



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:38 AM UTC

PDB ID : 7CS5 / pdb_00007cs5
Title : IiPLR1 with NADP⁺ and (-)pinorexinol
Authors : Shao, K.; Zhang, P.
Deposited on : 2020-08-14
Resolution : 2.19 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

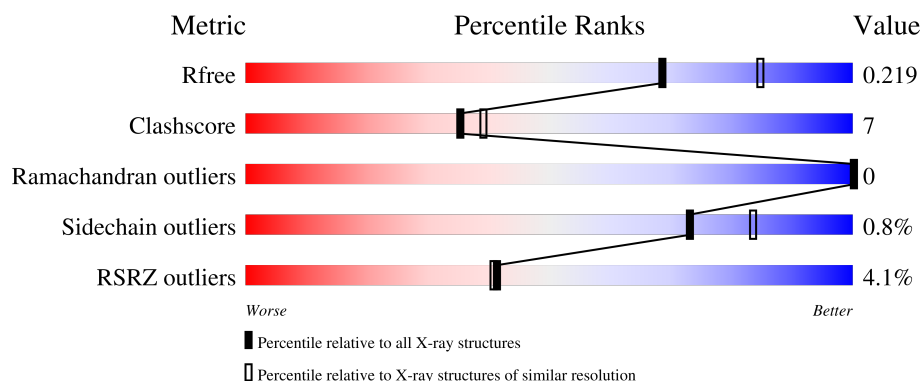
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	317	
1	B	317	
1	C	317	
1	D	317	
1	E	317	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	317	 3% 82% 7% 10%

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:

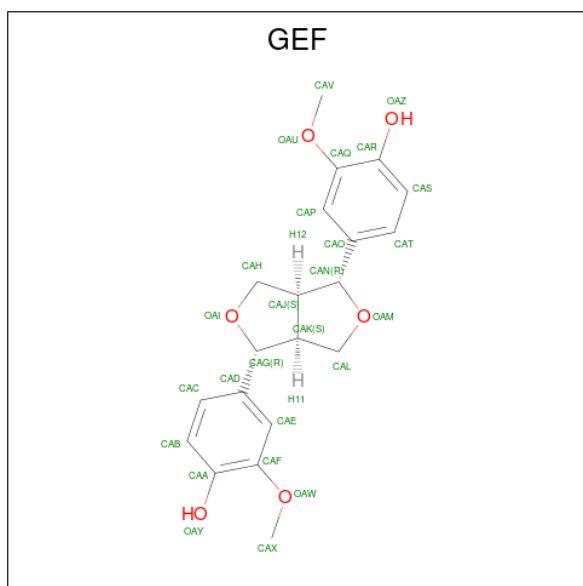
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GEF	B	401	-	X	-	-
2	GEF	C	401	-	X	X	-
2	GEF	D	401	-	X	-	-
2	GEF	E	401	-	X	X	-
2	GEF	F	401	-	X	-	-

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 Pinorexinol-laricresinol reductase.

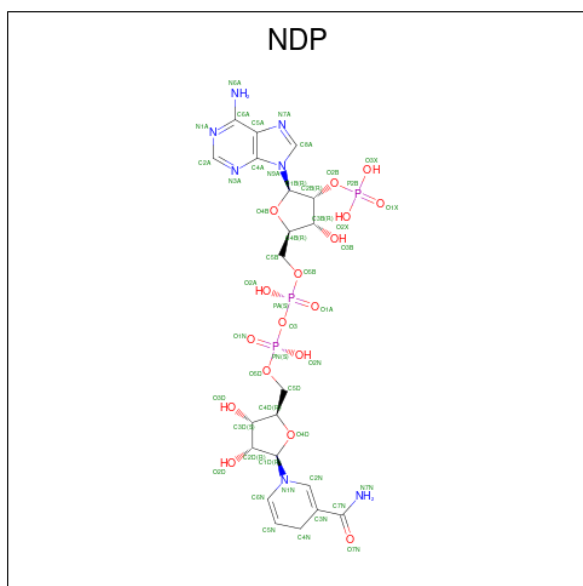
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	285	Total 2243	C 1426	N 379	O 429	S 9	0	0	0
1	A	284	Total 2234	C 1421	N 377	O 427	S 9	0	0	0
1	F	285	Total 2237	C 1422	N 377	O 429	S 9	0	0	0
1	D	285	Total 2243	C 1426	N 379	O 429	S 9	0	0	0
1	C	285	Total 2243	C 1426	N 379	O 429	S 9	0	0	0
1	B	290	Total 2286	C 1454	N 387	O 436	S 9	0	0	0

- Molecule 2 is 4-[(3R,3aS,6R,6aS)-6-(3-methoxy-4-oxidanyl-phenyl)-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan-3-yl]-2-methoxy-phenol (CCD ID: GEF) (formula: C₂₀H₂₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total 26	C 20	O 6	0	0
2	A	1	Total 26	C 20	O 6	0	0
2	F	1	Total 26	C 20	O 6	0	0
2	D	1	Total 26	C 20	O 6	0	0
2	C	1	Total 26	C 20	O 6	0	0
2	B	1	Total 26	C 20	O 6	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	E	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0
3	A	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0
3	F	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0
3	D	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0
3	C	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		

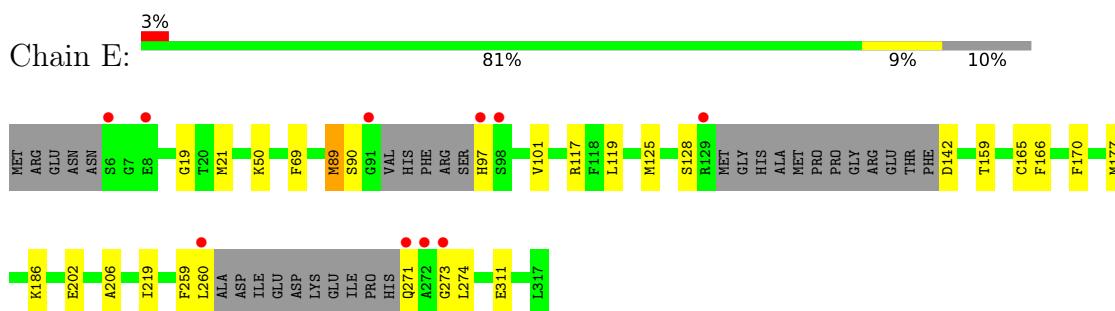
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	193	Total	O	0	0
			193	193		
4	A	156	Total	O	0	0
			156	156		
4	F	175	Total	O	0	0
			175	175		
4	D	178	Total	O	0	0
			178	178		
4	C	202	Total	O	0	0
			202	202		
4	B	201	Total	O	0	0
			201	201		

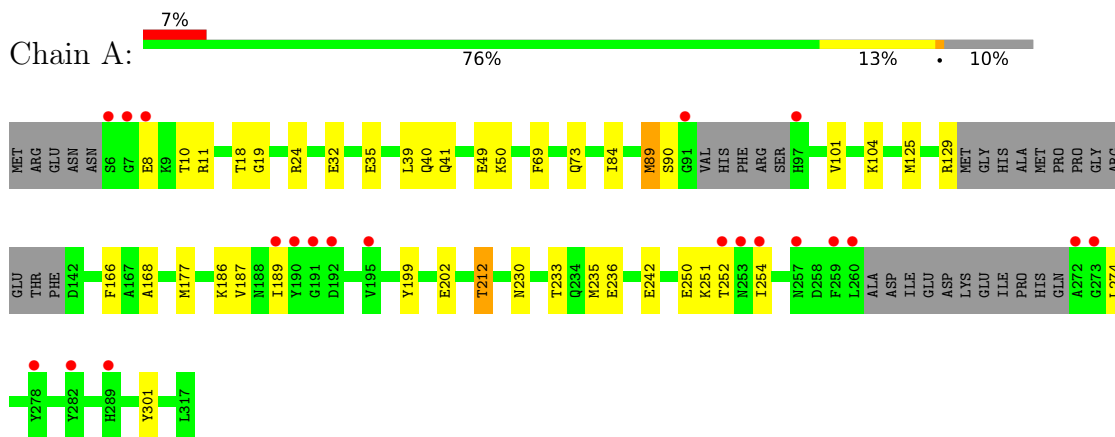
3 Residue-property plots [i](#)

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

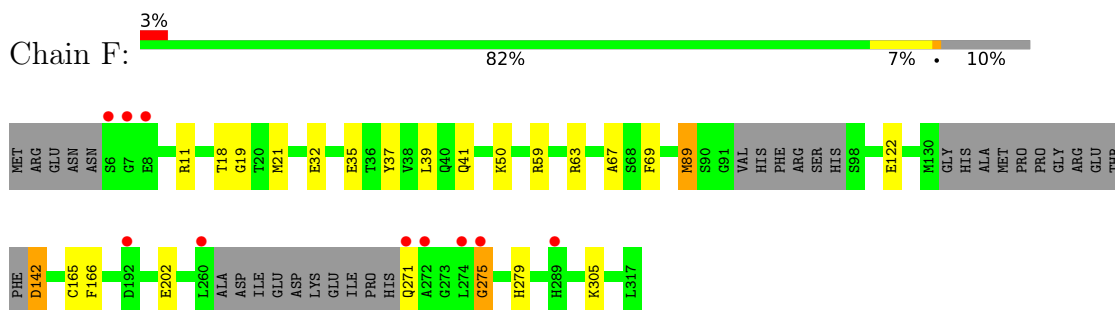
- Molecule 1: Pinoresinol-lariciresinol reductase



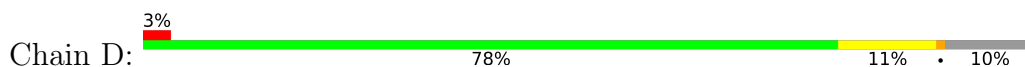
- Molecule 1: Pinoresinol-lariciresinol reductase

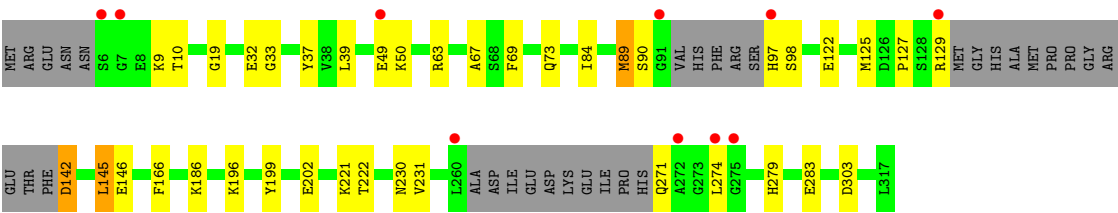


- Molecule 1: Pinoresinol-lariciresinol reductase

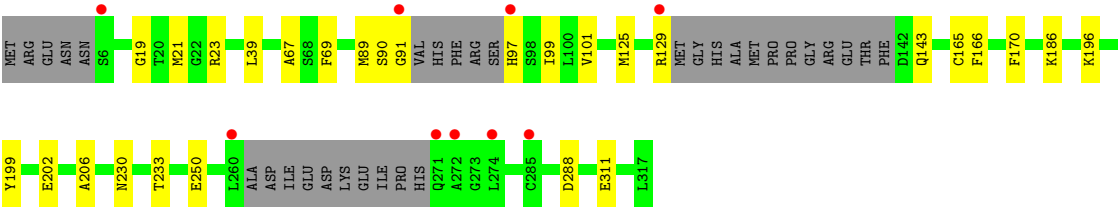
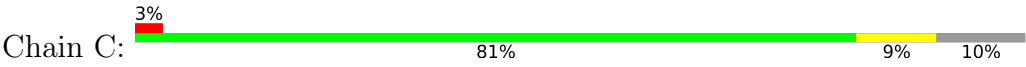


- Molecule 1: Pinoresinol-lariciresinol reductase

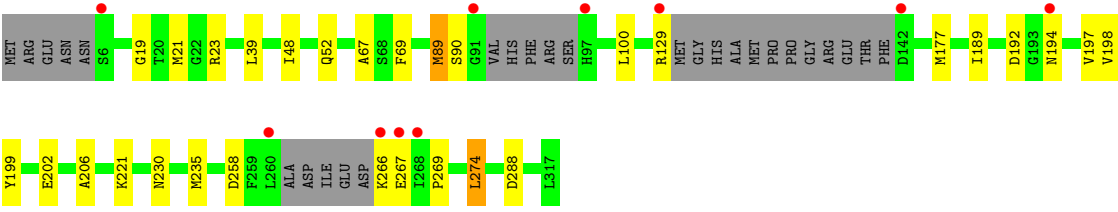
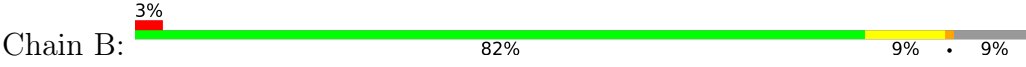




● Molecule 1: Pinoresinol-lariciresinol reductase



● Molecule 1: Pinoresinol-lariciresinol reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	244.95Å 244.95Å 75.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.50 – 2.19 39.50 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.50-2.19) 96.1 (39.50-2.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.10_2155, PHENIX 1.10_2155	Depositor
R, R_{free}	0.183 , 0.220 0.184 , 0.219	Depositor DCC
R_{free} test set	2007 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15191	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7928e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

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

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	0.34	0/2271	0.51	0/3067
1	B	0.38	0/2325	0.55	2/3140 (0.1%)
1	C	0.33	0/2280	0.52	0/3079
1	D	0.35	1/2280 (0.0%)	0.52	0/3079
1	E	0.34	0/2280	0.51	0/3079
1	F	0.35	1/2273 (0.0%)	0.52	0/3069
All	All	0.35	2/13709 (0.0%)	0.52	2/18513 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	122	GLU	CA-C	5.86	1.55	1.52
1	F	122	GLU	CA-C	5.31	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	LEU	CA-C-N	-5.79	110.07	121.41
1	B	274	LEU	C-N-CA	-5.79	110.07	121.41

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	128	SER	Peptide
1	F	275	GLY	Peptide

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	2234	0	2240	46	0
1	B	2286	0	2292	25	0
1	C	2243	0	2248	26	0
1	D	2243	0	2248	43	0
1	E	2243	0	2248	24	0
1	F	2237	0	2242	21	0
2	A	26	0	0	3	0
2	B	26	0	0	5	0
2	C	26	0	0	9	0
2	D	26	0	0	3	0
2	E	26	0	0	9	0
2	F	26	0	0	5	0
3	A	48	26	26	11	0
3	B	48	26	26	6	0
3	C	48	26	26	3	0
3	D	48	26	26	8	0
3	E	48	26	26	7	0
3	F	48	26	26	10	0
4	A	156	0	0	4	0
4	B	201	0	0	3	0
4	C	202	0	0	4	0
4	D	178	0	0	12	0
4	E	193	0	0	5	0
4	F	175	0	0	4	0
All	All	15035	156	13674	204	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 7.

