



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:58 AM UTC

PDB ID : 7CS4 / pdb_00007cs4
Title : IiPLR1 with NADP⁺ and (+)pinoreosinol
Authors : Shao, K.; Zhang, P.
Deposited on : 2020-08-14
Resolution : 2.31 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)
Xtrriage (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

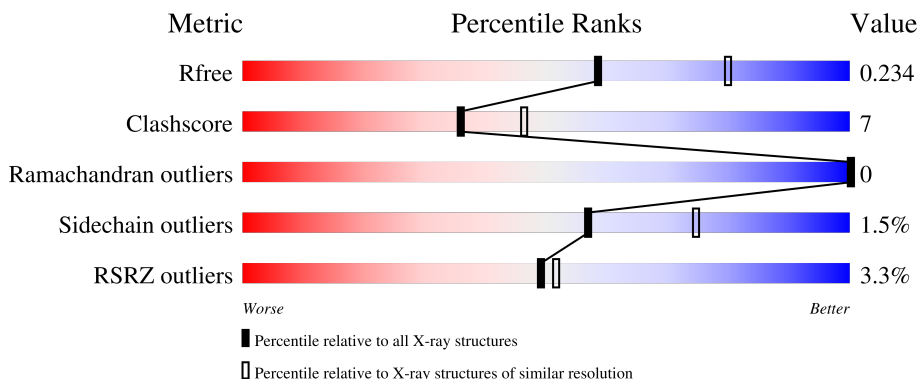
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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.



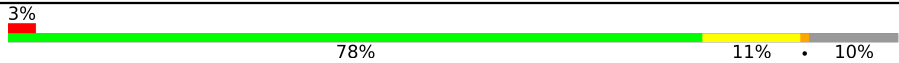
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	317	 7% 74% 14% • 11%
1	B	317	 2% 79% 12% 8%
1	C	317	 2% 82% 8% 10%
1	D	317	 3% 75% 15% • 10%
1	E	317	 2% 80% 9% 10%

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Mol	Chain	Length	Quality of chain
1	F	317	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '3%', a large green segment labeled '78%', a yellow segment labeled '11%', and a small grey segment at the end labeled '10%'.</p>

2 Entry composition [i](#)

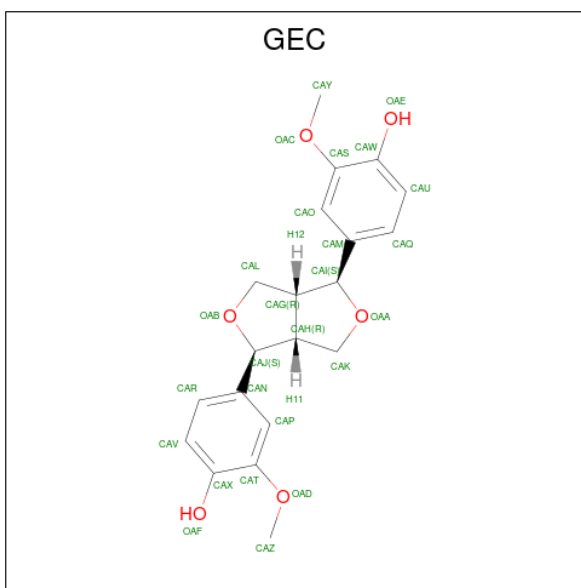
There are 4 unique types of molecules in this entry. The entry contains 14481 atoms, of which 156 are hydrogens and 0 are deuteriums.

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 Pinorexinol-lariciresinol reductase.

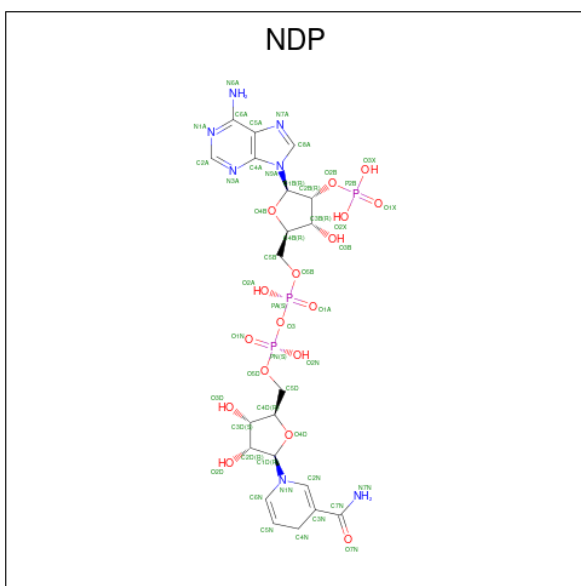
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	284	Total	C	N	O	S	0	0	0
			2232	1420	376	427	9			
1	A	283	Total	C	N	O	S	0	0	0
			2222	1415	373	425	9			
1	F	286	Total	C	N	O	S	0	0	0
			2244	1427	378	429	10			
1	D	286	Total	C	N	O	S	0	0	0
			2250	1430	380	431	9			
1	C	284	Total	C	N	O	S	0	0	0
			2231	1419	375	428	9			
1	B	291	Total	C	N	O	S	0	0	0
			2291	1457	387	438	9			

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



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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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

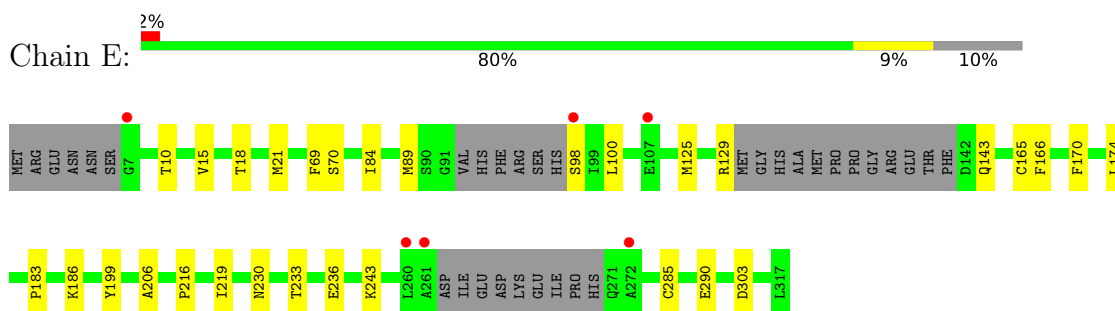
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	80	Total	O	0	0
			80	80		
4	A	64	Total	O	0	0
			64	64		
4	F	54	Total	O	0	0
			54	54		
4	D	56	Total	O	0	0
			56	56		
4	C	65	Total	O	0	0
			65	65		
4	B	92	Total	O	0	0
			92	92		

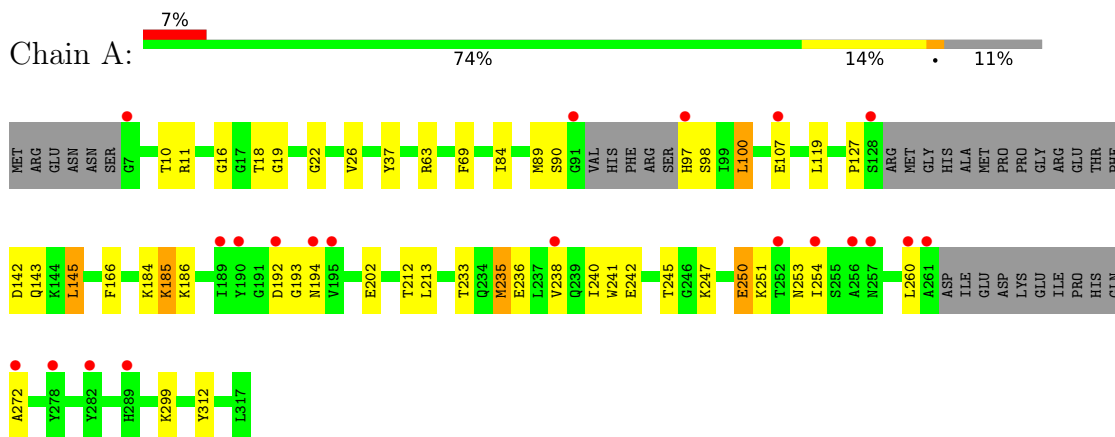
3 Residue-property plots [i](#)

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.

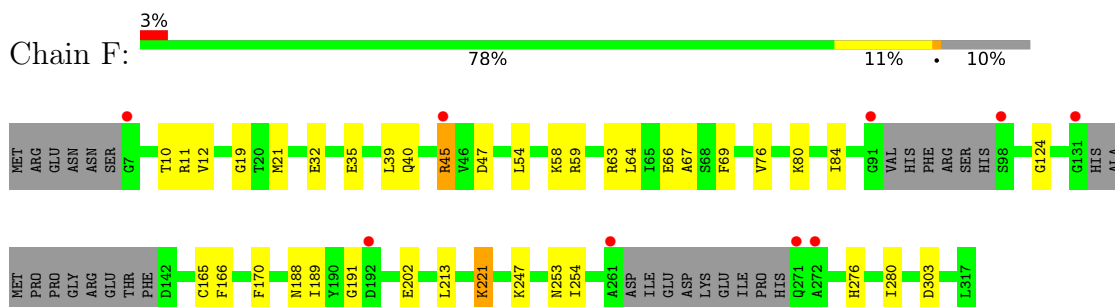
- Molecule 1: Pinoresinol-lariciresinol reductase



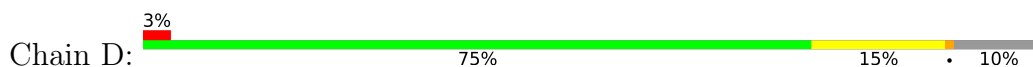
- Molecule 1: Pinoresinol-lariciresinol reductase

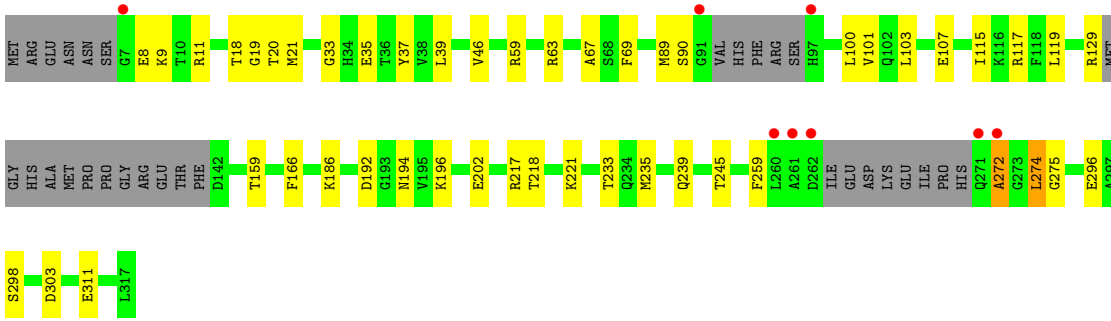


- Molecule 1: Pinoresinol-lariciresinol reductase

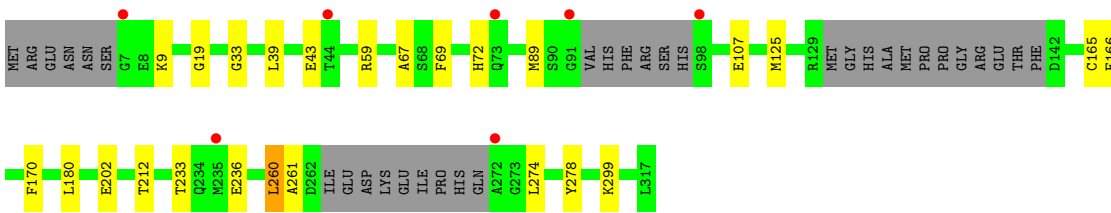
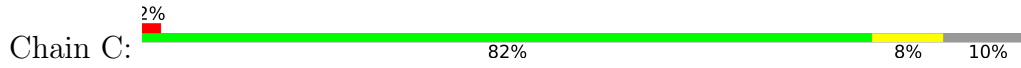


- Molecule 1: Pinoresinol-lariciresinol reductase

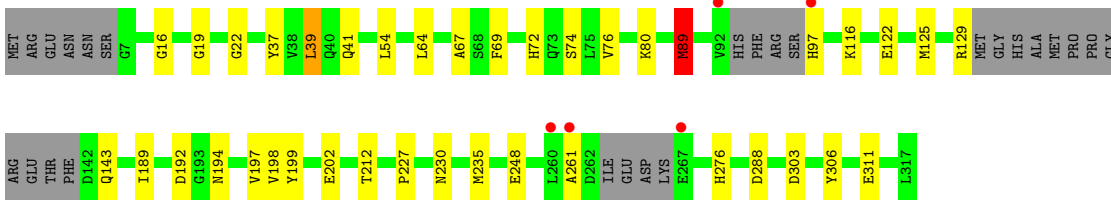
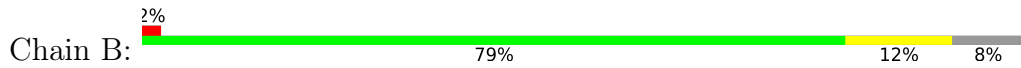




• Molecule 1: Pinoresinol-lariciresinol reductase



• Molecule 1: Pinoresinol-lariciresinol reductase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	244.92Å 244.92Å 75.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.66 – 2.31 48.66 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.66-2.31) 88.9 (48.66-2.31)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.32Å)	Xtrriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.202 , 0.231 0.205 , 0.234	Depositor DCC
R_{free} test set	1997 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtrriage
Anisotropy	0.537	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14481	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.31 % 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 9.5983e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GEC, 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	0.40	0/2259	0.60	1/3052 (0.0%)
1	B	0.40	0/2330	0.56	0/3149
1	C	0.39	0/2267	0.54	0/3062
1	D	0.36	0/2287	0.53	0/3089
1	E	0.37	0/2268	0.52	0/3063
1	F	0.37	0/2280	0.53	0/3078
All	All	0.38	0/13691	0.55	1/18493 (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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	GLU	CA-CB-CG	5.90	125.90	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	89	MET	Peptide
1	C	261	ALA	Peptide
1	D	272	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2222	0	2227	55	1
1	B	2291	0	2292	29	1
1	C	2231	0	2237	20	0
1	D	2250	0	2252	36	0
1	E	2232	0	2241	21	0
1	F	2244	0	2253	30	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
2	C	26	0	0	0	0
2	D	26	0	0	0	0
2	E	26	0	0	0	0
2	F	26	0	0	1	0
3	A	48	26	25	13	0
3	B	48	26	26	4	0
3	C	48	26	25	6	0
3	D	48	26	25	11	0
3	E	48	26	26	4	0
3	F	48	26	25	8	0
4	A	64	0	0	4	0
4	B	92	0	0	6	0
4	C	65	0	0	3	0
4	D	56	0	0	6	0
4	E	80	0	0	3	0
4	F	54	0	0	6	0
All	All	14325	156	13654	200	1

