



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:34 AM UTC

PDB ID : 7CS7 / pdb_00007cs7
Title : IiPLR1 with NADP⁺ and (+)secoisolariciresinol
Authors : Shao, K.; Zhang, P.
Deposited on : 2020-08-14
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

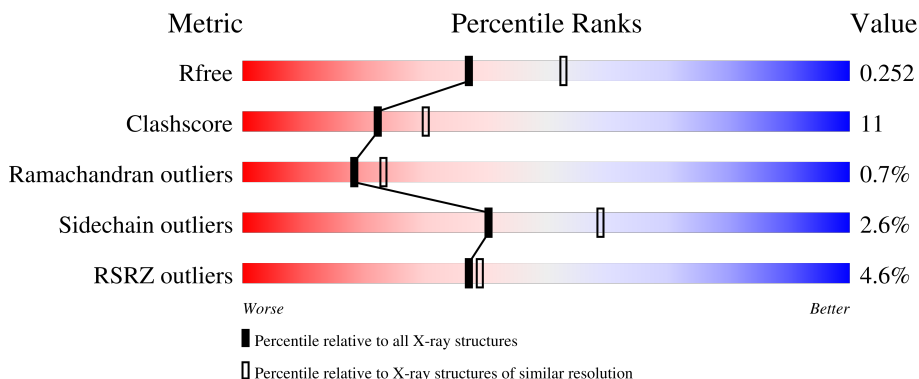
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



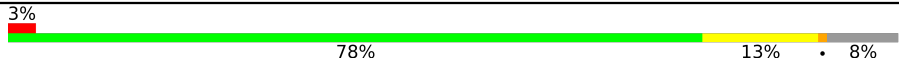
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	317	 3% 76% 11% • 10%
1	B	317	 9% 71% 18% • 9%
1	C	317	 3% 74% 14% • 10%
1	D	317	 3% 70% 19% • 11%
1	E	317	 3% 78% 11% • 10%

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Mol	Chain	Length	Quality of chain
1	F	317	 <p>3% 78% 13% 8%</p>

2 Entry composition [i](#)

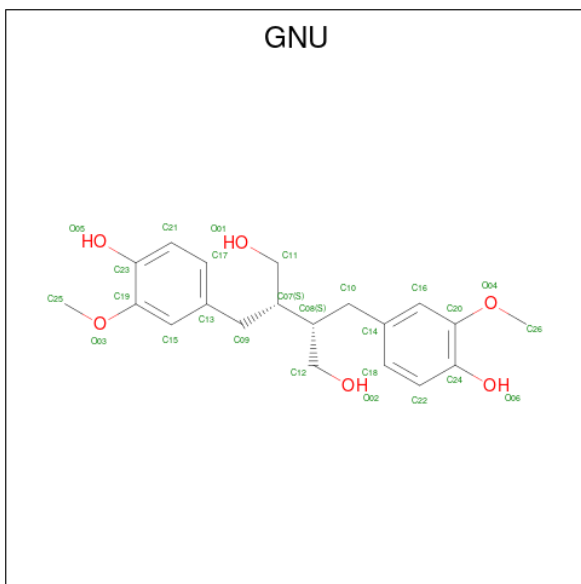
There are 4 unique types of molecules in this entry. The entry contains 15020 atoms, of which 312 are hydrogens and 0 are deuteriums.

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.

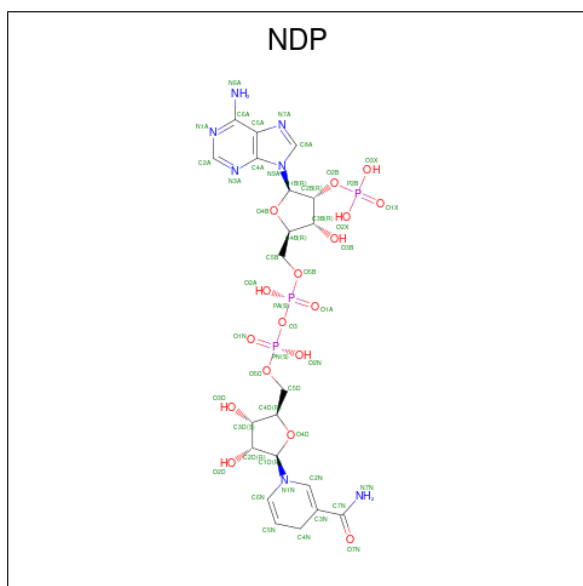
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	Total 2243	C 1426	N 379	O 429	S 9	0	0	0
1	B	287	Total 2263	C 1441	N 383	O 430	S 9	0	0	0
1	C	284	Total 2233	C 1420	N 376	O 428	S 9	0	0	0
1	D	283	Total 2229	C 1418	N 375	O 427	S 9	0	0	0
1	E	286	Total 2247	C 1428	N 380	O 430	S 9	0	0	0
1	F	293	Total 2308	C 1469	N 392	O 438	S 9	0	0	0

- Molecule 2 is (2S,3S)-2,3-bis[(3-methoxy-4-oxidanyl-phenyl)methyl]butane-1,4-diol (CCD ID: GNU) (formula: C₂₀H₂₆O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			52	20	26	6		
2	B	1	Total	C	H	O	0	0
			52	20	26	6		
2	C	1	Total	C	H	O	0	0
			52	20	26	6		
2	D	1	Total	C	H	O	0	0
			52	20	26	6		
2	E	1	Total	C	H	O	0	0
			52	20	26	6		
2	F	1	Total	C	H	O	0	0
			52	20	26	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	A	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	B	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		
3	D	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	E	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	F	1	74	21	26	7	17	3	0	0

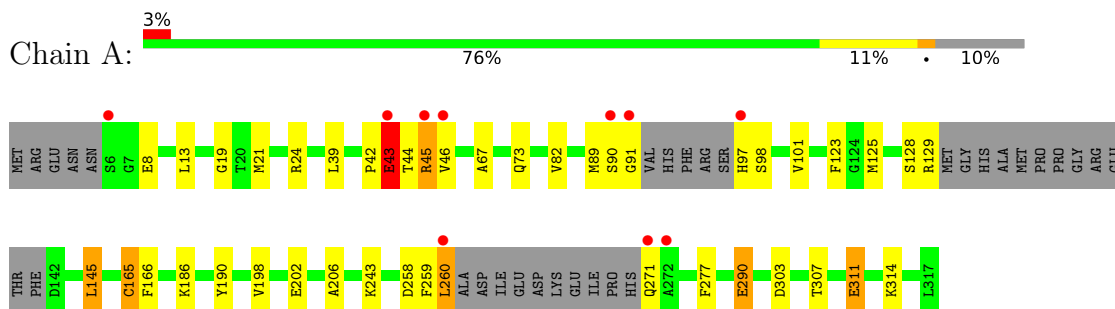
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	141	141	141	0	0
4	B	124	124	124	0	0
4	C	103	103	103	0	0
4	D	102	102	102	0	0
4	E	133	133	133	0	0
4	F	138	138	138	0	0

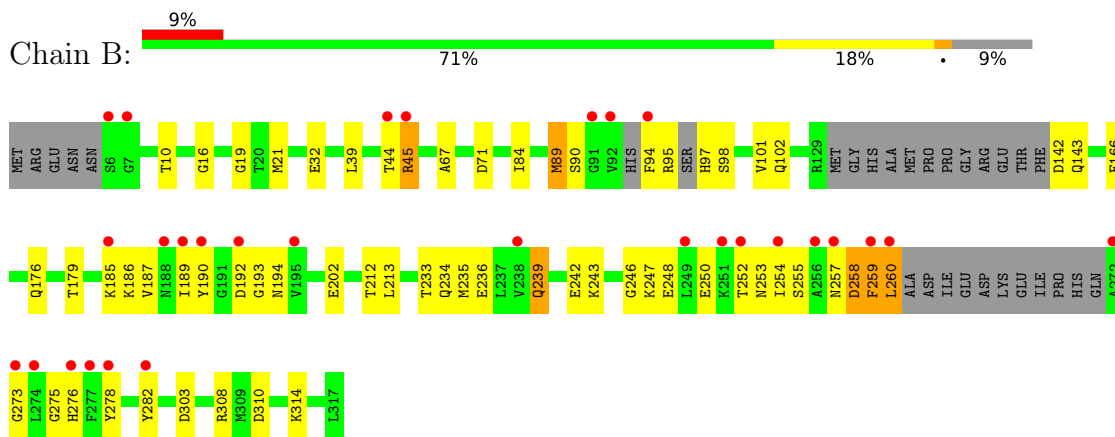
3 Residue-property plots [i](#)

