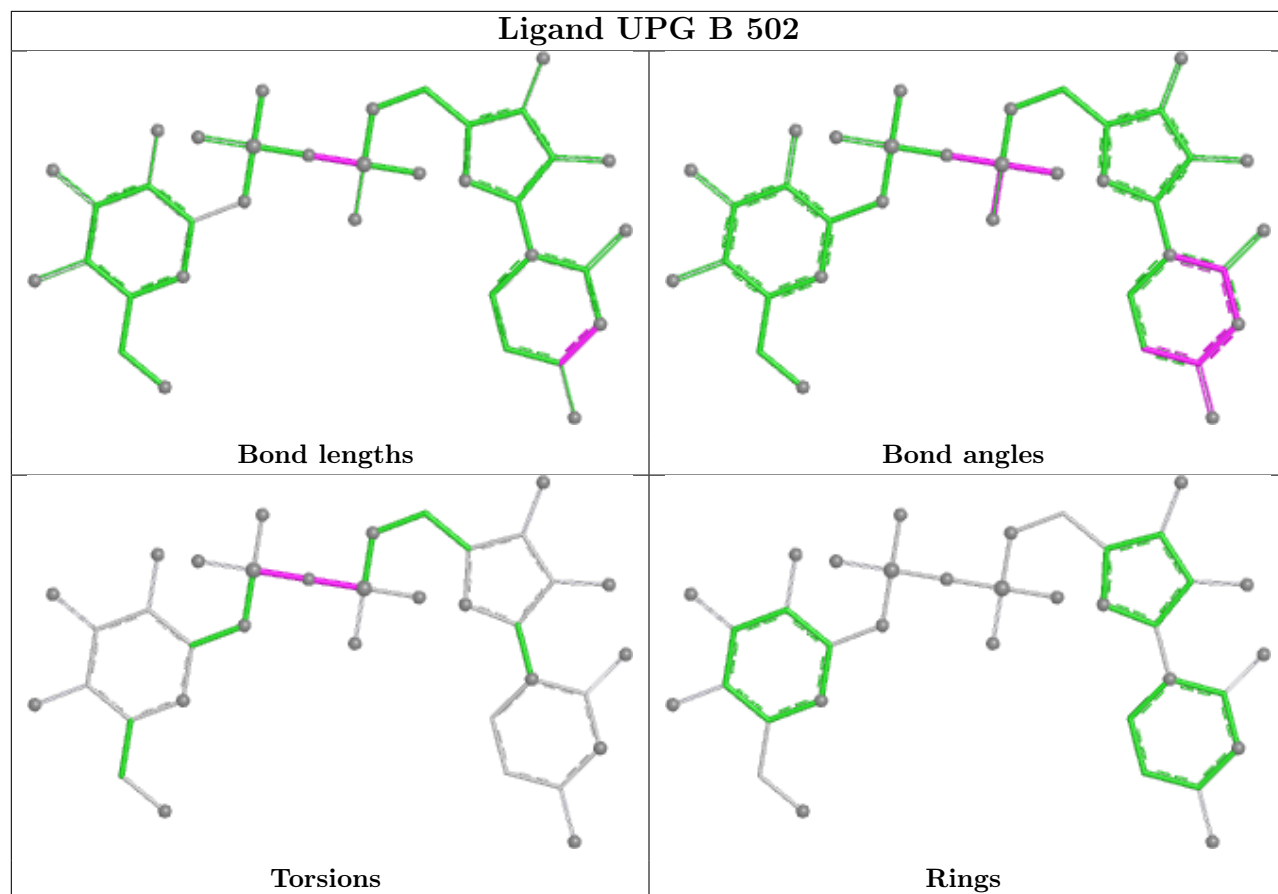


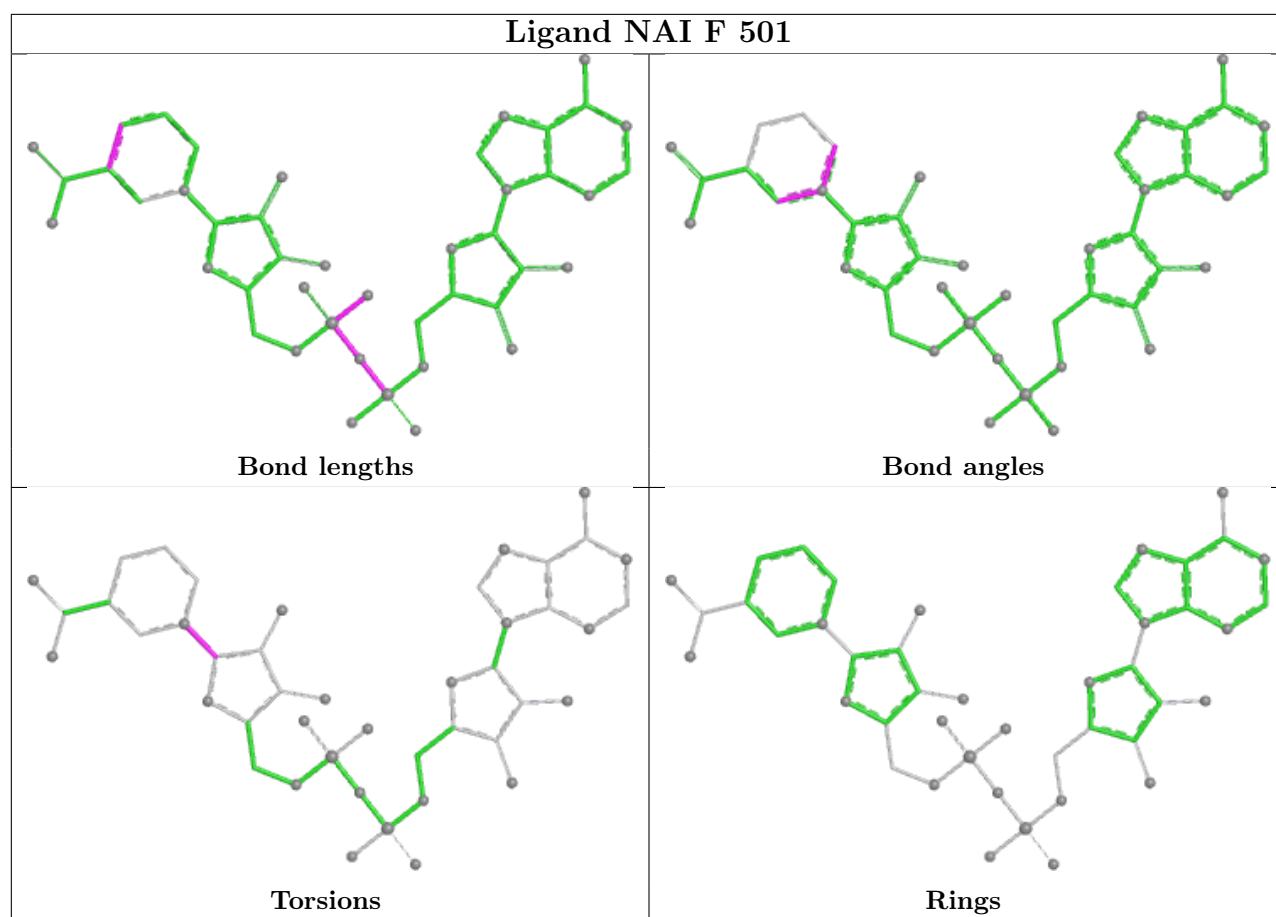


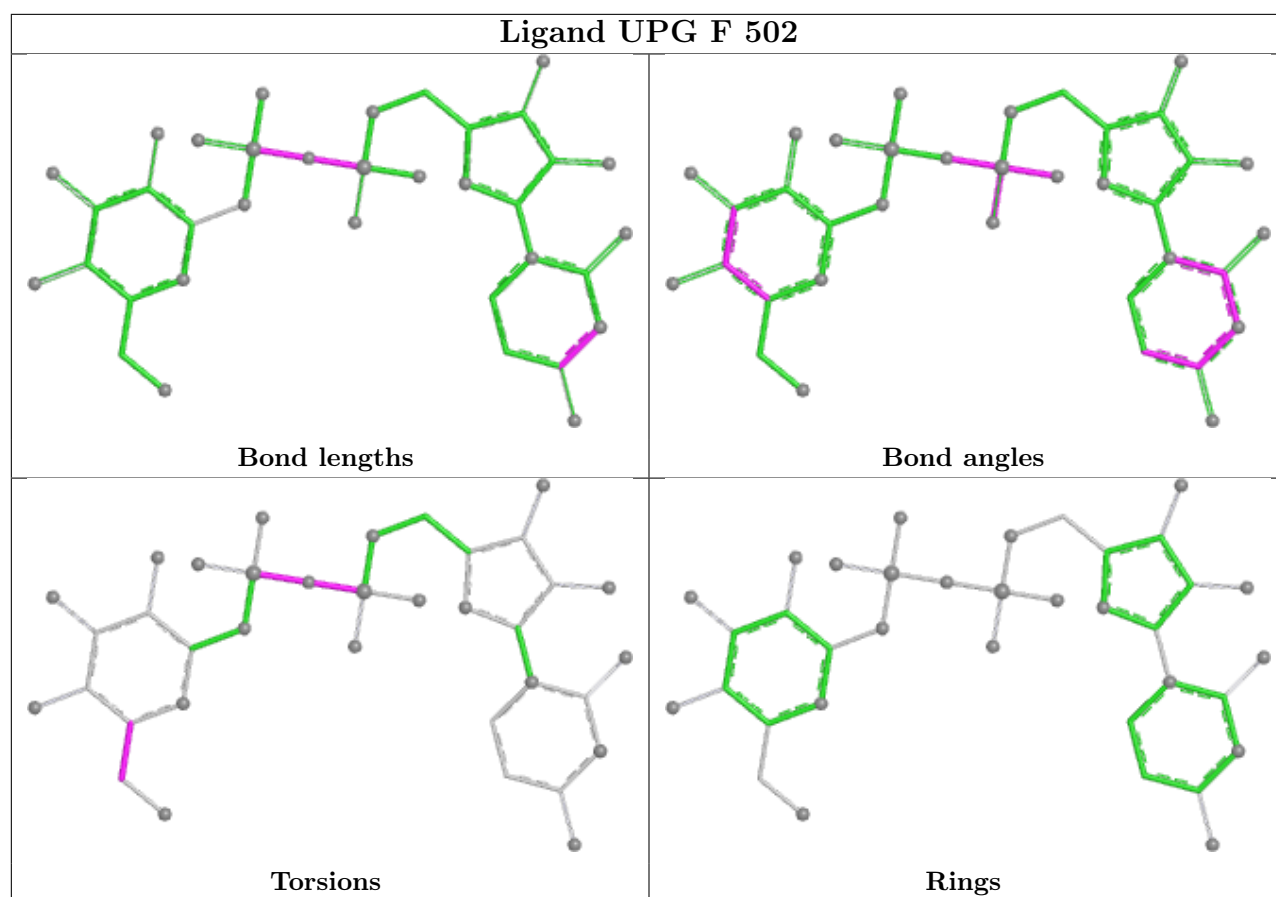


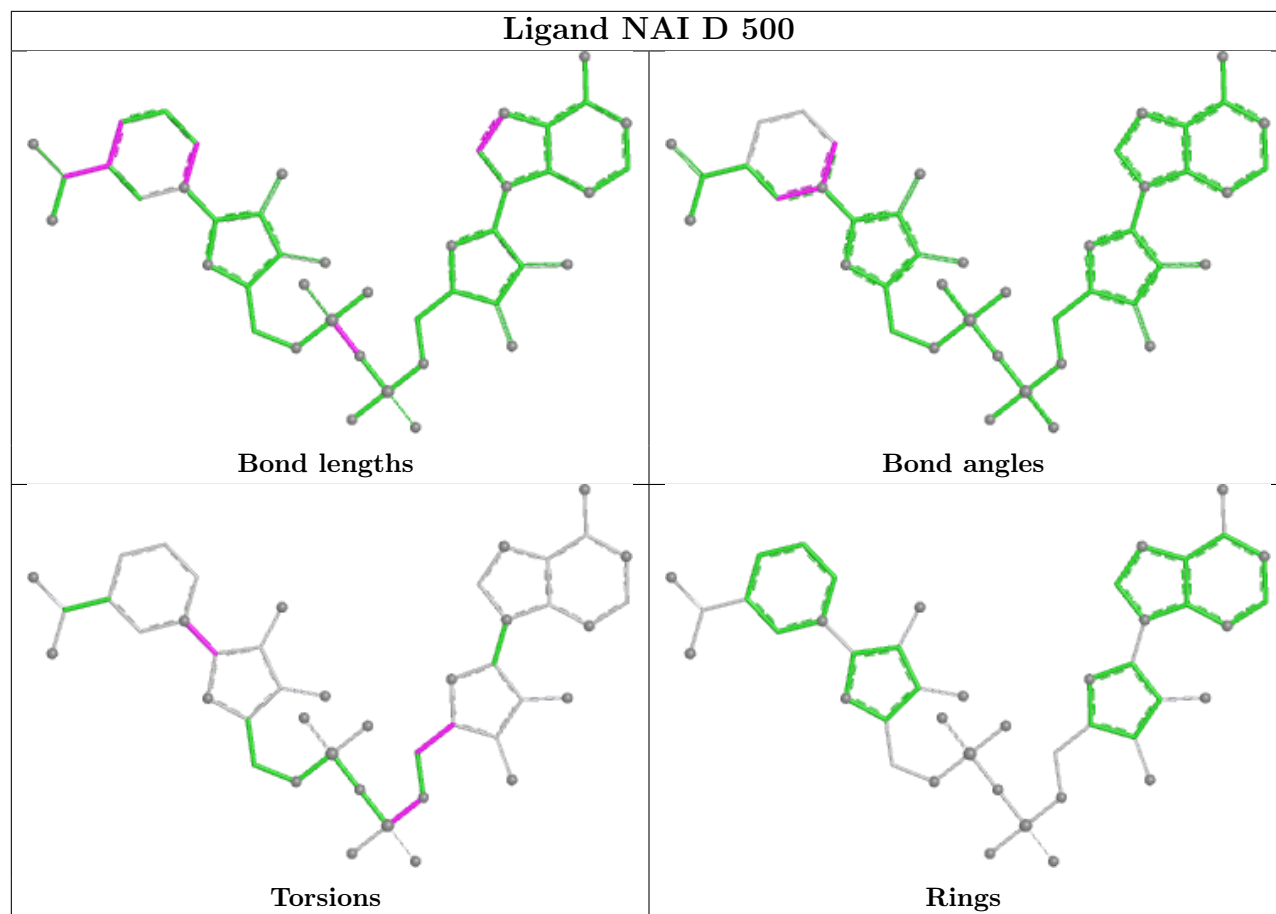


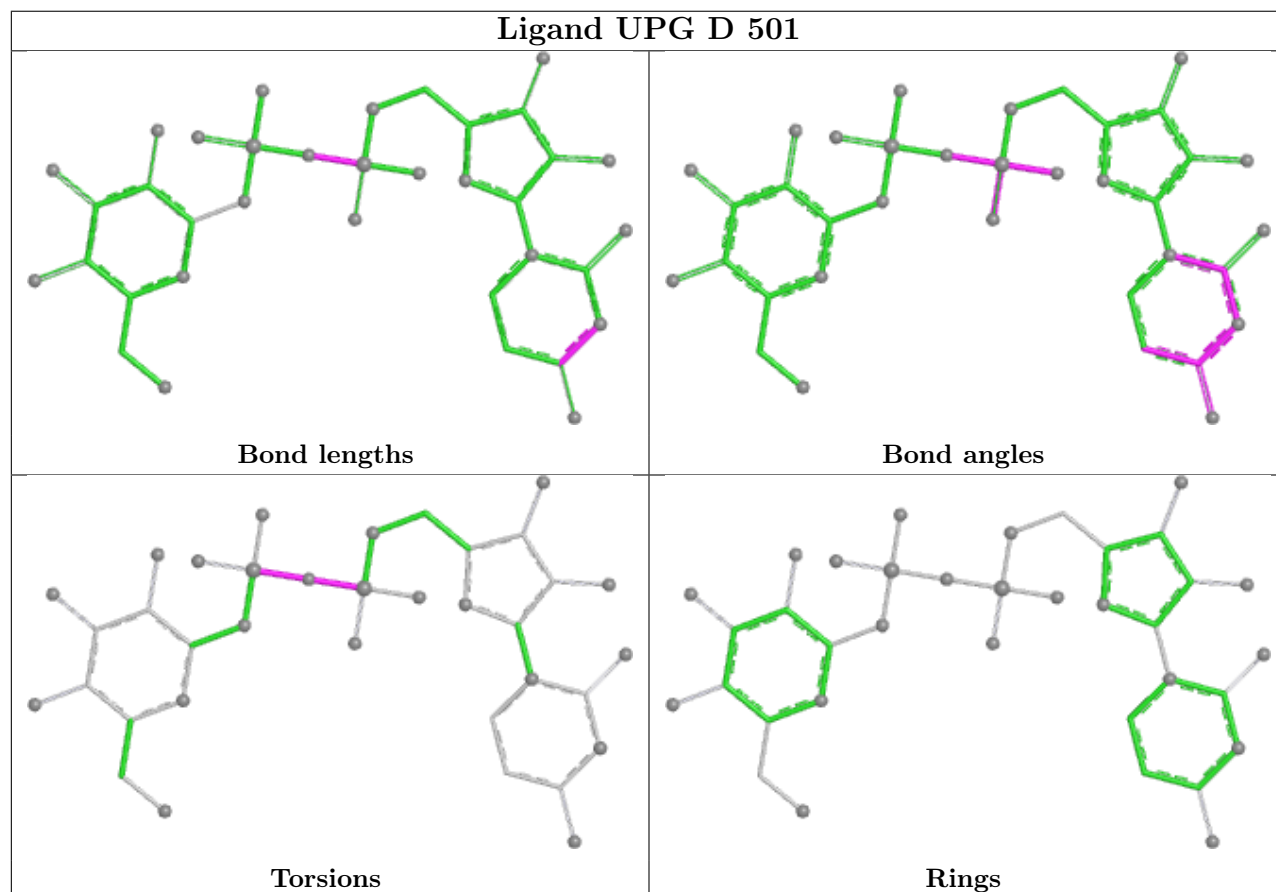
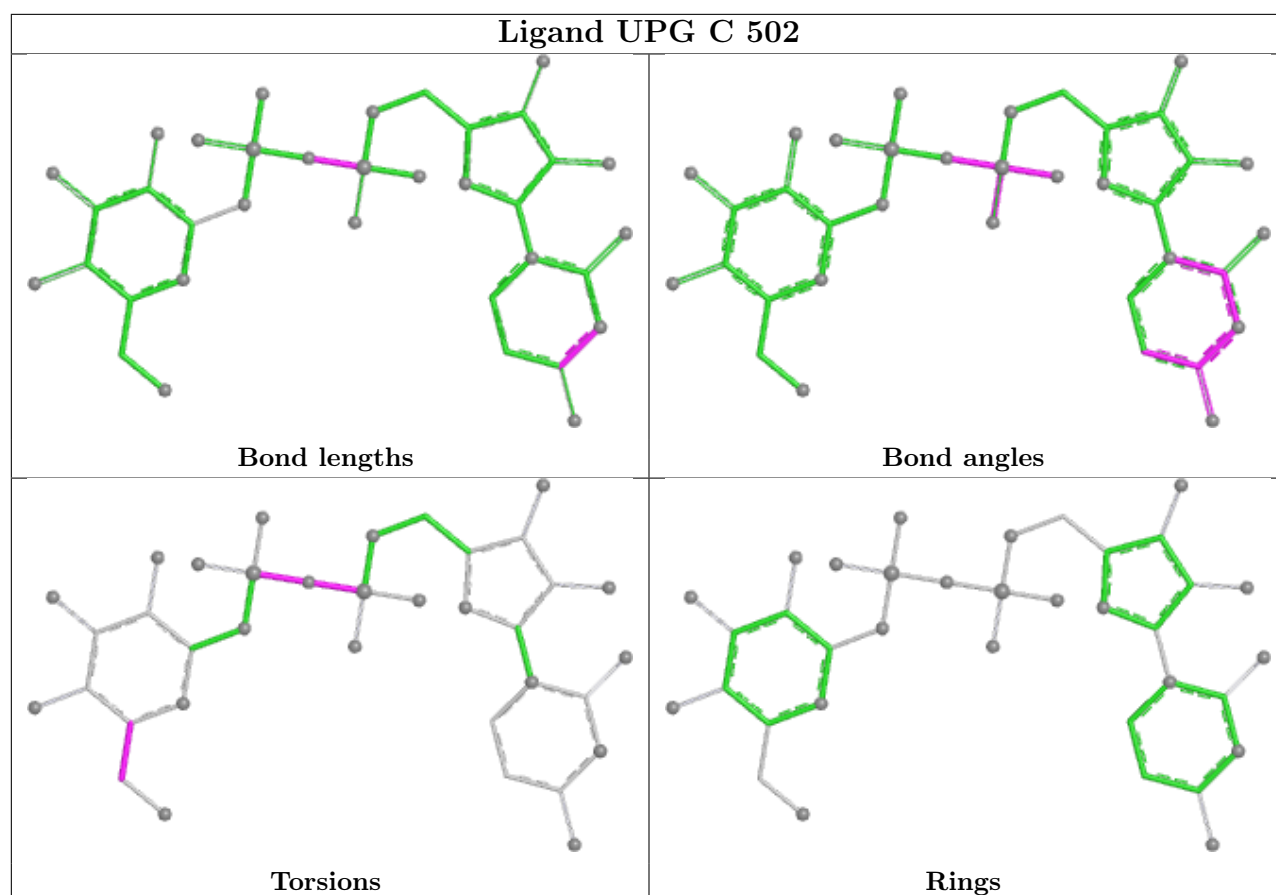












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	459/494 (92%)	0.14	5 (1%) 78 79	38, 66, 107, 141	0
1	B	459/494 (92%)	0.11	7 (1%) 72 73	38, 63, 98, 136	0
1	C	459/494 (92%)	0.05	10 (2%) 62 64	42, 62, 96, 123	0
1	D	459/494 (92%)	0.39	20 (4%) 39 41	43, 70, 113, 138	0