All (204) 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:401:GEF:OAM	2:E:401:GEF:CAN	1.89	1.18
2:F:401:GEF:OAM	2:F:401:GEF:CAN	1.87	1.14
2:B:401:GEF:OAM	2:B:401:GEF:CAN	1.92	1.07
2:C:401:GEF:CAN	2:C:401:GEF:OAM	1.83	1.06
2:C:401:GEF:OAM	2:C:401:GEF:CAO	2.09	1.00
2:C:401:GEF:CAO	2:C:401:GEF:CAL	2.42	0.97
2:E:401:GEF:OAM	2:E:401:GEF:CAO	2.14	0.95
2:F:401:GEF:OAM	2:F:401:GEF:CAO	2.14	0.95
1:D:221:LYS:HE3	1:D:222:THR:H	1.33	0.94
2:E:401:GEF:CAO	2:E:401:GEF:CAL	2.45	0.92
1:A:125:MET:H	2:A:401:GEF:CAV	1.82	0.92
1:F:39:LEU:HD11	1:F:67:ALA:HB3	1.52	0.89
1:C:129:ARG:NH2	1:C:288:ASP:OD1	2.05	0.89
1:D:274:LEU:HD21	1:B:269:PRO:HD3	1.53	0.89
2:F:401:GEF:CAO	2:F:401:GEF:CAL	2.51	0.88
1:D:142:ASP:N	4:D:503:HOH:O	2.08	0.87
1:D:39:LEU:HD11	1:D:67:ALA:HB3	1.57	0.84
2:B:401:GEF:OAM	2:B:401:GEF:CAO	2.26	0.83
1:F:142:ASP:N	4:F:501:HOH:O	2.12	0.82
1:E:271:GLN:N	4:E:502:HOH:O	2.15	0.79
1:C:97:HIS:N	1:C:143:GLN:OE1	2.16	0.78
1:D:142:ASP:OD1	4:D:501:HOH:O	2.03	0.77
2:B:401:GEF:CAO	2:B:401:GEF:CAL	2.63	0.76
1:D:125:MET:H	2:D:401:GEF:CAV	1.99	0.76
1:A:125:MET:HE3	1:A:129:ARG:HH22	1.50	0.75
1:B:21:MET:CE	1:B:206:ALA:HB2	2.16	0.74
1:A:19:GLY:HA3	3:A:402:NDP:H52A	1.69	0.74
1:D:49:GLU:OE2	4:D:502:HOH:O	2.07	0.73
1:A:125:MET:N	2:A:401:GEF:CAV	2.52	0.73
1:D:221:LYS:HE3	1:D:222:THR:N	2.04	0.72
1:D:19:GLY:HA3	3:D:402:NDP:H52A	1.72	0.71
1:C:129:ARG:HH22	1:C:288:ASP:CG	1.97	0.71
1:A:10:THR:HG21	1:A:84:ILE:HD12	1.72	0.70
1:D:125:MET:HG3	2:D:401:GEF:CAV	2.21	0.69
1:C:311:GLU:OE1	4:C:501:HOH:O	2.09	0.69
1:B:202:GLU:OE2	4:B:501:HOH:O	2.10	0.69
1:F:305:LYS:HE3	1:F:305:LYS:HA	1.74	0.69
1:A:202:GLU:H	1:A:202:GLU:CD	2.01	0.69
1:C:91:GLY:CA	1:C:99:ILE:HG12	2.23	0.68
1:F:305:LYS:HA	1:F:305:LYS:CE	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:LYS:HE2	4:D:508:HOH:O	1.93	0.68
1:B:177:MET:HE1	1:B:274:LEU:HD23	1.76	0.67
1:B:221:LYS:NZ	4:B:504:HOH:O	2.28	0.67
1:E:259:PHE:O	1:E:260:LEU:HB2	1.92	0.67
1:F:202:GLU:H	1:F:202:GLU:CD	2.04	0.66
1:A:73:GLN:OE1	4:A:501:HOH:O	2.14	0.66
1:C:186:LYS:NZ	1:C:250:GLU:OE2	2.18	0.65
1:E:125:MET:HG3	2:E:401:GEF:CAV	2.26	0.65
1:E:273:GLY:HA3	4:E:651:HOH:O	1.96	0.65
1:F:19:GLY:HA3	3:F:402:NDP:H52A	1.77	0.65
1:E:166:PHE:HB3	1:E:202:GLU:OE1	1.97	0.65
1:E:177:MET:HE1	1:E:274:LEU:HD23	1.80	0.64
1:D:63:ARG:NH1	4:D:507:HOH:O	2.25	0.64
1:C:91:GLY:HA3	1:C:99:ILE:HG12	1.79	0.64
1:E:142:ASP:OD1	4:E:501:HOH:O	2.15	0.63
1:D:125:MET:N	2:D:401:GEF:CAV	2.62	0.62
1:D:279:HIS:ND1	1:D:283:GLU:OE1	2.21	0.62
1:A:90:SER:HB3	3:A:402:NDP:O1A	1.99	0.62
1:A:242:GLU:OE2	1:A:251:LYS:NZ	2.33	0.62
2:B:401:GEF:CAN	3:B:402:NDP:H42N	2.30	0.62
1:B:21:MET:HE1	1:B:206:ALA:HB2	1.82	0.61
2:E:401:GEF:CAN	3:E:402:NDP:H42N	2.31	0.61
1:A:18:THR:OG1	3:A:402:NDP:O1X	2.18	0.61
1:D:271:GLN:HB2	1:D:274:LEU:HD12	1.82	0.61
1:A:50:LYS:HE3	3:A:402:NDP:O3X	2.00	0.60
1:D:202:GLU:H	1:D:202:GLU:CD	2.09	0.60
1:A:254:ILE:H	1:A:254:ILE:HD12	1.65	0.60
1:E:311:GLU:OE1	4:E:503:HOH:O	2.17	0.60
1:C:165:CYS:HB3	1:C:170:PHE:CD2	2.37	0.60
1:B:39:LEU:HD11	1:B:67:ALA:HB3	1.84	0.59
1:D:146:GLU:OE1	4:D:504:HOH:O	2.16	0.59
1:C:125:MET:H	2:C:401:GEF:CAV	2.15	0.59
1:E:125:MET:H	2:E:401:GEF:CAV	2.16	0.59
1:F:271:GLN:N	4:F:506:HOH:O	2.35	0.59
1:E:69:PHE:CD1	3:E:402:NDP:H2A	2.38	0.59
1:C:21:MET:CE	1:C:206:ALA:HB2	2.33	0.59
1:A:39:LEU:HD23	1:A:40:GLN:N	2.18	0.59
1:F:166:PHE:H	3:F:402:NDP:H72N	1.51	0.58
1:E:186:LYS:HE2	4:E:536:HOH:O	2.03	0.58
1:C:125:MET:N	2:C:401:GEF:CAV	2.67	0.58
1:C:69:PHE:CD2	3:C:402:NDP:H2A	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HD3	1:A:187:VAL:N	2.19	0.57
1:E:125:MET:N	2:E:401:GEF:CAV	2.67	0.57
1:D:69:PHE:CD2	3:D:402:NDP:H2A	2.40	0.57
2:F:401:GEF:CAL	2:F:401:GEF:CAT	2.82	0.57
2:C:401:GEF:CAN	3:C:402:NDP:H42N	2.35	0.56
1:E:69:PHE:CE1	3:E:402:NDP:H2A	2.40	0.56
1:F:37:TYR:CE1	1:F:63:ARG:HD2	2.41	0.56
1:C:91:GLY:HA2	1:C:99:ILE:HG12	1.87	0.56
1:A:186:LYS:HZ1	1:A:250:GLU:HG2	1.69	0.56
1:D:97:HIS:N	4:D:513:HOH:O	2.37	0.56
2:F:401:GEF:CAN	3:F:402:NDP:H42N	2.36	0.56
1:A:39:LEU:HD23	1:A:39:LEU:C	2.31	0.55
1:A:166:PHE:H	3:A:402:NDP:H72N	1.53	0.55
1:D:166:PHE:H	3:D:402:NDP:H72N	1.53	0.55
1:D:196:LYS:HD2	1:D:231:VAL:HG12	1.87	0.55
1:B:69:PHE:CD2	3:B:402:NDP:H2A	2.42	0.55
1:E:259:PHE:O	1:E:260:LEU:CB	2.57	0.53
1:B:39:LEU:CD1	1:B:67:ALA:HB3	2.38	0.53
1:D:69:PHE:CE2	3:D:402:NDP:H2A	2.45	0.52
1:A:8:GLU:HA	1:A:8:GLU:OE2	2.09	0.52
1:C:91:GLY:HA3	1:C:99:ILE:CG1	2.38	0.52
1:B:90:SER:HB3	3:B:402:NDP:O1A	2.10	0.51
2:C:401:GEF:CAV	2:C:401:GEF:OAZ	2.59	0.51
1:F:275:GLY:O	1:F:279:HIS:CD2	2.64	0.51
1:D:73:GLN:HG3	4:D:518:HOH:O	2.09	0.51
1:A:32:GLU:OE1	4:A:502:HOH:O	2.19	0.51
1:A:186:LYS:NZ	1:A:250:GLU:HG2	2.26	0.51
1:C:196:LYS:HE3	1:C:233:THR:HG23	1.93	0.51
1:A:125:MET:HE3	1:A:129:ARG:NH2	2.24	0.50
1:D:89:MET:HA	3:D:402:NDP:H51A	1.94	0.50
1:A:69:PHE:O	1:A:104:LYS:HD3	2.12	0.50
1:A:233:THR:HG23	1:A:236:GLU:OE2	2.12	0.50
1:D:9:LYS:HD3	1:D:33:GLY:O	2.12	0.50
1:F:59:ARG:HD2	4:F:504:HOH:O	2.11	0.49
1:A:10:THR:CG2	1:A:84:ILE:HD12	2.41	0.49
1:D:90:SER:HB3	3:D:402:NDP:O1A	2.12	0.49
1:D:127:PRO:HB2	1:D:145:LEU:HD13	1.94	0.49
1:D:39:LEU:CD1	1:D:67:ALA:HB3	2.36	0.48
1:F:21:MET:HE3	1:F:166:PHE:CZ	2.49	0.48
2:E:401:GEF:CAL	2:E:401:GEF:CAT	2.91	0.48
1:A:177:MET:HE1	1:A:274:LEU:HD23	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:LEU:HD11	1:C:67:ALA:HB3	1.96	0.48
1:A:69:PHE:CD2	3:A:402:NDP:H2A	2.49	0.48
1:A:89:MET:HA	3:A:402:NDP:H51A	1.96	0.48
1:A:49:GLU:OE2	1:B:23:ARG:NH1	2.46	0.48
1:A:252:THR:HG22	1:A:254:ILE:HD12	1.96	0.48
1:A:69:PHE:CE2	3:A:402:NDP:H2A	2.49	0.47
2:A:401:GEF:CAV	2:A:401:GEF:OAZ	2.62	0.47
1:A:11:ARG:HG2	1:A:35:GLU:HB3	1.95	0.47
1:B:258:ASP:OD2	4:B:503:HOH:O	2.20	0.47
1:D:32:GLU:OE2	4:D:505:HOH:O	2.20	0.47
1:D:50:LYS:HE3	3:D:402:NDP:O3X	2.15	0.47
1:F:11:ARG:HG2	1:F:35:GLU:HB3	1.97	0.47
1:F:69:PHE:CD2	3:F:402:NDP:H2A	2.50	0.47
1:A:254:ILE:H	1:A:254:ILE:CD1	2.28	0.47
1:F:89:MET:CE	3:F:402:NDP:H1B	2.44	0.46
1:D:303:ASP:OD1	1:D:303:ASP:N	2.44	0.46
1:C:97:HIS:O	1:C:101:VAL:HG23	2.16	0.46
1:C:202:GLU:OE2	4:C:502:HOH:O	2.21	0.46
1:A:254:ILE:HD12	1:A:254:ILE:N	2.31	0.46
1:B:19:GLY:HA3	3:B:402:NDP:H52A	1.97	0.46
1:B:192:ASP:HB2	1:B:194:ASN:OD1	2.16	0.46
2:C:401:GEF:CAL	2:C:401:GEF:CAT	2.93	0.45
1:D:73:GLN:NE2	4:D:518:HOH:O	2.49	0.45
1:C:166:PHE:HB3	1:C:202:GLU:OE1	2.15	0.45
1:E:21:MET:CE	1:E:206:ALA:HB2	2.46	0.45
1:A:89:MET:HB3	1:A:89:MET:HE3	1.33	0.45
1:C:199:TYR:O	1:C:230:ASN:HB3	2.16	0.45
1:C:288:ASP:OD2	4:C:503:HOH:O	2.21	0.45
1:F:18:THR:OG1	3:F:402:NDP:O1X	2.32	0.45
1:E:165:CYS:HB3	1:E:170:PHE:CD2	2.52	0.44
1:D:37:TYR:CE1	1:D:63:ARG:HD2	2.51	0.44
1:B:69:PHE:CE2	3:B:402:NDP:H2A	2.52	0.44
1:B:189:ILE:HG13	1:B:235:MET:HE1	1.98	0.44
2:B:401:GEF:CAL	2:B:401:GEF:CAT	2.95	0.44
1:A:186:LYS:HZ3	1:A:250:GLU:C	2.23	0.44
1:A:189:ILE:HG13	1:A:235:MET:HE1	1.98	0.44
1:D:129:ARG:HB2	4:D:542:HOH:O	2.17	0.44
1:E:19:GLY:HA3	3:E:402:NDP:H52A	2.00	0.44
3:A:402:NDP:P2B	3:A:402:NDP:HO3A	2.39	0.44
1:B:100:LEU:HD23	1:B:100:LEU:HA	1.86	0.43
1:B:199:TYR:O	1:B:230:ASN:HB3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:NH1	1:B:288:ASP:OD1	2.51	0.43
1:A:41:GLN:HE22	3:A:402:NDP:C2A	2.31	0.43
2:E:401:GEF:CAV	2:E:401:GEF:OAZ	2.67	0.42
1:F:41:GLN:OE1	3:F:402:NDP:H2A	2.19	0.42
1:A:168:ALA:HB1	1:B:48:ILE:CD1	2.49	0.42
1:D:186:LYS:HB3	4:D:620:HOH:O	2.19	0.42
1:A:186:LYS:HE2	1:A:250:GLU:HG2	2.01	0.42
1:A:212:THR:HA	1:A:301:TYR:OH	2.18	0.42
1:B:221:LYS:HB3	1:B:221:LYS:HE3	1.71	0.42
1:D:221:LYS:HD2	1:D:221:LYS:HA	1.80	0.42
1:E:117:ARG:NH2	1:E:219:ILE:HG12	2.35	0.42
1:E:119:LEU:HG	1:E:159:THR:HB	2.01	0.42
1:D:49:GLU:OE1	1:C:23:ARG:NH1	2.53	0.42
1:E:90:SER:HB3	3:E:402:NDP:O1A	2.19	0.42
1:A:125:MET:HE2	1:A:129:ARG:HH12	1.85	0.42
1:D:10:THR:HG21	1:D:84:ILE:HD12	2.01	0.42
1:D:89:MET:H	1:D:89:MET:HG2	1.75	0.41
1:E:97:HIS:O	1:E:101:VAL:HG23	2.20	0.41
1:F:32:GLU:OE1	4:F:502:HOH:O	2.20	0.41
1:E:50:LYS:HE3	3:E:402:NDP:O3X	2.20	0.41
1:F:50:LYS:HE3	3:F:402:NDP:O3X	2.20	0.41
1:D:89:MET:HB3	1:D:89:MET:HE3	1.42	0.41
1:F:165:CYS:HA	3:F:402:NDP:H72N	1.85	0.41
1:D:199:TYR:O	1:D:230:ASN:HB3	2.20	0.41
1:C:165:CYS:HA	3:C:402:NDP:H72N	1.86	0.41
1:B:197:VAL:HG12	1:B:198:VAL:N	2.36	0.41
1:B:266:LYS:HB2	1:B:267:GLU:H	1.73	0.41
1:C:125:MET:HG3	2:C:401:GEF:CAV	2.51	0.41
1:E:166:PHE:H	3:E:402:NDP:H72N	1.63	0.41
1:F:69:PHE:CE2	3:F:402:NDP:H2A	2.56	0.41
1:A:41:GLN:NE2	4:A:506:HOH:O	2.40	0.40
1:D:90:SER:O	1:D:98:SER:HB3	2.21	0.40
1:D:166:PHE:CD2	3:D:402:NDP:H41N	2.56	0.40
1:B:89:MET:HA	3:B:402:NDP:H51A	2.03	0.40
1:A:199:TYR:O	1:A:230:ASN:HB3	2.21	0.40
1:C:19:GLY:HA3	4:C:543:HOH:O	2.21	0.40
1:E:89:MET:HE2	1:E:89:MET:HB3	1.83	0.40
1:A:24:ARG:NH2	1:B:52:GLN:OE1	2.47	0.40
1:A:41:GLN:HE22	3:A:402:NDP:H2A	1.87	0.40
1:A:73:GLN:HG2	4:A:605:HOH:O	2.21	0.40
1:C:90:SER:O	1:C:91:GLY:C	2.65	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	276/317 (87%)	267 (97%)	9 (3%)	0	100	100
1	B	282/317 (89%)	275 (98%)	7 (2%)	0	100	100
1	C	277/317 (87%)	270 (98%)	7 (2%)	0	100	100
1	D	277/317 (87%)	272 (98%)	5 (2%)	0	100	100
1	E	277/317 (87%)	274 (99%)	3 (1%)	0	100	100
1	F	277/317 (87%)	271 (98%)	6 (2%)	0	100	100
All	All	1666/1902 (88%)	1629 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/271 (89%)	239 (99%)	3 (1%)	63	75
1	B	248/271 (92%)	247 (100%)	1 (0%)	84	91
1	C	243/271 (90%)	242 (100%)	1 (0%)	84	91
1	D	243/271 (90%)	240 (99%)	3 (1%)	63	75
1	E	243/271 (90%)	242 (100%)	1 (0%)	84	91
1	F	242/271 (89%)	240 (99%)	2 (1%)	73	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1461/1626 (90%)	1450 (99%)	11 (1%)	73	83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	89	MET
1	A	89	MET
1	A	101	VAL
1	A	212	THR
1	F	89	MET
1	F	142	ASP
1	D	89	MET
1	D	142	ASP
1	D	145	LEU
1	C	89	MET
1	B	89	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	52	GLN
1	A	41	GLN
1	A	276	HIS
1	F	40	GLN
1	F	52	GLN
1	D	73	GLN
1	B	81	GLN
1	B	143	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	NDP	A	402	-	51,52,52	3.43	19 (37%)	71,80,80	2.48	22 (30%)
2	GEF	A	401	-	29,29,29	3.21	9 (31%)	42,42,42	8.16	20 (47%)
3	NDP	D	402	-	51,52,52	3.43	21 (41%)	71,80,80	2.53	23 (32%)
3	NDP	B	402	-	51,52,52	3.19	19 (37%)	71,80,80	2.33	20 (28%)
2	GEF	F	401	-	29,29,29	6.79	12 (41%)	42,42,42	9.60	31 (73%)
3	NDP	E	402	-	51,52,52	3.33	19 (37%)	71,80,80	2.35	21 (29%)
2	GEF	E	401	-	29,29,29	7.06	11 (37%)	42,42,42	9.65	30 (71%)
2	GEF	B	401	-	29,29,29	7.47	11 (37%)	42,42,42	9.77	31 (73%)
3	NDP	F	402	-	51,52,52	3.23	17 (33%)	71,80,80	2.24	19 (26%)
3	NDP	C	402	-	51,52,52	3.34	20 (39%)	71,80,80	2.36	21 (29%)
2	GEF	C	401	-	29,29,29	6.65	11 (37%)	42,42,42	9.46	28 (66%)
2	GEF	D	401	-	29,29,29	3.04	9 (31%)	42,42,42	8.34	27 (64%)

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	NDP	A	402	-	-	7/34/77/77	0/5/5/5
2	GEF	A	401	-	-	8/12/34/34	0/4/4/4
3	NDP	D	402	-	-	4/34/77/77	0/5/5/5
3	NDP	B	402	-	-	4/34/77/77	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GEF	F	401	-	-	5/12/34/34	0/4/4/4
3	NDP	E	402	-	-	4/34/77/77	0/5/5/5
2	GEF	E	401	-	-	8/12/34/34	0/4/4/4
2	GEF	B	401	-	-	5/12/34/34	0/4/4/4
3	NDP	F	402	-	-	5/34/77/77	0/5/5/5
3	NDP	C	402	-	-	2/34/77/77	0/5/5/5
2	GEF	C	401	-	-	8/12/34/34	0/4/4/4
2	GEF	D	401	-	-	8/12/34/34	0/4/4/4