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

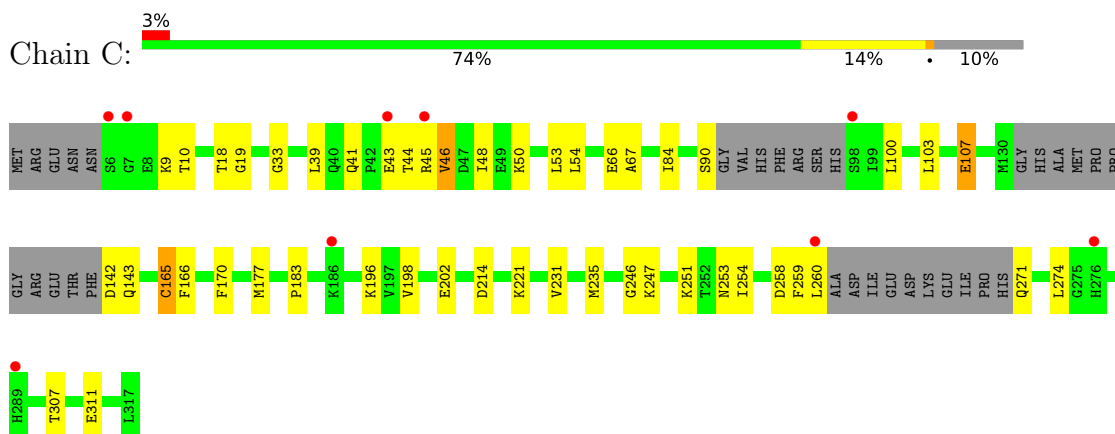
- Molecule 1: Pinoresinol-lariciresinol reductase



- Molecule 1: Pinoresinol-lariciresinol reductase

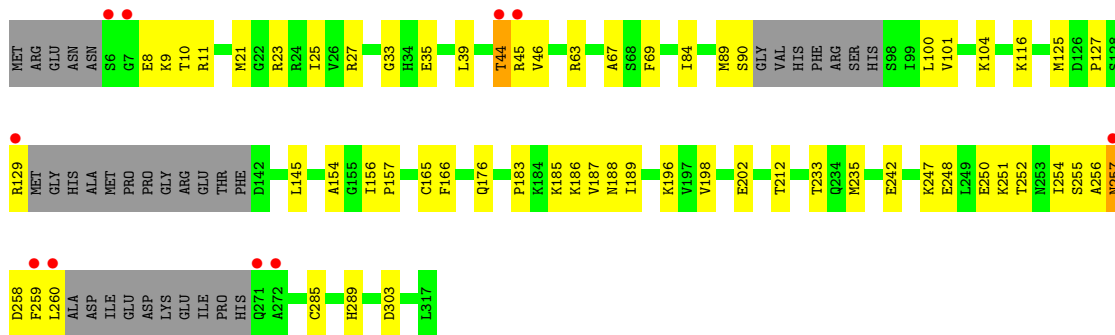


- Molecule 1: Pinoresinol-lariciresinol reductase



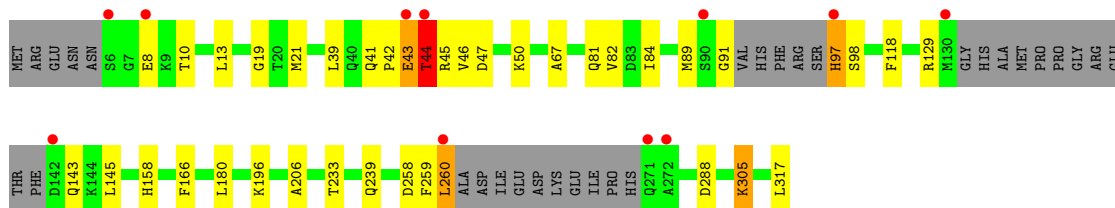
- Molecule 1: Pinoresinol-lariciresinol reductase

Chain D: 3% 70% 19% 11%



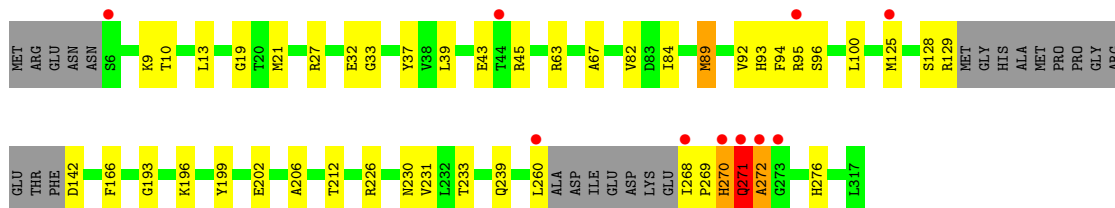
- Molecule 1: Pinoresinol-lariciresinol reductase

Chain E: 3% 78% 11% 10%



- Molecule 1: Pinoresinol-lariciresinol reductase

Chain F: 3% 78% 13% 8%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	243.61Å 243.61Å 76.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.25 – 2.30 32.25 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (32.25-2.30) 91.9 (32.25-2.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.197 , 0.252 0.198 , 0.252	Depositor DCC
R_{free} test set	1994 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtrriage
Anisotropy	0.540	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15020	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 31.31 % 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 1.1300e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNU, 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	0.36	0/2280	0.56	0/3079
1	B	0.33	0/2300	0.54	0/3104
1	C	0.33	0/2269	0.52	0/3064
1	D	0.32	0/2265	0.51	0/3059
1	E	0.36	0/2284	0.53	0/3084
1	F	0.36	0/2349	0.56	0/3175
All	All	0.34	0/13747	0.54	0/18565

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	A	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	HIS	Peptide
1	E	44	THR	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	2243	0	2248	38	0
1	B	2263	0	2270	67	0
1	C	2233	0	2239	45	0
1	D	2229	0	2238	53	0
1	E	2247	0	2249	41	0
1	F	2308	0	2312	40	0
2	A	26	26	0	0	0
2	B	26	26	0	0	0
2	C	26	26	0	1	0
2	D	26	26	0	2	0
2	E	26	26	0	1	0
2	F	26	26	0	2	0
3	A	48	26	25	9	0
3	B	48	26	26	6	0
3	C	48	26	25	7	0
3	D	48	26	24	12	0
3	E	48	26	25	6	0
3	F	48	26	23	2	0
4	A	141	0	0	7	0
4	B	124	0	0	11	0
4	C	103	0	0	9	0
4	D	102	0	0	4	0
4	E	133	0	0	7	0
4	F	138	0	0	8	0
All	All	14708	312	13704	294	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 11.