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 (200) 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)
3:F:402:NDP:O4D	3:F:402:NDP:C1D	1.64	1.17
1:D:217:ARG:O	1:D:221:LYS:NZ	1.87	1.06
1:A:186:LYS:HE3	1:A:250:GLU:HG2	1.51	0.93
1:A:236:GLU:O	1:A:240:ILE:HD12	1.73	0.89
1:A:233:THR:HG23	1:A:236:GLU:H	1.41	0.83
1:E:98:SER:N	4:E:501:HOH:O	2.11	0.81
1:A:193:GLY:O	1:A:233:THR:OG1	1.99	0.81
1:B:311:GLU:OE1	4:B:501:HOH:O	1.97	0.81
1:D:235:MET:O	1:D:239:GLN:HG3	1.80	0.81
1:A:233:THR:HG22	1:A:236:GLU:OE1	1.81	0.81
1:B:303:ASP:OD1	4:B:502:HOH:O	1.99	0.79
1:A:186:LYS:HA	1:A:186:LYS:HE2	1.65	0.79
1:D:202:GLU:OE1	4:D:501:HOH:O	1.99	0.79
1:D:39:LEU:HD11	1:D:67:ALA:HB3	1.66	0.78
1:F:19:GLY:HA3	3:F:402:NDP:H52A	1.65	0.77
1:F:35:GLU:OE2	1:F:63:ARG:NH1	2.18	0.77
1:D:19:GLY:HA3	3:D:402:NDP:H52A	1.67	0.76
1:A:186:LYS:CE	1:A:250:GLU:HG2	2.16	0.75
1:F:39:LEU:HD11	1:F:67:ALA:HB3	1.69	0.75
1:A:19:GLY:HA3	3:A:402:NDP:H52A	1.69	0.74
1:A:242:GLU:HA	1:A:245:THR:CG2	2.17	0.73
1:A:241:TRP:O	1:A:245:THR:HG22	1.88	0.73
1:A:142:ASP:N	4:A:502:HOH:O	2.21	0.73
1:A:186:LYS:HE3	1:A:250:GLU:CG	2.18	0.73
1:C:202:GLU:OE2	4:C:501:HOH:O	2.08	0.70
1:F:221:LYS:HE3	4:F:549:HOH:O	1.91	0.70
1:D:311:GLU:OE1	4:D:502:HOH:O	2.09	0.70
1:A:202:GLU:H	1:A:202:GLU:CD	2.00	0.70
1:D:59:ARG:NH1	4:D:504:HOH:O	2.19	0.70
1:E:21:MET:HE1	1:E:206:ALA:HB2	1.75	0.68
1:A:90:SER:HB3	3:A:402:NDP:O1A	1.93	0.68
1:E:18:THR:OG1	3:E:402:NDP:O1X	2.11	0.67
1:D:69:PHE:CE2	3:D:402:NDP:H2A	2.30	0.67
1:D:259:PHE:CE2	1:D:274:LEU:HD13	2.30	0.66
1:D:103:LEU:O	1:D:107:GLU:HG3	1.96	0.66
1:F:59:ARG:HD3	4:F:501:HOH:O	1.96	0.64
1:F:166:PHE:H	3:F:402:NDP:H72N	1.46	0.64
1:F:124:GLY:HA3	2:F:401:GEC:OAF	1.98	0.64
1:D:18:THR:OG1	3:D:402:NDP:O1X	2.15	0.63
1:A:312:TYR:OH	4:A:501:HOH:O	2.14	0.63
1:E:21:MET:CE	1:E:206:ALA:HB2	2.29	0.62
1:C:69:PHE:CD1	3:C:402:NDP:H2A	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:THR:OG1	3:A:402:NDP:O1X	2.17	0.61
1:A:127:PRO:HB2	1:A:145:LEU:HD13	1.82	0.61
1:C:59:ARG:NH2	4:C:503:HOH:O	2.33	0.61
1:F:202:GLU:H	1:F:202:GLU:CD	2.07	0.61
1:B:39:LEU:HD11	1:B:67:ALA:HB3	1.82	0.61
1:D:69:PHE:CD2	3:D:402:NDP:H2A	2.35	0.61
1:F:54:LEU:HD22	1:F:64:LEU:HD22	1.82	0.61
1:D:90:SER:HB3	3:D:402:NDP:O1A	2.02	0.59
1:B:97:HIS:N	1:B:143:GLN:HE22	2.00	0.59
1:A:10:THR:HG21	1:A:84:ILE:HD12	1.86	0.58
1:A:192:ASP:OD2	1:A:194:ASN:ND2	2.36	0.58
1:A:235:MET:HA	1:A:238:VAL:HG12	1.85	0.58
1:B:69:PHE:CE2	3:B:402:NDP:H2A	2.39	0.57
1:A:166:PHE:H	3:A:402:NDP:H72N	1.50	0.57
1:D:202:GLU:H	1:D:202:GLU:CD	2.12	0.57
1:B:74:SER:O	4:B:503:HOH:O	2.17	0.57
1:B:129:ARG:NH1	1:B:288:ASP:OD2	2.35	0.57
1:D:186:LYS:NZ	1:B:261:ALA:O	2.37	0.57
1:A:245:THR:HG23	1:A:247:LYS:H	1.68	0.57
1:B:202:GLU:H	1:B:202:GLU:CD	2.12	0.57
1:A:69:PHE:CE2	3:A:402:NDP:H2A	2.40	0.56
1:E:69:PHE:CE2	3:E:402:NDP:H2A	2.39	0.56
1:F:10:THR:HG21	1:F:84:ILE:HD12	1.87	0.56
1:A:186:LYS:HZ1	1:A:251:LYS:N	2.03	0.56
1:A:69:PHE:CD2	3:A:402:NDP:H2A	2.41	0.56
1:A:16:GLY:O	1:A:22:GLY:HA3	2.06	0.56
1:C:260:LEU:HD13	1:C:278:TYR:CE1	2.40	0.56
1:D:9:LYS:HD3	1:D:33:GLY:O	2.06	0.56
3:B:402:NDP:P2B	3:B:402:NDP:O3B	2.63	0.56
1:D:166:PHE:H	3:D:402:NDP:H72N	1.51	0.56
1:A:299:LYS:HE2	4:A:514:HOH:O	2.06	0.55
1:D:245:THR:OG1	4:D:503:HOH:O	2.18	0.55
1:D:303:ASP:OD1	1:D:303:ASP:N	2.39	0.55
1:E:69:PHE:CD2	3:E:402:NDP:H2A	2.42	0.55
1:A:260:LEU:HD12	1:A:260:LEU:H	1.72	0.55
1:C:43:GLU:HA	4:C:508:HOH:O	2.07	0.54
1:F:21:MET:HE3	1:F:166:PHE:CZ	2.42	0.54
1:F:59:ARG:NH2	4:F:502:HOH:O	2.27	0.54
1:C:233:THR:OG1	1:C:236:GLU:HG3	2.08	0.54
1:D:296:GLU:OE1	1:D:298:SER:OG	2.26	0.54
1:A:184:LYS:O	1:A:247:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:PRO:O	1:E:219:ILE:HG22	2.07	0.53
1:D:192:ASP:HB2	1:D:194:ASN:OD1	2.09	0.53
1:A:260:LEU:HD12	1:A:260:LEU:N	2.24	0.53
1:D:37:TYR:CE2	1:D:63:ARG:HD2	2.44	0.53
1:A:242:GLU:HA	1:A:245:THR:HG22	1.91	0.52
1:A:100:LEU:HD13	1:A:143:GLN:HB3	1.91	0.52
1:A:186:LYS:HZ1	1:A:250:GLU:C	2.18	0.52
1:A:235:MET:HA	1:A:238:VAL:CG1	2.39	0.52
3:D:402:NDP:O3B	3:D:402:NDP:P2B	2.68	0.52
1:B:69:PHE:CD2	3:B:402:NDP:H2A	2.46	0.51
1:D:129:ARG:NH1	4:D:507:HOH:O	2.43	0.51
3:A:402:NDP:P2B	3:A:402:NDP:O3B	2.69	0.51
1:D:196:LYS:HE2	1:D:233:THR:HG23	1.92	0.51
1:F:11:ARG:HG2	1:F:35:GLU:HB3	1.93	0.51
1:C:9:LYS:HE2	1:C:33:GLY:O	2.11	0.51
1:E:166:PHE:H	3:E:402:NDP:H72N	1.57	0.51
1:C:39:LEU:HD11	1:C:67:ALA:HB3	1.92	0.51
3:F:402:NDP:O3B	3:F:402:NDP:O1X	2.28	0.50
1:A:186:LYS:NZ	1:A:250:GLU:C	2.69	0.50
1:E:233:THR:OG1	1:E:236:GLU:HG3	2.12	0.50
1:C:69:PHE:CE1	3:C:402:NDP:H2A	2.47	0.50
1:A:90:SER:O	1:A:98:SER:OG	2.28	0.50
1:F:58:LYS:NZ	4:F:507:HOH:O	2.45	0.50
1:E:165:CYS:HB3	1:E:170:PHE:CD2	2.46	0.50
1:B:189:ILE:HG13	1:B:235:MET:HE1	1.93	0.50
1:F:69:PHE:CE2	3:F:402:NDP:H2A	2.47	0.50
1:D:272:ALA:HB1	1:D:275:GLY:H	1.77	0.50
1:D:218:THR:HA	1:D:221:LYS:NZ	2.28	0.48
1:E:303:ASP:OD1	1:E:303:ASP:N	2.37	0.48
1:B:122:GLU:OE1	4:B:504:HOH:O	2.20	0.48
1:B:89:MET:HB3	1:B:89:MET:HE3	1.42	0.48
1:F:303:ASP:OD1	1:F:303:ASP:N	2.39	0.48
1:B:125:MET:HE1	1:B:276:HIS:ND1	2.28	0.48
1:D:119:LEU:HG	1:D:159:THR:HB	1.96	0.47
1:A:89:MET:HE1	3:A:402:NDP:N3A	2.30	0.47
1:D:89:MET:O	3:D:402:NDP:H52N	2.14	0.47
3:D:402:NDP:P2B	3:D:402:NDP:HO3A	2.37	0.47
1:C:125:MET:HE3	1:C:125:MET:HB3	1.88	0.47
3:F:402:NDP:O3B	3:F:402:NDP:P2B	2.73	0.47
1:D:11:ARG:HG2	1:D:35:GLU:HB3	1.96	0.47
1:E:125:MET:HE3	1:E:285:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLY:HA3	3:C:402:NDP:H52A	1.97	0.47
1:B:16:GLY:O	1:B:22:GLY:HA3	2.15	0.47
1:F:165:CYS:HA	3:F:402:NDP:H72N	1.79	0.47
1:B:248:GLU:OE2	4:B:505:HOH:O	2.20	0.46
3:D:402:NDP:O2N	4:D:505:HOH:O	2.21	0.46
1:E:10:THR:HG21	1:E:84:ILE:HD12	1.97	0.46
1:F:32:GLU:HG2	4:F:508:HOH:O	2.15	0.46
1:D:89:MET:HE2	1:D:101:VAL:HG11	1.98	0.46
1:B:39:LEU:CD1	1:B:67:ALA:HB3	2.44	0.45
1:A:186:LYS:HE2	1:A:186:LYS:CA	2.38	0.45
1:B:76:VAL:O	1:B:80:LYS:HG3	2.16	0.45
1:D:46:VAL:HG13	1:C:180:LEU:HD21	1.98	0.45
1:C:274:LEU:O	1:C:274:LEU:HD23	2.17	0.45
1:A:186:LYS:NZ	1:A:250:GLU:HG2	2.32	0.45
1:D:35:GLU:HG2	1:D:37:TYR:CE1	2.52	0.45
1:B:116:LYS:NZ	4:B:515:HOH:O	2.49	0.45
1:E:174:LEU:HD12	1:E:183:PRO:HD2	1.99	0.45
1:B:194:ASN:OD1	1:B:194:ASN:N	2.50	0.44
3:A:402:NDP:P2B	3:A:402:NDP:HO3A	2.39	0.44
1:F:69:PHE:CD2	3:F:402:NDP:H2A	2.53	0.44
1:B:192:ASP:HB2	1:B:194:ASN:CG	2.42	0.44
1:E:100:LEU:HG	1:E:143:GLN:HG2	1.98	0.44
1:E:129:ARG:O	4:E:503:HOH:O	2.21	0.44
1:A:89:MET:O	3:A:402:NDP:H52N	2.18	0.44
1:A:166:PHE:CD1	3:A:402:NDP:H41N	2.53	0.44
3:A:402:NDP:O1X	3:A:402:NDP:O3B	2.36	0.43
1:B:197:VAL:HG12	1:B:198:VAL:N	2.34	0.43
1:E:186:LYS:HE3	1:E:186:LYS:HB2	1.57	0.43
1:A:84:ILE:HD13	1:A:213:LEU:O	2.19	0.43
1:F:45:ARG:HG3	1:F:47:ASP:HB2	2.00	0.43
1:B:39:LEU:HD21	1:B:41:GLN:HG2	2.00	0.43
1:A:233:THR:HG23	1:A:236:GLU:N	2.20	0.43
1:C:260:LEU:CD1	1:C:278:TYR:CE1	3.01	0.43
1:B:227:PRO:HB2	1:B:306:TYR:CE1	2.54	0.43
1:F:59:ARG:NH1	4:F:501:HOH:O	2.14	0.42
1:A:119:LEU:HD12	1:A:119:LEU:N	2.33	0.42
1:A:235:MET:HE3	1:A:235:MET:HB2	1.74	0.42
1:F:191:GLY:O	1:F:253:ASN:HB3	2.19	0.42
1:D:221:LYS:HB2	1:D:221:LYS:HE2	1.72	0.42
1:C:72:HIS:CE1	1:C:107:GLU:HG2	2.55	0.42
1:C:166:PHE:H	3:C:402:NDP:H72N	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLY:O	1:A:26:VAL:HG23	2.19	0.42
1:D:117:ARG:HD3	1:D:159:THR:OG1	2.19	0.42
1:B:192:ASP:HB2	1:B:194:ASN:OD1	2.19	0.42
1:E:15:VAL:HG12	1:E:89:MET:SD	2.59	0.42
1:A:236:GLU:O	1:A:240:ILE:CD1	2.58	0.42
1:F:40:GLN:O	1:F:66:GLU:HA	2.20	0.42
1:B:19:GLY:HA3	3:B:402:NDP:H52A	2.01	0.42
1:B:199:TYR:O	1:B:230:ASN:HB3	2.20	0.42
1:F:12:VAL:HA	1:F:84:ILE:O	2.20	0.42
1:D:115:ILE:HD13	1:D:115:ILE:HA	1.88	0.41
1:E:89:MET:HE3	1:E:89:MET:HB3	1.92	0.41
1:A:185:LYS:HB3	1:A:185:LYS:HE2	1.79	0.41
1:A:186:LYS:HE2	1:A:250:GLU:O	2.20	0.41
1:F:165:CYS:HB3	1:F:170:PHE:CD2	2.56	0.41
1:F:188:ASN:HB3	1:F:254:ILE:HD13	2.02	0.41
1:A:37:TYR:CE2	1:A:63:ARG:HD2	2.55	0.41
1:F:276:HIS:O	1:F:280:ILE:HG13	2.20	0.41
1:C:69:PHE:HD1	3:C:402:NDP:H2A	1.83	0.41
1:A:253:ASN:O	1:A:254:ILE:C	2.63	0.41
1:B:54:LEU:HD22	1:B:64:LEU:HD22	2.01	0.41
1:E:129:ARG:HB2	4:E:503:HOH:O	2.21	0.41
1:A:242:GLU:HA	1:A:245:THR:HG21	2.02	0.41
1:A:242:GLU:CA	1:A:245:THR:HG22	2.51	0.41
1:F:84:ILE:HD13	1:F:213:LEU:O	2.21	0.41
1:F:189:ILE:O	1:F:253:ASN:HA	2.21	0.41
1:D:21:MET:HE3	1:D:166:PHE:CZ	2.56	0.41
3:D:402:NDP:O5D	3:D:402:NDP:H6N	2.21	0.41
1:C:89:MET:O	3:C:402:NDP:H52N	2.21	0.41
1:C:299:LYS:HD3	1:C:299:LYS:HA	1.75	0.41
1:C:165:CYS:HB3	1:C:170:PHE:CD2	2.56	0.40
1:E:199:TYR:O	1:E:230:ASN:HB3	2.22	0.40
1:F:76:VAL:O	1:F:80:LYS:HG3	2.22	0.40
1:A:166:PHE:CD2	3:A:402:NDP:C7N	3.04	0.40
1:A:272:ALA:HA	4:A:519:HOH:O	2.21	0.40
1:B:72:HIS:O	1:B:76:VAL:HG23	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:NH2	1:B:37:TYR:OH[6_545]	2.05	0.15

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	275/317 (87%)	268 (98%)	7 (2%)	0	100	100
1	B	283/317 (89%)	275 (97%)	8 (3%)	0	100	100
1	C	276/317 (87%)	269 (98%)	7 (2%)	0	100	100
1	D	278/317 (88%)	270 (97%)	8 (3%)	0	100	100
1	E	276/317 (87%)	271 (98%)	5 (2%)	0	100	100
1	F	278/317 (88%)	274 (99%)	4 (1%)	0	100	100
All	All	1666/1902 (88%)	1627 (98%)	39 (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	240/271 (89%)	233 (97%)	7 (3%)	37	55
1	B	248/271 (92%)	245 (99%)	3 (1%)	63	79
1	C	241/271 (89%)	239 (99%)	2 (1%)	73	86
1	D	243/271 (90%)	239 (98%)	4 (2%)	55	73
1	E	241/271 (89%)	238 (99%)	3 (1%)	63	79
1	F	242/271 (89%)	239 (99%)	3 (1%)	63	79
All	All	1455/1626 (90%)	1433 (98%)	22 (2%)	57	75