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	GEF	OAM-CAN	28.92	1.92	1.43
2	E	401	GEF	OAM-CAN	26.97	1.89	1.43
2	F	401	GEF	OAM-CAN	26.03	1.87	1.43
2	C	401	GEF	OAM-CAN	23.73	1.83	1.43
2	B	401	GEF	CAJ-CAN	-14.09	1.25	1.54
2	E	401	GEF	CAJ-CAN	-13.98	1.26	1.54
2	F	401	GEF	CAJ-CAN	-12.99	1.28	1.54
2	C	401	GEF	CAJ-CAN	-12.76	1.28	1.54
2	B	401	GEF	CAJ-CAK	-10.77	1.28	1.55
2	E	401	GEF	CAJ-CAK	-10.55	1.29	1.55
2	B	401	GEF	OAI-CAH	-10.30	1.21	1.43
2	B	401	GEF	OAI-CAG	10.03	1.60	1.43
2	C	401	GEF	CAJ-CAK	-9.80	1.30	1.55
2	A	401	GEF	OAI-CAG	-9.66	1.27	1.43
2	D	401	GEF	OAI-CAG	-9.54	1.27	1.43
2	C	401	GEF	OAI-CAH	-9.46	1.23	1.43
2	C	401	GEF	OAI-CAG	9.16	1.59	1.43
2	C	401	GEF	CAO-CAN	-9.02	1.35	1.51
3	D	402	NDP	O4B-C1B	8.97	1.62	1.42
2	F	401	GEF	CAJ-CAK	-8.89	1.33	1.55
2	E	401	GEF	OAI-CAG	8.89	1.58	1.43
2	C	401	GEF	CAD-CAG	-8.82	1.36	1.51
3	F	402	NDP	C2B-C1B	-8.79	1.31	1.53
3	C	402	NDP	O4D-C1D	8.71	1.62	1.42
2	F	401	GEF	OAI-CAG	8.70	1.58	1.43
3	C	402	NDP	O4B-C1B	8.70	1.62	1.42
3	B	402	NDP	O4D-C1D	8.63	1.61	1.42
3	E	402	NDP	O4D-C1D	8.62	1.61	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	NDP	C2B-C1B	-8.62	1.31	1.53
2	E	401	GEF	CAD-CAG	-8.55	1.36	1.51
2	B	401	GEF	OAM-CAL	8.50	1.62	1.43
3	F	402	NDP	O4B-C1B	8.46	1.61	1.42
3	A	402	NDP	O4B-C1B	8.44	1.61	1.42
3	B	402	NDP	C2B-C1B	-8.37	1.32	1.53
3	D	402	NDP	C2B-C1B	-8.29	1.32	1.53
3	A	402	NDP	O4D-C1D	8.24	1.61	1.42
2	F	401	GEF	OAM-CAL	8.17	1.61	1.43
3	C	402	NDP	C2B-C1B	-8.16	1.33	1.53
3	A	402	NDP	PA-O3	8.05	1.68	1.59
2	E	401	GEF	OAI-CAH	-7.92	1.26	1.43
3	F	402	NDP	O4D-C1D	7.91	1.60	1.42
2	F	401	GEF	OAI-CAH	-7.87	1.27	1.43
3	A	402	NDP	C2B-C1B	-7.82	1.33	1.53
3	E	402	NDP	O4B-C1B	7.81	1.60	1.42
2	C	401	GEF	OAM-CAL	7.79	1.60	1.43
3	D	402	NDP	O4D-C1D	7.76	1.59	1.42
3	B	402	NDP	O4B-C1B	7.75	1.59	1.42
2	F	401	GEF	CAD-CAG	-7.70	1.38	1.51
2	B	401	GEF	CAD-CAG	-7.45	1.38	1.51
2	E	401	GEF	CAO-CAN	-7.45	1.38	1.51
2	F	401	GEF	CAO-CAN	-7.24	1.38	1.51
3	E	402	NDP	C2D-C1D	-7.06	1.31	1.53
3	C	402	NDP	C6N-C5N	7.00	1.54	1.33
3	A	402	NDP	C6N-C5N	6.93	1.54	1.33
3	D	402	NDP	PA-O3	6.91	1.67	1.59
3	A	402	NDP	C2D-C1D	-6.89	1.31	1.53
2	A	401	GEF	CAK-CAG	6.88	1.68	1.54
3	F	402	NDP	C6N-C5N	6.88	1.54	1.33
3	D	402	NDP	C2D-C1D	-6.82	1.32	1.53
3	C	402	NDP	C2D-C1D	-6.82	1.32	1.53
3	D	402	NDP	C6N-C5N	6.75	1.53	1.33
3	B	402	NDP	C2D-C1D	-6.73	1.32	1.53
2	B	401	GEF	CAO-CAN	-6.72	1.39	1.51
3	D	402	NDP	O4B-C4B	-6.70	1.30	1.45
2	E	401	GEF	OAM-CAL	6.70	1.58	1.43
3	F	402	NDP	C2D-C1D	-6.67	1.32	1.53
2	F	401	GEF	CAH-CAJ	-6.63	1.40	1.53
3	E	402	NDP	O4B-C4B	-6.48	1.30	1.45
3	E	402	NDP	C6N-C5N	6.43	1.52	1.33
2	A	401	GEF	CAO-CAN	-6.40	1.40	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NDP	C6N-C5N	6.36	1.52	1.33
3	A	402	NDP	O4B-C4B	-6.33	1.30	1.45
3	C	402	NDP	O4B-C4B	-6.25	1.31	1.45
2	D	401	GEF	CAK-CAG	6.22	1.66	1.54
2	E	401	GEF	CAK-CAG	6.22	1.66	1.54
2	B	401	GEF	CAK-CAG	6.21	1.66	1.54
2	E	401	GEF	CAH-CAJ	-6.18	1.41	1.53
3	B	402	NDP	O4B-C4B	-6.15	1.31	1.45
3	C	402	NDP	PA-O3	5.85	1.65	1.59
3	A	402	NDP	O4D-C4D	-5.76	1.32	1.45
3	B	402	NDP	PA-O3	5.73	1.65	1.59
2	F	401	GEF	CAK-CAG	5.65	1.65	1.54
2	D	401	GEF	CAJ-CAK	5.62	1.68	1.55
3	D	402	NDP	C2N-C3N	5.58	1.50	1.35
3	D	402	NDP	O4D-C4D	-5.55	1.32	1.45
3	E	402	NDP	O4D-C4D	-5.46	1.32	1.45
2	D	401	GEF	CAO-CAN	-5.45	1.41	1.51
2	A	401	GEF	CAJ-CAK	5.38	1.68	1.55
2	A	401	GEF	CAD-CAG	-5.23	1.42	1.51
2	C	401	GEF	CAK-CAG	5.18	1.64	1.54
2	C	401	GEF	CAH-CAJ	-5.13	1.43	1.53
3	F	402	NDP	O4B-C4B	-5.10	1.33	1.45
3	E	402	NDP	C2N-C3N	5.10	1.49	1.35
2	B	401	GEF	CAH-CAJ	-5.05	1.43	1.53
3	A	402	NDP	C2N-C3N	5.02	1.49	1.35
2	D	401	GEF	CAD-CAG	-5.00	1.42	1.51
3	F	402	NDP	O4D-C4D	-4.98	1.33	1.45
3	F	402	NDP	C2N-C3N	4.88	1.48	1.35
3	C	402	NDP	C2N-C3N	4.87	1.48	1.35
3	C	402	NDP	O4D-C4D	-4.75	1.34	1.45
3	E	402	NDP	PA-O3	4.57	1.64	1.59
3	D	402	NDP	C6A-N6A	4.55	1.45	1.34
3	C	402	NDP	C6A-N6A	4.49	1.45	1.34
3	A	402	NDP	C6A-N6A	4.41	1.45	1.34
3	B	402	NDP	O4D-C4D	-4.36	1.35	1.45
3	F	402	NDP	C5A-C4A	-4.30	1.31	1.39
3	F	402	NDP	PA-O3	4.29	1.64	1.59
3	F	402	NDP	C6A-N6A	4.29	1.45	1.34
3	B	402	NDP	C2N-C3N	4.27	1.46	1.35
3	C	402	NDP	PN-O3	4.11	1.63	1.59
2	D	401	GEF	OAM-CAN	4.10	1.50	1.43
3	E	402	NDP	C6A-N6A	4.02	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NDP	C6A-N6A	3.93	1.44	1.34
3	A	402	NDP	C6N-N1N	3.90	1.46	1.37
3	A	402	NDP	C5A-C4A	-3.78	1.32	1.39
3	E	402	NDP	PN-O3	3.71	1.63	1.59
2	A	401	GEF	OAM-CAL	-3.66	1.36	1.43
3	E	402	NDP	C7N-N7N	3.64	1.43	1.33
3	D	402	NDP	C5A-C4A	-3.63	1.32	1.39
3	F	402	NDP	C7N-N7N	3.63	1.43	1.33
3	E	402	NDP	C5A-C4A	-3.61	1.32	1.39
2	A	401	GEF	OAM-CAN	3.60	1.49	1.43
3	E	402	NDP	O2D-C2D	3.55	1.51	1.43
3	D	402	NDP	O2D-C2D	3.48	1.51	1.43
3	F	402	NDP	O2D-C2D	3.47	1.51	1.43
3	F	402	NDP	C6N-N1N	3.44	1.45	1.37
3	A	402	NDP	O2D-C2D	3.36	1.51	1.43
3	B	402	NDP	C5A-C4A	-3.34	1.33	1.39
3	C	402	NDP	C7N-N7N	3.33	1.43	1.33
3	B	402	NDP	C7N-N7N	3.33	1.43	1.33
3	C	402	NDP	C5A-C4A	-3.29	1.33	1.39
2	A	401	GEF	CAL-CAK	3.25	1.59	1.53
2	D	401	GEF	OAM-CAL	-3.04	1.37	1.43
3	A	402	NDP	C7N-N7N	3.04	1.42	1.33
3	D	402	NDP	C6N-N1N	2.96	1.44	1.37
3	E	402	NDP	C6N-N1N	2.86	1.44	1.37
3	D	402	NDP	C4N-C5N	2.82	1.56	1.49
3	B	402	NDP	O2D-C2D	2.79	1.49	1.43
3	D	402	NDP	C4N-C3N	2.71	1.55	1.50
3	D	402	NDP	C7N-N7N	2.69	1.41	1.33
3	A	402	NDP	C4N-C5N	2.68	1.56	1.49
3	C	402	NDP	O2D-C2D	2.68	1.49	1.43
3	B	402	NDP	PN-O3	2.65	1.62	1.59
2	B	401	GEF	CAL-CAK	2.63	1.57	1.53
3	E	402	NDP	C5A-C6A	-2.63	1.33	1.41
3	B	402	NDP	C6N-N1N	2.61	1.43	1.37
3	E	402	NDP	C4N-C5N	2.61	1.55	1.49
3	D	402	NDP	C2A-N3A	2.60	1.38	1.33
2	E	401	GEF	CAL-CAK	2.60	1.57	1.53
3	D	402	NDP	C8A-N7A	2.57	1.36	1.31
3	C	402	NDP	C2A-N3A	2.55	1.38	1.33
3	C	402	NDP	C6N-N1N	2.53	1.43	1.37
3	A	402	NDP	C2A-N3A	2.52	1.38	1.33
2	A	401	GEF	OAI-CAH	-2.47	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NDP	C4N-C5N	2.46	1.55	1.49
3	F	402	NDP	PN-O3	2.45	1.62	1.59
3	E	402	NDP	C2A-N3A	2.44	1.38	1.33
3	C	402	NDP	P2B-O2B	2.42	1.63	1.59
2	D	401	GEF	OAI-CAH	-2.39	1.38	1.43
2	D	401	GEF	CAL-CAK	2.36	1.57	1.53
3	C	402	NDP	O3D-C3D	-2.36	1.37	1.43
3	B	402	NDP	C5A-C6A	-2.35	1.34	1.41
3	A	402	NDP	C4N-C3N	2.27	1.54	1.50
3	A	402	NDP	PA-O5B	2.21	1.68	1.59
2	C	401	GEF	CAT-CAO	2.20	1.42	1.39
3	C	402	NDP	C4N-C5N	2.15	1.54	1.49
3	F	402	NDP	C5A-C6A	-2.12	1.35	1.41
3	C	402	NDP	C5A-C6A	-2.12	1.35	1.41
3	D	402	NDP	PA-O5B	2.11	1.67	1.59
2	F	401	GEF	CAL-CAK	2.10	1.56	1.53
3	E	402	NDP	P2B-O2B	2.08	1.63	1.59
3	D	402	NDP	C5B-C4B	2.08	1.57	1.51
3	B	402	NDP	C5B-C4B	2.07	1.57	1.51
3	D	402	NDP	O7N-C7N	-2.04	1.19	1.24
3	B	402	NDP	C2A-N3A	2.02	1.37	1.33
3	F	402	NDP	C4N-C5N	2.02	1.54	1.49
2	F	401	GEF	CAT-CAO	2.01	1.42	1.39
3	A	402	NDP	O7N-C7N	-2.01	1.19	1.24