All (294) 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:D:402:NDP:O4D	3:D:402:NDP:C1D	1.64	1.27
3:E:402:NDP:O4D	3:E:402:NDP:C1D	1.63	1.13
1:C:19:GLY:HA3	3:C:402:NDP:H52A	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASP:N	4:B:501:HOH:O	1.97	0.97
1:F:268:ILE:HG22	1:F:269:PRO:HD3	1.48	0.93
1:C:39:LEU:HD11	1:C:67:ALA:HB3	1.50	0.92
1:A:42:PRO:HB2	1:A:45:ARG:HH22	1.34	0.91
1:F:239:GLN:NE2	4:F:502:HOH:O	2.05	0.89
1:E:260:LEU:HD13	1:E:260:LEU:H	1.39	0.85
1:A:91:GLY:O	4:A:501:HOH:O	1.94	0.83
1:F:270:HIS:HA	1:F:271:GLN:HB3	1.60	0.83
1:F:27:ARG:NH1	4:F:503:HOH:O	2.12	0.82
1:B:19:GLY:HA3	3:B:402:NDP:H52A	1.62	0.81
1:F:21:MET:CE	1:F:206:ALA:HB2	2.10	0.81
1:A:45:ARG:H	1:A:45:ARG:HD3	1.46	0.81
1:E:45:ARG:H	1:E:45:ARG:HD2	1.45	0.81
1:A:19:GLY:HA3	3:A:402:NDP:H52A	1.62	0.81
1:B:39:LEU:HD11	1:B:67:ALA:HB3	1.63	0.80
1:C:100:LEU:HD21	1:C:143:GLN:HG2	1.62	0.80
1:F:21:MET:HE1	1:F:206:ALA:HB2	1.63	0.80
1:B:233:THR:HG22	1:B:236:GLU:OE1	1.82	0.79
1:B:95:ARG:HA	1:B:143:GLN:CD	2.07	0.78
1:D:10:THR:HG21	1:D:84:ILE:HD12	1.65	0.78
1:B:258:ASP:OD1	4:B:502:HOH:O	2.02	0.77
1:E:91:GLY:O	4:E:501:HOH:O	2.02	0.77
1:B:257:ASN:N	4:B:502:HOH:O	2.17	0.75
1:B:185:LYS:NZ	1:B:250:GLU:OE2	2.19	0.75
1:A:73:GLN:OE1	4:A:502:HOH:O	2.05	0.75
1:C:44:THR:HG21	1:C:54:LEU:CD1	2.17	0.75
1:B:247:LYS:NZ	1:B:248:GLU:O	2.18	0.75
1:B:233:THR:HG23	1:B:236:GLU:H	1.51	0.74
1:F:202:GLU:OE2	4:F:501:HOH:O	2.04	0.74
1:C:44:THR:HG21	1:C:54:LEU:HD12	1.68	0.73
1:C:235:MET:HE1	1:C:251:LYS:HE2	1.71	0.73
1:A:260:LEU:HD22	1:A:260:LEU:H	1.53	0.71
1:F:93:HIS:ND1	1:F:271:GLN:O	2.24	0.71
1:C:45:ARG:NH2	4:C:501:HOH:O	1.95	0.70
1:A:202:GLU:OE2	4:A:503:HOH:O	2.09	0.69
1:C:260:LEU:H	1:C:260:LEU:HD22	1.58	0.69
1:A:42:PRO:O	1:A:44:THR:N	2.26	0.69
1:B:44:THR:HG23	1:B:45:ARG:HD3	1.74	0.69
1:C:271:GLN:HB2	1:C:274:LEU:HD12	1.75	0.69
1:D:8:GLU:OE2	1:D:8:GLU:HA	1.92	0.69
1:F:19:GLY:HA3	3:F:402:NDP:H52A	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:PRO:O	4:D:501:HOH:O	2.11	0.68
1:E:42:PRO:HD2	1:E:43:GLU:HG2	1.76	0.68
1:D:44:THR:HG22	1:D:45:ARG:HG3	1.75	0.68
1:E:39:LEU:HD11	1:E:67:ALA:HB3	1.73	0.68
1:B:44:THR:O	1:B:45:ARG:HG3	1.94	0.68
1:B:193:GLY:O	1:B:233:THR:OG1	2.11	0.68
1:E:305:LYS:NZ	4:E:505:HOH:O	2.25	0.68
1:D:185:LYS:NZ	1:D:250:GLU:OE1	2.27	0.67
1:F:271:GLN:HA	4:F:512:HOH:O	1.94	0.67
1:E:19:GLY:HA3	3:E:402:NDP:H52A	1.76	0.67
1:D:166:PHE:HB3	1:D:202:GLU:OE1	1.95	0.66
1:D:258:ASP:O	1:D:260:LEU:HD22	1.96	0.66
1:D:166:PHE:H	3:D:402:NDP:H72N	1.41	0.66
1:D:257:ASN:OD1	4:D:502:HOH:O	2.14	0.66
1:A:39:LEU:HD11	1:A:67:ALA:HB3	1.79	0.65
1:F:270:HIS:HA	1:F:271:GLN:CB	2.22	0.65
1:D:202:GLU:OE2	4:D:503:HOH:O	2.15	0.65
1:C:9:LYS:HD3	1:C:33:GLY:O	1.97	0.64
1:B:94:PHE:N	4:B:508:HOH:O	2.29	0.64
1:C:214:ASP:OD2	4:C:502:HOH:O	2.14	0.64
1:E:21:MET:CE	1:E:206:ALA:HB2	2.27	0.64
1:A:43:GLU:O	1:A:43:GLU:HG2	1.99	0.62
1:B:98:SER:O	1:B:101:VAL:HG12	1.98	0.62
1:C:165:CYS:HB2	1:C:198:VAL:O	1.99	0.62
1:A:43:GLU:O	1:A:43:GLU:CG	2.48	0.61
1:C:235:MET:HE1	1:C:251:LYS:CE	2.30	0.61
1:F:10:THR:HG21	1:F:84:ILE:HD12	1.81	0.61
1:D:39:LEU:HD11	1:D:67:ALA:HB3	1.81	0.61
1:B:275:GLY:N	4:B:505:HOH:O	2.24	0.61
1:E:44:THR:HG21	4:E:553:HOH:O	2.01	0.61
1:B:19:GLY:CA	3:B:402:NDP:H52A	2.31	0.60
1:D:9:LYS:HD2	1:D:33:GLY:O	2.01	0.60
1:C:196:LYS:HD2	1:C:231:VAL:HG12	1.82	0.60
1:E:97:HIS:N	1:E:143:GLN:HE22	2.00	0.60
1:B:202:GLU:CD	1:B:202:GLU:H	2.08	0.60
1:C:45:ARG:NH2	1:C:66:GLU:OE1	2.34	0.60
1:D:257:ASN:N	4:D:502:HOH:O	2.35	0.60
1:E:258:ASP:O	1:E:260:LEU:N	2.35	0.60
1:F:94:PHE:HZ	1:F:125:MET:HE1	1.67	0.59
1:B:254:ILE:HG23	1:B:258:ASP:HB2	1.84	0.59
1:D:186:LYS:HE2	1:D:252:THR:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PHE:O	3:A:402:NDP:H2N	2.01	0.59
1:C:100:LEU:HD21	1:C:143:GLN:CG	2.32	0.59
1:B:186:LYS:HG2	1:B:250:GLU:HB3	1.84	0.59
1:A:165:CYS:HB2	1:A:198:VAL:O	2.03	0.59
1:E:41:GLN:OE1	4:E:502:HOH:O	2.16	0.58
1:B:90:SER:OG	3:B:402:NDP:H8A	2.03	0.58
1:C:246:GLY:C	1:C:247:LYS:HD2	2.28	0.58
1:C:170:PHE:HE2	3:C:402:NDP:N7N	2.01	0.58
1:B:190:TYR:HD2	1:B:234:GLN:OE1	1.86	0.58
1:C:221:LYS:NZ	4:C:504:HOH:O	2.19	0.58
1:F:94:PHE:HB3	1:F:142:ASP:HB3	1.86	0.58
1:B:278:TYR:CD1	1:B:282:TYR:HB2	2.39	0.57
1:E:10:THR:HG21	1:E:84:ILE:HD12	1.87	0.57
1:B:242:GLU:HG2	1:B:247:LYS:O	2.05	0.57
1:C:18:THR:OG1	3:C:402:NDP:O1X	2.08	0.57
1:F:43:GLU:HG2	4:F:623:HOH:O	2.05	0.57
3:A:402:NDP:O1X	3:A:402:NDP:O3B	2.23	0.57
1:D:35:GLU:OE2	1:D:63:ARG:NH1	2.38	0.57
1:B:16:GLY:N	4:B:514:HOH:O	2.39	0.56
1:C:10:THR:HG21	1:C:84:ILE:HD12	1.87	0.56
1:D:186:LYS:HE2	1:D:252:THR:CB	2.34	0.56
1:F:92:VAL:O	2:F:401:GNU:O01	2.24	0.56
1:A:307:THR:HG23	1:A:311:GLU:HG2	1.88	0.56
1:C:271:GLN:NE2	4:C:511:HOH:O	2.39	0.56
1:B:314:LYS:NZ	4:B:512:HOH:O	2.36	0.55
1:F:271:GLN:O	1:F:272:ALA:HB3	2.06	0.55
1:A:166:PHE:H	3:A:402:NDP:H72N	1.54	0.55
1:E:45:ARG:H	1:E:45:ARG:CD	2.19	0.55
1:E:44:THR:OG1	1:E:46:VAL:HG22	2.07	0.55
1:D:129:ARG:HH12	1:D:289:HIS:CD2	2.23	0.55
1:D:196:LYS:HD3	1:D:233:THR:HG23	1.89	0.55
1:E:97:HIS:N	4:E:510:HOH:O	2.40	0.55
1:D:255:SER:HB3	1:D:258:ASP:OD2	2.07	0.54
1:F:196:LYS:HE2	1:F:233:THR:HG23	1.88	0.54
1:B:254:ILE:CG2	1:B:258:ASP:HB2	2.37	0.54
1:C:177:MET:HE1	1:C:274:LEU:CD2	2.37	0.54
1:F:125:MET:HE2	1:F:276:HIS:CD2	2.42	0.54
1:F:268:ILE:CG2	1:F:269:PRO:HD3	2.29	0.54
1:C:66:GLU:HG2	4:C:501:HOH:O	2.06	0.54
1:C:166:PHE:CD1	3:C:402:NDP:H41N	2.42	0.54
1:E:41:GLN:HB3	1:E:43:GLU:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ASN:C	1:C:254:ILE:HD12	2.33	0.54
1:A:13:LEU:HB2	1:A:82:VAL:HG11	1.90	0.53
1:B:95:ARG:O	1:B:143:GLN:NE2	2.42	0.53
1:F:269:PRO:O	1:F:270:HIS:CB	2.56	0.53
1:B:278:TYR:HD1	1:B:282:TYR:HB2	1.73	0.53
1:B:258:ASP:O	1:B:260:LEU:HD13	2.08	0.53
1:D:89:MET:O	3:D:402:NDP:H52N	2.07	0.53
1:B:189:ILE:O	1:B:253:ASN:HA	2.09	0.53
1:C:177:MET:HE1	1:C:274:LEU:HD21	1.90	0.53
1:D:166:PHE:HB2	3:D:402:NDP:N7N	2.24	0.53
1:B:176:GLN:NE2	1:B:187:VAL:HG23	2.24	0.53
1:D:90:SER:HA	3:D:402:NDP:PA	2.48	0.53
1:B:44:THR:HG22	4:B:510:HOH:O	2.08	0.52
1:C:166:PHE:HB3	1:C:202:GLU:OE2	2.09	0.52
1:D:186:LYS:HE2	1:D:252:THR:OG1	2.09	0.52
1:E:129:ARG:NH2	1:E:288:ASP:OD2	2.42	0.52
1:A:42:PRO:HB2	1:A:45:ARG:NH2	2.16	0.51
1:D:89:MET:HE2	1:D:101:VAL:CG1	2.40	0.51
1:F:226:ARG:NH1	4:F:504:HOH:O	2.27	0.51
1:E:89:MET:O	3:E:402:NDP:H52N	2.11	0.51
1:A:190:TYR:CE2	1:A:277:PHE:HE2	2.29	0.51
1:E:196:LYS:HE3	1:E:233:THR:HG23	1.93	0.51
1:E:260:LEU:H	1:E:260:LEU:CD1	2.18	0.51
1:F:32:GLU:HG3	4:F:515:HOH:O	2.11	0.51
1:C:183:PRO:O	4:C:503:HOH:O	2.19	0.50