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	70	SER
1	E	243	LYS
1	E	290	GLU
1	A	97	HIS
1	A	100	LEU
1	A	107	GLU
1	A	145	LEU
1	A	185	LYS
1	A	212	THR
1	A	235	MET
1	F	45	ARG
1	F	221	LYS
1	F	247	LYS
1	D	8	GLU
1	D	20	THR
1	D	100	LEU
1	D	274	LEU
1	C	212	THR
1	C	260	LEU
1	B	39	LEU
1	B	89	MET
1	B	212	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	253	ASN
1	E	279	HIS
1	E	289	HIS
1	A	40	GLN
1	B	253	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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
2	GEC	B	401	-	29,29,29	3.20	10 (34%)	42,42,42	2.35	18 (42%)
3	NDP	B	402	-	51,52,52	3.53	23 (45%)	71,80,80	2.69	24 (33%)
2	GEC	D	401	-	29,29,29	2.60	10 (34%)	42,42,42	2.30	13 (30%)
3	NDP	D	402	-	51,52,52	3.66	24 (47%)	71,80,80	2.69	27 (38%)
2	GEC	C	401	-	29,29,29	2.63	9 (31%)	42,42,42	2.15	12 (28%)
2	GEC	F	401	-	29,29,29	2.91	9 (31%)	42,42,42	2.39	16 (38%)
2	GEC	A	401	-	29,29,29	2.32	10 (34%)	42,42,42	1.92	13 (30%)
3	NDP	C	402	-	51,52,52	3.43	22 (43%)	71,80,80	2.50	26 (36%)
3	NDP	F	402	-	51,52,52	3.81	24 (47%)	71,80,80	2.60	29 (40%)
3	NDP	A	402	-	51,52,52	3.66	22 (43%)	71,80,80	2.57	30 (42%)
3	NDP	E	402	-	51,52,52	3.39	18 (35%)	71,80,80	2.62	27 (38%)
2	GEC	E	401	-	29,29,29	2.43	8 (27%)	42,42,42	1.97	12 (28%)

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	GEC	B	401	-	-	0/12/34/34	0/4/4/4
3	NDP	B	402	-	-	6/34/77/77	0/5/5/5
2	GEC	D	401	-	-	0/12/34/34	0/4/4/4
3	NDP	D	402	-	-	3/34/77/77	0/5/5/5

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

All (189) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NDP	PA-O3	10.67	1.71	1.59
3	A	402	NDP	PA-O3	10.58	1.70	1.59
3	F	402	NDP	C2B-C1B	-10.52	1.27	1.53
3	A	402	NDP	C2B-C1B	-9.71	1.29	1.53
3	F	402	NDP	O4D-C1D	9.62	1.64	1.42
3	F	402	NDP	PA-O3	9.59	1.69	1.59
3	D	402	NDP	C2B-C1B	-9.51	1.29	1.53
3	E	402	NDP	C2B-C1B	-9.47	1.29	1.53
3	F	402	NDP	O4B-C1B	9.21	1.63	1.42
3	D	402	NDP	O4B-C1B	9.19	1.63	1.42
3	C	402	NDP	O4B-C1B	9.18	1.63	1.42
3	B	402	NDP	C2B-C1B	-9.06	1.30	1.53
3	D	402	NDP	PA-O3	9.01	1.69	1.59
3	A	402	NDP	O4B-C1B	8.68	1.62	1.42
3	C	402	NDP	O4D-C1D	8.47	1.61	1.42
3	C	402	NDP	C2B-C1B	-8.45	1.32	1.53
3	D	402	NDP	O4D-C1D	8.45	1.61	1.42
3	A	402	NDP	O4D-C1D	8.15	1.60	1.42
3	B	402	NDP	O4D-C1D	8.14	1.60	1.42
3	B	402	NDP	O4B-C1B	8.08	1.60	1.42
3	E	402	NDP	PA-O3	7.90	1.68	1.59
3	E	402	NDP	C2D-C1D	-7.77	1.29	1.53
3	E	402	NDP	O4B-C1B	7.77	1.60	1.42
3	C	402	NDP	C2D-C1D	-7.76	1.29	1.53
3	E	402	NDP	O4D-C1D	7.76	1.59	1.42
2	F	401	GEC	CAN-CAJ	-7.65	1.38	1.51
3	F	402	NDP	C6N-C5N	7.64	1.56	1.33
2	C	401	GEC	CAN-CAJ	-7.58	1.38	1.51
3	A	402	NDP	C2D-C1D	-7.58	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NDP	C2D-C1D	-7.33	1.30	1.53
2	D	401	GEC	CAN-CAJ	-6.92	1.39	1.51
3	D	402	NDP	C2D-C1D	-6.84	1.32	1.53
3	F	402	NDP	C2D-C1D	-6.81	1.32	1.53
3	A	402	NDP	O4B-C4B	-6.81	1.29	1.45
2	F	401	GEC	CAM-CAI	-6.72	1.39	1.51
3	C	402	NDP	C6N-C5N	6.57	1.53	1.33
2	A	401	GEC	CAN-CAJ	-6.53	1.40	1.51
3	D	402	NDP	C6N-C5N	6.50	1.53	1.33
3	E	402	NDP	C6N-C5N	6.46	1.53	1.33
2	E	401	GEC	CAN-CAJ	-6.39	1.40	1.51
3	B	402	NDP	O4B-C4B	-6.33	1.30	1.45
2	B	401	GEC	OAB-CAL	-6.31	1.30	1.43
3	C	402	NDP	PA-O3	6.25	1.66	1.59
3	C	402	NDP	O4B-C4B	-6.19	1.31	1.45
2	F	401	GEC	CAG-CAI	-6.14	1.41	1.54
3	D	402	NDP	O4B-C4B	-6.07	1.31	1.45
3	A	402	NDP	C6N-C5N	5.97	1.51	1.33
2	B	401	GEC	CAL-CAG	-5.91	1.42	1.53
2	B	401	GEC	OAA-CAI	-5.91	1.34	1.43
2	C	401	GEC	CAM-CAI	-5.89	1.41	1.51
3	B	402	NDP	C6N-C5N	5.88	1.51	1.33
3	E	402	NDP	O4D-C4D	-5.84	1.32	1.45
3	D	402	NDP	C2N-C3N	5.75	1.51	1.35
2	B	401	GEC	CAN-CAJ	-5.72	1.41	1.51
3	D	402	NDP	C6A-N6A	5.57	1.48	1.34
3	A	402	NDP	O4D-C4D	-5.55	1.32	1.45
3	F	402	NDP	C2N-C3N	5.54	1.50	1.35
3	E	402	NDP	O4B-C4B	-5.53	1.32	1.45
3	F	402	NDP	O4B-C4B	-5.49	1.32	1.45
2	E	401	GEC	CAM-CAI	-5.41	1.41	1.51
2	A	401	GEC	CAM-CAI	-5.40	1.41	1.51
2	B	401	GEC	CAM-CAI	-5.33	1.42	1.51
3	F	402	NDP	O4D-C4D	-5.27	1.33	1.45
2	D	401	GEC	CAM-CAI	-5.27	1.42	1.51
3	E	402	NDP	C2N-C3N	5.18	1.49	1.35
2	B	401	GEC	OAB-CAJ	-5.10	1.35	1.43
3	C	402	NDP	O4D-C4D	-5.07	1.33	1.45
3	A	402	NDP	C2N-C3N	5.06	1.49	1.35
3	C	402	NDP	C6A-N6A	4.87	1.46	1.34
3	B	402	NDP	O4D-C4D	-4.83	1.34	1.45
3	C	402	NDP	C2N-C3N	4.83	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NDP	C6A-N6A	4.79	1.46	1.34
3	D	402	NDP	O4D-C4D	-4.71	1.34	1.45
2	D	401	GEC	CAG-CAI	-4.71	1.44	1.54
2	B	401	GEC	OAA-CAK	-4.67	1.33	1.43
3	A	402	NDP	C6A-N6A	4.61	1.46	1.34
2	F	401	GEC	CAH-CAJ	-4.60	1.45	1.54
2	B	401	GEC	CAK-CAH	-4.59	1.44	1.53
3	B	402	NDP	C2N-C3N	4.43	1.47	1.35
3	E	402	NDP	C6A-N6A	4.32	1.45	1.34
2	F	401	GEC	CAK-CAH	-4.29	1.45	1.53
3	F	402	NDP	C6A-N6A	4.27	1.45	1.34
2	F	401	GEC	OAA-CAI	-4.24	1.36	1.43
3	A	402	NDP	O2D-C2D	4.20	1.53	1.43
2	C	401	GEC	OAA-CAI	-4.15	1.37	1.43
2	B	401	GEC	CAH-CAJ	-4.11	1.46	1.54
3	F	402	NDP	O2D-C2D	4.11	1.53	1.43
3	F	402	NDP	C7N-N7N	4.10	1.45	1.33
2	D	401	GEC	OAA-CAI	-4.08	1.37	1.43
2	D	401	GEC	CAK-CAH	-4.02	1.45	1.53
2	E	401	GEC	CAL-CAG	-3.95	1.45	1.53
2	E	401	GEC	CAG-CAI	-3.92	1.46	1.54
2	A	401	GEC	OAB-CAJ	-3.91	1.37	1.43
2	C	401	GEC	CAH-CAJ	-3.89	1.46	1.54
3	F	402	NDP	C5A-C4A	-3.81	1.32	1.39
3	D	402	NDP	O2D-C2D	3.79	1.52	1.43
2	E	401	GEC	CAK-CAH	-3.70	1.46	1.53
3	A	402	NDP	C5A-C4A	-3.64	1.32	1.39
2	B	401	GEC	CAG-CAI	-3.52	1.47	1.54
2	D	401	GEC	CAH-CAJ	-3.50	1.47	1.54
2	C	401	GEC	CAL-CAG	-3.48	1.46	1.53
2	C	401	GEC	CAG-CAI	-3.48	1.47	1.54
3	D	402	NDP	C2A-N3A	3.46	1.40	1.33
3	B	402	NDP	C5A-C4A	-3.44	1.32	1.39
3	B	402	NDP	C7N-N7N	3.44	1.43	1.33
2	A	401	GEC	OAB-CAL	-3.44	1.36	1.43
3	D	402	NDP	C8A-N7A	3.41	1.38	1.31
2	E	401	GEC	OAB-CAJ	-3.39	1.38	1.43
3	E	402	NDP	C5A-C4A	-3.39	1.33	1.39
3	D	402	NDP	C4N-C3N	3.34	1.56	1.50
3	E	402	NDP	C7N-N7N	3.28	1.42	1.33
2	C	401	GEC	OAB-CAL	-3.26	1.36	1.43
3	A	402	NDP	C7N-N7N	3.23	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402	NDP	PN-O3	3.20	1.63	1.59
2	A	401	GEC	CAG-CAI	-3.19	1.47	1.54
3	D	402	NDP	C5A-C4A	-3.12	1.33	1.39
3	C	402	NDP	C7N-N7N	3.10	1.42	1.33
2	F	401	GEC	CAL-CAG	-3.09	1.47	1.53
3	C	402	NDP	C2A-N3A	3.06	1.39	1.33
3	E	402	NDP	O2D-C2D	3.05	1.50	1.43
3	B	402	NDP	O2D-C2D	3.04	1.50	1.43
3	F	402	NDP	C8A-N7A	2.98	1.37	1.31
3	C	402	NDP	C5A-C4A	-2.97	1.33	1.39
3	B	402	NDP	C4N-C5N	2.94	1.56	1.49
2	C	401	GEC	OAB-CAJ	-2.93	1.39	1.43
3	C	402	NDP	C8A-N7A	2.93	1.37	1.31
3	D	402	NDP	C7N-N7N	2.88	1.41	1.33
3	E	402	NDP	C2A-N3A	2.75	1.38	1.33
2	D	401	GEC	CAL-CAG	-2.75	1.47	1.53
2	C	401	GEC	CAK-CAH	-2.74	1.47	1.53
2	F	401	GEC	OAB-CAL	-2.73	1.38	1.43
2	D	401	GEC	OAA-CAK	-2.70	1.38	1.43
3	C	402	NDP	O2D-C2D	2.70	1.49	1.43
3	B	402	NDP	PN-O3	2.69	1.62	1.59
2	D	401	GEC	OAB-CAL	-2.68	1.38	1.43
3	F	402	NDP	O3D-C3D	-2.67	1.36	1.43
3	B	402	NDP	PN-O5D	2.67	1.69	1.59
3	A	402	NDP	O3D-C3D	-2.64	1.36	1.43
3	F	402	NDP	C6N-N1N	2.64	1.43	1.37
2	F	401	GEC	OAB-CAJ	-2.64	1.39	1.43
3	C	402	NDP	O3B-C3B	-2.62	1.36	1.43
2	E	401	GEC	CAH-CAJ	-2.62	1.49	1.54
3	D	402	NDP	O3D-C3D	-2.60	1.36	1.43
2	A	401	GEC	OAA-CAK	-2.55	1.38	1.43
3	E	402	NDP	C5A-C6A	-2.54	1.33	1.41
3	F	402	NDP	C5A-C6A	-2.52	1.34	1.41
2	D	401	GEC	OAB-CAJ	-2.52	1.39	1.43
3	D	402	NDP	PN-O5D	2.49	1.69	1.59
2	A	401	GEC	CAH-CAJ	-2.47	1.49	1.54
3	F	402	NDP	O7N-C7N	-2.45	1.18	1.24
3	A	402	NDP	C4N-C5N	2.45	1.55	1.49
3	F	402	NDP	C2A-N1A	2.41	1.38	1.33
3	B	402	NDP	C5A-C6A	-2.41	1.34	1.41
3	E	402	NDP	C6N-N1N	2.41	1.43	1.37
3	A	402	NDP	C8A-N7A	2.38	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NDP	C2A-N3A	2.36	1.38	1.33
3	F	402	NDP	C4N-C5N	2.35	1.55	1.49
3	E	402	NDP	C4N-C3N	2.35	1.54	1.50
3	D	402	NDP	C4N-C5N	2.33	1.55	1.49
3	D	402	NDP	O7N-C7N	-2.32	1.19	1.24
2	A	401	GEC	CAL-CAG	-2.31	1.48	1.53
3	B	402	NDP	C8A-N7A	2.31	1.36	1.31
3	F	402	NDP	C5D-C4D	2.27	1.58	1.51
2	E	401	GEC	OAB-CAL	-2.26	1.39	1.43
3	C	402	NDP	O3D-C3D	-2.24	1.37	1.43
3	D	402	NDP	C5A-C6A	-2.23	1.34	1.41
3	C	402	NDP	PA-O2A	-2.21	1.45	1.55
3	C	402	NDP	C6N-N1N	2.18	1.42	1.37
3	B	402	NDP	C6N-N1N	2.17	1.42	1.37
3	E	402	NDP	C8A-N7A	2.16	1.35	1.31
3	C	402	NDP	C5A-C6A	-2.15	1.35	1.41
3	A	402	NDP	C5A-C6A	-2.14	1.35	1.41
3	B	402	NDP	O3D-C3D	-2.14	1.37	1.43
3	C	402	NDP	C4N-C3N	2.12	1.54	1.50
3	F	402	NDP	C5B-C4B	2.11	1.57	1.51
3	D	402	NDP	C6N-N1N	2.10	1.42	1.37
3	B	402	NDP	C2A-N3A	2.08	1.37	1.33
3	A	402	NDP	C4N-C3N	2.08	1.53	1.50
3	A	402	NDP	C6N-N1N	2.08	1.42	1.37
2	A	401	GEC	CAK-CAH	-2.06	1.49	1.53
2	A	401	GEC	OAD-CAT	-2.06	1.33	1.37
3	B	402	NDP	C2A-N1A	2.06	1.37	1.33
3	D	402	NDP	O2B-C2B	2.05	1.51	1.44
3	A	402	NDP	C8A-N9A	-2.04	1.34	1.37
3	C	402	NDP	O2B-C2B	2.03	1.51	1.44
3	A	402	NDP	PN-O5D	2.03	1.67	1.59
3	F	402	NDP	P2B-O3X	-2.02	1.47	1.54
3	B	402	NDP	C5B-C4B	2.01	1.57	1.51
3	D	402	NDP	C2A-N1A	2.01	1.37	1.33