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GEF	OAM-CAN-CAJ	-30.34	72.24	104.73
2	B	401	GEF	OAM-CAL-CAK	-30.04	65.44	105.56
2	D	401	GEF	OAI-CAG-CAK	-29.52	73.11	104.73
2	A	401	GEF	OAI-CAG-CAK	-29.04	73.63	104.73
2	E	401	GEF	OAM-CAL-CAK	-28.45	67.56	105.56
2	F	401	GEF	OAM-CAN-CAJ	-27.80	74.96	104.73
2	F	401	GEF	OAM-CAL-CAK	-27.60	68.69	105.56
2	E	401	GEF	OAM-CAN-CAO	-26.98	80.40	110.39
2	C	401	GEF	OAM-CAL-CAK	-26.89	69.64	105.56
2	F	401	GEF	OAM-CAN-CAO	-26.81	80.59	110.39
2	C	401	GEF	OAM-CAN-CAO	-26.70	80.71	110.39
2	E	401	GEF	OAM-CAN-CAJ	-26.60	76.24	104.73
2	C	401	GEF	OAM-CAN-CAJ	-25.16	77.79	104.73
2	B	401	GEF	OAM-CAN-CAO	-23.42	84.35	110.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	GEF	OAM-CAL-CAK	-21.64	76.66	105.56
2	D	401	GEF	CAH-CAJ-CAK	-21.52	74.81	103.24
2	A	401	GEF	OAM-CAL-CAK	-21.40	76.97	105.56
2	C	401	GEF	CAL-CAK-CAG	21.24	148.46	114.53
2	A	401	GEF	CAH-CAJ-CAK	-20.88	75.66	103.24
2	E	401	GEF	CAL-CAK-CAG	20.35	147.04	114.53
2	F	401	GEF	CAL-CAK-CAG	19.58	145.81	114.53
2	B	401	GEF	CAL-CAK-CAG	18.21	143.62	114.53
2	C	401	GEF	CAH-OAI-CAG	-17.39	70.81	106.43
2	E	401	GEF	CAH-OAI-CAG	-16.24	73.18	106.43
2	C	401	GEF	OAI-CAH-CAJ	16.14	127.12	105.56
2	B	401	GEF	OAI-CAH-CAJ	16.12	127.09	105.56
2	B	401	GEF	CAH-OAI-CAG	-16.08	73.51	106.43
2	F	401	GEF	CAH-OAI-CAG	-15.64	74.41	106.43
2	B	401	GEF	CAK-CAJ-CAN	14.61	127.03	103.10
2	A	401	GEF	CAK-CAJ-CAN	-14.59	79.21	103.10
2	D	401	GEF	CAK-CAJ-CAN	-14.59	79.21	103.10
2	E	401	GEF	OAI-CAH-CAJ	13.38	123.43	105.56
2	F	401	GEF	CAK-CAJ-CAN	13.33	124.93	103.10
2	F	401	GEF	OAI-CAH-CAJ	12.91	122.81	105.56
2	E	401	GEF	CAK-CAJ-CAN	11.86	122.53	103.10
2	C	401	GEF	CAK-CAJ-CAN	11.83	122.47	103.10
2	A	401	GEF	CAO-CAN-CAJ	-11.28	99.58	115.90
2	D	401	GEF	CAO-CAN-CAJ	-10.90	100.13	115.90
2	A	401	GEF	CAH-CAJ-CAN	10.50	131.31	114.53
2	D	401	GEF	OAI-CAH-CAJ	9.85	118.72	105.56
2	D	401	GEF	CAH-CAJ-CAN	9.69	130.02	114.53
2	A	401	GEF	OAI-CAH-CAJ	9.60	118.38	105.56
2	D	401	GEF	CAV-OAU-CAQ	9.23	131.05	117.51
2	D	401	GEF	OAI-CAG-CAD	-8.73	100.69	110.39
2	F	401	GEF	CAP-CAO-CAN	-8.71	100.67	119.88
2	A	401	GEF	OAI-CAG-CAD	-8.58	100.85	110.39
2	C	401	GEF	CAH-CAJ-CAN	8.55	128.18	114.53
2	E	401	GEF	CAO-CAN-CAJ	8.41	128.06	115.90
2	F	401	GEF	CAT-CAO-CAN	8.34	136.19	120.62
2	D	401	GEF	OAU-CAQ-CAR	8.32	127.02	114.55
2	F	401	GEF	OAI-CAG-CAK	-8.30	95.84	104.73
2	B	401	GEF	CAO-CAN-CAJ	8.27	127.86	115.90
2	A	401	GEF	OAU-CAQ-CAR	7.90	126.40	114.55
2	E	401	GEF	CAP-CAO-CAN	-7.82	102.63	119.88
2	B	401	GEF	OAI-CAG-CAK	-7.80	96.38	104.73
2	F	401	GEF	CAC-CAD-CAG	7.64	134.88	120.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	GEF	CAO-CAN-CAJ	7.61	126.91	115.90
2	F	401	GEF	CAH-CAJ-CAN	7.55	126.59	114.53
3	B	402	NDP	N3A-C2A-N1A	-7.40	117.39	128.58
2	D	401	GEF	CAT-CAO-CAN	7.36	134.35	120.62
2	E	401	GEF	CAH-CAJ-CAN	7.35	126.26	114.53
2	A	401	GEF	CAT-CAO-CAN	7.32	134.28	120.62
2	A	401	GEF	OAM-CAN-CAJ	7.29	112.55	104.73
2	D	401	GEF	CAL-CAK-CAJ	7.20	112.76	103.24
3	A	402	NDP	N3A-C2A-N1A	-7.17	117.73	128.58
2	E	401	GEF	OAU-CAQ-CAR	7.15	125.28	114.55
2	C	401	GEF	CAJ-CAK-CAG	-7.11	91.46	103.10
3	A	402	NDP	O4B-C4B-C3B	-7.10	91.06	105.15
2	E	401	GEF	CAJ-CAK-CAG	-7.10	91.48	103.10
2	F	401	GEF	CAJ-CAK-CAG	-7.04	91.58	103.10
2	D	401	GEF	OAM-CAN-CAJ	6.90	112.12	104.73
2	C	401	GEF	CAO-CAN-CAJ	6.83	125.78	115.90
2	A	401	GEF	CAL-CAK-CAJ	6.78	112.21	103.24
2	B	401	GEF	CAH-CAJ-CAN	6.76	125.33	114.53
2	B	401	GEF	CAC-CAD-CAG	6.72	133.16	120.62
2	E	401	GEF	CAT-CAO-CAN	6.64	133.02	120.62
3	C	402	NDP	C5A-C4A-N3A	-6.62	117.60	126.72
2	A	401	GEF	OAU-CAQ-CAP	-6.56	112.78	124.08
3	D	402	NDP	C5A-C4A-N3A	-6.54	117.71	126.72
3	A	402	NDP	C5A-C4A-N3A	-6.48	117.80	126.72
2	D	401	GEF	OAU-CAQ-CAP	-6.47	112.94	124.08
2	B	401	GEF	CAP-CAO-CAN	-6.45	105.64	119.88
3	D	402	NDP	O4B-C4B-C3B	-6.44	92.37	105.15
3	D	402	NDP	N3A-C2A-N1A	-6.39	118.91	128.58
2	E	401	GEF	OAI-CAG-CAK	-6.38	97.90	104.73
3	F	402	NDP	C5A-C4A-N3A	-6.36	117.95	126.72
3	C	402	NDP	N3A-C2A-N1A	-6.31	119.03	128.58
2	E	401	GEF	CAC-CAD-CAG	6.31	132.40	120.62
2	A	401	GEF	CAL-CAK-CAG	6.27	124.55	114.53
2	C	401	GEF	OAU-CAQ-CAR	6.23	123.90	114.55
2	C	401	GEF	CAC-CAD-CAG	6.21	132.22	120.62
2	C	401	GEF	CAP-CAO-CAN	-6.18	106.25	119.88
3	F	402	NDP	N3A-C2A-N1A	-6.11	119.33	128.58
2	F	401	GEF	CAE-CAD-CAG	-6.00	106.65	119.88
2	A	401	GEF	CAP-CAO-CAN	-5.99	106.67	119.88
3	F	402	NDP	O4B-C4B-C3B	-5.95	93.34	105.15
3	E	402	NDP	N6A-C6A-N1A	-5.87	105.30	118.38
3	E	402	NDP	C5A-C4A-N3A	-5.87	118.64	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GEF	CAJ-CAK-CAG	-5.87	93.49	103.10
2	B	401	GEF	OAI-CAG-CAD	-5.77	103.98	110.39
3	E	402	NDP	N3A-C2A-N1A	-5.75	119.88	128.58
2	C	401	GEF	CAE-CAD-CAG	-5.74	107.22	119.88
2	B	401	GEF	CAT-CAO-CAN	5.70	131.26	120.62
3	D	402	NDP	N6A-C6A-N1A	-5.63	105.83	118.38
3	C	402	NDP	O4B-C4B-C3B	-5.58	94.08	105.15
3	E	402	NDP	O4B-C4B-C3B	-5.57	94.10	105.15
2	D	401	GEF	CAP-CAO-CAN	-5.56	107.62	119.88
2	E	401	GEF	CAE-CAD-CAG	-5.55	107.63	119.88
3	B	402	NDP	C5A-C4A-N3A	-5.50	119.14	126.72
3	B	402	NDP	O4B-C4B-C3B	-5.45	94.33	105.15
3	A	402	NDP	N6A-C6A-N1A	-5.41	106.33	118.38
3	B	402	NDP	N6A-C6A-N1A	-5.40	106.35	118.38
2	D	401	GEF	CAL-CAK-CAG	5.33	123.05	114.53
2	B	401	GEF	CAE-CAD-CAG	-5.33	108.13	119.88
2	E	401	GEF	OAI-CAG-CAD	-5.25	104.55	110.39
3	F	402	NDP	N6A-C6A-N1A	-5.21	106.78	118.38
2	B	401	GEF	CAL-CAK-CAJ	5.20	110.11	103.24
3	B	402	NDP	O4B-C1B-N9A	-5.13	98.24	108.09
3	C	402	NDP	N6A-C6A-N1A	-5.12	106.97	118.38
3	D	402	NDP	N3A-C4A-N9A	5.11	135.85	127.17
2	E	401	GEF	CAV-OAU-CAQ	5.06	124.94	117.51
3	A	402	NDP	O4B-C1B-N9A	-5.01	98.47	108.09
2	E	401	GEF	CAL-OAM-CAN	-4.98	96.24	106.43
3	E	402	NDP	O2N-PN-O3	4.94	120.62	107.27
3	E	402	NDP	O4B-C1B-N9A	-4.91	98.67	108.09
3	D	402	NDP	N9A-C8A-N7A	-4.90	106.98	113.94
3	C	402	NDP	N3A-C4A-N9A	4.85	135.42	127.17
3	F	402	NDP	N3A-C4A-N9A	4.84	135.40	127.17
2	C	401	GEF	CAT-CAO-CAN	4.82	129.62	120.62
3	A	402	NDP	N3A-C4A-N9A	4.79	135.31	127.17
3	A	402	NDP	C2A-N3A-C4A	4.78	123.50	111.83
2	C	401	GEF	CAL-OAM-CAN	-4.75	96.70	106.43
2	E	401	GEF	CAQ-CAP-CAO	4.75	127.19	119.86
2	C	401	GEF	OAI-CAG-CAK	-4.71	99.69	104.73
3	D	402	NDP	O4B-C1B-N9A	-4.60	99.25	108.09
2	E	401	GEF	CAL-CAK-CAJ	4.60	109.32	103.24
3	D	402	NDP	O2N-PN-O3	4.57	119.62	107.27
2	A	401	GEF	CAV-OAU-CAQ	4.57	124.21	117.51
3	D	402	NDP	C4A-N9A-C1B	-4.51	116.08	126.63
2	C	401	GEF	CAT-CAO-CAP	-4.50	113.52	118.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NDP	N3A-C4A-N9A	4.49	134.81	127.17
3	E	402	NDP	C4A-N9A-C1B	-4.42	116.30	126.63
3	B	402	NDP	C4A-N9A-C1B	-4.42	116.30	126.63
2	F	401	GEF	CAV-OAU-CAQ	-4.40	111.07	117.51
2	C	401	GEF	OAI-CAG-CAD	-4.37	105.54	110.39
2	A	401	GEF	OAM-CAN-CAO	4.35	115.23	110.39
3	C	402	NDP	O4B-C1B-N9A	-4.32	99.79	108.09
3	E	402	NDP	C3N-C2N-N1N	-4.29	116.91	123.20
2	B	401	GEF	CAP-CAQ-CAR	-4.24	115.76	120.04
3	E	402	NDP	N3A-C4A-N9A	4.23	134.36	127.17
3	B	402	NDP	C2A-N3A-C4A	4.21	122.11	111.83
3	C	402	NDP	O2N-PN-O3	4.20	118.64	107.27
3	F	402	NDP	C4A-N9A-C1B	-4.18	116.86	126.63
2	B	401	GEF	CAD-CAG-CAK	4.17	121.93	115.90
2	C	401	GEF	CAV-OAU-CAQ	4.17	123.63	117.51
2	D	401	GEF	OAM-CAN-CAO	4.16	115.02	110.39
3	D	402	NDP	C2A-N3A-C4A	4.16	121.99	111.83
3	F	402	NDP	C2A-N3A-C4A	4.10	121.84	111.83
3	C	402	NDP	C4A-N9A-C1B	-4.09	117.06	126.63
3	C	402	NDP	C2A-N3A-C4A	4.08	121.80	111.83
2	E	401	GEF	CAP-CAQ-CAR	-4.05	115.96	120.04
3	E	402	NDP	C1B-N9A-C8A	4.01	135.99	127.09
2	E	401	GEF	CAT-CAO-CAP	-4.01	114.09	118.74
2	F	401	GEF	CAL-OAM-CAN	-4.00	98.23	106.43
2	B	401	GEF	CAV-OAU-CAQ	-3.97	111.69	117.51
2	C	401	GEF	CAQ-CAP-CAO	3.97	125.99	119.86
3	F	402	NDP	N9A-C8A-N7A	-3.94	108.35	113.94
2	B	401	GEF	CAL-OAM-CAN	-3.89	98.47	106.43
2	B	401	GEF	CAH-CAJ-CAK	-3.88	98.12	103.24
2	F	401	GEF	CAT-CAO-CAP	-3.87	114.25	118.74
3	C	402	NDP	N9A-C8A-N7A	-3.86	108.45	113.94
3	A	402	NDP	N9A-C8A-N7A	-3.83	108.51	113.94
3	D	402	NDP	O4B-C1B-C2B	-3.81	100.03	106.59
3	B	402	NDP	C1B-N9A-C8A	3.80	135.53	127.09
2	C	401	GEF	CAH-CAJ-CAK	-3.79	98.23	103.24
3	F	402	NDP	C3N-C2N-N1N	-3.70	117.78	123.20
2	B	401	GEF	CAQ-CAP-CAO	3.69	125.56	119.86
2	A	401	GEF	CAC-CAD-CAG	3.68	127.50	120.62
3	A	402	NDP	C4A-N9A-C1B	-3.68	118.04	126.63
3	A	402	NDP	O2N-PN-O3	3.66	117.17	107.27
2	F	401	GEF	CAQ-CAP-CAO	3.65	125.50	119.86
3	F	402	NDP	O4B-C1B-N9A	-3.65	101.08	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	NDP	C3N-C2N-N1N	-3.64	117.86	123.20
2	F	401	GEF	CAB-CAC-CAD	-3.61	117.58	121.18
3	E	402	NDP	C5A-C6A-N6A	3.59	132.17	123.29
2	F	401	GEF	CAL-CAK-CAJ	3.56	107.94	103.24
3	A	402	NDP	O4B-C1B-C2B	-3.55	100.47	106.59
3	A	402	NDP	C3N-C2N-N1N	-3.54	118.00	123.20
2	B	401	GEF	CAT-CAO-CAP	-3.51	114.67	118.74
3	F	402	NDP	C1B-N9A-C8A	3.50	134.86	127.09
3	D	402	NDP	C4A-N9A-C8A	3.50	109.41	105.74
2	D	401	GEF	CAC-CAD-CAG	3.49	127.14	120.62
3	C	402	NDP	C1B-N9A-C8A	3.49	134.83	127.09
2	A	401	GEF	CAX-OAW-CAF	-3.39	112.54	117.51
2	D	401	GEF	CAX-OAW-CAF	-3.38	112.56	117.51
3	E	402	NDP	C2A-N3A-C4A	3.37	120.06	111.83
3	B	402	NDP	N9A-C8A-N7A	-3.36	109.17	113.94
3	B	402	NDP	C3N-C2N-N1N	-3.34	118.29	123.20
3	D	402	NDP	C1B-N9A-C8A	3.34	134.50	127.09
2	A	401	GEF	CAE-CAD-CAG	-3.31	112.59	119.88
3	D	402	NDP	C3N-C2N-N1N	-3.24	118.45	123.20
3	E	402	NDP	N9A-C8A-N7A	-3.21	109.38	113.94
3	C	402	NDP	C6A-C5A-C4A	3.19	121.54	117.18
3	D	402	NDP	O2B-P2B-O1X	-3.18	98.01	109.33
3	B	402	NDP	C5A-C6A-N6A	3.17	131.15	123.29
3	B	402	NDP	O3X-P2B-O2B	3.16	118.17	105.85
2	F	401	GEF	CAE-CAF-CAA	-3.16	116.85	120.04
2	F	401	GEF	OAI-CAG-CAD	-3.16	106.89	110.39
2	C	401	GEF	CAL-CAK-CAJ	3.16	107.41	103.24
2	E	401	GEF	CAB-CAC-CAD	-3.14	118.05	121.18
3	E	402	NDP	O2B-C2B-C3B	-3.14	100.41	111.68
3	E	402	NDP	C6A-C5A-C4A	3.12	121.44	117.18
2	E	401	GEF	OAU-CAQ-CAP	-3.09	118.76	124.08
3	B	402	NDP	O2B-C2B-C3B	-3.06	100.70	111.68
3	D	402	NDP	O3X-P2B-O2B	3.06	117.76	105.85
2	E	401	GEF	CAS-CAT-CAO	-3.02	118.17	121.18
3	C	402	NDP	C5A-C6A-N6A	3.01	130.74	123.29
2	D	401	GEF	CAQ-CAP-CAO	3.00	124.49	119.86
2	D	401	GEF	CAE-CAD-CAG	-2.97	113.32	119.88
2	C	401	GEF	CAP-CAQ-CAR	-2.96	117.06	120.04
3	E	402	NDP	O3X-P2B-O2B	2.95	117.36	105.85
2	C	401	GEF	OAU-CAQ-CAP	-2.93	119.03	124.08
2	B	401	GEF	OAY-CAA-CAF	-2.90	113.32	120.13
2	F	401	GEF	CAP-CAQ-CAR	-2.89	117.12	120.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	GEF	CAF-CAE-CAD	2.85	124.27	119.86
2	F	401	GEF	CAX-OAW-CAF	-2.85	113.34	117.51
3	E	402	NDP	O2B-P2B-O1X	-2.84	99.20	109.33
3	D	402	NDP	C5A-C6A-N6A	2.83	130.30	123.29
3	B	402	NDP	O4B-C1B-C2B	-2.81	101.76	106.59
3	C	402	NDP	O3X-P2B-O2B	2.80	116.77	105.85
3	D	402	NDP	O2B-C2B-C3B	-2.80	101.64	111.68
3	A	402	NDP	C1B-N9A-C8A	2.79	133.30	127.09
3	A	402	NDP	C4B-O4B-C1B	-2.79	103.31	109.47
3	A	402	NDP	C4A-N9A-C8A	2.77	108.65	105.74
3	C	402	NDP	P2B-O2B-C2B	2.73	130.73	123.43
3	C	402	NDP	O3B-C3B-C2B	-2.68	103.67	111.19
2	F	401	GEF	CAH-CAJ-CAK	-2.68	99.71	103.24
2	E	401	GEF	CAE-CAF-CAA	-2.68	117.34	120.04
3	B	402	NDP	O2N-PN-O3	2.63	114.37	107.27
3	C	402	NDP	O4B-C1B-C2B	-2.63	102.07	106.59
3	F	402	NDP	C6A-C5A-C4A	2.61	120.75	117.18
2	D	401	GEF	CAS-CAR-CAQ	-2.56	116.65	119.55
3	F	402	NDP	C5A-C6A-N6A	2.56	129.62	123.29
3	A	402	NDP	C5A-C6A-N1A	2.53	123.94	117.51
3	A	402	NDP	C5A-C6A-N6A	2.52	129.53	123.29
3	B	402	NDP	C4B-O4B-C1B	-2.51	103.93	109.47
2	E	401	GEF	CAD-CAG-CAK	2.49	119.50	115.90
2	B	401	GEF	OAY-CAA-CAB	2.46	125.98	119.36
3	C	402	NDP	C4B-O4B-C1B	-2.45	104.06	109.47
3	D	402	NDP	C5A-C6A-N1A	2.42	123.67	117.51
3	F	402	NDP	C4A-N9A-C8A	2.42	108.28	105.74
3	A	402	NDP	O2A-PA-O3	-2.40	100.78	107.27
3	F	402	NDP	C5A-C6A-N1A	2.40	123.60	117.51
3	F	402	NDP	C4B-O4B-C1B	-2.34	104.31	109.47
2	B	401	GEF	CAB-CAC-CAD	-2.33	118.85	121.18
3	A	402	NDP	O3X-P2B-O2B	2.33	114.92	105.85
2	F	401	GEF	OAY-CAA-CAF	-2.32	114.67	120.13
3	A	402	NDP	O3B-C3B-C2B	-2.32	104.68	111.19
3	E	402	NDP	C4B-O4B-C1B	-2.32	104.34	109.47
3	B	402	NDP	C4A-N9A-C8A	2.32	108.17	105.74
3	D	402	NDP	C6A-C5A-C4A	2.30	120.33	117.18
3	D	402	NDP	C4B-O4B-C1B	-2.30	104.40	109.47
3	A	402	NDP	O2B-P2B-O1X	-2.29	101.19	109.33
2	C	401	GEF	OAY-CAA-CAF	-2.28	114.78	120.13
3	F	402	NDP	O4D-C1D-N1N	-2.28	103.74	108.08
2	C	401	GEF	CAB-CAC-CAD	-2.26	118.92	121.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	GEF	CAJ-CAK-CAG	2.26	106.80	103.10
2	B	401	GEF	OAU-CAQ-CAP	2.25	127.95	124.08
3	C	402	NDP	C4A-N9A-C8A	2.25	108.10	105.74
2	C	401	GEF	CAD-CAG-CAK	2.23	119.12	115.90
2	B	401	GEF	CAE-CAF-CAA	-2.23	117.80	120.04
3	D	402	NDP	C5A-N7A-C8A	2.22	106.94	103.45
2	D	401	GEF	CAS-CAT-CAO	-2.20	118.99	121.18
2	E	401	GEF	OAY-CAA-CAF	-2.18	115.00	120.13
2	F	401	GEF	CAC-CAB-CAA	2.17	122.67	120.50
3	E	402	NDP	O4B-C1B-C2B	-2.17	102.86	106.59
3	A	402	NDP	O3B-C3B-C4B	2.15	117.27	111.08
3	E	402	NDP	C6A-C5A-N7A	-2.15	127.95	132.09
2	D	401	GEF	CAD-CAG-CAK	2.14	118.99	115.90
2	B	401	GEF	CAF-CAE-CAD	2.12	123.14	119.86
3	F	402	NDP	O4B-C1B-C2B	-2.11	102.95	106.59
2	F	401	GEF	OAY-CAA-CAB	2.11	125.03	119.36
2	E	401	GEF	CAT-CAS-CAR	2.10	122.60	120.50
3	F	402	NDP	O2N-PN-O3	2.10	112.94	107.27
3	B	402	NDP	C3N-C7N-N7N	-2.08	113.98	117.67
3	E	402	NDP	O3B-C3B-C2B	-2.07	105.38	111.19
2	B	401	GEF	OAW-CAF-CAE	2.07	127.64	124.08
3	C	402	NDP	C5A-N7A-C8A	2.04	106.65	103.45
3	B	402	NDP	O3B-C3B-C2B	-2.03	105.49	111.19
2	D	401	GEF	OAY-CAA-CAF	-2.03	115.37	120.13
2	F	401	GEF	OAW-CAF-CAA	2.02	117.58	114.55
2	D	401	GEF	OAZ-CAR-CAS	2.01	124.76	119.36
3	D	402	NDP	O3D-C3D-C2D	-2.00	105.40	111.82