1:B:44:THR:C	1:B:45:ARG:HG3	2.35	0.50
1:B:190:TYR:CD2	1:B:234:GLN:OE1	2.64	0.50
1:C:142:ASP:N	4:C:516:HOH:O	2.44	0.50
1:D:89:MET:HE2	1:D:101:VAL:HG11	1.92	0.50
1:D:23:ARG:O	1:D:27:ARG:HG3	2.12	0.50
1:B:166:PHE:H	3:B:402:NDP:H72N	1.60	0.49
1:D:69:PHE:O	1:D:104:LYS:HD3	2.12	0.49
1:E:47:ASP:OD2	1:E:50:LYS:HD2	2.11	0.49
1:E:42:PRO:O	1:E:43:GLU:C	2.56	0.49
1:E:239:GLN:OE1	4:E:503:HOH:O	2.20	0.49
1:D:166:PHE:N	3:D:402:NDP:H72N	2.09	0.49
2:C:401:GNU:C09	3:C:402:NDP:H42N	2.43	0.49
1:A:89:MET:O	3:A:402:NDP:H52N	2.12	0.49
1:B:89:MET:HE1	1:B:102:GLN:CG	2.43	0.49
1:D:254:ILE:HD12	1:D:254:ILE:N	2.27	0.49
1:A:166:PHE:CD1	3:A:402:NDP:C7N	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:SER:HB2	1:B:258:ASP:OD1	2.12	0.49
1:F:270:HIS:N	4:F:512:HOH:O	2.39	0.49
1:B:273:GLY:HA2	4:B:554:HOH:O	2.12	0.48
1:B:239:GLN:NE2	4:B:516:HOH:O	2.43	0.48
1:D:189:ILE:HD12	1:D:235:MET:CE	2.43	0.48
1:C:45:ARG:NH1	4:C:501:HOH:O	2.43	0.48
1:D:166:PHE:CD2	3:D:402:NDP:C7N	2.96	0.48
1:A:45:ARG:O	1:A:46:VAL:C	2.56	0.48
1:F:94:PHE:CZ	1:F:125:MET:HE1	2.46	0.48
1:D:165:CYS:HB2	1:D:198:VAL:O	2.13	0.48
1:B:21:MET:HE3	1:B:166:PHE:CZ	2.49	0.48
1:B:192:ASP:OD1	1:B:192:ASP:O	2.31	0.48
1:F:271:GLN:O	1:F:272:ALA:CB	2.62	0.48
1:F:13:LEU:HB2	1:F:82:VAL:HG11	1.96	0.48
1:D:11:ARG:HG2	1:D:35:GLU:HB3	1.95	0.47
1:C:271:GLN:N	4:C:511:HOH:O	2.47	0.47
1:E:45:ARG:CD	1:E:45:ARG:N	2.77	0.47
1:A:44:THR:O	1:A:46:VAL:N	2.48	0.47
1:F:93:HIS:HB2	1:F:95:ARG:O	2.15	0.47
1:D:176:GLN:CD	1:D:187:VAL:HG23	2.39	0.47
1:C:103:LEU:O	1:C:107:GLU:HG2	2.15	0.47
1:C:170:PHE:HE2	3:C:402:NDP:H71N	1.62	0.47
1:C:254:ILE:HD12	1:C:254:ILE:N	2.30	0.47
1:A:98:SER:O	1:A:101:VAL:HB	2.15	0.47
1:F:39:LEU:HD11	1:F:67:ALA:HB3	1.97	0.47
1:A:258:ASP:O	1:A:260:LEU:HD13	2.15	0.46
1:B:166:PHE:CD2	3:B:402:NDP:H41N	2.50	0.46
1:C:41:GLN:O	1:C:44:THR:HB	2.14	0.46
1:C:46:VAL:O	1:C:46:VAL:HG13	2.14	0.46
1:D:89:MET:O	3:D:402:NDP:H3D	2.16	0.46
1:B:89:MET:HE2	1:B:89:MET:H	1.81	0.46
1:B:235:MET:SD	1:B:239:GLN:OE1	2.74	0.46
1:D:154:ALA:HB3	1:D:156:ILE:HD12	1.97	0.46
1:A:290:GLU:HG3	4:A:504:HOH:O	2.15	0.46
1:C:258:ASP:O	1:C:260:LEU:N	2.48	0.46
1:A:259:PHE:O	1:A:260:LEU:C	2.58	0.46
1:D:188:ASN:OD1	1:D:254:ILE:HD11	2.16	0.46
1:A:128:SER:HA	1:A:145:LEU:HD11	1.97	0.46
1:B:303:ASP:OD1	1:B:303:ASP:N	2.47	0.46
1:C:254:ILE:HG23	1:C:258:ASP:HB2	1.97	0.46
1:E:97:HIS:CG	1:E:98:SER:H	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:GLU:H	1:E:43:GLU:CD	2.22	0.46
1:A:303:ASP:OD1	1:A:303:ASP:N	2.43	0.46
1:A:90:SER:HA	3:A:402:NDP:O3	2.15	0.45
1:B:10:THR:HG21	1:B:84:ILE:HD12	1.99	0.45
1:B:97:HIS:HA	1:B:143:GLN:HE22	1.81	0.45
1:F:128:SER:O	1:F:129:ARG:HB3	2.16	0.45
1:C:166:PHE:CD2	3:C:402:NDP:O7N	2.70	0.45
1:E:81:GLN:NE2	4:E:504:HOH:O	2.21	0.45
1:E:97:HIS:N	1:E:97:HIS:HD1	2.14	0.45
1:B:258:ASP:OD1	1:B:258:ASP:N	2.49	0.45
1:D:21:MET:HE2	1:D:25:ILE:HD11	1.99	0.45
1:D:89:MET:O	1:D:90:SER:C	2.60	0.45
1:B:194:ASN:HA	1:B:233:THR:OG1	2.17	0.45
1:D:90:SER:OG	3:D:402:NDP:H8A	2.17	0.45
1:E:44:THR:OG1	1:E:46:VAL:CG2	2.64	0.45
1:C:45:ARG:HG3	1:C:45:ARG:HH11	1.82	0.44
1:D:303:ASP:OD2	1:D:303:ASP:N	2.50	0.44
1:A:166:PHE:CD2	3:A:402:NDP:H41N	2.52	0.44
1:F:89:MET:HE3	1:F:89:MET:HB3	1.40	0.44
1:F:100:LEU:HD23	1:F:100:LEU:HA	1.75	0.44
1:A:314:LYS:NZ	4:A:520:HOH:O	2.50	0.44
3:D:402:NDP:O5D	3:D:402:NDP:H6N	2.17	0.44
1:D:116:LYS:O	1:D:157:PRO:HG2	2.18	0.44
1:B:243:LYS:HA	1:B:243:LYS:HD2	1.76	0.44
1:D:90:SER:HA	3:D:402:NDP:O3	2.18	0.44
1:E:145:LEU:HD12	1:E:145:LEU:HA	1.82	0.44
1:A:21:MET:CE	1:A:206:ALA:HB2	2.47	0.44
1:B:190:TYR:HD1	1:B:259:PHE:CE1	2.36	0.44
1:B:194:ASN:O	1:B:194:ASN:OD1	2.36	0.44
1:C:307:THR:HG23	1:C:311:GLU:HG2	1.99	0.44
1:A:24:ARG:NH1	4:A:522:HOH:O	2.51	0.43
1:F:202:GLU:CD	1:F:202:GLU:H	2.27	0.43
2:F:401:GNU:O02	2:F:401:GNU:C11	2.67	0.43
1:F:37:TYR:CE2	1:F:63:ARG:HD2	2.54	0.43
1:B:84:ILE:HD13	1:B:213:LEU:O	2.18	0.43
1:D:125:MET:HE3	1:D:285:CYS:SG	2.58	0.43
1:D:196:LYS:HD3	1:D:233:THR:CG2	2.49	0.43
1:F:268:ILE:N	1:F:269:PRO:CD	2.81	0.43
1:B:260:LEU:HD13	1:B:260:LEU:N	2.34	0.42
1:A:43:GLU:HA	1:A:45:ARG:NE	2.35	0.42
1:A:186:LYS:HE2	1:A:186:LYS:HB2	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:TYR:O	1:F:230:ASN:HB3	2.20	0.42
1:B:308:ARG:HB2	1:B:310:ASP:OD1	2.20	0.42
2:D:401:GNU:O01	2:D:401:GNU:C13	2.67	0.42
3:D:402:NDP:O3B	3:D:402:NDP:P2B	2.78	0.42
1:A:125:MET:HE3	1:A:125:MET:HB2	1.98	0.42
1:B:260:LEU:HD22	1:B:260:LEU:H	1.84	0.42
1:D:44:THR:C	1:D:45:ARG:HG3	2.45	0.42
1:B:89:MET:HE1	1:B:102:GLN:HG3	2.01	0.42
1:E:43:GLU:O	1:E:44:THR:C	2.62	0.42
1:E:44:THR:C	1:E:46:VAL:H	2.28	0.42
1:E:97:HIS:N	1:E:143:GLN:NE2	2.67	0.42
1:D:145:LEU:HD12	1:D:145:LEU:HA	1.92	0.42
1:E:13:LEU:HB2	1:E:82:VAL:HG11	2.02	0.42
1:B:166:PHE:CD1	3:B:402:NDP:C7N	3.03	0.41
1:B:252:THR:O	1:B:252:THR:HG22	2.20	0.41
1:C:90:SER:O	1:C:90:SER:OG	2.21	0.41
1:C:246:GLY:O	1:C:247:LYS:HD2	2.19	0.41
1:F:193:GLY:O	1:F:233:THR:HB	2.20	0.41
1:B:254:ILE:HG23	1:B:258:ASP:CB	2.49	0.41
1:B:255:SER:HB2	4:B:502:HOH:O	2.19	0.41
1:B:242:GLU:O	1:B:246:GLY:N	2.49	0.41
1:E:166:PHE:CD2	3:E:402:NDP:H41N	2.55	0.41
1:F:196:LYS:HD2	1:F:231:VAL:HG12	2.03	0.41
1:B:190:TYR:O	1:B:193:GLY:N	2.53	0.41
1:B:95:ARG:HA	1:B:143:GLN:OE1	2.19	0.41
1:F:9:LYS:HG2	1:F:33:GLY:O	2.20	0.41
1:F:166:PHE:CD2	3:F:402:NDP:H41N	2.55	0.41
1:D:46:VAL:HG13	1:E:180:LEU:HD21	2.02	0.41
1:D:255:SER:OG	1:D:256:ALA:N	2.53	0.41
1:A:44:THR:O	1:A:45:ARG:C	2.64	0.41
3:A:402:NDP:HO3A	3:A:402:NDP:P2B	2.43	0.41
1:D:248:GLU:HG3	1:D:251:LYS:HZ1	1.86	0.41
2:E:401:GNU:C09	3:E:402:NDP:H42N	2.51	0.41
1:B:89:MET:HB2	1:B:89:MET:HE3	1.27	0.41
1:D:242:GLU:HG2	1:D:247:LYS:O	2.21	0.40
1:E:118:PHE:O	1:E:158:HIS:HA	2.21	0.40
1:E:317:LEU:HA	1:E:317:LEU:HD23	1.86	0.40
1:C:44:THR:HG21	1:C:54:LEU:HD11	1.99	0.40
1:D:189:ILE:HD12	1:D:235:MET:HE1	2.02	0.40
2:D:401:GNU:O01	2:D:401:GNU:C15	2.69	0.40
1:E:21:MET:HE1	1:E:206:ALA:HB2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LYS:HE3	4:A:629:HOH:O	2.21	0.40
1:B:71:ASP:OD1	1:B:71:ASP:C	2.64	0.40
1:D:127:PRO:C	1:D:129:ARG:H	2.30	0.40
1:E:166:PHE:CD1	3:E:402:NDP:C7N	3.04	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	277/317 (87%)	267 (96%)	8 (3%)	2 (1%)	18 23
1	B	277/317 (87%)	267 (96%)	9 (3%)	1 (0%)	30 38
1	C	276/317 (87%)	268 (97%)	7 (2%)	1 (0%)	30 38
1	D	275/317 (87%)	265 (96%)	9 (3%)	1 (0%)	30 38
1	E	278/317 (88%)	269 (97%)	6 (2%)	3 (1%)	11 13
1	F	287/317 (90%)	274 (96%)	9 (3%)	4 (1%)	9 9
All	All	1670/1902 (88%)	1610 (96%)	48 (3%)	12 (1%)	18 23