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NDP	O4B-C4B-C3B	-8.95	87.39	105.15
3	D	402	NDP	O4B-C4B-C3B	-8.33	88.62	105.15
3	C	402	NDP	O4B-C4B-C3B	-7.24	90.78	105.15
3	F	402	NDP	O4B-C4B-C3B	-7.24	90.79	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NDP	N3A-C2A-N1A	-6.89	118.15	128.58
3	C	402	NDP	N3A-C2A-N1A	-6.75	118.37	128.58
3	E	402	NDP	N3A-C2A-N1A	-6.64	118.53	128.58
3	B	402	NDP	N3A-C2A-N1A	-6.63	118.54	128.58
3	C	402	NDP	C5A-C4A-N3A	-6.55	117.69	126.72
3	E	402	NDP	O4B-C4B-C3B	-6.53	92.18	105.15
2	D	401	GEC	OAA-CAI-CAG	-6.43	97.85	104.73
3	A	402	NDP	C5A-C4A-N3A	-6.35	117.97	126.72
2	F	401	GEC	OAA-CAI-CAG	-6.17	98.13	104.73
2	B	401	GEC	OAB-CAJ-CAH	-6.06	98.24	104.73
3	E	402	NDP	N6A-C6A-N1A	-6.03	104.95	118.38
2	C	401	GEC	OAA-CAI-CAG	-6.00	98.31	104.73
3	A	402	NDP	O4B-C4B-C3B	-5.91	93.41	105.15
2	B	401	GEC	OAA-CAI-CAG	-5.84	98.48	104.73
2	D	401	GEC	CAL-CAG-CAI	-5.84	105.21	114.53
3	F	402	NDP	N3A-C2A-N1A	-5.82	119.78	128.58
3	F	402	NDP	C5A-C4A-N3A	-5.77	118.77	126.72
3	B	402	NDP	N6A-C6A-N1A	-5.72	105.63	118.38
2	A	401	GEC	OAB-CAJ-CAH	-5.69	98.63	104.73
3	D	402	NDP	O3B-C3B-C2B	-5.65	95.38	111.19
3	C	402	NDP	N6A-C6A-N1A	-5.63	105.85	118.38
3	F	402	NDP	C3N-C2N-N1N	-5.57	115.03	123.20
3	D	402	NDP	N6A-C6A-N1A	-5.51	106.09	118.38
3	B	402	NDP	C5A-C4A-N3A	-5.45	119.22	126.72
3	F	402	NDP	N6A-C6A-N1A	-5.45	106.25	118.38
3	E	402	NDP	C4A-N9A-C1B	-5.44	113.91	126.63
3	E	402	NDP	C5A-C4A-N3A	-5.33	119.37	126.72
3	B	402	NDP	C4A-N9A-C1B	-5.31	114.20	126.63
2	F	401	GEC	CAL-CAG-CAI	-5.29	106.08	114.53
2	C	401	GEC	OAB-CAJ-CAN	-5.29	104.51	110.39
3	D	402	NDP	N3A-C2A-N1A	-5.22	120.68	128.58
3	B	402	NDP	N9A-C8A-N7A	-5.22	106.53	113.94
3	A	402	NDP	N6A-C6A-N1A	-5.21	106.77	118.38
3	D	402	NDP	C4A-N9A-C1B	-5.18	114.52	126.63
3	C	402	NDP	O2N-PN-O3	5.17	121.25	107.27
2	E	401	GEC	OAB-CAJ-CAN	-5.16	104.66	110.39
3	B	402	NDP	O4B-C1B-C2B	-5.15	97.73	106.59
3	F	402	NDP	C4A-N9A-C1B	-5.11	114.68	126.63
3	B	402	NDP	O4B-C1B-N9A	-5.08	98.33	108.09
3	A	402	NDP	O2N-PN-O3	5.05	120.94	107.27
2	B	401	GEC	CAL-CAG-CAI	-5.03	106.49	114.53
2	A	401	GEC	OAA-CAI-CAG	-5.00	99.38	104.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	NDP	N9A-C8A-N7A	-4.98	106.86	113.94
2	F	401	GEC	OAB-CAJ-CAH	-4.95	99.43	104.73
2	E	401	GEC	CAL-CAG-CAI	-4.89	106.72	114.53
3	D	402	NDP	C5A-C4A-N3A	-4.84	120.05	126.72
3	B	402	NDP	N3A-C4A-N9A	4.84	135.40	127.17
3	B	402	NDP	C4A-N9A-C8A	4.68	110.65	105.74
3	A	402	NDP	N3A-C4A-N9A	4.68	135.12	127.17
3	C	402	NDP	C4A-N9A-C1B	-4.66	115.74	126.63
2	C	401	GEC	CAL-CAG-CAI	-4.66	107.09	114.53
3	E	402	NDP	O2N-PN-O3	4.62	119.75	107.27
3	E	402	NDP	O4B-C1B-N9A	-4.59	99.28	108.09
2	D	401	GEC	OAB-CAJ-CAH	-4.57	99.84	104.73
3	F	402	NDP	N3A-C4A-N9A	4.52	134.85	127.17
3	A	402	NDP	C2A-N3A-C4A	4.49	122.79	111.83
3	C	402	NDP	C1B-N9A-C8A	4.46	137.00	127.09
3	A	402	NDP	C4A-N9A-C1B	-4.43	116.28	126.63
3	F	402	NDP	N9A-C8A-N7A	-4.39	107.70	113.94
3	E	402	NDP	C1B-N9A-C8A	4.33	136.71	127.09
2	D	401	GEC	CAK-CAH-CAJ	-4.32	107.64	114.53
3	D	402	NDP	C3N-C2N-N1N	-4.28	116.92	123.20
3	D	402	NDP	O2N-PN-O3	4.27	118.80	107.27
3	C	402	NDP	N3A-C4A-N9A	4.26	134.41	127.17
3	E	402	NDP	C3N-C2N-N1N	-4.25	116.96	123.20
3	C	402	NDP	C2A-N3A-C4A	4.25	122.21	111.83
3	F	402	NDP	O3B-C3B-C2B	-4.25	99.30	111.19
3	D	402	NDP	O4B-C1B-C2B	-4.19	99.38	106.59
2	E	401	GEC	OAB-CAJ-CAH	-4.16	100.28	104.73
3	E	402	NDP	N9A-C8A-N7A	-4.16	108.03	113.94
3	E	402	NDP	N3A-C4A-N9A	4.16	134.24	127.17
3	E	402	NDP	O3X-P2B-O2B	4.14	121.99	105.85
2	F	401	GEC	CAK-CAH-CAJ	-4.13	107.94	114.53
2	E	401	GEC	OAA-CAI-CAG	-4.08	100.36	104.73
3	A	402	NDP	O2A-PA-O3	-4.04	96.36	107.27
2	D	401	GEC	OAB-CAJ-CAN	-3.97	105.98	110.39
3	D	402	NDP	C4A-N9A-C8A	3.95	109.88	105.74
3	F	402	NDP	O2D-C2D-C3D	-3.92	99.25	111.82
3	F	402	NDP	C1B-N9A-C8A	3.91	135.77	127.09
3	D	402	NDP	C5A-C6A-N6A	3.90	132.93	123.29
3	B	402	NDP	C2A-N3A-C4A	3.84	121.21	111.83
3	D	402	NDP	C1B-N9A-C8A	3.83	135.59	127.09
3	E	402	NDP	C2A-N3A-C4A	3.83	121.17	111.83
3	D	402	NDP	O2A-PA-O3	-3.79	97.02	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GEC	OAB-CAJ-CAN	-3.77	106.20	110.39
2	C	401	GEC	OAB-CAJ-CAH	-3.75	100.72	104.73
2	F	401	GEC	OAB-CAJ-CAN	-3.74	106.24	110.39
3	A	402	NDP	N9A-C8A-N7A	-3.73	108.64	113.94
3	F	402	NDP	O2N-PN-O3	3.70	117.27	107.27
3	B	402	NDP	C3N-C2N-N1N	-3.70	117.77	123.20
3	F	402	NDP	C2A-N3A-C4A	3.68	120.81	111.83
2	B	401	GEC	CAK-CAH-CAJ	-3.67	108.67	114.53
3	D	402	NDP	N3A-C4A-N9A	3.65	133.38	127.17
3	A	402	NDP	C1B-N9A-C8A	3.65	135.19	127.09
3	B	402	NDP	C1B-N9A-C8A	3.63	135.14	127.09
3	D	402	NDP	O4B-C1B-N9A	-3.63	101.12	108.09
3	F	402	NDP	C4A-N9A-C8A	3.61	109.53	105.74
2	F	401	GEC	OAB-CAL-CAG	-3.60	100.75	105.56
2	F	401	GEC	OAA-CAK-CAH	-3.59	100.77	105.56
3	A	402	NDP	C3N-C2N-N1N	-3.58	117.95	123.20
3	E	402	NDP	O3-PA-O1A	3.56	121.42	110.70
3	D	402	NDP	O3D-C3D-C2D	-3.54	100.48	111.82
3	F	402	NDP	O7N-C7N-C3N	-3.54	114.23	120.90
2	F	401	GEC	CAM-CAI-CAG	-3.51	110.81	115.90
3	C	402	NDP	C3N-C2N-N1N	-3.49	118.08	123.20
3	D	402	NDP	C6A-C5A-C4A	3.47	121.92	117.18
3	C	402	NDP	O3X-P2B-O2B	3.47	119.35	105.85
3	E	402	NDP	C4A-N9A-C8A	3.45	109.36	105.74
3	D	402	NDP	O2D-C2D-C3D	-3.41	100.89	111.82
2	F	401	GEC	CAY-OAC-CAS	-3.38	112.56	117.51
3	B	402	NDP	C5A-C6A-N6A	3.33	131.54	123.29
3	C	402	NDP	O4B-C1B-N9A	-3.30	101.76	108.09
3	A	402	NDP	O3B-C3B-C2B	-3.28	101.99	111.19
2	B	401	GEC	CAR-CAN-CAJ	-3.25	114.55	120.62
3	B	402	NDP	O2B-C2B-C3B	-3.25	100.01	111.68
3	B	402	NDP	O3X-P2B-O2B	3.24	118.48	105.85
2	A	401	GEC	CAL-CAG-CAI	-3.24	109.36	114.53
3	A	402	NDP	O4B-C1B-N9A	-3.23	101.88	108.09
3	A	402	NDP	O4B-C1B-C2B	-3.23	101.03	106.59
3	E	402	NDP	C5A-C6A-N6A	3.23	131.27	123.29
2	B	401	GEC	CAP-CAN-CAJ	3.20	126.94	119.88
3	F	402	NDP	O2A-PA-O3	-3.16	98.74	107.27
2	A	401	GEC	OAB-CAJ-CAN	-3.15	106.89	110.39
3	C	402	NDP	N9A-C8A-N7A	-3.14	109.48	113.94
3	D	402	NDP	O2B-C2B-C3B	-3.14	100.42	111.68
2	A	401	GEC	OAA-CAI-CAM	3.13	113.88	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	GEC	OAA-CAK-CAH	-3.09	101.43	105.56
2	B	401	GEC	OAB-CAL-CAG	-3.08	101.44	105.56
3	B	402	NDP	O3-PN-O1N	3.04	119.86	110.70
2	E	401	GEC	CAK-CAH-CAJ	-3.01	109.72	114.53
2	F	401	GEC	CAR-CAN-CAJ	-3.00	115.01	120.62
3	B	402	NDP	O2A-PA-O3	-2.98	99.22	107.27
2	D	401	GEC	CAO-CAM-CAI	2.97	126.42	119.88
2	D	401	GEC	OAA-CAI-CAM	2.95	113.68	110.39
3	B	402	NDP	O3B-C3B-C2B	-2.95	102.92	111.19
3	E	402	NDP	O4B-C1B-C2B	-2.93	101.53	106.59
2	B	401	GEC	CAO-CAM-CAI	2.93	126.34	119.88
2	D	401	GEC	CAQ-CAM-CAI	-2.92	115.16	120.62
3	D	402	NDP	O3-PN-O1N	2.91	119.45	110.70
2	B	401	GEC	OAA-CAI-CAM	2.89	113.61	110.39
2	F	401	GEC	OAC-CAS-CAW	2.89	118.89	114.55
3	A	402	NDP	PN-O5D-C5D	-2.87	104.89	121.35
3	A	402	NDP	P2B-O2B-C2B	-2.86	115.78	123.43
3	C	402	NDP	C5A-C6A-N6A	2.86	130.37	123.29
2	C	401	GEC	CAK-CAH-CAJ	-2.85	109.97	114.53
2	B	401	GEC	CAZ-OAD-CAT	-2.84	113.34	117.51
3	E	402	NDP	O3B-C3B-C2B	-2.84	103.24	111.19
3	E	402	NDP	PN-O5D-C5D	-2.82	105.20	121.35
3	C	402	NDP	O3D-C3D-C4D	-2.81	103.01	111.08
3	F	402	NDP	C5A-C6A-N6A	2.78	130.17	123.29
3	E	402	NDP	O2D-C2D-C1D	-2.78	100.53	110.10
3	F	402	NDP	O4B-C1B-N9A	-2.78	102.75	108.09
3	A	402	NDP	C2D-C3D-C4D	2.76	107.94	102.61
3	A	402	NDP	O3-PN-O1N	2.75	118.99	110.70
3	C	402	NDP	O4B-C1B-C2B	-2.74	101.87	106.59
2	D	401	GEC	OAB-CAL-CAG	-2.72	101.93	105.56
2	E	401	GEC	CAO-CAM-CAI	2.68	125.79	119.88
3	E	402	NDP	O2B-C2B-C3B	-2.68	102.07	111.68
3	F	402	NDP	O3D-C3D-C2D	-2.68	103.24	111.82
2	C	401	GEC	OAB-CAL-CAG	-2.66	102.01	105.56
3	A	402	NDP	C4A-N9A-C8A	2.64	108.51	105.74
3	A	402	NDP	O2B-C2B-C3B	-2.63	102.23	111.68
3	A	402	NDP	O5D-C5D-C4D	-2.63	100.04	108.99
3	A	402	NDP	O3X-P2B-O2B	2.60	115.97	105.85
3	E	402	NDP	O3X-P2B-O1X	-2.59	100.74	110.83
2	F	401	GEC	CAQ-CAU-CAW	-2.55	117.95	120.50
3	F	402	NDP	C6A-C5A-C4A	2.54	120.64	117.18
2	C	401	GEC	CAZ-OAD-CAT	-2.52	113.82	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	GEC	CAY-OAC-CAS	-2.51	113.83	117.51
3	C	402	NDP	O2B-P2B-O1X	-2.49	100.45	109.33
3	B	402	NDP	C5A-N7A-C8A	2.49	107.36	103.45
3	F	402	NDP	O2B-C2B-C1B	-2.48	101.32	110.05
3	C	402	NDP	C3N-C7N-N7N	-2.48	113.26	117.67
2	B	401	GEC	OAA-CAK-CAH	-2.47	102.26	105.56
3	C	402	NDP	C5A-C6A-N1A	2.47	123.79	117.51
3	E	402	NDP	C5A-C6A-N1A	2.47	123.78	117.51
2	C	401	GEC	CAP-CAN-CAJ	2.46	125.31	119.88
2	B	401	GEC	CAQ-CAM-CAI	-2.45	116.04	120.62
3	C	402	NDP	O3-PN-O1N	2.43	118.02	110.70
3	D	402	NDP	C2A-N3A-C4A	2.42	117.74	111.83
3	A	402	NDP	C5A-C6A-N6A	2.42	129.28	123.29
3	A	402	NDP	C5A-C6A-N1A	2.41	123.64	117.51
2	E	401	GEC	CAP-CAN-CAJ	2.41	125.19	119.88
3	E	402	NDP	O4D-C4D-C5D	-2.40	101.65	109.33
3	F	402	NDP	O4B-C1B-C2B	-2.40	102.46	106.59
2	A	401	GEC	OAB-CAL-CAG	-2.39	102.37	105.56
3	F	402	NDP	C5D-C4D-C3D	-2.39	106.61	115.21
3	F	402	NDP	C5A-C6A-N1A	2.39	123.57	117.51
2	C	401	GEC	CAR-CAN-CAJ	-2.38	116.18	120.62
3	A	402	NDP	O2D-C2D-C3D	-2.38	104.19	111.82
2	F	401	GEC	OAC-CAS-CAO	-2.37	120.00	124.08
3	C	402	NDP	PN-O5D-C5D	-2.36	107.81	121.35
3	F	402	NDP	C2D-C3D-C4D	2.34	107.14	102.61
3	B	402	NDP	C3N-C7N-N7N	-2.32	113.55	117.67
2	A	401	GEC	CAM-CAI-CAG	-2.31	112.55	115.90
2	E	401	GEC	CAZ-OAD-CAT	-2.30	114.14	117.51
3	F	402	NDP	O4D-C1D-N1N	-2.30	103.70	108.08
2	F	401	GEC	CAG-CAH-CAJ	-2.29	99.36	103.10
3	D	402	NDP	C5A-N7A-C8A	2.28	107.04	103.45
3	A	402	NDP	O3D-C3D-C2D	-2.28	104.51	111.82
2	B	401	GEC	CAN-CAJ-CAH	2.28	119.19	115.90
2	E	401	GEC	CAQ-CAM-CAI	-2.27	116.38	120.62
2	E	401	GEC	CAR-CAN-CAJ	-2.27	116.38	120.62
3	A	402	NDP	O5D-PN-O1N	-2.27	99.94	108.94
2	E	401	GEC	CAY-OAC-CAS	-2.26	114.19	117.51
3	D	402	NDP	O2B-P2B-O1X	-2.26	101.29	109.33
3	D	402	NDP	C2D-C3D-C4D	2.25	106.96	102.61
2	B	401	GEC	CAP-CAT-CAX	-2.25	117.78	120.04
3	B	402	NDP	O3D-C3D-C4D	-2.23	104.67	111.08
3	E	402	NDP	C3N-C7N-N7N	-2.23	113.71	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	GEC	OAD-CAT-CAX	2.23	117.89	114.55
3	F	402	NDP	O7N-C7N-N7N	2.22	127.88	122.89
3	C	402	NDP	O3B-C3B-C4B	-2.22	104.71	111.08
2	C	401	GEC	CAQ-CAU-CAW	-2.21	118.28	120.50
2	E	401	GEC	OAD-CAT-CAX	2.20	117.85	114.55
3	B	402	NDP	C6A-C5A-C4A	2.17	120.15	117.18
3	C	402	NDP	O2D-C2D-C1D	-2.17	102.64	110.10
2	A	401	GEC	CAO-CAM-CAI	2.17	124.65	119.88
2	A	401	GEC	CAG-CAH-CAJ	-2.16	99.57	103.10
3	E	402	NDP	O2A-PA-O1A	-2.16	102.42	112.44
2	A	401	GEC	CAQ-CAM-CAI	-2.15	116.60	120.62
3	C	402	NDP	O2B-C2B-C3B	-2.15	103.95	111.68
2	D	401	GEC	CAR-CAN-CAJ	-2.15	116.60	120.62
3	C	402	NDP	C6A-C5A-C4A	2.15	120.11	117.18
2	A	401	GEC	OAD-CAT-CAX	2.14	117.76	114.55
2	B	401	GEC	OAD-CAT-CAX	2.14	117.75	114.55
2	C	401	GEC	OAC-CAS-CAW	2.13	117.75	114.55
3	E	402	NDP	O2N-PN-O5D	-2.13	97.90	107.57
3	D	402	NDP	P2B-O2B-C2B	-2.12	117.78	123.43
2	F	401	GEC	CAP-CAN-CAJ	2.12	124.54	119.88
2	C	401	GEC	OAD-CAT-CAX	2.10	117.69	114.55
3	C	402	NDP	PA-O5B-C5B	-2.09	109.39	121.35
3	B	402	NDP	C5A-C6A-N1A	2.08	122.80	117.51
3	D	402	NDP	PN-O5D-C5D	-2.08	109.42	121.35
2	B	401	GEC	CAV-CAX-CAT	2.06	121.89	119.55
2	D	401	GEC	CAR-CAV-CAX	-2.05	118.45	120.50
2	F	401	GEC	CAR-CAV-CAX	-2.05	118.45	120.50
3	A	402	NDP	O2B-C2B-C1B	-2.04	102.87	110.05
3	F	402	NDP	PN-O5D-C5D	-2.04	109.67	121.35
3	F	402	NDP	P2B-O2B-C2B	-2.03	118.00	123.43
3	A	402	NDP	O3D-C3D-C4D	-2.02	105.27	111.08
2	A	401	GEC	CAP-CAN-CAJ	2.02	124.34	119.88
2	B	401	GEC	CAG-CAH-CAJ	-2.01	99.82	103.10