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	402	NDP	C5B-O5B-PA-O2A
3	E	402	NDP	C5B-O5B-PA-O3
3	A	402	NDP	C5B-O5B-PA-O2A
3	A	402	NDP	C5B-O5B-PA-O3
3	D	402	NDP	C5B-O5B-PA-O2A
3	D	402	NDP	C5B-O5B-PA-O3
3	B	402	NDP	C5B-O5B-PA-O2A
2	E	401	GEF	CAR-CAQ-OAU-CAV
2	A	401	GEF	CAR-CAQ-OAU-CAV
2	D	401	GEF	CAR-CAQ-OAU-CAV

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	401	GEF	CAR-CAQ-OAU-CAV
2	E	401	GEF	CAP-CAQ-OAU-CAV
2	A	401	GEF	CAP-CAQ-OAU-CAV
2	D	401	GEF	CAP-CAQ-OAU-CAV
2	C	401	GEF	CAP-CAQ-OAU-CAV
2	F	401	GEF	CAC-CAD-CAG-CAK
2	B	401	GEF	CAC-CAD-CAG-CAK
2	E	401	GEF	CAE-CAD-CAG-CAK
2	B	401	GEF	CAE-CAD-CAG-CAK
2	A	401	GEF	CAJ-CAN-CAO-CAT
2	F	401	GEF	CAE-CAD-CAG-CAK
2	E	401	GEF	CAC-CAD-CAG-CAK
2	A	401	GEF	CAC-CAD-CAG-CAK
2	D	401	GEF	CAJ-CAN-CAO-CAT
2	C	401	GEF	OAM-CAN-CAO-CAP
2	A	401	GEF	OAM-CAN-CAO-CAP
2	A	401	GEF	CAE-CAD-CAG-CAK
2	F	401	GEF	CAJ-CAN-CAO-CAP
2	D	401	GEF	CAE-CAD-CAG-CAK
2	C	401	GEF	CAE-CAD-CAG-CAK
2	B	401	GEF	CAJ-CAN-CAO-CAP
2	D	401	GEF	OAM-CAN-CAO-CAP
2	C	401	GEF	CAC-CAD-CAG-OAI
2	E	401	GEF	CAJ-CAN-CAO-CAP
2	D	401	GEF	CAC-CAD-CAG-CAK
2	C	401	GEF	CAJ-CAN-CAO-CAP
2	C	401	GEF	CAC-CAD-CAG-CAK
2	E	401	GEF	CAC-CAD-CAG-OAI
2	D	401	GEF	CAJ-CAN-CAO-CAP
2	E	401	GEF	OAM-CAN-CAO-CAP
2	A	401	GEF	CAJ-CAN-CAO-CAP
3	B	402	NDP	C5B-O5B-PA-O3
2	C	401	GEF	CAE-CAD-CAG-OAI
3	C	402	NDP	O4D-C1D-N1N-C2N
2	A	401	GEF	OAM-CAN-CAO-CAT
3	E	402	NDP	O4D-C1D-N1N-C2N
3	F	402	NDP	O4D-C1D-N1N-C2N
3	D	402	NDP	O4D-C1D-N1N-C2N
3	A	402	NDP	O4D-C1D-N1N-C2N
3	B	402	NDP	O4D-C1D-N1N-C2N
3	E	402	NDP	C2D-C1D-N1N-C2N
3	A	402	NDP	C2B-O2B-P2B-O1X

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	F	402	NDP	C2B-O2B-P2B-O1X
2	D	401	GEF	OAM-CAN-CAO-CAT
2	B	401	GEF	OAM-CAN-CAO-CAP
3	A	402	NDP	C2D-C1D-N1N-C2N
2	E	401	GEF	CAE-CAD-CAG-OAI
3	D	402	NDP	C2D-C1D-N1N-C2N
3	C	402	NDP	C2D-C1D-N1N-C2N
2	F	401	GEF	OAM-CAN-CAO-CAP
2	F	401	GEF	CAC-CAD-CAG-OAI
2	B	401	GEF	CAC-CAD-CAG-OAI
3	F	402	NDP	C2D-C1D-N1N-C2N
3	B	402	NDP	C2D-C1D-N1N-C2N
3	A	402	NDP	C2B-O2B-P2B-O2X
3	F	402	NDP	C2B-O2B-P2B-O2X
3	F	402	NDP	C2B-O2B-P2B-O3X
3	A	402	NDP	PN-O3-PA-O2A

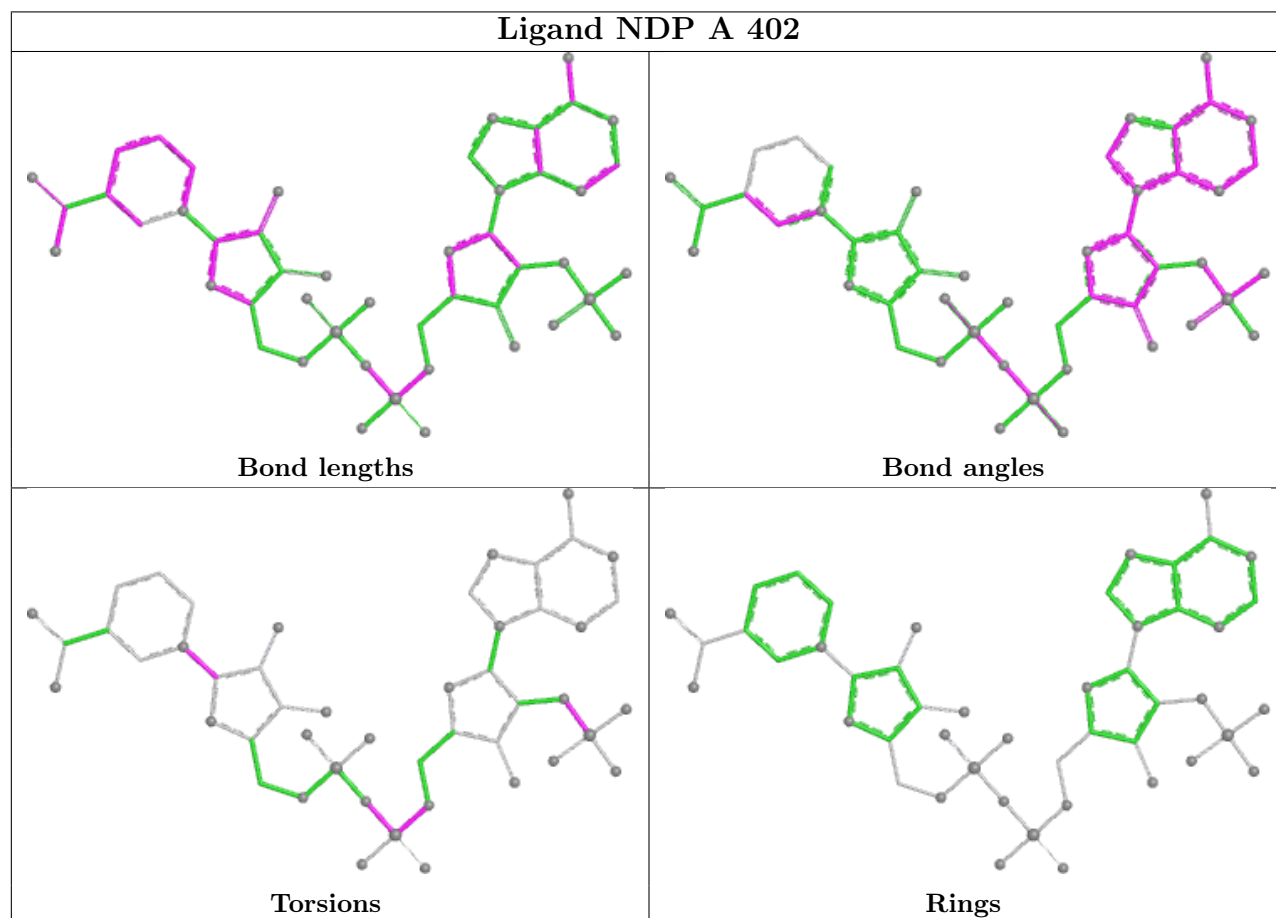
There are no ring outliers.

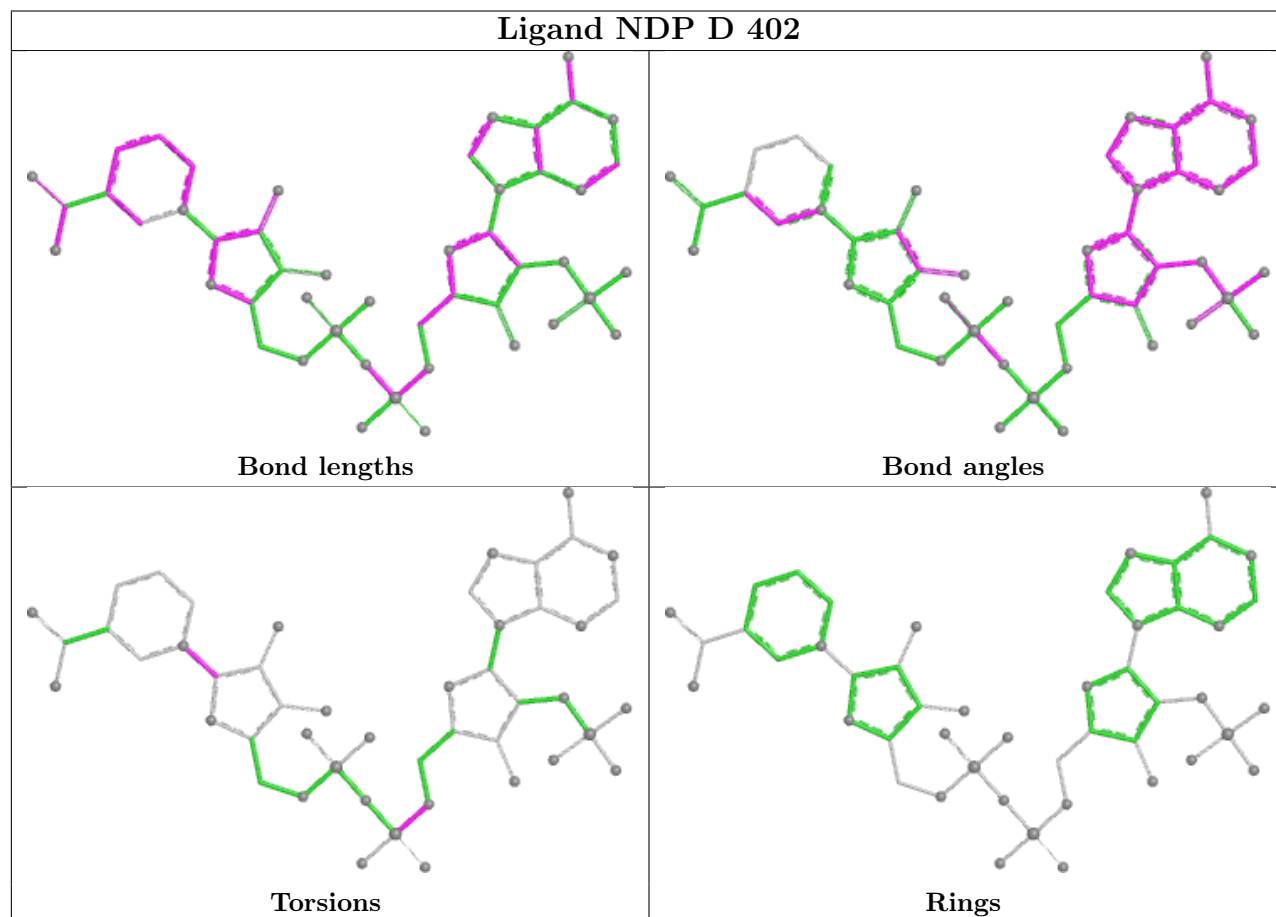
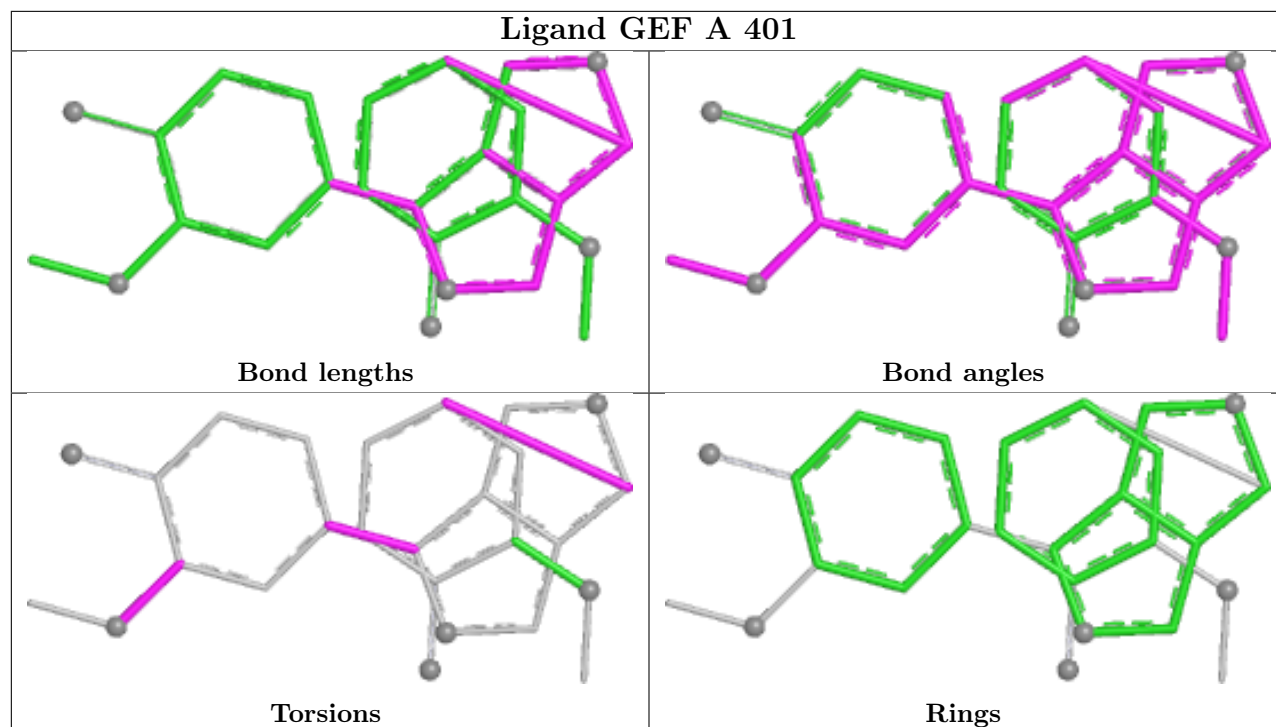
12 monomers are involved in 75 short contacts:

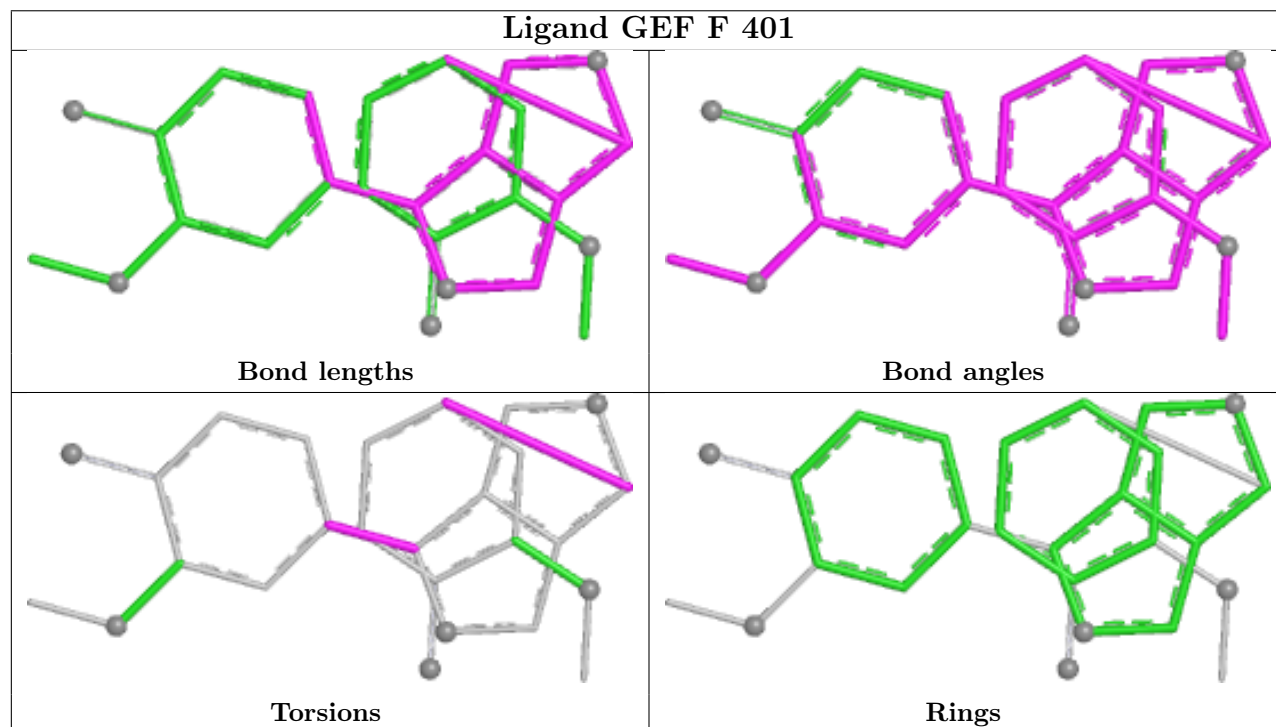
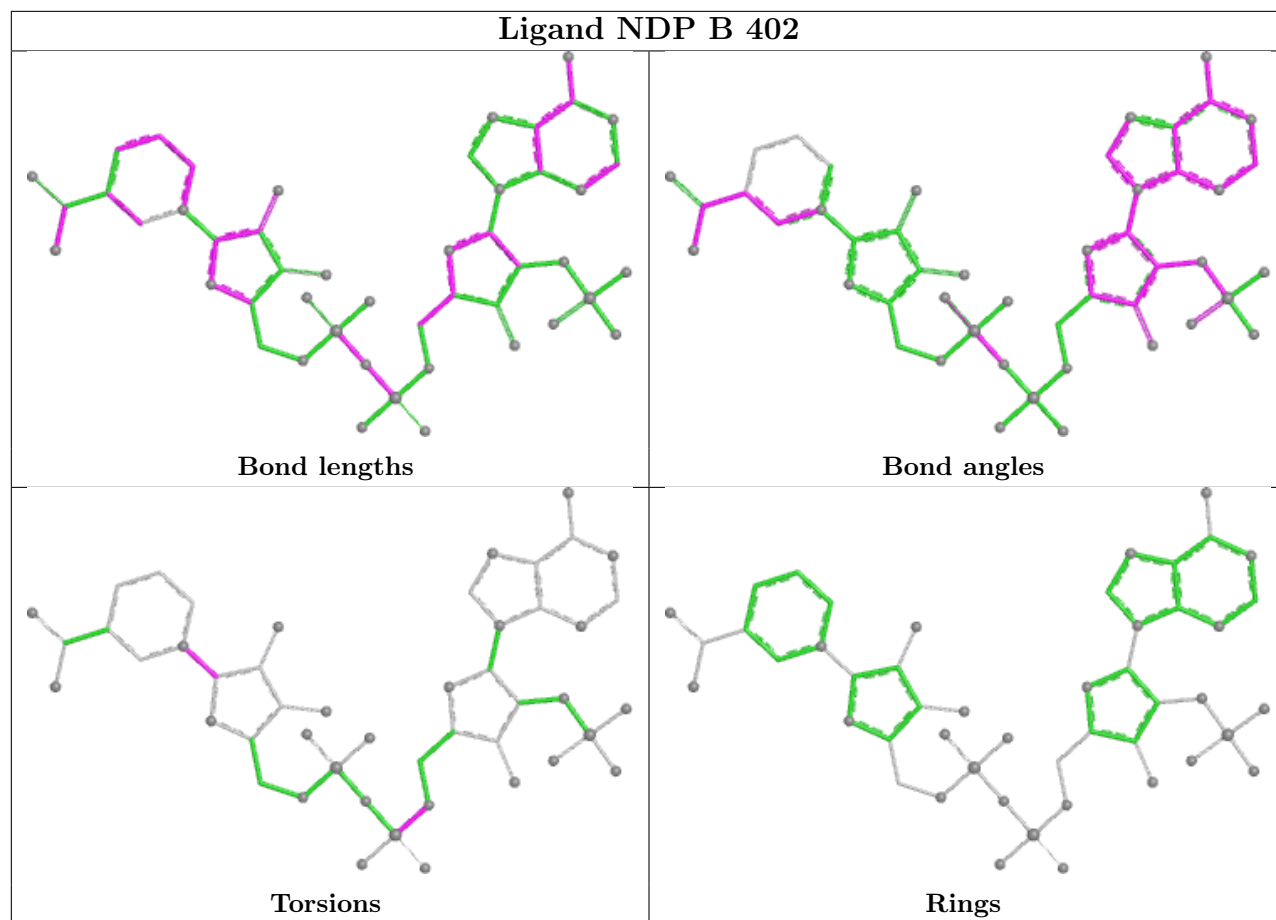
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	NDP	11	0
2	A	401	GEF	3	0
3	D	402	NDP	8	0
3	B	402	NDP	6	0
2	F	401	GEF	5	0
3	E	402	NDP	7	0
2	E	401	GEF	9	0
2	B	401	GEF	5	0
3	F	402	NDP	10	0
3	C	402	NDP	3	0
2	C	401	GEF	9	0
2	D	401	GEF	3	0

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

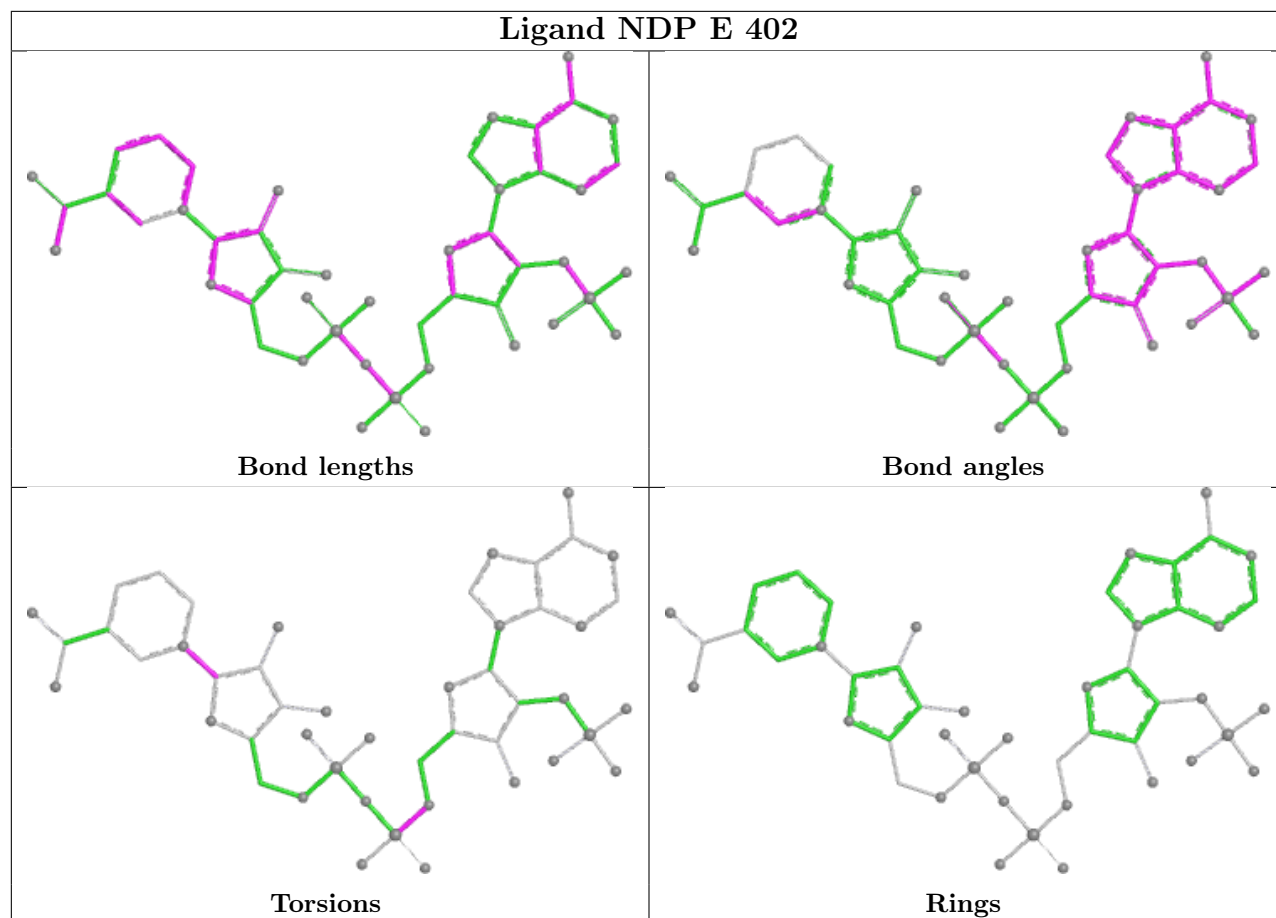
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



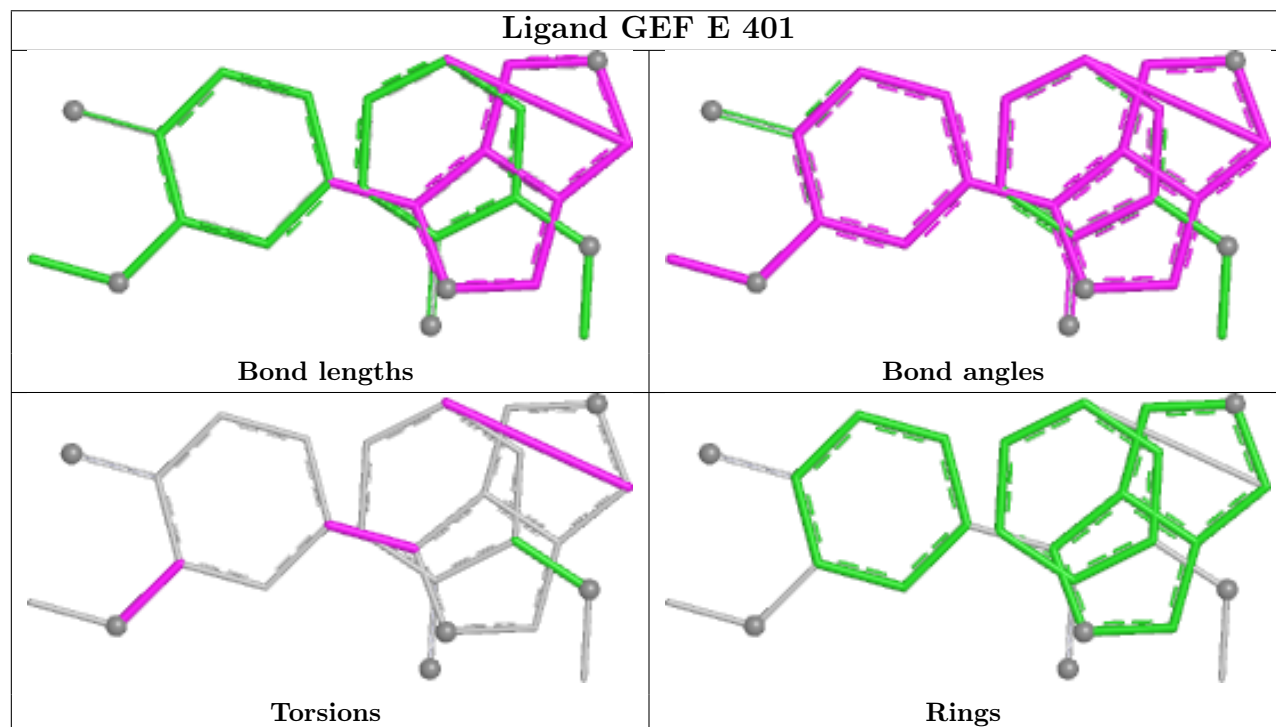


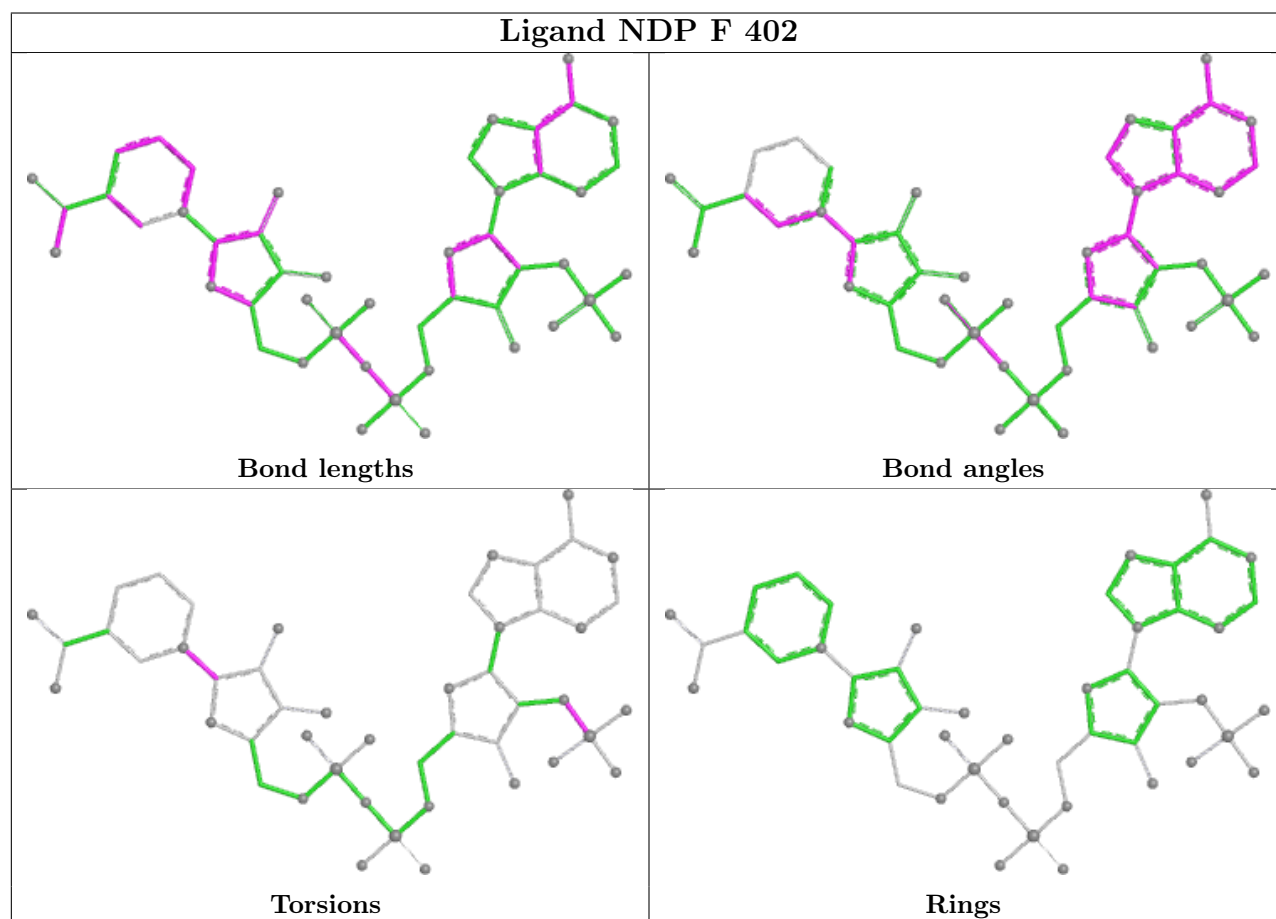
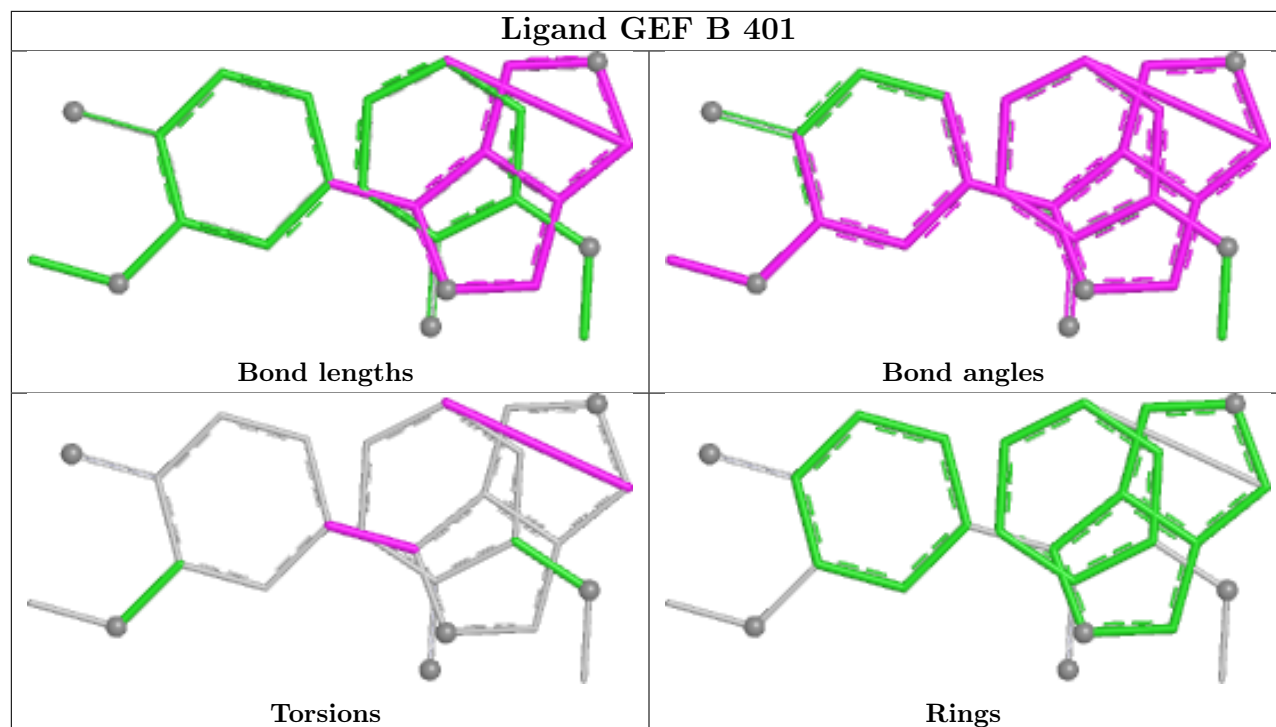