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	45	ARG
1	F	270	HIS
1	C	259	PHE
1	E	43	GLU
1	E	259	PHE
1	E	44	THR
1	F	271	GLN

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Mol	Chain	Res	Type
1	F	272	ALA
1	D	259	PHE
1	B	259	PHE
1	F	45	ARG

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	243/271 (90%)	234 (96%)	9 (4%)	30	45
1	B	245/271 (90%)	236 (96%)	9 (4%)	30	45
1	C	242/271 (89%)	235 (97%)	7 (3%)	37	55
1	D	242/271 (89%)	238 (98%)	4 (2%)	53	72
1	E	243/271 (90%)	239 (98%)	4 (2%)	55	73
1	F	250/271 (92%)	245 (98%)	5 (2%)	48	67
All	All	1465/1626 (90%)	1427 (97%)	38 (3%)	40	59

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	43	GLU
1	A	129	ARG
1	A	145	LEU
1	A	165	CYS
1	A	260	LEU
1	A	271	GLN
1	A	290	GLU
1	A	311	GLU
1	B	32	GLU
1	B	45	ARG
1	B	89	MET
1	B	179	THR
1	B	212	THR

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Mol	Chain	Res	Type
1	B	239	GLN
1	B	258	ASP
1	B	260	LEU
1	B	276	HIS
1	C	43	GLU
1	C	46	VAL
1	C	48	ILE
1	C	50	LYS
1	C	53	LEU
1	C	107	GLU
1	C	165	CYS
1	D	44	THR
1	D	100	LEU
1	D	212	THR
1	D	257	ASN
1	E	8	GLU
1	E	97	HIS
1	E	260	LEU
1	E	305	LYS
1	F	89	MET
1	F	96	SER
1	F	212	THR
1	F	260	LEU
1	F	271	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	41	GLN
1	A	97	HIS
1	B	81	GLN
1	B	194	ASN
1	C	52	GLN
1	C	73	GLN
1	C	239	GLN
1	D	40	GLN
1	D	41	GLN
1	E	41	GLN
1	E	239	GLN
1	F	40	GLN
1	F	271	GLN