There are no chirality outliers.

All (27) 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	F	402	NDP	C5B-O5B-PA-O3
3	D	402	NDP	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
3	C	402	NDP	C5B-O5B-PA-O3
3	B	402	NDP	C5B-O5B-PA-O2A
3	B	402	NDP	C5B-O5B-PA-O3
2	F	401	GEC	CAO-CAS-OAC-CAY
2	F	401	GEC	CAW-CAS-OAC-CAY
3	A	402	NDP	C5B-O5B-PA-O3
3	B	402	NDP	C3B-C4B-C5B-O5B
3	E	402	NDP	O4D-C1D-N1N-C2N
3	F	402	NDP	O4D-C1D-N1N-C2N
3	A	402	NDP	O4D-C1D-N1N-C2N
3	D	402	NDP	O4D-C1D-N1N-C2N
3	C	402	NDP	O4D-C1D-N1N-C2N
3	B	402	NDP	O4D-C1D-N1N-C2N
3	B	402	NDP	C2N-C3N-C7N-N7N
3	F	402	NDP	C2B-O2B-P2B-O1X
3	E	402	NDP	C2D-C1D-N1N-C2N
3	A	402	NDP	C2D-C1D-N1N-C2N
3	D	402	NDP	C2D-C1D-N1N-C2N
3	C	402	NDP	C2D-C1D-N1N-C2N
3	C	402	NDP	C3B-C4B-C5B-O5B
3	B	402	NDP	C2D-C1D-N1N-C2N
3	A	402	NDP	C2B-O2B-P2B-O3X
3	F	402	NDP	C2B-O2B-P2B-O2X

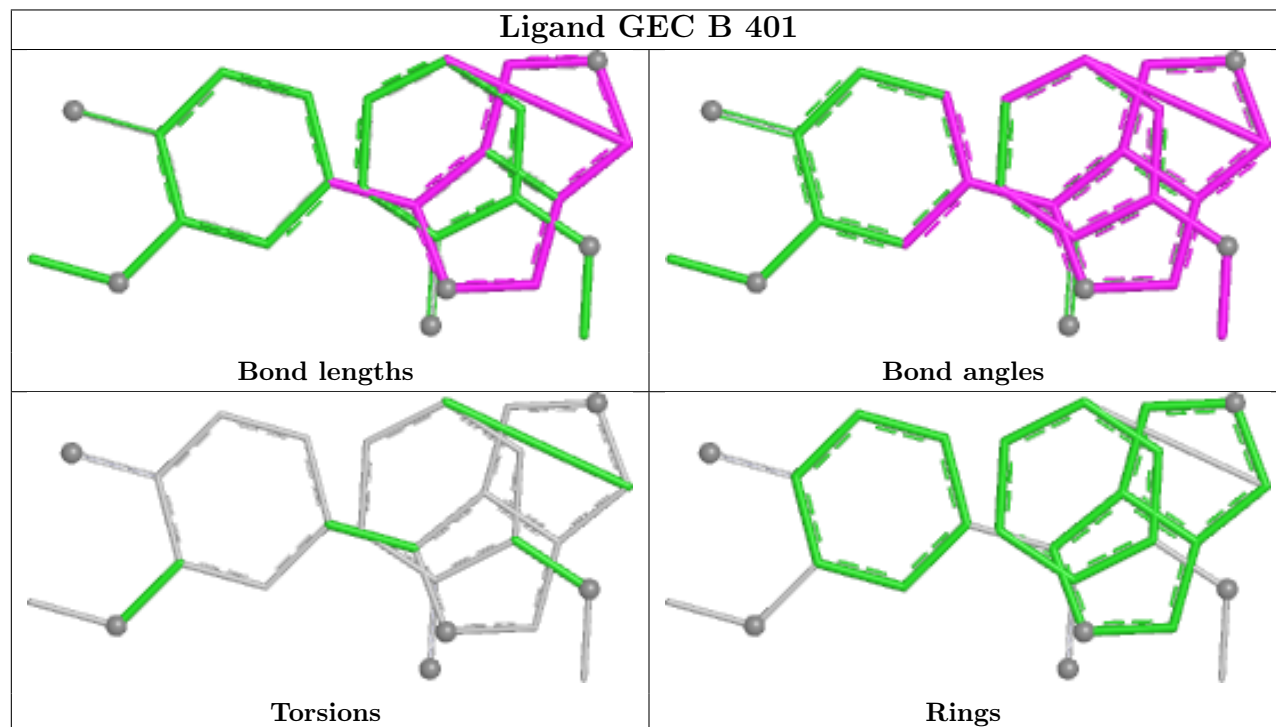
There are no ring outliers.

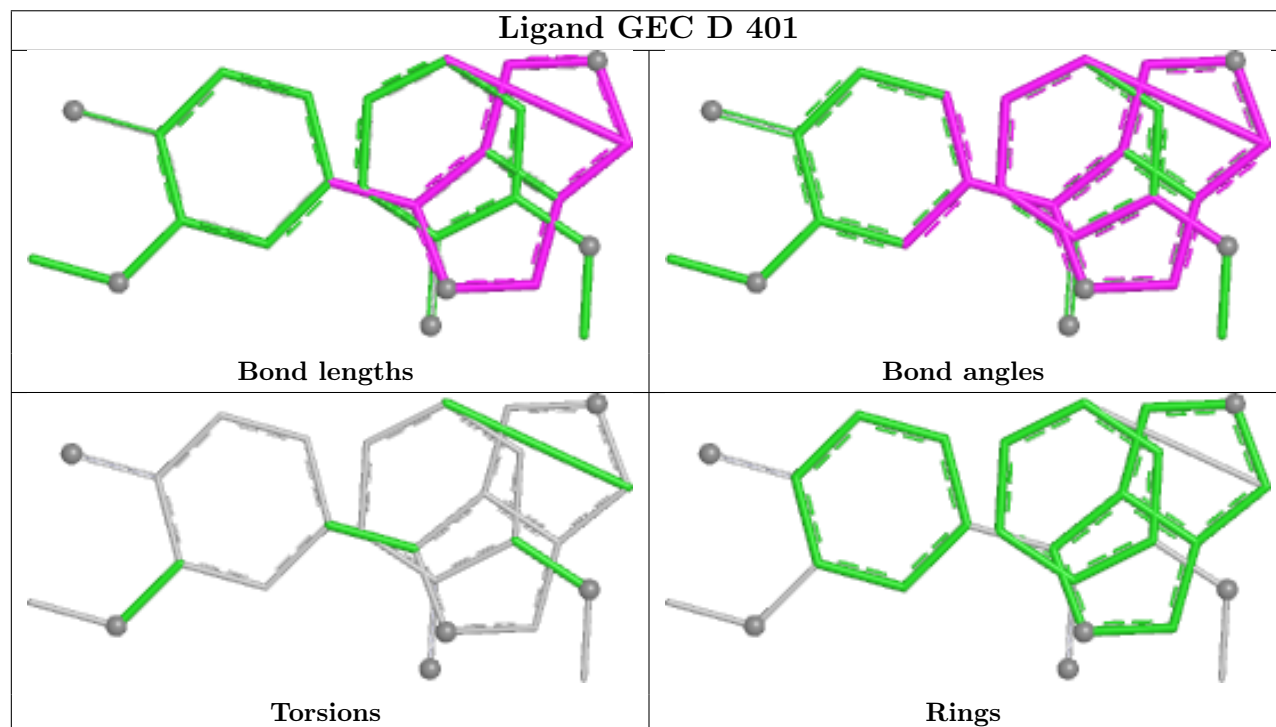
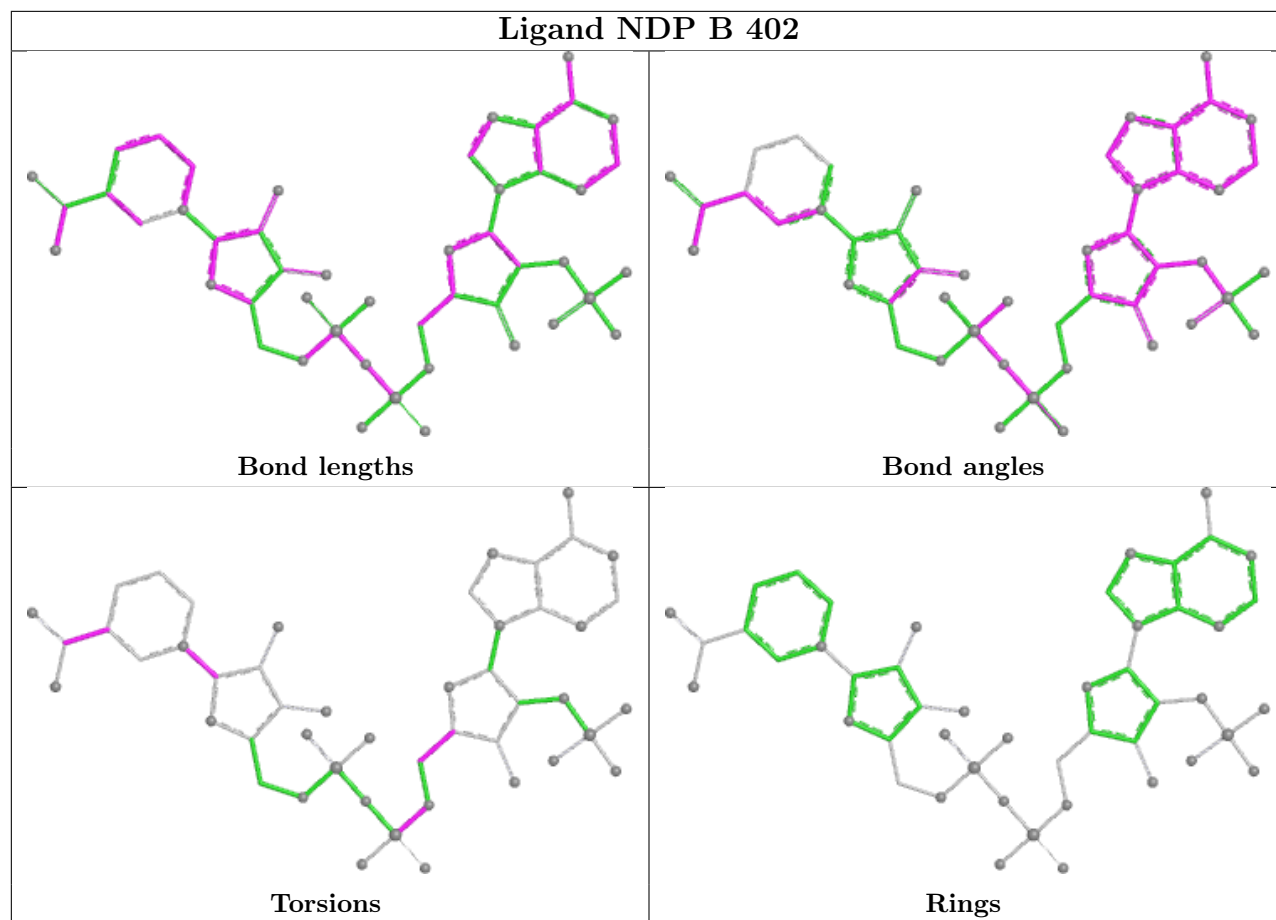
7 monomers are involved in 47 short contacts:

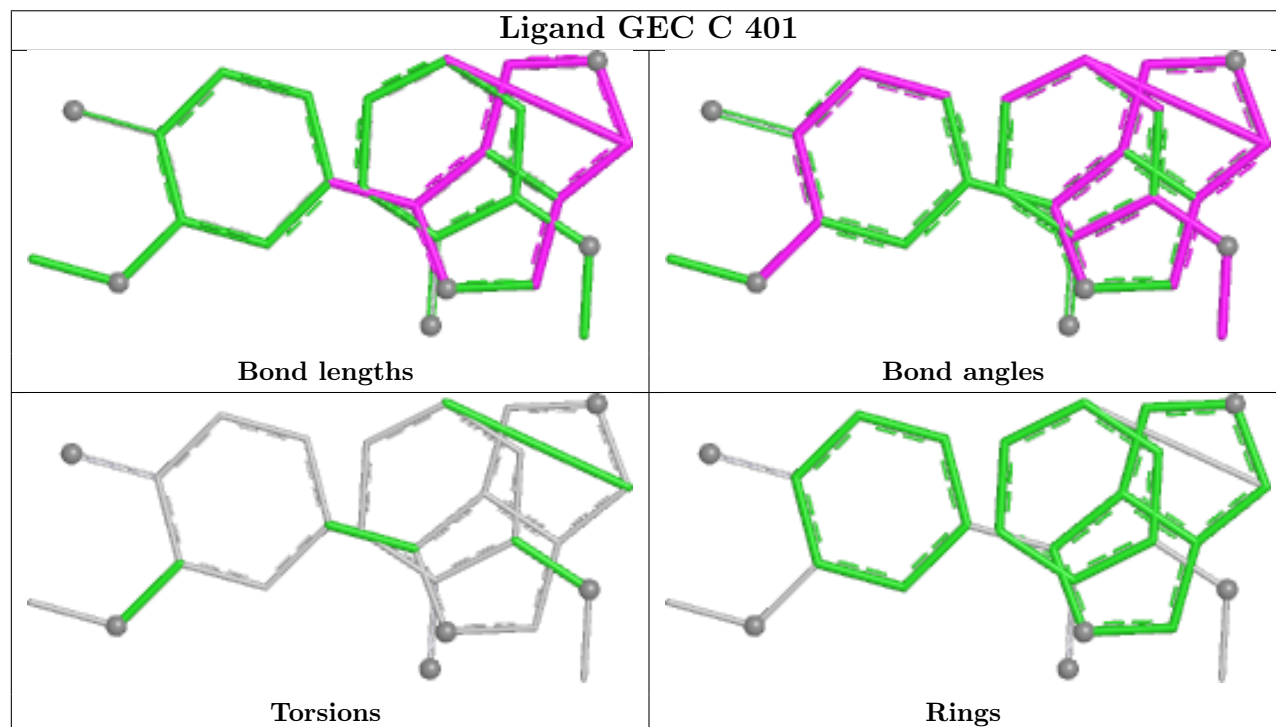
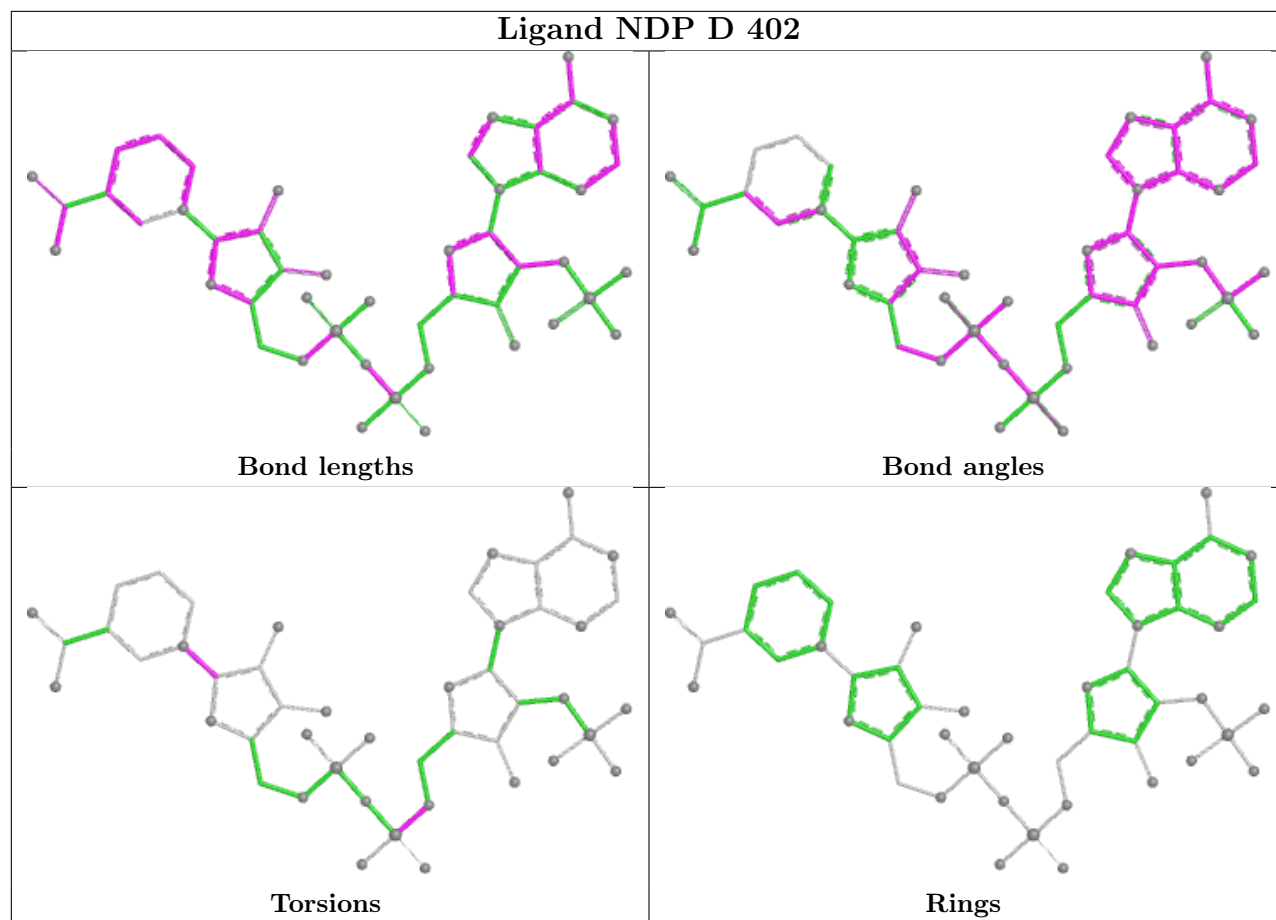
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	NDP	4	0
3	D	402	NDP	11	0
2	F	401	GEC	1	0
3	C	402	NDP	6	0
3	F	402	NDP	8	0
3	A	402	NDP	13	0
3	E	402	NDP	4	0

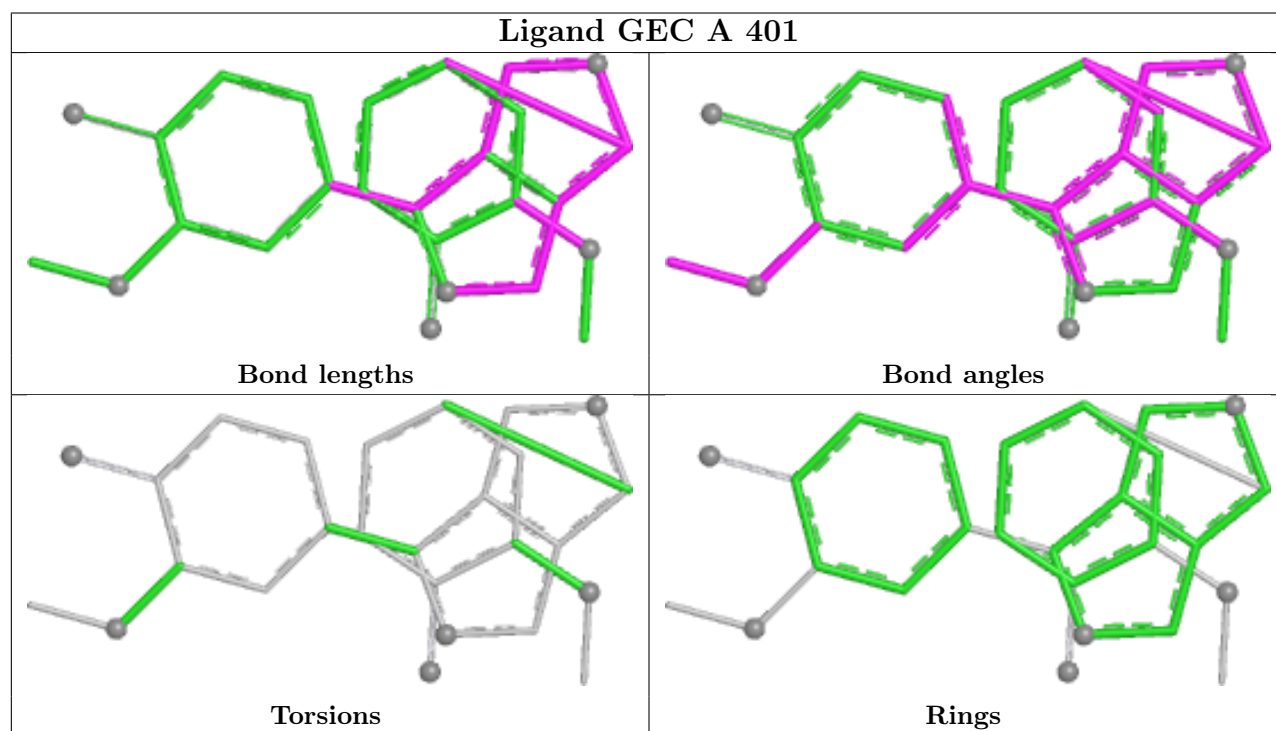
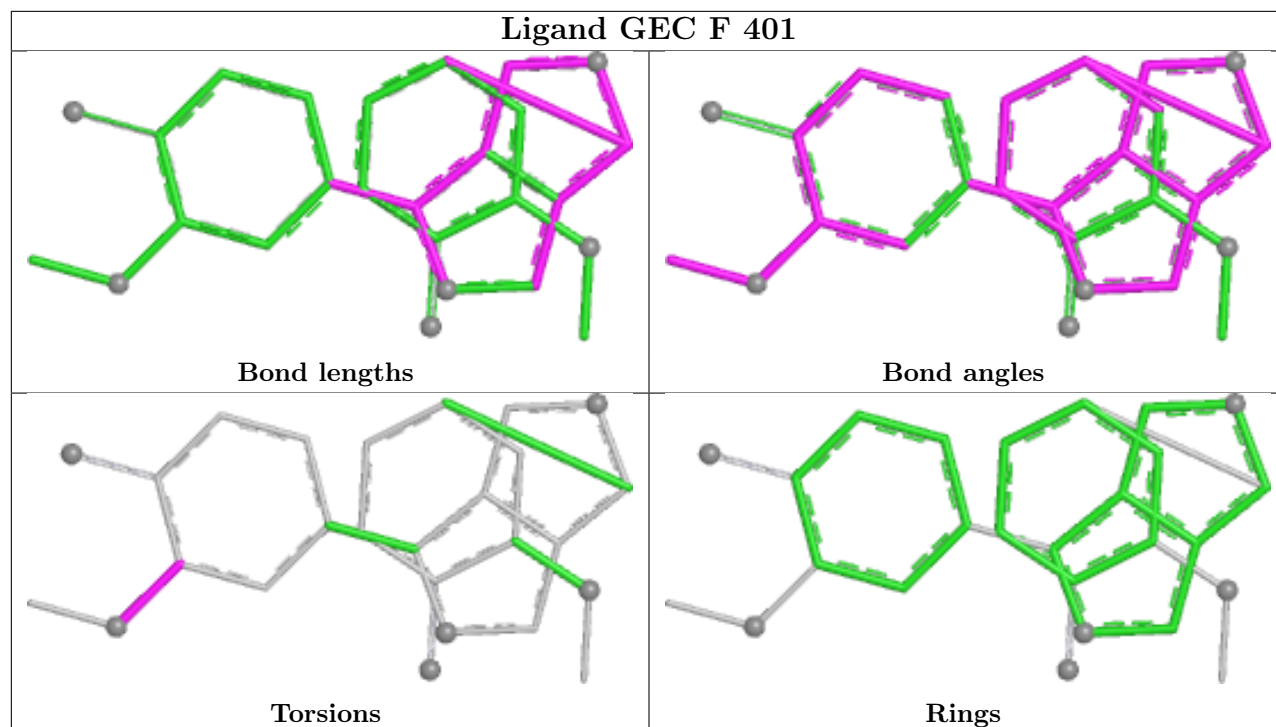
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

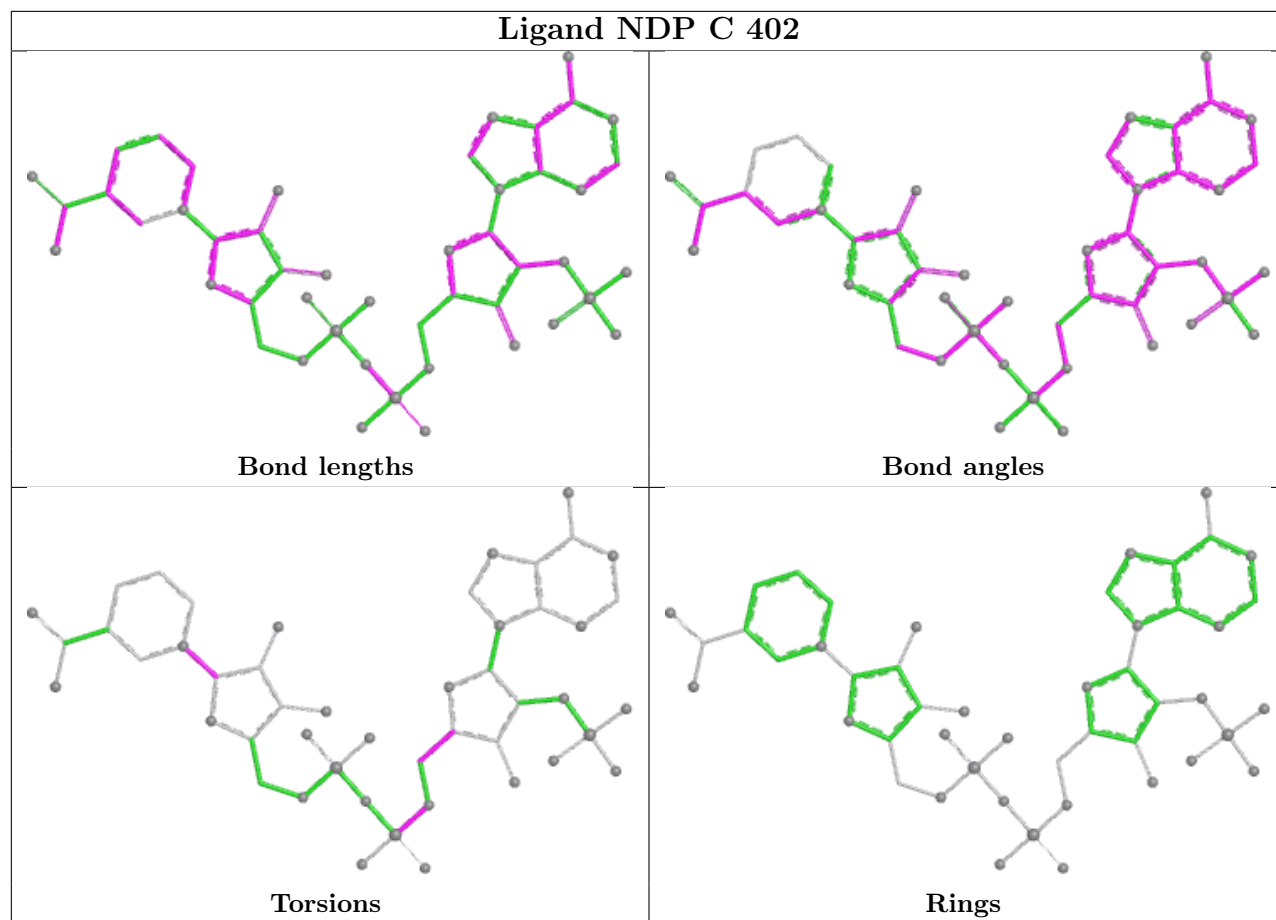
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