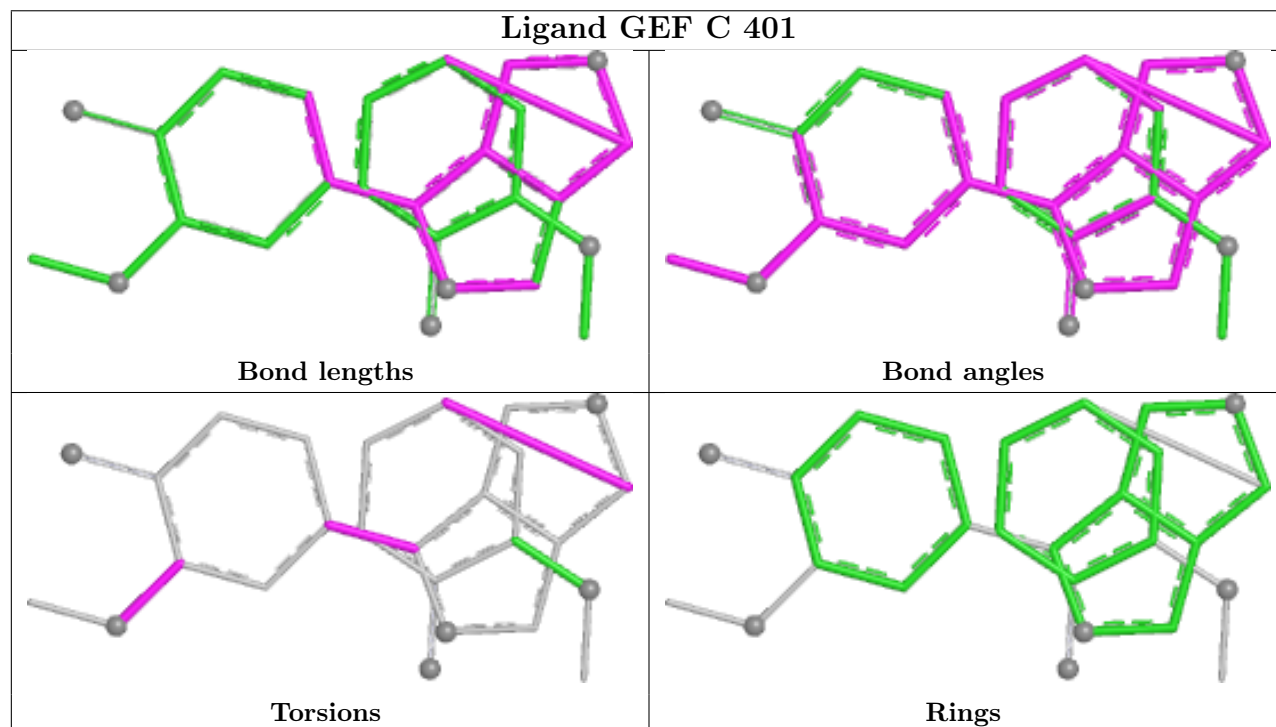
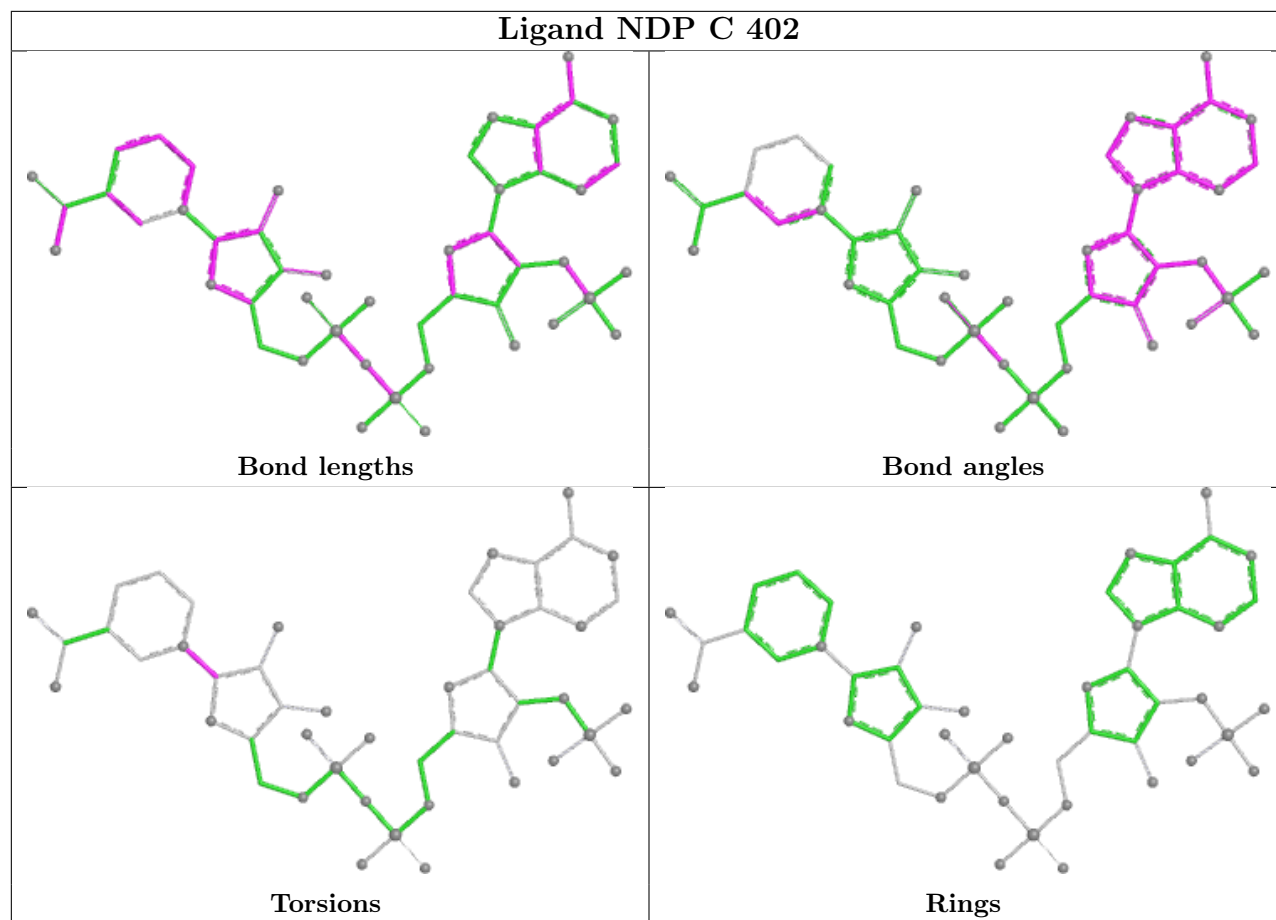
Ligand NDP E 402

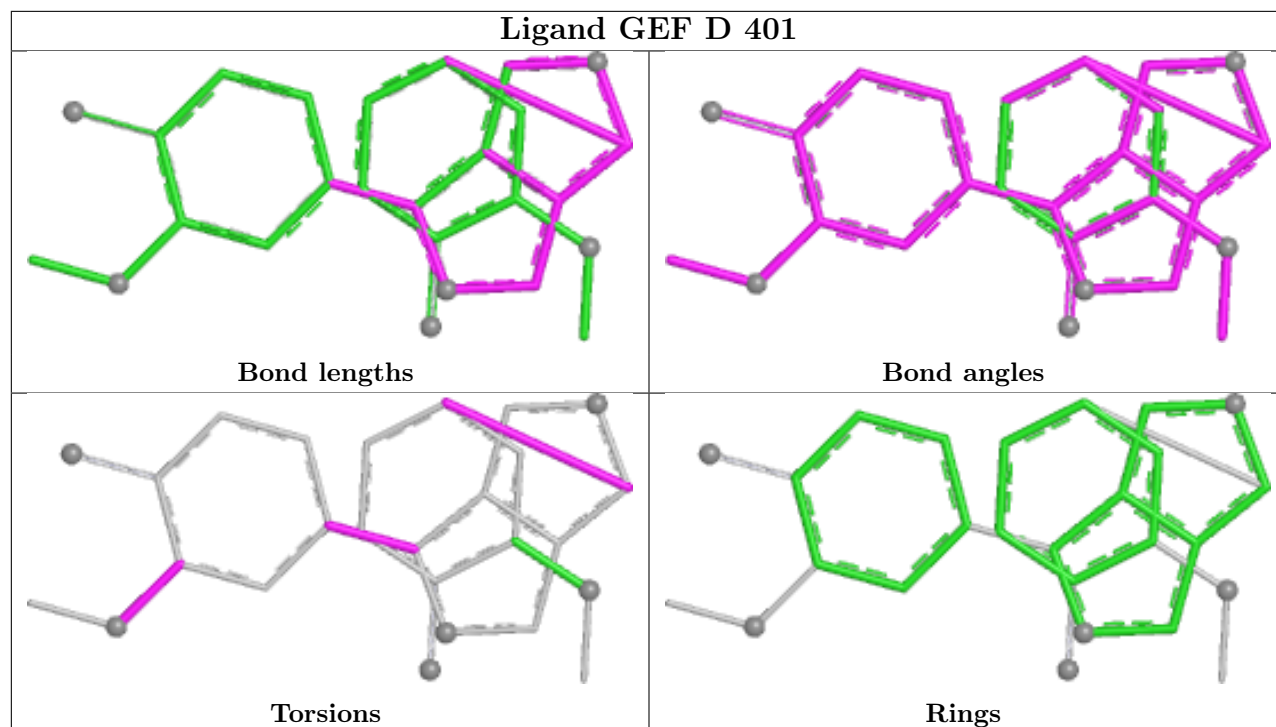


Ligand GEF E 401









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	284/317 (89%)	0.12	21 (7%)	20 20	17, 29, 55, 83	0
1	B	290/317 (91%)	-0.30	10 (3%)	48 47	17, 25, 42, 70	0
1	C	285/317 (89%)	-0.25	9 (3%)	50 49	18, 26, 44, 63	0
1	D	285/317 (89%)	-0.03	10 (3%)	47 46	21, 30, 46, 81	0
1	E	285/317 (89%)	-0.25	10 (3%)	47 46	18, 27, 46, 76	0
1	F	285/317 (89%)	0.02	10 (3%)	47 46	20, 31, 53, 83	0
All	All	1714/1902 (90%)	-0.12	70 (4%)	41 41	17, 28, 51, 83	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	6	SER	8.3
1	A	6	SER	8.2
1	D	6	SER	8.0
1	D	7	GLY	7.9
1	E	272	ALA	7.7
1	A	7	GLY	7.5
1	E	260	LEU	6.7
1	A	260	LEU	5.8
1	F	7	GLY	5.6
1	C	91	GLY	5.5
1	C	260	LEU	5.4
1	A	272	ALA	5.0
1	F	275	GLY	4.7
1	D	97	HIS	4.4
1	B	260	LEU	4.4
1	A	91	GLY	4.2
1	E	271	GLN	4.1
1	E	97	HIS	4.0
1	B	97	HIS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	266	LYS	3.8
1	D	272	ALA	3.8
1	C	97	HIS	3.7
1	C	272	ALA	3.6
1	D	91	GLY	3.6
1	D	260	LEU	3.5
1	F	260	LEU	3.3
1	B	268	ILE	3.2
1	B	267	GLU	3.2
1	A	97	HIS	3.1
1	E	273	GLY	3.0
1	A	289	HIS	3.0
1	B	129	ARG	3.0
1	A	259	PHE	2.9
1	F	274	LEU	2.9
1	A	253	ASN	2.9
1	F	272	ALA	2.8
1	A	252	THR	2.8
1	A	257	ASN	2.8
1	B	142	ASP	2.8
1	A	254	ILE	2.7
1	E	91	GLY	2.7
1	B	6	SER	2.7
1	E	6	SER	2.6
1	A	8	GLU	2.6
1	C	6	SER	2.6
1	D	275	GLY	2.5
1	F	192	ASP	2.5
1	D	129	ARG	2.5
1	E	98	SER	2.4
1	E	129	ARG	2.4
1	C	274	LEU	2.4
1	A	282	TYR	2.3
1	A	192	ASP	2.3
1	E	8	GLU	2.3
1	F	8	GLU	2.3
1	C	271	GLN	2.3
1	C	129	ARG	2.3
1	F	271	GLN	2.2
1	C	285	CYS	2.2
1	A	195	VAL	2.2
1	D	49	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	274	LEU	2.1
1	A	273	GLY	2.1
1	B	194	ASN	2.1
1	A	278	TYR	2.1
1	F	289	HIS	2.1
1	A	191	GLY	2.1
1	A	189	ILE	2.1
1	A	190	TYR	2.0
1	B	91	GLY	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.