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
3	NDP	C	402	-	51,52,52	3.84	25 (49%)	71,80,80	1.95	12 (16%)
2	GNU	C	401	-	27,27,27	1.07	2 (7%)	32,36,36	0.95	2 (6%)
3	NDP	B	402	-	51,52,52	3.53	23 (45%)	71,80,80	1.90	14 (19%)
3	NDP	F	402	-	51,52,52	3.51	22 (43%)	71,80,80	1.97	16 (22%)
2	GNU	B	401	-	27,27,27	1.06	3 (11%)	32,36,36	1.05	2 (6%)
2	GNU	D	401	-	27,27,27	1.27	2 (7%)	32,36,36	1.37	5 (15%)
2	GNU	E	401	-	27,27,27	1.19	3 (11%)	32,36,36	1.24	3 (9%)
3	NDP	E	402	-	51,52,52	3.71	22 (43%)	71,80,80	1.86	12 (16%)
3	NDP	A	402	-	51,52,52	3.73	24 (47%)	71,80,80	1.89	12 (16%)
3	NDP	D	402	-	51,52,52	3.77	23 (45%)	71,80,80	1.90	15 (21%)
2	GNU	A	401	-	27,27,27	1.00	3 (11%)	32,36,36	1.35	5 (15%)
2	GNU	F	401	-	27,27,27	1.16	3 (11%)	32,36,36	1.51	3 (9%)

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	C	402	-	-	8/34/77/77	0/5/5/5
2	GNU	C	401	-	-	4/20/20/20	0/2/2/2
3	NDP	B	402	-	-	4/34/77/77	0/5/5/5
3	NDP	F	402	-	-	6/34/77/77	0/5/5/5
2	GNU	B	401	-	-	4/20/20/20	0/2/2/2
2	GNU	D	401	-	-	4/20/20/20	0/2/2/2
2	GNU	E	401	-	-	8/20/20/20	0/2/2/2
3	NDP	E	402	-	-	2/34/77/77	0/5/5/5
3	NDP	A	402	-	-	6/34/77/77	0/5/5/5
3	NDP	D	402	-	-	10/34/77/77	0/5/5/5
2	GNU	A	401	-	-	0/20/20/20	0/2/2/2
2	GNU	F	401	-	-	5/20/20/20	0/2/2/2

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	NDP	O4D-C1D	9.50	1.64	1.42
3	E	402	NDP	O4D-C1D	9.37	1.63	1.42
3	A	402	NDP	O4D-C1D	9.19	1.63	1.42
3	C	402	NDP	O4D-C1D	9.15	1.63	1.42
3	C	402	NDP	C2B-C1B	-9.03	1.30	1.53
3	C	402	NDP	O4B-C1B	8.98	1.62	1.42
3	D	402	NDP	O4B-C1B	8.96	1.62	1.42
3	E	402	NDP	O4B-C1B	8.94	1.62	1.42
3	B	402	NDP	C2B-C1B	-8.71	1.31	1.53
3	E	402	NDP	C2B-C1B	-8.66	1.31	1.53
3	F	402	NDP	O4D-C1D	8.54	1.61	1.42
3	D	402	NDP	C2B-C1B	-8.52	1.32	1.53
3	A	402	NDP	O4B-C1B	8.49	1.61	1.42
3	B	402	NDP	O4D-C1D	8.48	1.61	1.42
3	F	402	NDP	O4B-C1B	8.26	1.61	1.42
3	A	402	NDP	C2B-C1B	-8.25	1.32	1.53
3	F	402	NDP	C2B-C1B	-8.12	1.33	1.53
3	B	402	NDP	O4B-C1B	8.01	1.60	1.42
3	C	402	NDP	PA-O3	7.89	1.68	1.59
3	C	402	NDP	PN-O3	7.84	1.68	1.59
3	D	402	NDP	PA-O3	7.70	1.67	1.59
3	A	402	NDP	PA-O3	7.68	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	NDP	C6N-C5N	7.41	1.55	1.33
3	A	402	NDP	PN-O3	7.37	1.67	1.59
3	C	402	NDP	C6N-C5N	7.35	1.55	1.33
3	D	402	NDP	C6N-C5N	7.23	1.55	1.33
3	A	402	NDP	C6N-C5N	7.21	1.55	1.33
3	B	402	NDP	C6N-C5N	7.18	1.55	1.33
3	E	402	NDP	PA-O3	7.05	1.67	1.59
3	F	402	NDP	C2D-C1D	-7.03	1.31	1.53
3	D	402	NDP	PN-O3	6.98	1.67	1.59
3	E	402	NDP	C2D-C1D	-6.97	1.31	1.53
3	F	402	NDP	C6N-C5N	6.82	1.54	1.33
3	A	402	NDP	C2D-C1D	-6.80	1.32	1.53
3	C	402	NDP	C2D-C1D	-6.79	1.32	1.53
3	B	402	NDP	C2D-C1D	-6.77	1.32	1.53
3	D	402	NDP	C2D-C1D	-6.75	1.32	1.53
3	F	402	NDP	O4B-C4B	-6.57	1.30	1.45
3	B	402	NDP	O4B-C4B	-6.48	1.30	1.45
3	A	402	NDP	O4B-C4B	-6.35	1.30	1.45
3	E	402	NDP	PN-O3	6.23	1.66	1.59
3	E	402	NDP	O4B-C4B	-6.21	1.31	1.45
3	E	402	NDP	O4D-C4D	-6.18	1.31	1.45
3	C	402	NDP	O4D-C4D	-6.17	1.31	1.45
3	B	402	NDP	O4D-C4D	-6.16	1.31	1.45
3	F	402	NDP	O4D-C4D	-6.15	1.31	1.45
3	D	402	NDP	O4D-C4D	-6.14	1.31	1.45
3	A	402	NDP	O4D-C4D	-6.12	1.31	1.45
3	C	402	NDP	O4B-C4B	-6.11	1.31	1.45
3	C	402	NDP	C2N-C3N	6.08	1.51	1.35
3	D	402	NDP	C2N-C3N	6.07	1.51	1.35
3	F	402	NDP	PA-O3	5.91	1.65	1.59
3	A	402	NDP	C2N-C3N	5.87	1.51	1.35
3	B	402	NDP	PN-O3	5.87	1.65	1.59
3	D	402	NDP	O4B-C4B	-5.76	1.32	1.45
3	E	402	NDP	C2N-C3N	5.68	1.50	1.35
3	B	402	NDP	C2N-C3N	5.64	1.50	1.35
3	D	402	NDP	C6A-N6A	5.57	1.48	1.34
3	F	402	NDP	C2N-C3N	5.56	1.50	1.35
3	C	402	NDP	C6A-N6A	5.44	1.48	1.34
3	B	402	NDP	PA-O3	5.38	1.65	1.59
3	F	402	NDP	PN-O3	5.37	1.65	1.59
3	E	402	NDP	C6A-N6A	5.18	1.47	1.34
3	B	402	NDP	C6A-N6A	5.13	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402	NDP	C6A-N6A	5.04	1.47	1.34
3	A	402	NDP	C6A-N6A	4.94	1.46	1.34
3	E	402	NDP	C7N-N7N	4.19	1.45	1.33
3	D	402	NDP	C7N-N7N	4.15	1.45	1.33
3	A	402	NDP	C7N-N7N	4.09	1.45	1.33
3	B	402	NDP	C7N-N7N	4.03	1.45	1.33
3	C	402	NDP	C7N-N7N	4.02	1.45	1.33
3	F	402	NDP	C7N-N7N	3.83	1.44	1.33
3	D	402	NDP	C6N-N1N	3.39	1.45	1.37
3	A	402	NDP	P2B-O2B	3.33	1.65	1.59
3	C	402	NDP	C6N-N1N	3.31	1.45	1.37
3	C	402	NDP	C4N-C5N	3.30	1.57	1.49
3	E	402	NDP	O2D-C2D	3.28	1.51	1.43
3	D	402	NDP	C4N-C5N	3.26	1.57	1.49
3	D	402	NDP	O2D-C2D	3.22	1.50	1.43
3	E	402	NDP	C6N-N1N	3.17	1.44	1.37
3	A	402	NDP	O2D-C2D	3.15	1.50	1.43
3	B	402	NDP	O2D-C2D	3.14	1.50	1.43
3	A	402	NDP	C6N-N1N	3.13	1.44	1.37
3	C	402	NDP	C4N-C3N	3.11	1.55	1.50
3	E	402	NDP	C4N-C5N	3.11	1.57	1.49
2	D	401	GNU	O03-C19	3.10	1.42	1.37
3	F	402	NDP	O2D-C2D	3.09	1.50	1.43
3	A	402	NDP	C4N-C5N	3.09	1.57	1.49
3	C	402	NDP	O2D-C2D	3.07	1.50	1.43
3	D	402	NDP	P2B-O2B	3.03	1.64	1.59
2	C	401	GNU	O04-C20	2.97	1.42	1.37
3	B	402	NDP	C4N-C5N	2.95	1.56	1.49
3	A	402	NDP	C7N-C3N	2.93	1.55	1.48
3	C	402	NDP	C7N-C3N	2.93	1.55	1.48
3	A	402	NDP	C4N-C3N	2.89	1.55	1.50
3	B	402	NDP	C6N-N1N	2.80	1.44	1.37
3	F	402	NDP	O3B-C3B	-2.79	1.36	1.43
2	E	401	GNU	O03-C19	2.76	1.41	1.37
3	E	402	NDP	C7N-C3N	2.73	1.54	1.48
2	D	401	GNU	O04-C20	2.72	1.41	1.37
3	B	402	NDP	C4N-C3N	2.67	1.55	1.50
3	B	402	NDP	C5A-C4A	-2.67	1.34	1.39
3	C	402	NDP	O3D-C3D	-2.66	1.36	1.43
3	D	402	NDP	O3B-C3B	-2.65	1.36	1.43
3	F	402	NDP	O3D-C3D	-2.63	1.36	1.43
3	A	402	NDP	O3D-C3D	-2.62	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	GNU	O03-C19	2.62	1.41	1.37
3	F	402	NDP	C6N-N1N	2.58	1.43	1.37
3	F	402	NDP	C5A-C4A	-2.58	1.34	1.39
2	B	401	GNU	O04-C20	2.55	1.41	1.37
3	D	402	NDP	C4N-C3N	2.54	1.54	1.50
3	E	402	NDP	C4N-C3N	2.54	1.54	1.50
3	F	402	NDP	C4N-C5N	2.53	1.55	1.49
3	E	402	NDP	O3B-C3B	-2.51	1.36	1.43
3	F	402	NDP	C4N-C3N	2.51	1.54	1.50
3	D	402	NDP	O3D-C3D	-2.50	1.36	1.43
3	F	402	NDP	C8A-N9A	-2.50	1.33	1.37
3	D	402	NDP	C7N-C3N	2.49	1.54	1.48
3	F	402	NDP	P2B-O2B	2.46	1.63	1.59
2	A	401	GNU	O04-C20	2.46	1.41	1.37
2	A	401	GNU	O03-C19	2.44	1.41	1.37
2	E	401	GNU	O05-C23	2.44	1.41	1.36
3	F	402	NDP	C5A-N7A	-2.42	1.34	1.39
2	B	401	GNU	O05-C23	2.42	1.41	1.36
3	E	402	NDP	P2B-O2B	2.41	1.63	1.59
3	B	402	NDP	C8A-N9A	-2.40	1.33	1.37
3	B	402	NDP	C5A-N7A	-2.39	1.34	1.39
3	C	402	NDP	PN-O5D	2.39	1.68	1.59
3	B	402	NDP	O3D-C3D	-2.37	1.37	1.43
3	D	402	NDP	O7N-C7N	-2.36	1.18	1.24
3	E	402	NDP	O3D-C3D	-2.36	1.37	1.43
2	F	401	GNU	O05-C23	2.30	1.41	1.36
3	C	402	NDP	O3B-C3B	-2.30	1.37	1.43
3	B	402	NDP	C7N-C3N	2.29	1.53	1.48
2	B	401	GNU	O06-C24	2.29	1.40	1.36
3	C	402	NDP	PA-O5B	2.26	1.68	1.59
2	E	401	GNU	O04-C20	2.26	1.40	1.37
3	A	402	NDP	O7N-C7N	-2.25	1.19	1.24
3	A	402	NDP	O3B-C3B	-2.24	1.37	1.43
3	C	402	NDP	C5A-C4A	-2.22	1.35	1.39
3	A	402	NDP	C5A-C4A	-2.19	1.35	1.39
3	C	402	NDP	O7N-C7N	-2.17	1.19	1.24
3	E	402	NDP	C5A-N7A	-2.16	1.35	1.39
3	C	402	NDP	C5D-C4D	2.16	1.58	1.51
3	B	402	NDP	O3B-C3B	-2.15	1.37	1.43
2	C	401	GNU	O06-C24	2.10	1.40	1.36
3	C	402	NDP	P2B-O2B	2.09	1.63	1.59
3	B	402	NDP	PA-O5B	2.08	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	NDP	O2B-C2B	2.07	1.51	1.44
3	A	402	NDP	C5A-N7A	-2.07	1.35	1.39
3	E	402	NDP	O7N-C7N	-2.04	1.19	1.24
2	A	401	GNU	O06-C24	2.03	1.40	1.36
2	F	401	GNU	O04-C20	2.01	1.40	1.37
3	A	402	NDP	PN-O5D	2.01	1.67	1.59
3	D	402	NDP	PN-O5D	2.01	1.67	1.59