1	E	456/494 (92%)	0.75	40 (8%) 15 17	49, 83, 122, 148	0
1	F	459/494 (92%)	-0.10	3 (0%) 84 85	40, 54, 79, 132	0
All	All	2751/2964 (92%)	0.22	85 (3%) 51 53	38, 65, 110, 148	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	14	TYR	4.3
1	E	48	PRO	4.1
1	F	382	HIS	4.0
1	D	53	TYR	4.0
1	D	1	MET	3.9
1	C	382	HIS	3.8
1	A	1	MET	3.8
1	A	382	HIS	3.8
1	B	382	HIS	3.8
1	C	1	MET	3.5
1	E	382	HIS	3.5
1	B	1	MET	3.5
1	B	73	THR	3.4
1	D	370	LYS	3.4
1	B	275	SER	3.3
1	E	6	LYS	3.2
1	D	183	ASP	3.1
1	E	81	GLU	3.1
1	E	51	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	342	THR	3.0
1	E	342	THR	3.0
1	E	12	ALA	3.0
1	E	53	TYR	2.9
1	C	323	PHE	2.9
1	E	67	LYS	2.9
1	F	289	GLU	2.8
1	A	73	THR	2.8
1	C	287	LEU	2.8
1	D	417	TRP	2.7
1	E	343	GLY	2.7
1	E	389	ASP	2.7
1	E	400	ASP	2.7
1	F	389	ASP	2.7
1	C	389	ASP	2.6
1	D	341	ASP	2.6
1	A	389	ASP	2.6
1	E	465	LYS	2.5
1	C	458	GLN	2.5
1	E	98	MET	2.5
1	C	440	ASP	2.5
1	D	267	LYS	2.5
1	D	93	THR	2.4
1	E	37	VAL	2.4
1	C	465	LYS	2.4
1	E	38	ASN	2.4
1	E	458	GLN	2.4
1	B	465	LYS	2.3
1	D	48	PRO	2.3
1	D	170	LYS	2.3
1	C	98	MET	2.3
1	D	371	VAL	2.3
1	D	382	HIS	2.3
1	D	465	LYS	2.3
1	E	398	SER	2.3
1	E	437	PHE	2.3
1	E	184	GLU	2.3
1	B	389	ASP	2.2
1	D	14	TYR	2.2
1	A	4	ILE	2.2
1	D	458	GLN	2.2
1	E	142	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	184	GLU	2.2
1	D	161	GLU	2.2
1	E	165	GLU	2.2
1	E	402	TYR	2.1
1	C	322	LEU	2.1
1	E	372	PRO	2.1
1	D	89	VAL	2.1
1	E	28	PRO	2.1
1	E	214	TRP	2.1
1	E	457	PHE	2.1
1	E	396	THR	2.1
1	E	454	THR	2.1
1	D	52	ILE	2.1
1	E	459	ILE	2.1
1	E	15	VAL	2.1
1	E	45	TRP	2.1
1	E	164	ALA	2.1
1	E	339	LYS	2.1
1	E	462	ILE	2.0
1	E	205	ARG	2.0
1	E	277	PHE	2.0
1	D	98	MET	2.0
1	E	169	ILE	2.0
1	E	427	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