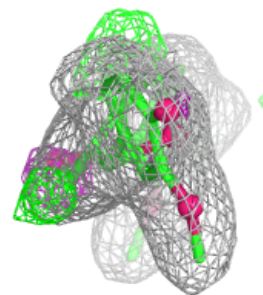
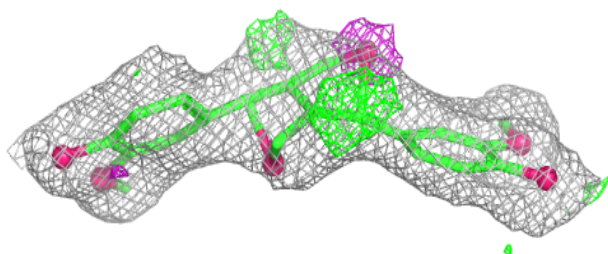
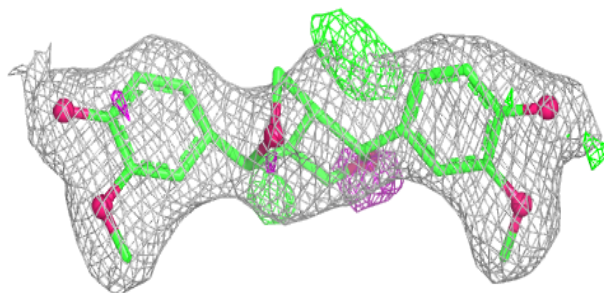
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GEF	F	401	26/26	0.86	0.13	35,45,54,57	0
2	GEF	A	401	26/26	0.88	0.13	31,39,50,51	0
2	GEF	E	401	26/26	0.88	0.12	28,37,44,48	0
2	GEF	D	401	26/26	0.88	0.12	29,40,53,56	0
2	GEF	C	401	26/26	0.90	0.11	25,34,43,44	0
2	GEF	B	401	26/26	0.90	0.14	24,36,50,53	0
3	NDP	D	402	48/48	0.93	0.09	26,34,49,62	0
3	NDP	A	402	48/48	0.95	0.09	20,30,44,57	0
3	NDP	E	402	48/48	0.95	0.08	22,33,46,57	0
3	NDP	B	402	48/48	0.95	0.08	17,27,44,53	0
3	NDP	C	402	48/48	0.96	0.07	20,28,44,54	0
3	NDP	F	402	48/48	0.96	0.07	23,33,42,51	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

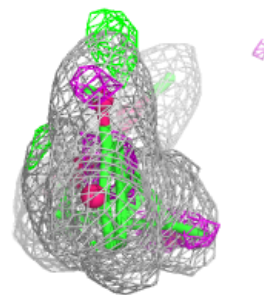
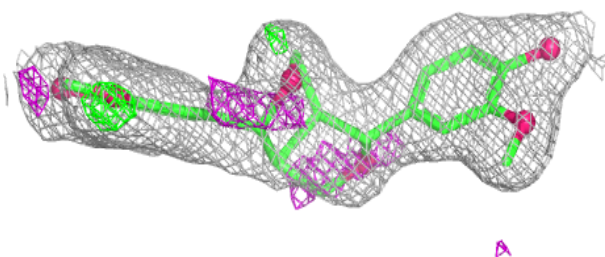
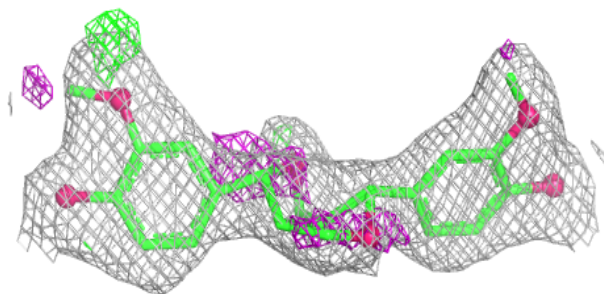
Electron density around GEF F 401:

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

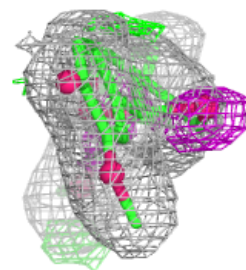
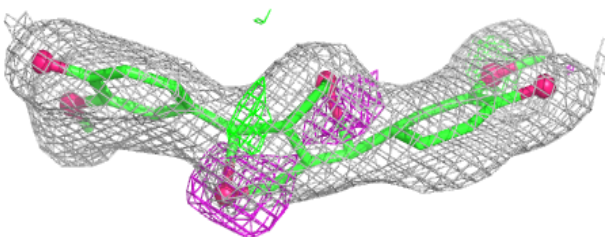
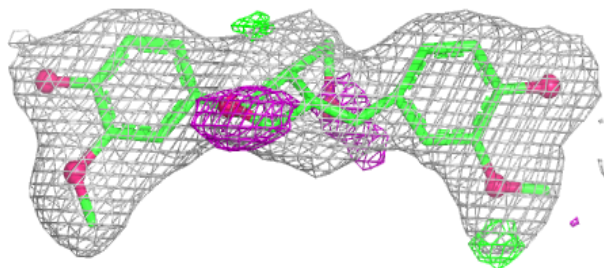


Electron density around GEF A 401:

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

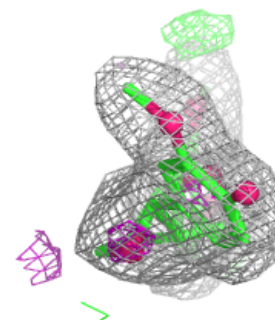
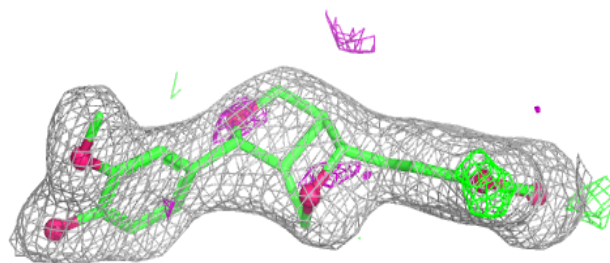
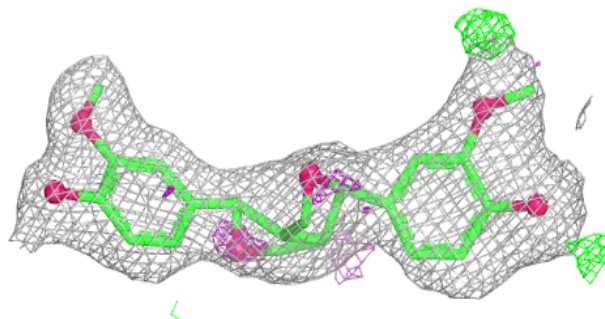
**Electron density around GEF E 401:**

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

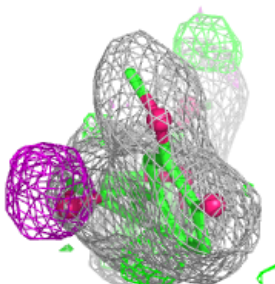
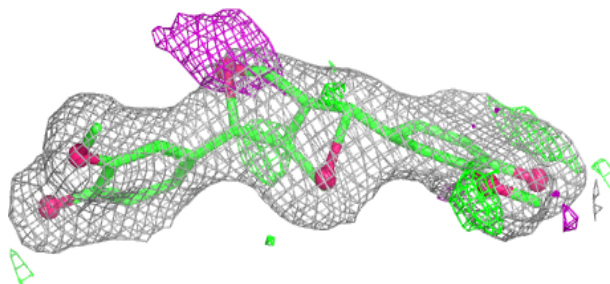
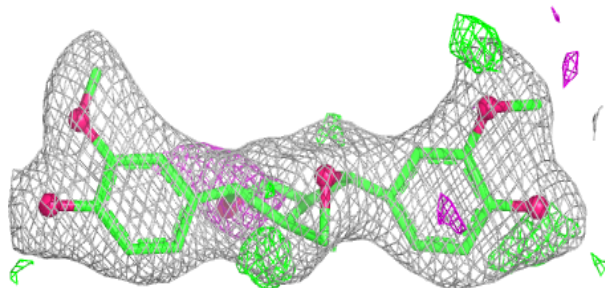


Electron density around GEF D 401:

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

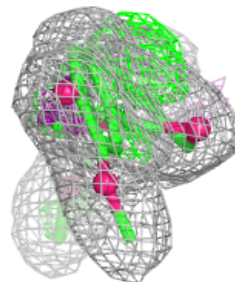
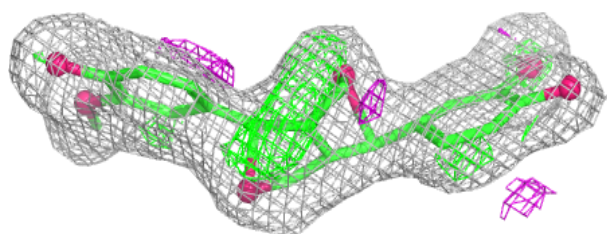
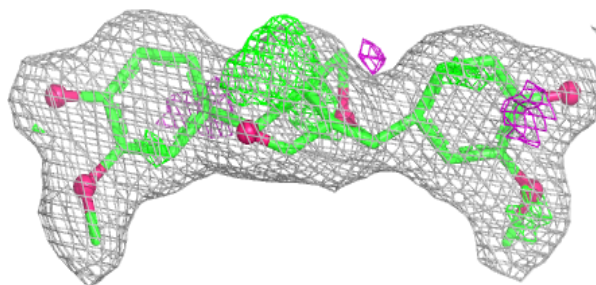
**Electron density around GEF C 401:**

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

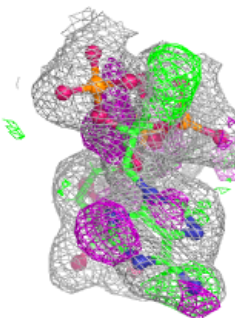
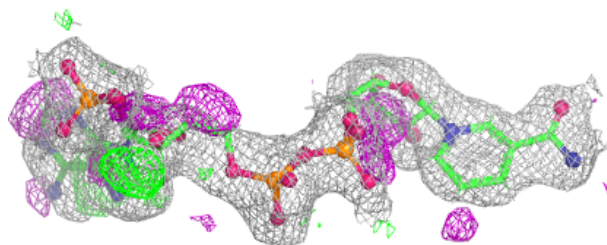
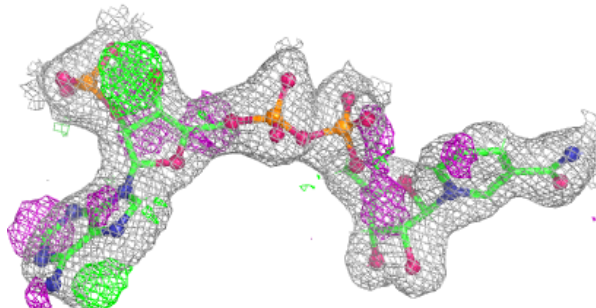


Electron density around GEF B 401:

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

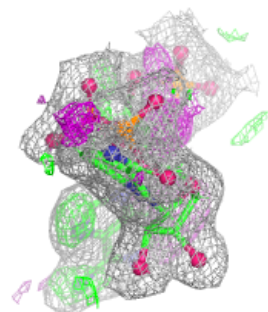
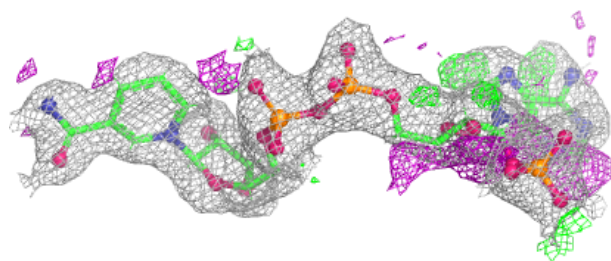
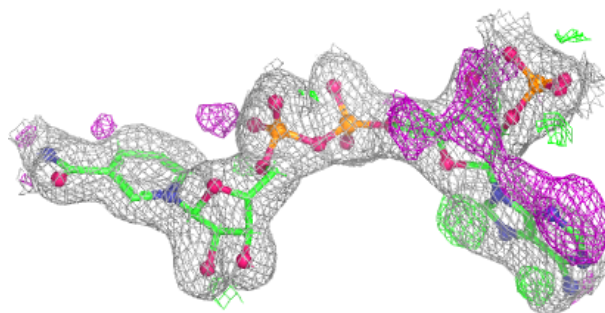
**Electron density around NDP D 402:**

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

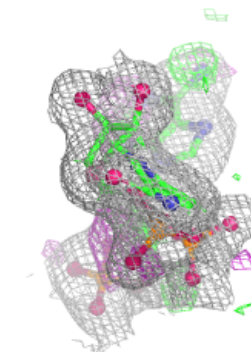
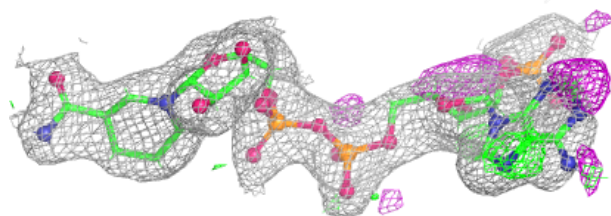
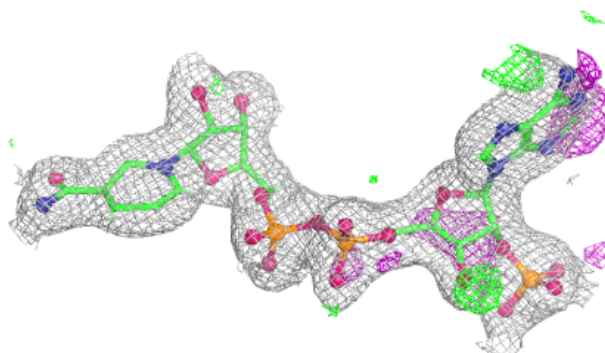


Electron density around NDP A 402:

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

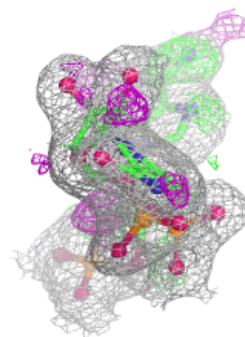
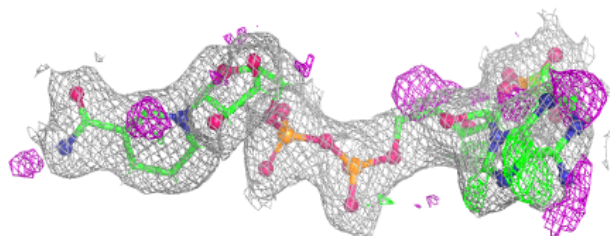
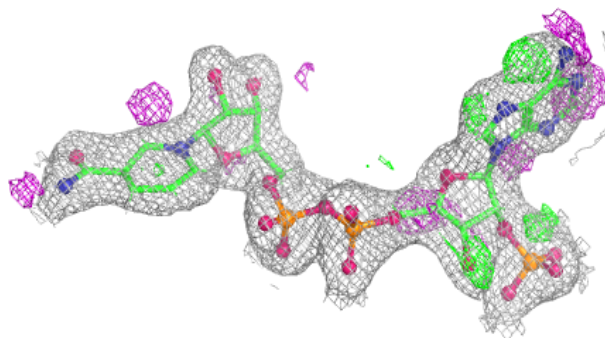
**Electron density around NDP E 402:**

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

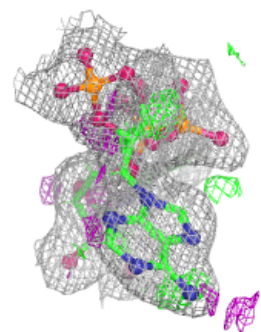
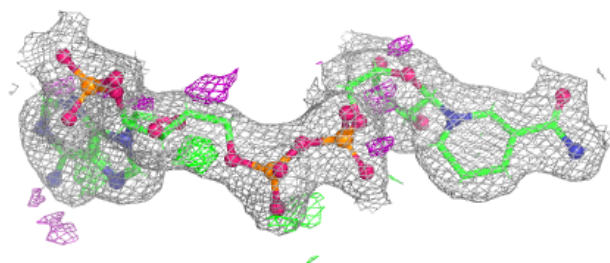
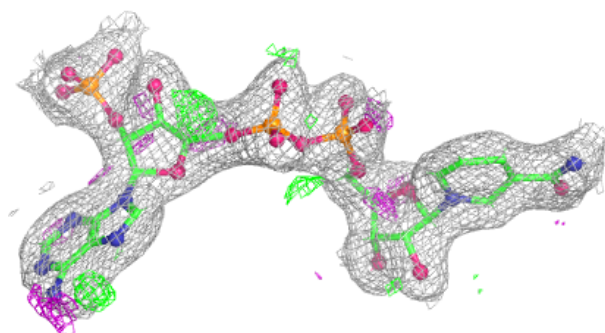


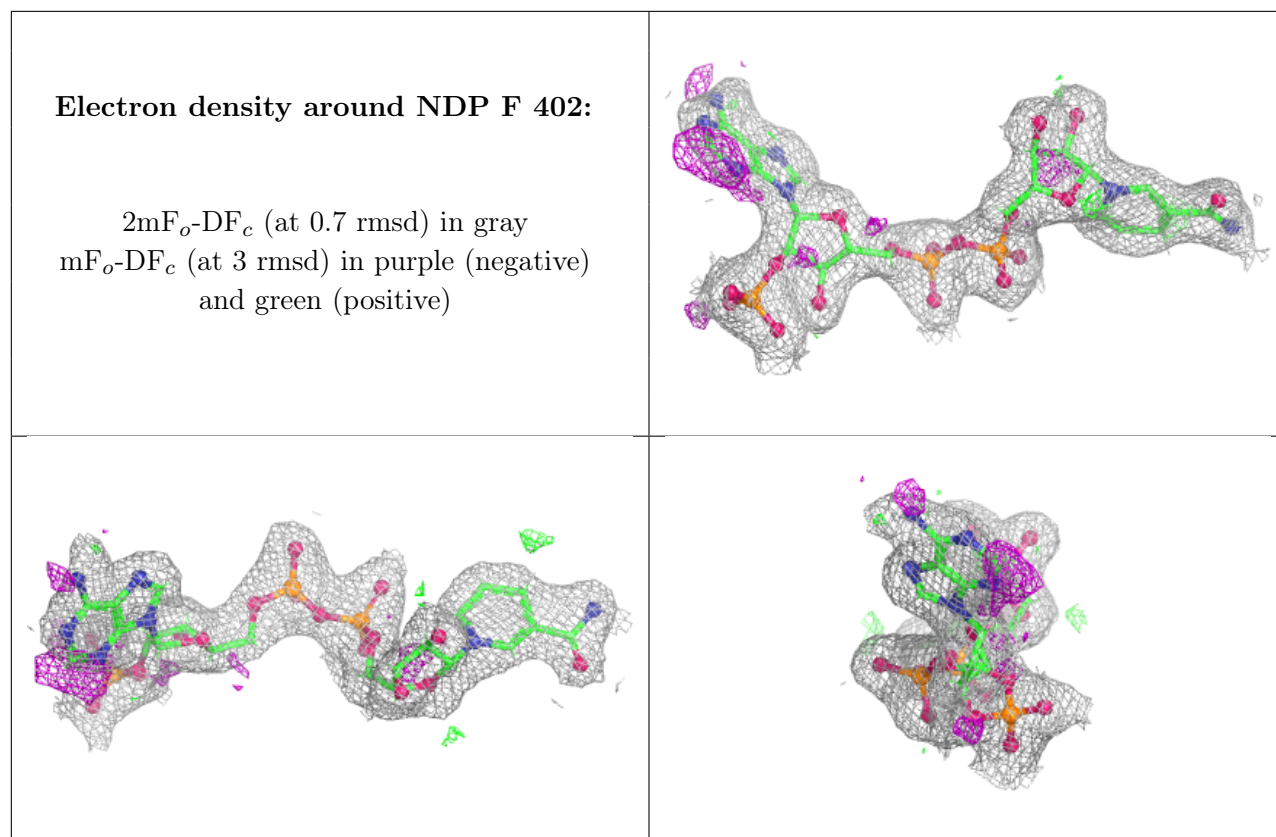
Electron density around NDP B 402:

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

**Electron density around NDP C 402:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.