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NDP	N6A-C6A-N1A	-6.21	104.56	118.38
3	C	402	NDP	C4A-N9A-C1B	-6.14	112.27	126.63
2	F	401	GNU	C10-C08-C12	-5.94	102.81	110.30
3	D	402	NDP	N6A-C6A-N1A	-5.84	105.38	118.38
3	E	402	NDP	C5A-C4A-N3A	-5.66	118.93	126.72
3	D	402	NDP	C5A-C4A-N3A	-5.59	119.02	126.72
3	F	402	NDP	C4A-N9A-C1B	-5.51	113.75	126.63
3	B	402	NDP	C5A-C4A-N3A	-5.35	119.35	126.72
3	C	402	NDP	N6A-C6A-N1A	-5.31	106.55	118.38
3	A	402	NDP	C4A-N9A-C1B	-5.25	114.36	126.63
3	A	402	NDP	C5A-C4A-N3A	-5.19	119.57	126.72
3	F	402	NDP	N3A-C2A-N1A	-5.18	120.74	128.58
3	B	402	NDP	N6A-C6A-N1A	-5.16	106.89	118.38
3	B	402	NDP	N3A-C2A-N1A	-5.15	120.78	128.58
3	C	402	NDP	N3A-C2A-N1A	-5.04	120.95	128.58
3	A	402	NDP	N3A-C2A-N1A	-4.99	121.03	128.58
3	D	402	NDP	N3A-C2A-N1A	-4.97	121.06	128.58
3	E	402	NDP	N6A-C6A-N1A	-4.97	107.31	118.38
3	E	402	NDP	N3A-C2A-N1A	-4.95	121.08	128.58
3	C	402	NDP	C1B-N9A-C8A	4.93	138.03	127.09
3	B	402	NDP	C4A-N9A-C1B	-4.87	115.23	126.63
3	F	402	NDP	N6A-C6A-N1A	-4.85	107.57	118.38
3	F	402	NDP	C5A-C4A-N3A	-4.71	120.23	126.72
3	F	402	NDP	O4B-C1B-N9A	-4.69	99.09	108.09
3	A	402	NDP	C1B-N9A-C8A	4.67	137.46	127.09
3	C	402	NDP	C5A-C4A-N3A	-4.63	120.34	126.72
3	D	402	NDP	C4A-N9A-C1B	-4.57	115.94	126.63
3	E	402	NDP	C4A-N9A-C1B	-4.56	115.96	126.63
3	D	402	NDP	C5A-C6A-N6A	4.56	134.58	123.29
3	A	402	NDP	C5A-C6A-N6A	4.48	134.37	123.29
3	F	402	NDP	C1B-N9A-C8A	4.40	136.86	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	NDP	N3A-C4A-N9A	4.39	134.63	127.17
3	C	402	NDP	N9A-C8A-N7A	-4.36	107.74	113.94
3	F	402	NDP	N9A-C8A-N7A	-4.20	107.97	113.94
3	B	402	NDP	N3A-C4A-N9A	4.13	134.19	127.17
3	B	402	NDP	N9A-C8A-N7A	-4.09	108.14	113.94
2	A	401	GNU	C26-O04-C20	4.05	123.45	117.51
3	D	402	NDP	C1B-N9A-C8A	4.04	136.07	127.09
3	B	402	NDP	C1B-N9A-C8A	4.00	135.98	127.09
3	C	402	NDP	C5A-C6A-N6A	3.89	132.91	123.29
3	A	402	NDP	N9A-C8A-N7A	-3.88	108.44	113.94
3	D	402	NDP	N3A-C4A-N9A	3.85	133.71	127.17
3	B	402	NDP	C5A-C6A-N6A	3.81	132.72	123.29
3	E	402	NDP	C1B-N9A-C8A	3.81	135.54	127.09
3	E	402	NDP	C5A-C6A-N6A	3.78	132.64	123.29
3	E	402	NDP	N9A-C8A-N7A	-3.78	108.58	113.94
2	D	401	GNU	C26-O04-C20	3.72	122.98	117.51
3	C	402	NDP	C4A-N9A-C8A	3.71	109.64	105.74
3	D	402	NDP	N9A-C8A-N7A	-3.70	108.69	113.94
3	C	402	NDP	N3A-C4A-N9A	3.68	133.43	127.17
3	F	402	NDP	N3A-C4A-N9A	3.67	133.41	127.17
2	E	401	GNU	C14-C10-C08	-3.60	107.98	113.61
3	F	402	NDP	C5A-C6A-N6A	3.55	132.08	123.29
3	A	402	NDP	N3A-C4A-N9A	3.52	133.16	127.17
3	F	402	NDP	C4A-N9A-C8A	3.45	109.36	105.74
2	F	401	GNU	C26-O04-C20	3.34	122.41	117.51
3	D	402	NDP	C2A-N3A-C4A	3.26	119.80	111.83
2	D	401	GNU	C25-O03-C19	3.26	122.29	117.51
3	B	402	NDP	C2A-N3A-C4A	3.24	119.73	111.83
3	A	402	NDP	C2A-N3A-C4A	3.23	119.72	111.83
3	E	402	NDP	C2A-N3A-C4A	3.18	119.61	111.83
2	F	401	GNU	C14-C10-C08	-3.11	108.75	113.61
2	B	401	GNU	C13-C09-C07	3.08	118.41	113.61
3	C	402	NDP	C2A-N3A-C4A	3.06	119.30	111.83
3	F	402	NDP	C3N-C2N-N1N	-3.01	118.78	123.20
3	F	402	NDP	C2A-N3A-C4A	3.01	119.18	111.83
2	E	401	GNU	C10-C08-C12	-2.96	106.57	110.30
2	A	401	GNU	C25-O03-C19	2.92	121.79	117.51
3	B	402	NDP	C4A-N9A-C8A	2.85	108.73	105.74
3	D	402	NDP	C5A-N7A-C8A	2.84	107.92	103.45
3	E	402	NDP	C6A-C5A-C4A	2.78	120.98	117.18
3	B	402	NDP	C5A-N7A-C8A	2.72	107.73	103.45
3	E	402	NDP	C5A-N7A-C8A	2.62	107.56	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NDP	C5A-N7A-C8A	2.61	107.56	103.45
3	E	402	NDP	C4A-N9A-C8A	2.61	108.47	105.74
2	E	401	GNU	O04-C20-C24	2.60	118.45	114.55
2	A	401	GNU	O03-C19-C23	2.56	118.39	114.55
2	C	401	GNU	O04-C20-C24	2.55	118.38	114.55
3	C	402	NDP	C5A-N7A-C8A	2.51	107.40	103.45
2	B	401	GNU	O04-C20-C24	2.48	118.27	114.55
3	D	402	NDP	C6A-C5A-C4A	2.45	120.53	117.18
3	B	402	NDP	C6A-C5A-C4A	2.43	120.49	117.18
3	C	402	NDP	O2B-C2B-C1B	-2.41	101.59	110.05
2	A	401	GNU	O04-C20-C24	2.39	118.14	114.55
3	B	402	NDP	O5B-C5B-C4B	2.35	117.01	108.99
3	F	402	NDP	C5A-N7A-C8A	2.32	107.10	103.45
3	A	402	NDP	C4A-N9A-C8A	2.31	108.17	105.74
2	D	401	GNU	C10-C08-C12	-2.25	107.46	110.30
2	C	401	GNU	O03-C19-C23	2.24	117.91	114.55
3	F	402	NDP	C4B-O4B-C1B	-2.23	104.53	109.47
3	A	402	NDP	O4B-C1B-N9A	-2.23	103.80	108.09
3	D	402	NDP	C5B-C4B-C3B	-2.18	107.37	115.21
3	F	402	NDP	C6A-C5A-C4A	2.14	120.10	117.18
3	D	402	NDP	C3N-C2N-N1N	-2.14	120.07	123.20
3	D	402	NDP	C4A-C5A-N7A	-2.11	108.17	110.58
3	D	402	NDP	C4A-N9A-C8A	2.10	107.95	105.74
2	A	401	GNU	C09-C07-C11	-2.09	107.66	110.30
3	B	402	NDP	O4B-C1B-N9A	-2.09	104.08	108.09
3	F	402	NDP	C2B-C1B-N9A	2.04	117.12	113.75
2	D	401	GNU	C09-C13-C15	2.02	123.90	120.43
2	D	401	GNU	C09-C13-C17	-2.02	117.15	120.90