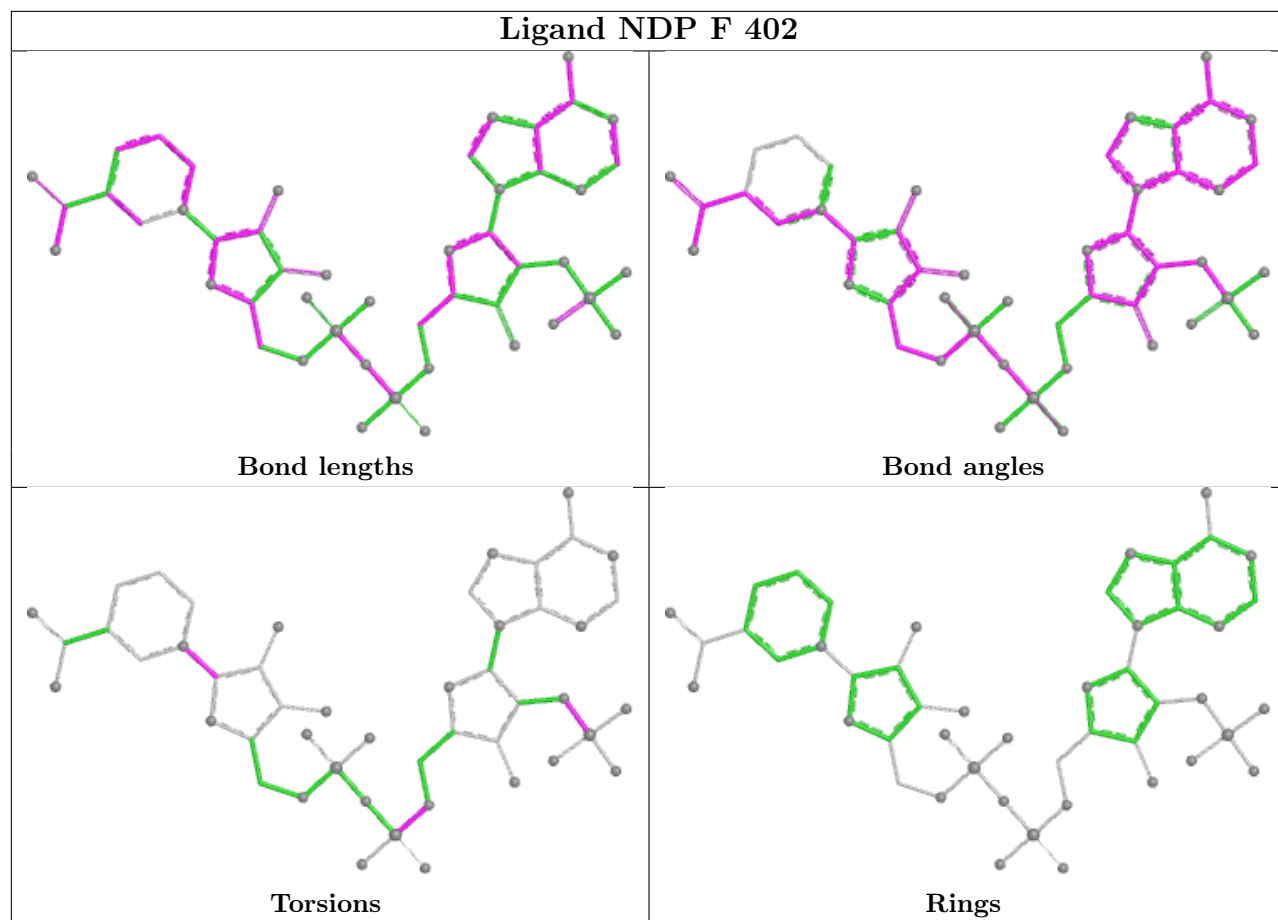


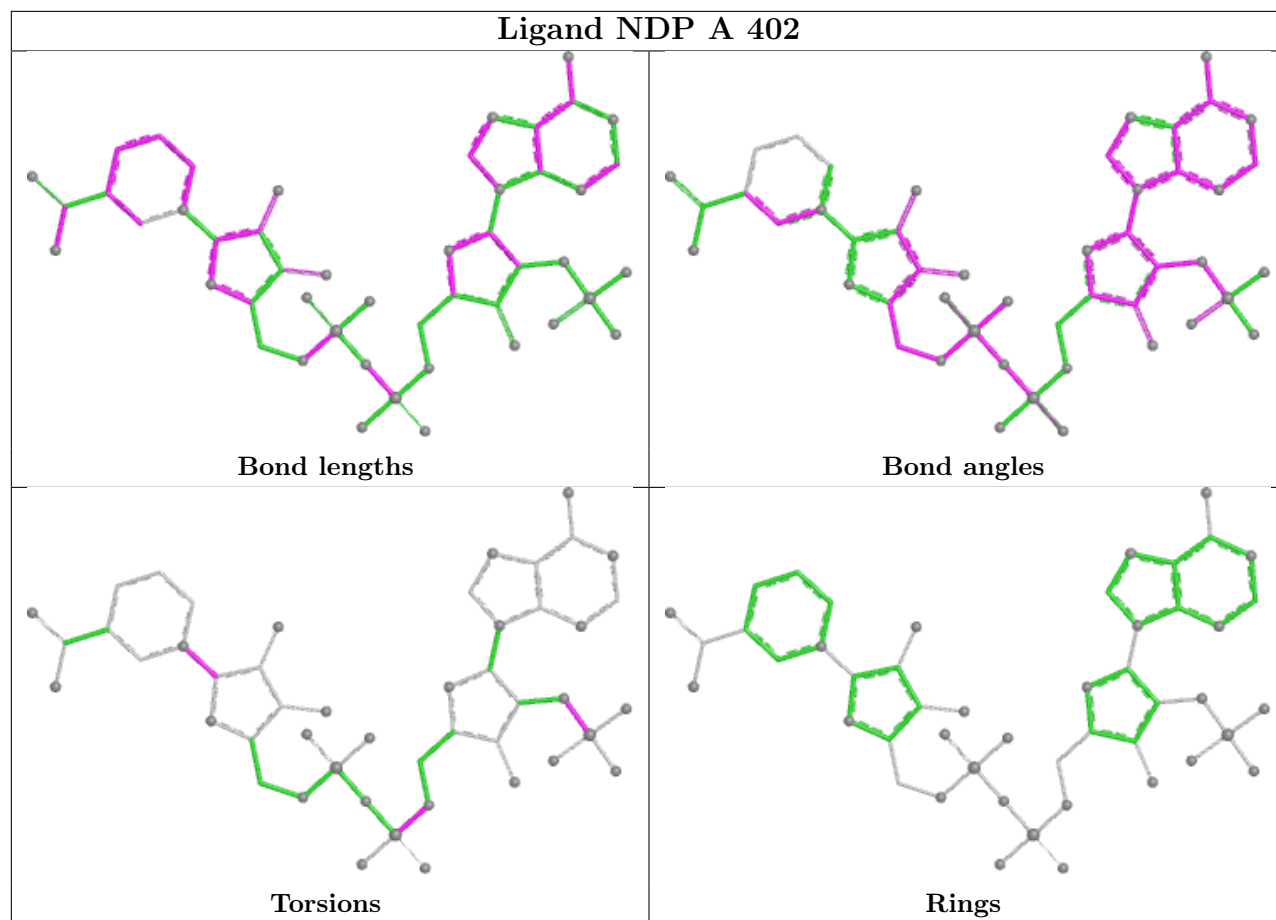


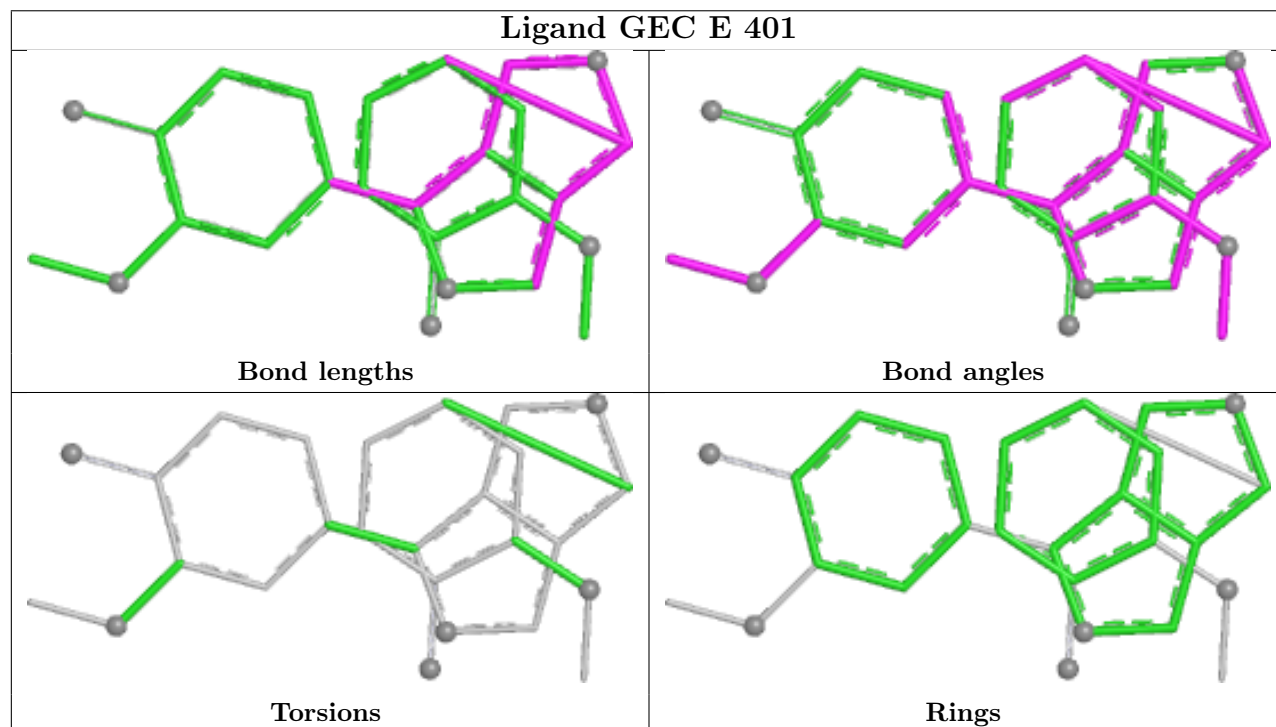
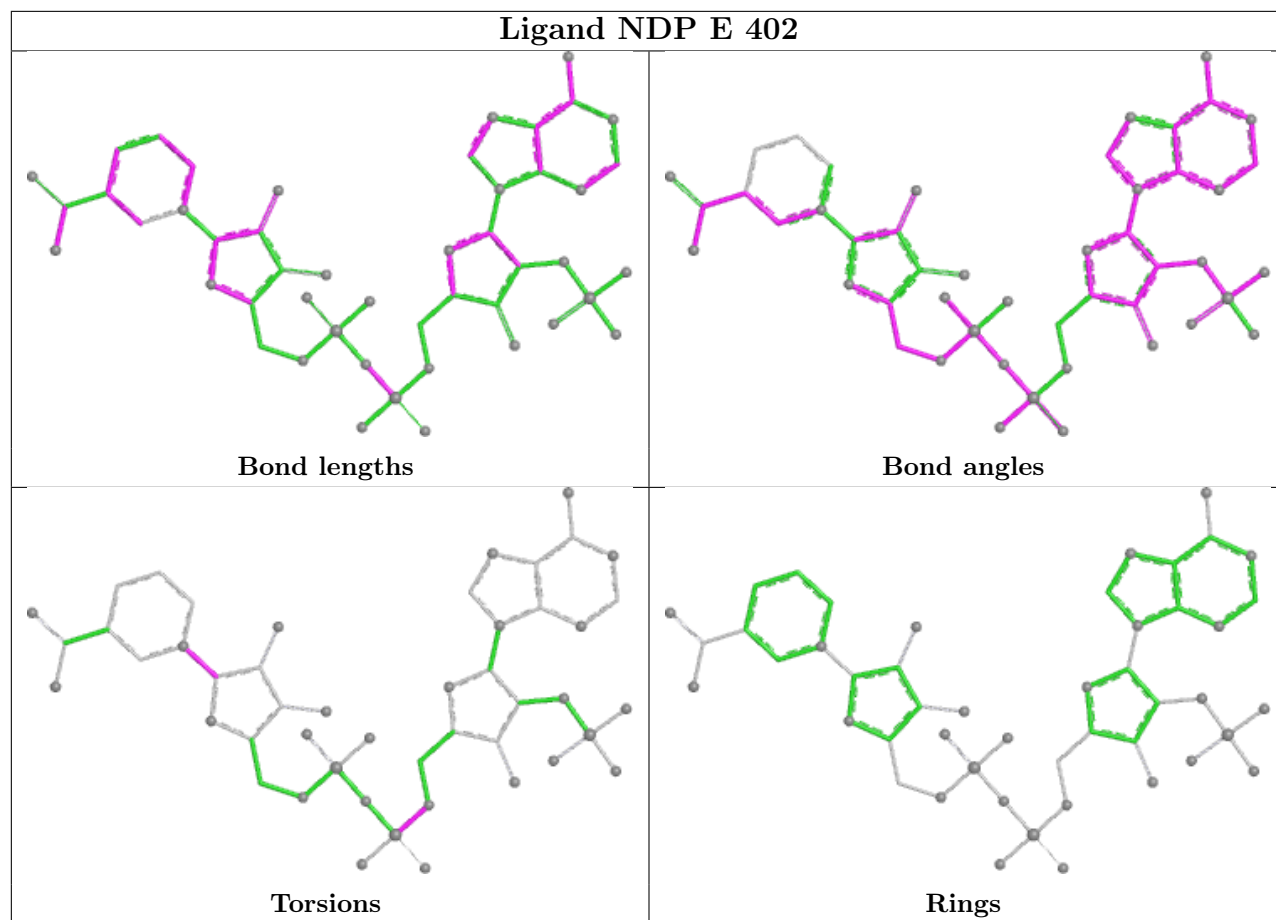












5.7 Other polymers [i](#)

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	283/317 (89%)	0.31	21 (7%) 20 22	28, 40, 69, 90	0
1	B	291/317 (91%)	-0.21	5 (1%) 69 70	26, 35, 52, 75	0
1	C	284/317 (89%)	-0.14	7 (2%) 58 60	29, 36, 54, 71	0
1	D	286/317 (90%)	0.04	8 (2%) 55 57	31, 41, 60, 94	0
1	E	284/317 (89%)	-0.14	6 (2%) 63 65	29, 38, 54, 70	0
1	F	286/317 (90%)	0.10	9 (3%) 51 53	31, 41, 63, 84	0
All	All	1714/1902 (90%)	-0.01	56 (3%) 49 51	26, 39, 62, 94	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	ALA	6.8
1	A	7	GLY	5.9
1	F	7	GLY	5.4
1	D	7	GLY	4.9
1	E	261	ALA	4.8
1	A	91	GLY	4.7
1	A	272	ALA	4.7
1	D	97	HIS	4.5
1	C	7	GLY	4.2
1	F	131	GLY	4.1
1	D	91	GLY	4.1
1	D	262	ASP	4.0
1	F	261	ALA	4.0
1	B	261	ALA	3.7
1	C	91	GLY	3.7
1	E	7	GLY	3.5
1	F	272	ALA	3.5
1	D	272	ALA	3.5
1	A	128	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	92	VAL	3.2
1	E	98	SER	3.2
1	A	260	LEU	3.2
1	A	107	GLU	3.1
1	D	271	GLN	2.9
1	A	257	ASN	2.9
1	A	190	TYR	2.8
1	A	189	ILE	2.7
1	A	282	TYR	2.7
1	C	44	THR	2.6
1	A	254	ILE	2.6
1	A	97	HIS	2.6
1	B	267	GLU	2.6
1	E	272	ALA	2.6
1	A	194	ASN	2.5
1	B	97	HIS	2.5
1	C	235	MET	2.5
1	A	278	TYR	2.4
1	D	261	ALA	2.4
1	C	272	ALA	2.4
1	D	260	LEU	2.4
1	A	289	HIS	2.4
1	E	260	LEU	2.3
1	A	256	ALA	2.3
1	F	98	SER	2.3
1	C	73	GLN	2.3
1	A	195	VAL	2.3
1	A	238	VAL	2.3
1	A	192	ASP	2.3
1	F	91	GLY	2.3
1	F	45	ARG	2.3
1	B	260	LEU	2.2
1	A	252	THR	2.2
1	F	192	ASP	2.1
1	F	271	GLN	2.1
1	C	98	SER	2.1
1	E	107	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

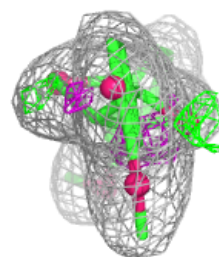
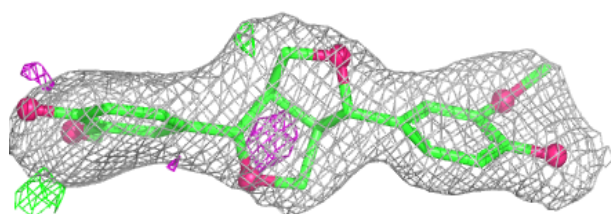
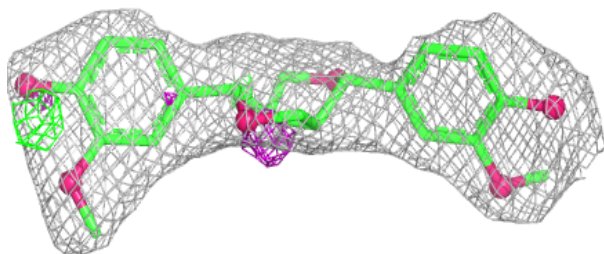
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GEC	F	401	26/26	0.87	0.14	42,57,63,64	0
2	GEC	D	401	26/26	0.90	0.12	46,52,58,59	0
2	GEC	C	401	26/26	0.90	0.10	35,44,49,51	0
2	GEC	A	401	26/26	0.91	0.11	41,48,55,58	0
2	GEC	E	401	26/26	0.91	0.11	35,47,56,57	0
2	GEC	B	401	26/26	0.92	0.09	27,32,37,42	0
3	NDP	D	402	48/48	0.92	0.09	36,47,61,81	0
3	NDP	E	402	48/48	0.94	0.08	29,41,51,61	0
3	NDP	B	402	48/48	0.94	0.08	24,34,50,61	0
3	NDP	C	402	48/48	0.95	0.07	29,40,54,69	0
3	NDP	A	402	48/48	0.95	0.08	30,38,48,62	0
3	NDP	F	402	48/48	0.96	0.07	33,44,56,61	0