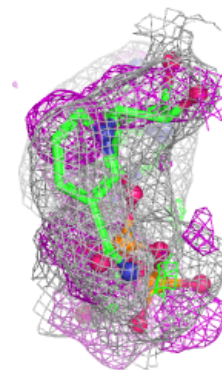
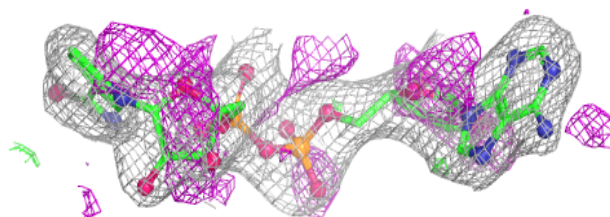
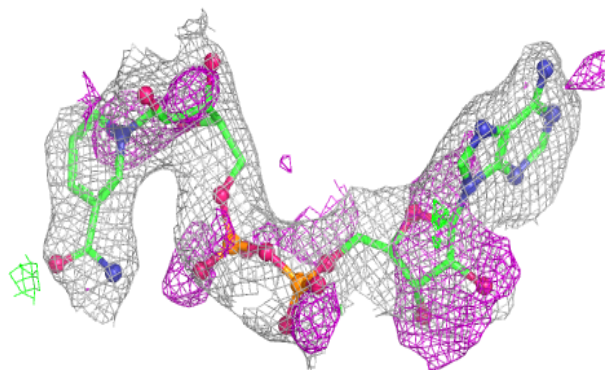
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAI	D	500	44/44	0.87	0.12	61,67,80,85	0
3	UPG	E	501	36/36	0.87	0.13	71,84,94,95	0
4	DMS	C	503	4/4	0.87	0.24	105,107,107,109	0
4	DMS	F	503	4/4	0.87	0.18	91,94,94,95	0
2	NAI	E	500	44/44	0.88	0.12	83,90,96,100	0
4	DMS	A	503	4/4	0.91	0.18	97,98,99,100	0
3	UPG	D	501	36/36	0.92	0.10	49,59,64,67	0
4	DMS	B	503	4/4	0.93	0.17	106,106,108,108	0
2	NAI	A	501	44/44	0.95	0.10	41,56,81,82	0
2	NAI	C	501	44/44	0.95	0.09	38,49,61,63	0
2	NAI	F	501	44/44	0.96	0.07	35,40,50,51	0
3	UPG	A	502	36/36	0.96	0.07	33,44,49,52	0
3	UPG	B	502	36/36	0.96	0.07	41,46,50,54	0
3	UPG	C	502	36/36	0.96	0.07	38,44,53,55	0
2	NAI	B	501	44/44	0.96	0.08	46,57,73,75	0
3	UPG	F	502	36/36	0.97	0.07	38,43,49,50	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.

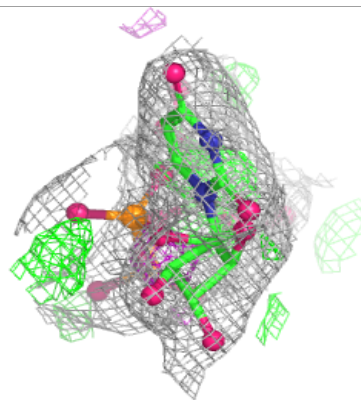
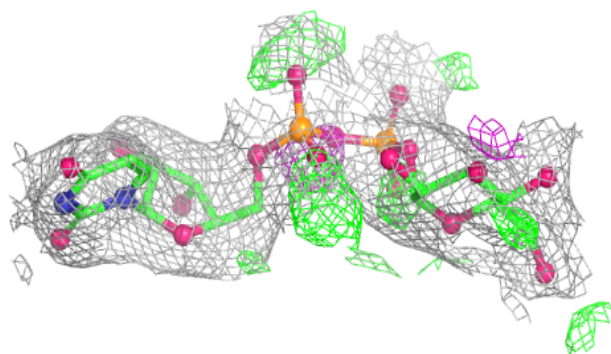
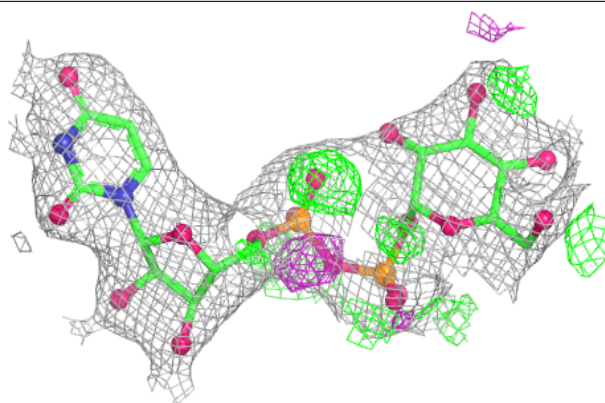
Electron density around NAI D 500:

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

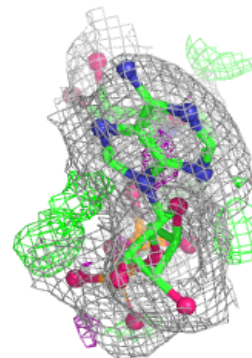
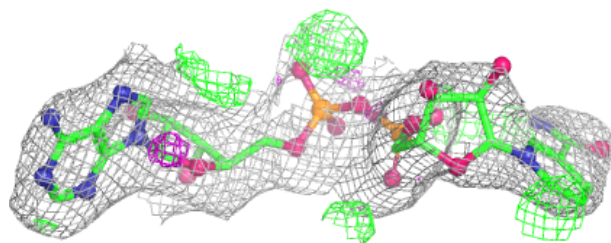
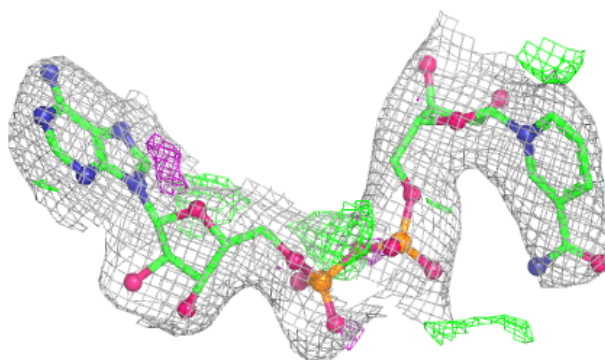


Electron density around UPG E 501:

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

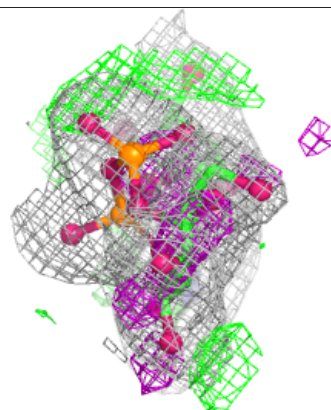
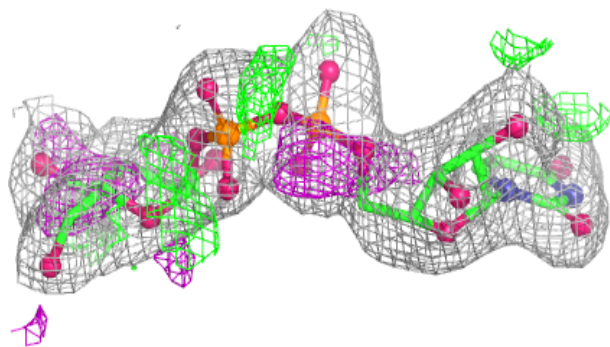
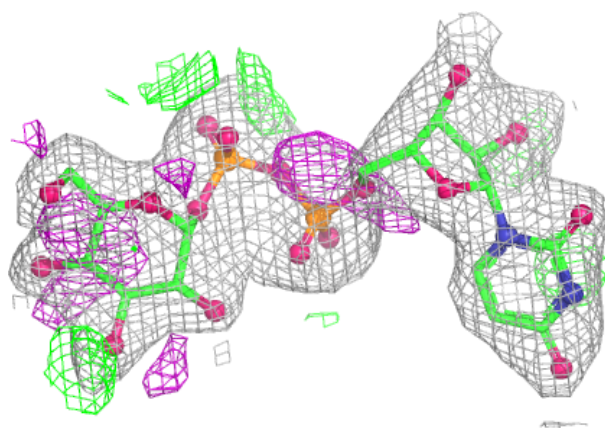
**Electron density around NAI E 500:**

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

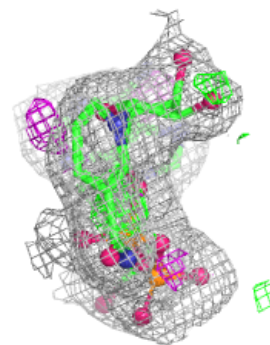
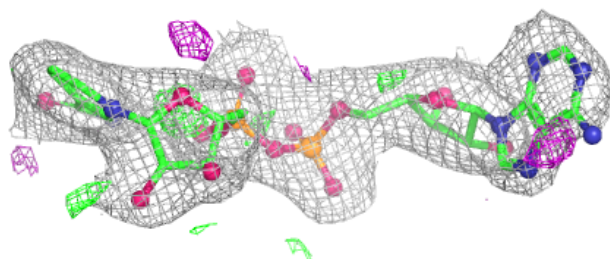
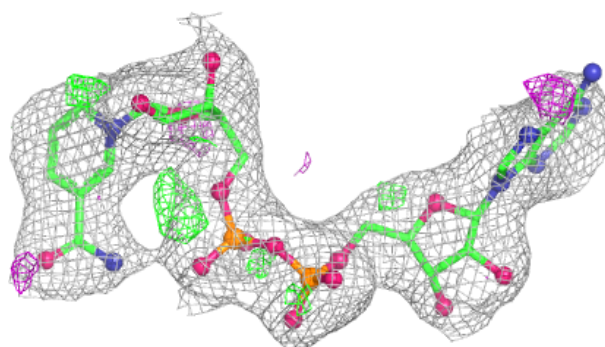


Electron density around UPG D 501:

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

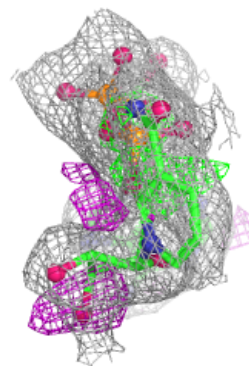
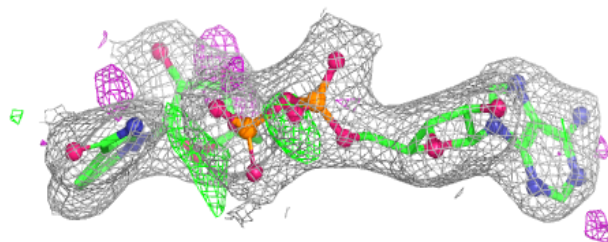
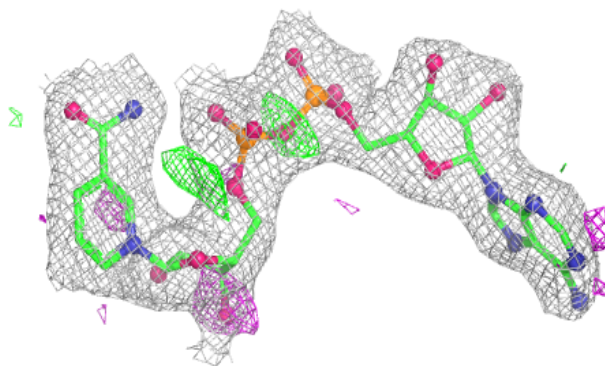
**Electron density around NAI A 501:**

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and green (positive)

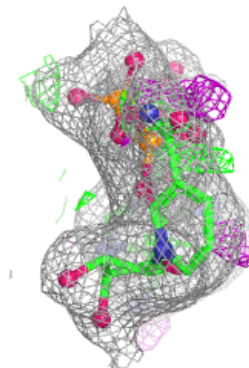
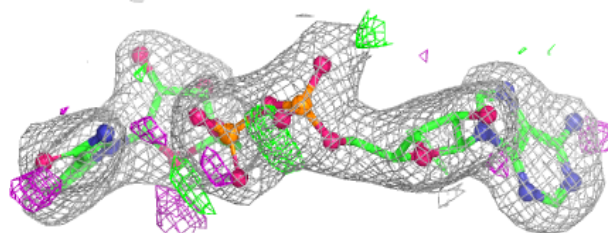
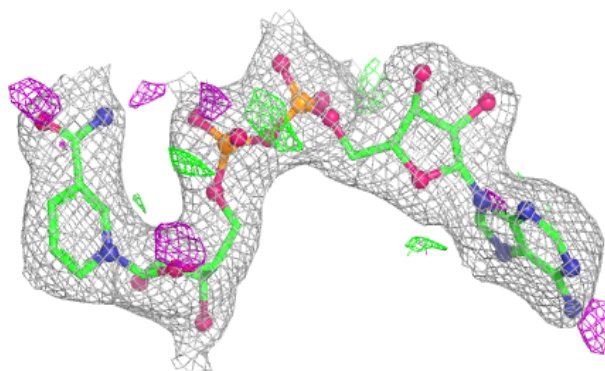


Electron density around NAI C 501:

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

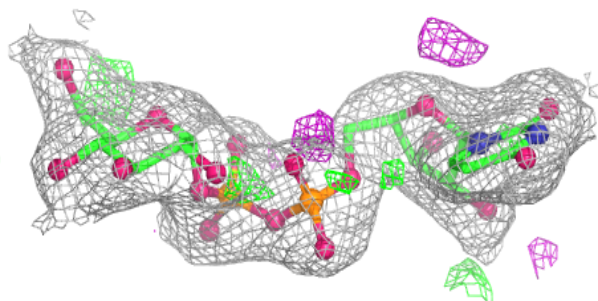
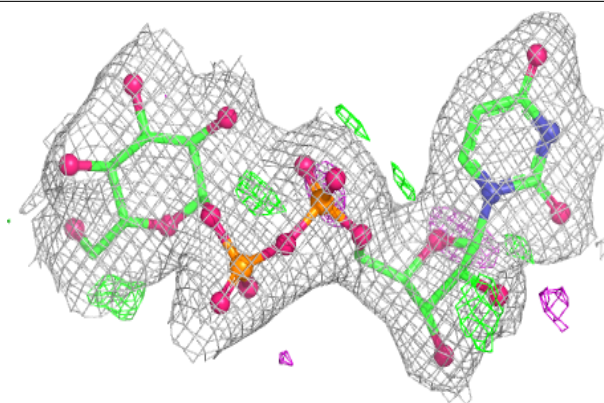
**Electron density around NAI F 501:**

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and green (positive)

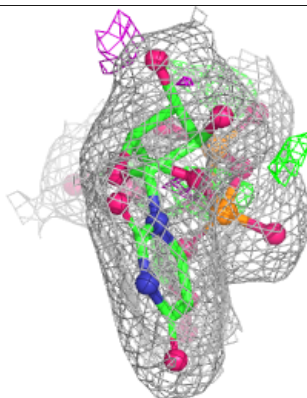
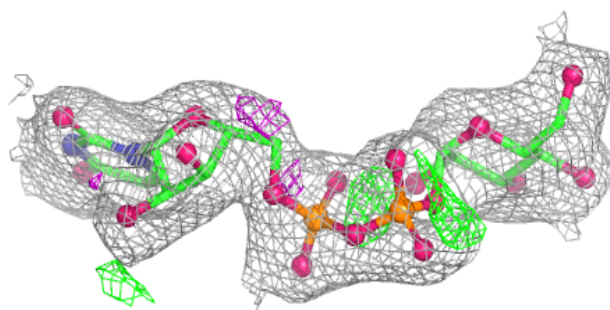
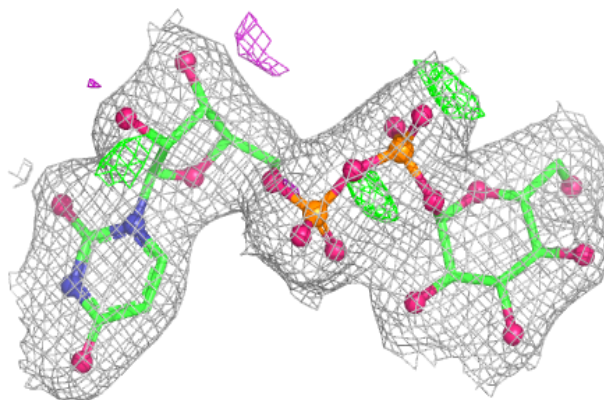


Electron density around UPG A 502:

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

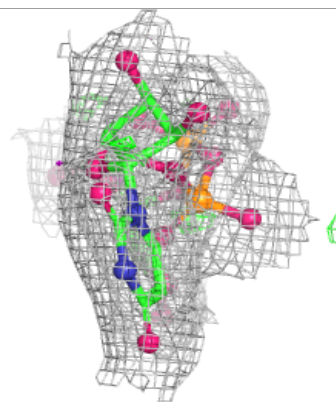
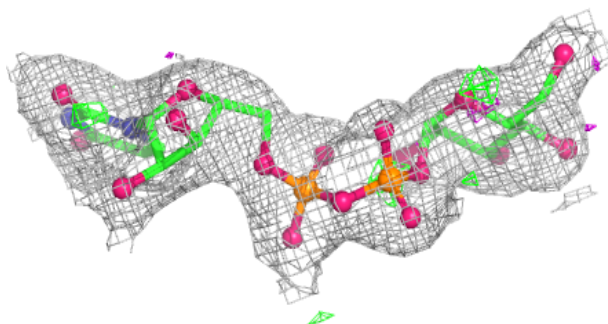
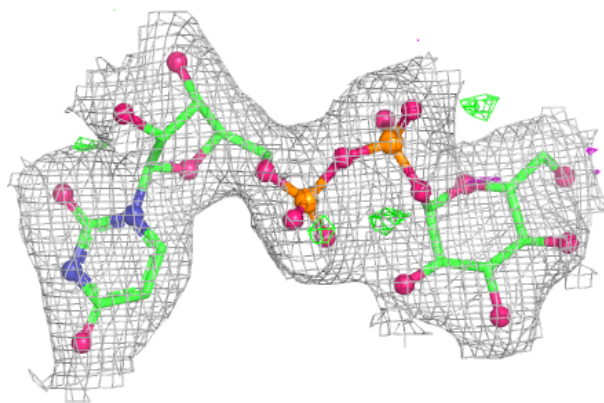
**Electron density around UPG B 502:**

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and green (positive)

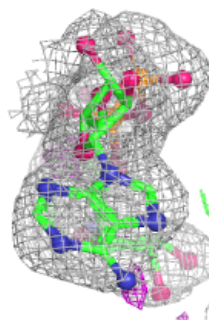
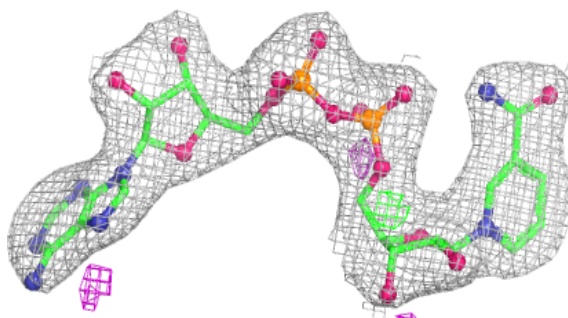


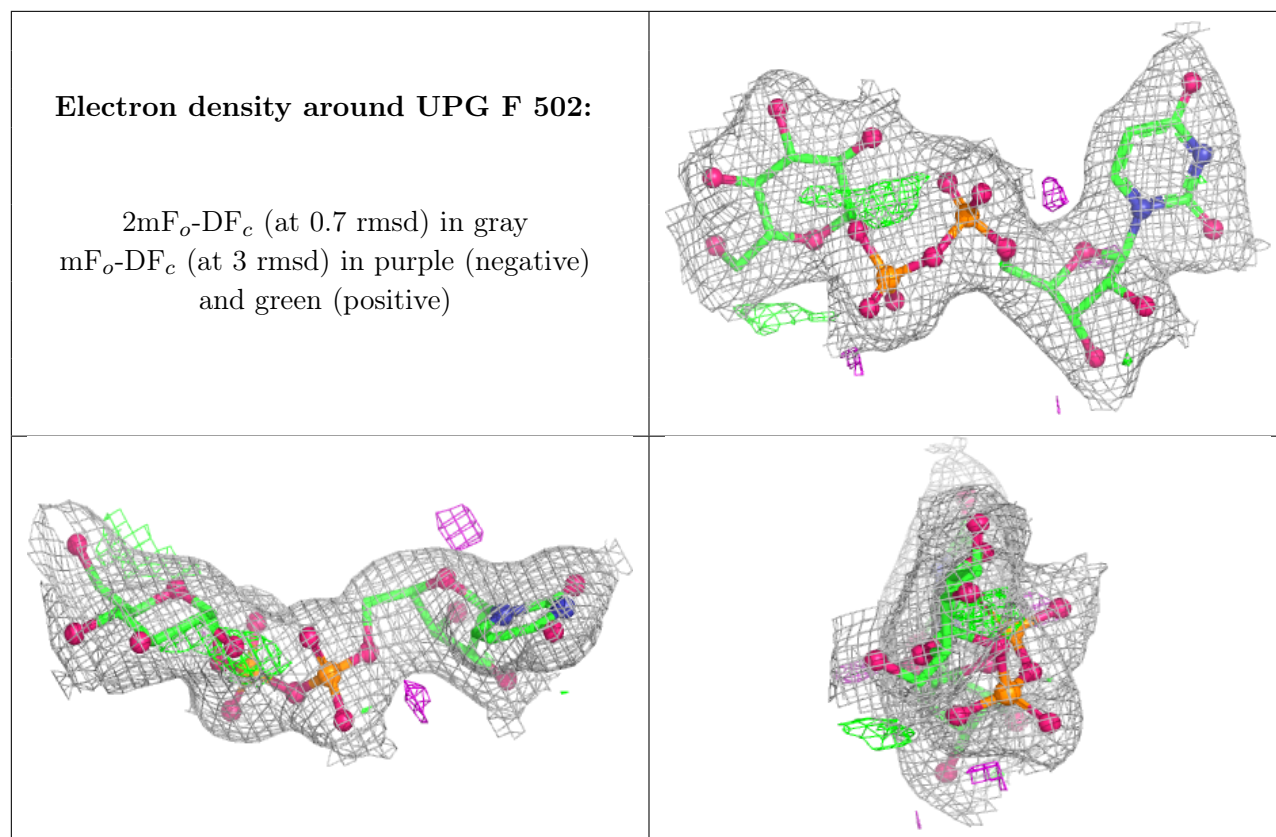
Electron density around UPG C 502:

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

**Electron density around NAI B 501:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.