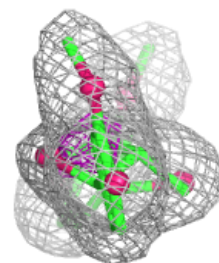
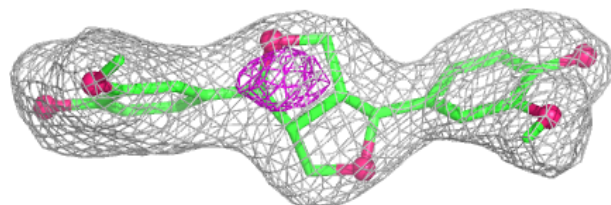
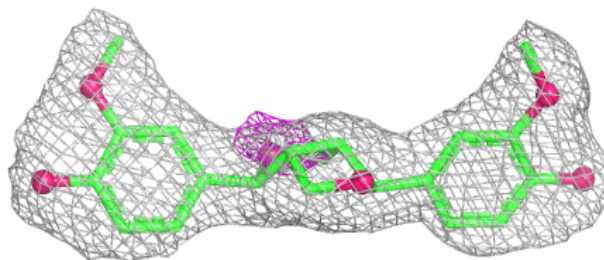
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

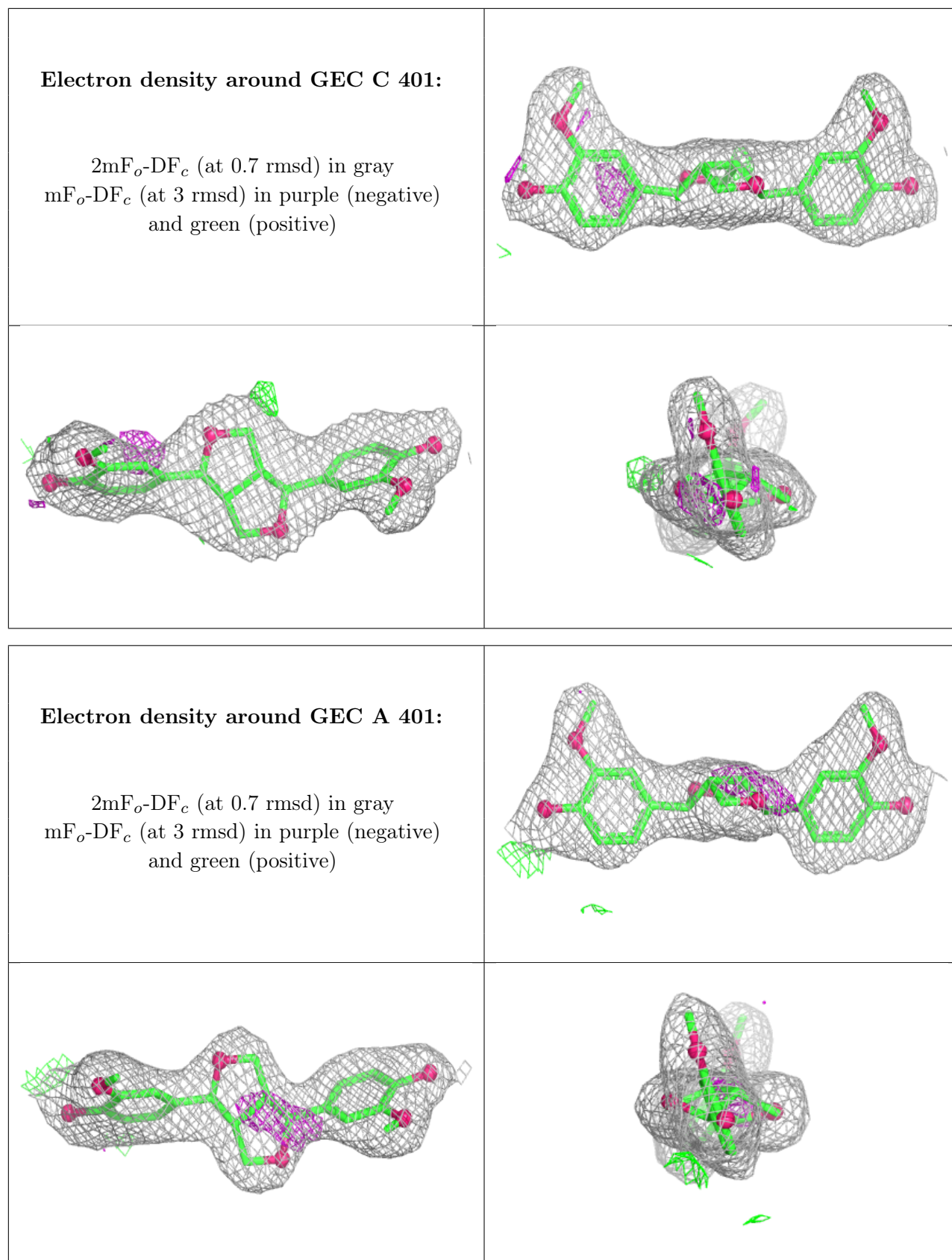
Electron density around GEC F 401:

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

**Electron density around GEC D 401:**

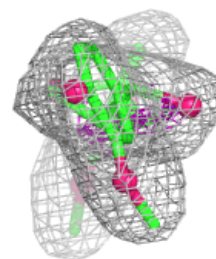
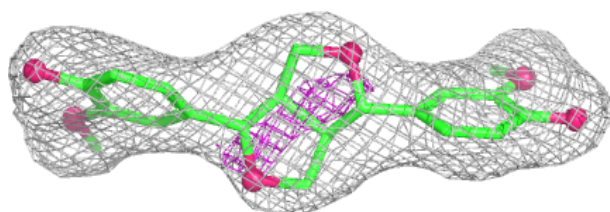
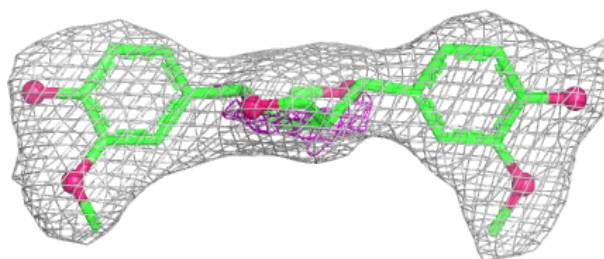
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



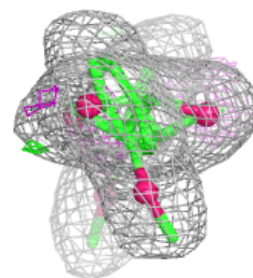
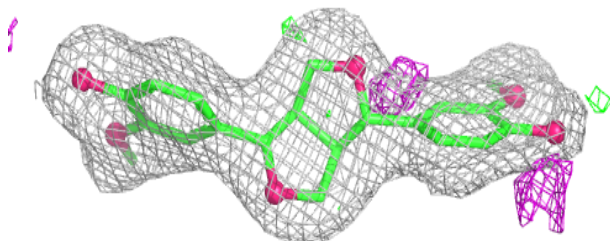
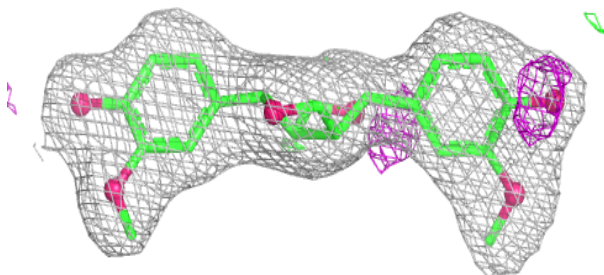


Electron density around GEC E 401:

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

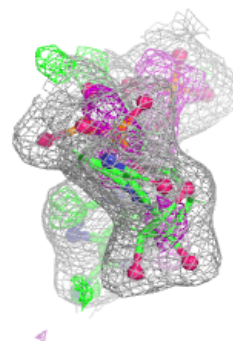
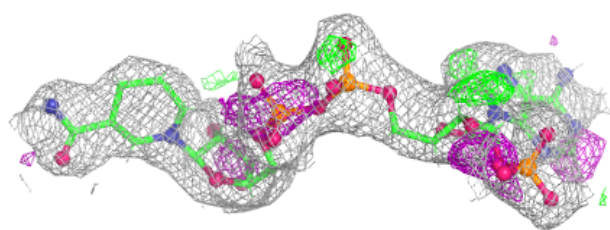
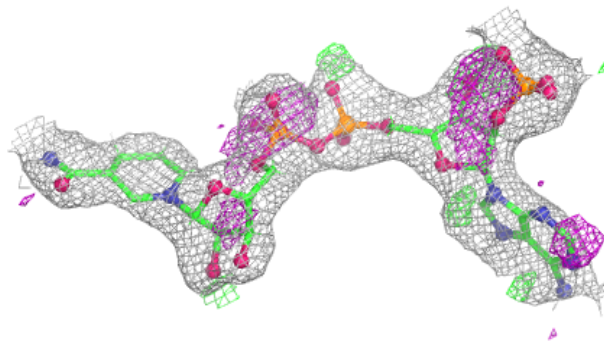
**Electron density around GEC B 401:**

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

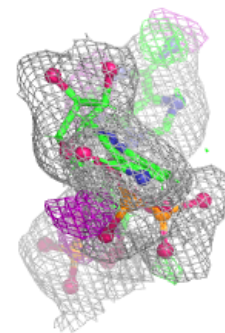
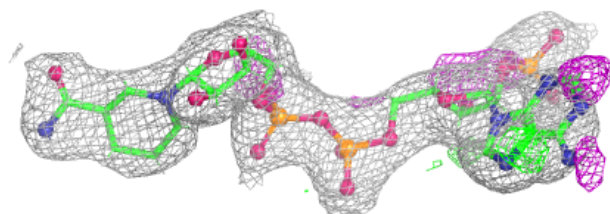
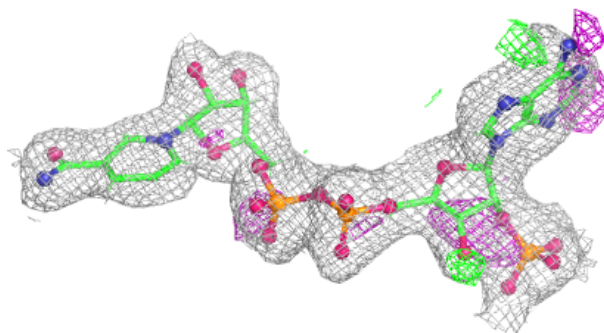


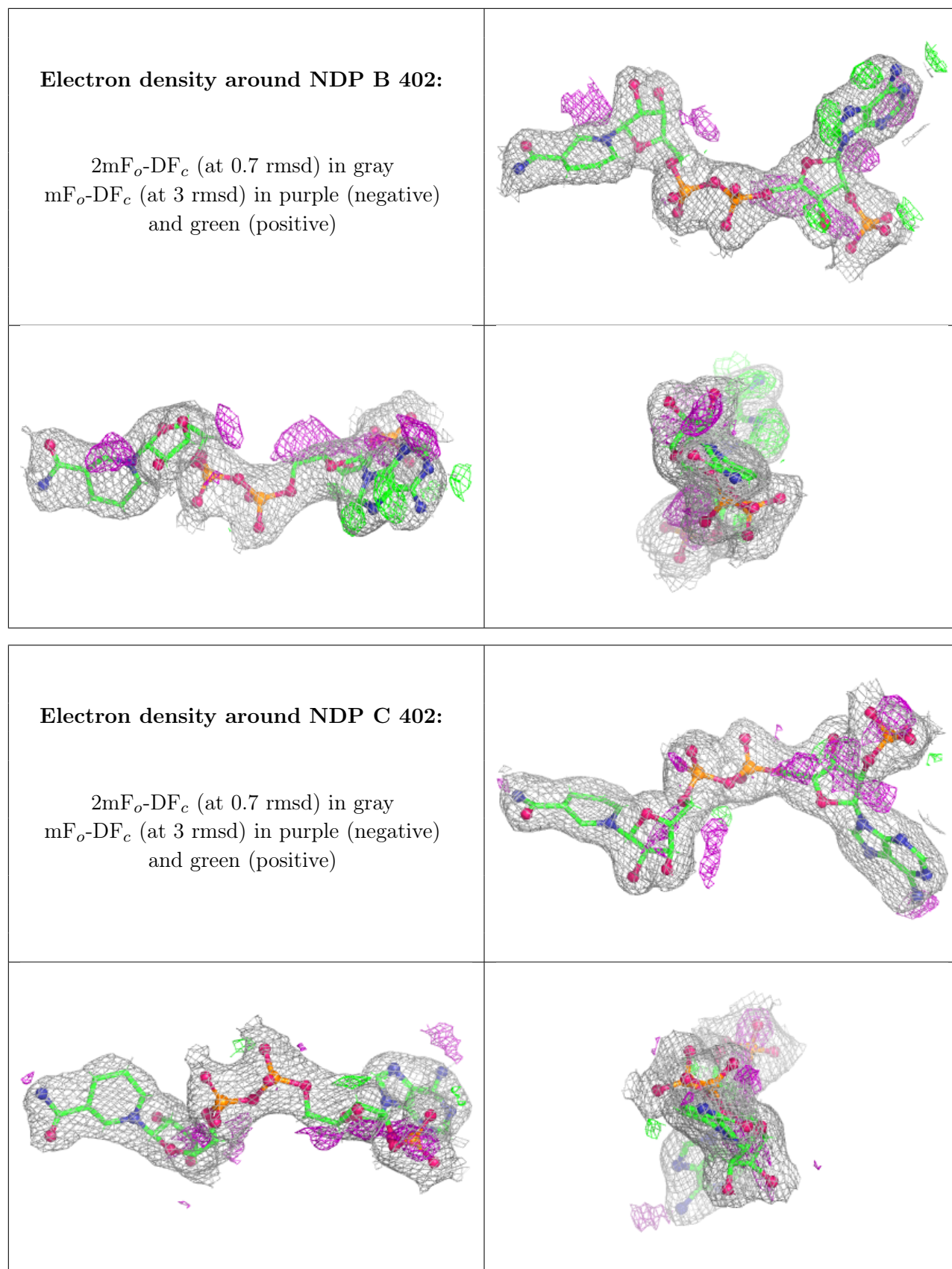
Electron density around NDP D 402:

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

**Electron density around NDP E 402:**

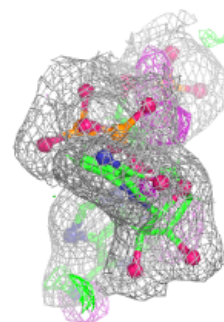
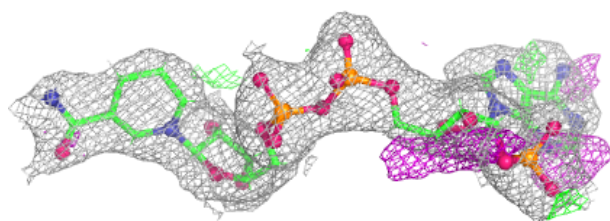
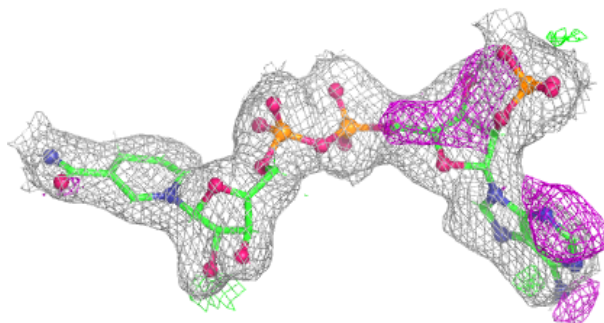
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



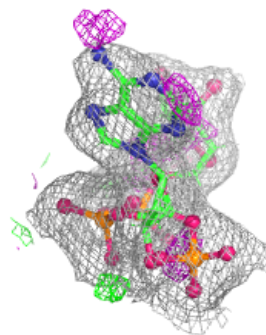
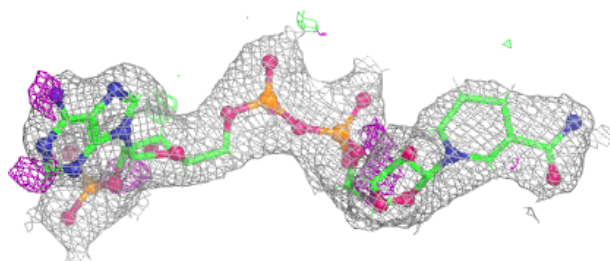
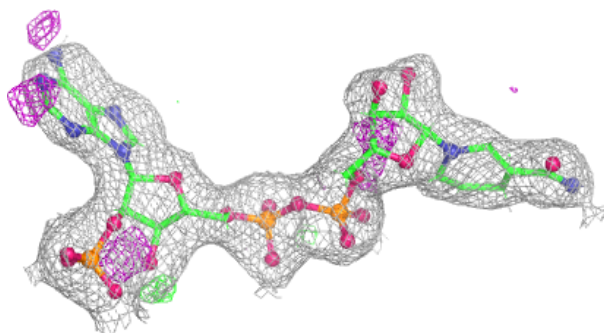


Electron density around NDP A 402:

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

**Electron density around NDP F 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.