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	GNU	C11-C07-C09-C13
2	F	401	GNU	C11-C07-C08-C12
3	C	402	NDP	C5D-O5D-PN-O3
3	C	402	NDP	C5D-O5D-PN-O1N
3	C	402	NDP	C2N-C3N-C7N-O7N
3	C	402	NDP	C2N-C3N-C7N-N7N
3	D	402	NDP	C5B-O5B-PA-O1A
3	D	402	NDP	C5B-O5B-PA-O3
3	F	402	NDP	C2N-C3N-C7N-O7N

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Mol	Chain	Res	Type	Atoms
2	C	401	GNU	C24-C20-O04-C26
2	E	401	GNU	C24-C20-O04-C26
2	D	401	GNU	C23-C19-O03-C25
3	D	402	NDP	C3B-C2B-O2B-P2B
2	C	401	GNU	C23-C19-O03-C25
2	E	401	GNU	C16-C20-O04-C26
2	C	401	GNU	C16-C20-O04-C26
2	D	401	GNU	C15-C19-O03-C25
2	C	401	GNU	C15-C19-O03-C25
3	A	402	NDP	C1B-C2B-O2B-P2B
3	F	402	NDP	C1B-C2B-O2B-P2B
3	A	402	NDP	C3B-C2B-O2B-P2B
3	B	402	NDP	C3B-C2B-O2B-P2B
3	F	402	NDP	C3B-C2B-O2B-P2B
3	D	402	NDP	C3B-C4B-C5B-O5B
3	B	402	NDP	C1B-C2B-O2B-P2B
2	E	401	GNU	C23-C19-O03-C25
3	D	402	NDP	O4D-C4D-C5D-O5D
2	E	401	GNU	C15-C19-O03-C25
3	D	402	NDP	O4B-C4B-C5B-O5B
3	F	402	NDP	C2N-C3N-C7N-N7N
2	E	401	GNU	C11-C07-C08-C12
2	B	401	GNU	C24-C20-O04-C26
3	A	402	NDP	C2D-C1D-N1N-C2N
2	E	401	GNU	C09-C07-C08-C10
2	F	401	GNU	C09-C07-C08-C10
3	C	402	NDP	C2B-O2B-P2B-O1X
2	F	401	GNU	C09-C07-C08-C12
2	B	401	GNU	C08-C07-C09-C13
2	F	401	GNU	C11-C07-C09-C13
3	C	402	NDP	C5D-O5D-PN-O2N
3	A	402	NDP	O4D-C1D-N1N-C2N
3	A	402	NDP	O4D-C1D-N1N-C6N
3	A	402	NDP	C2D-C1D-N1N-C6N
3	C	402	NDP	C2B-O2B-P2B-O2X
3	C	402	NDP	O4D-C1D-N1N-C2N
3	E	402	NDP	O4D-C1D-N1N-C2N
2	B	401	GNU	C16-C20-O04-C26
2	D	401	GNU	C07-C09-C13-C15
3	D	402	NDP	O4D-C1D-N1N-C2N
3	F	402	NDP	O4D-C1D-N1N-C2N
3	B	402	NDP	O4D-C1D-N1N-C2N

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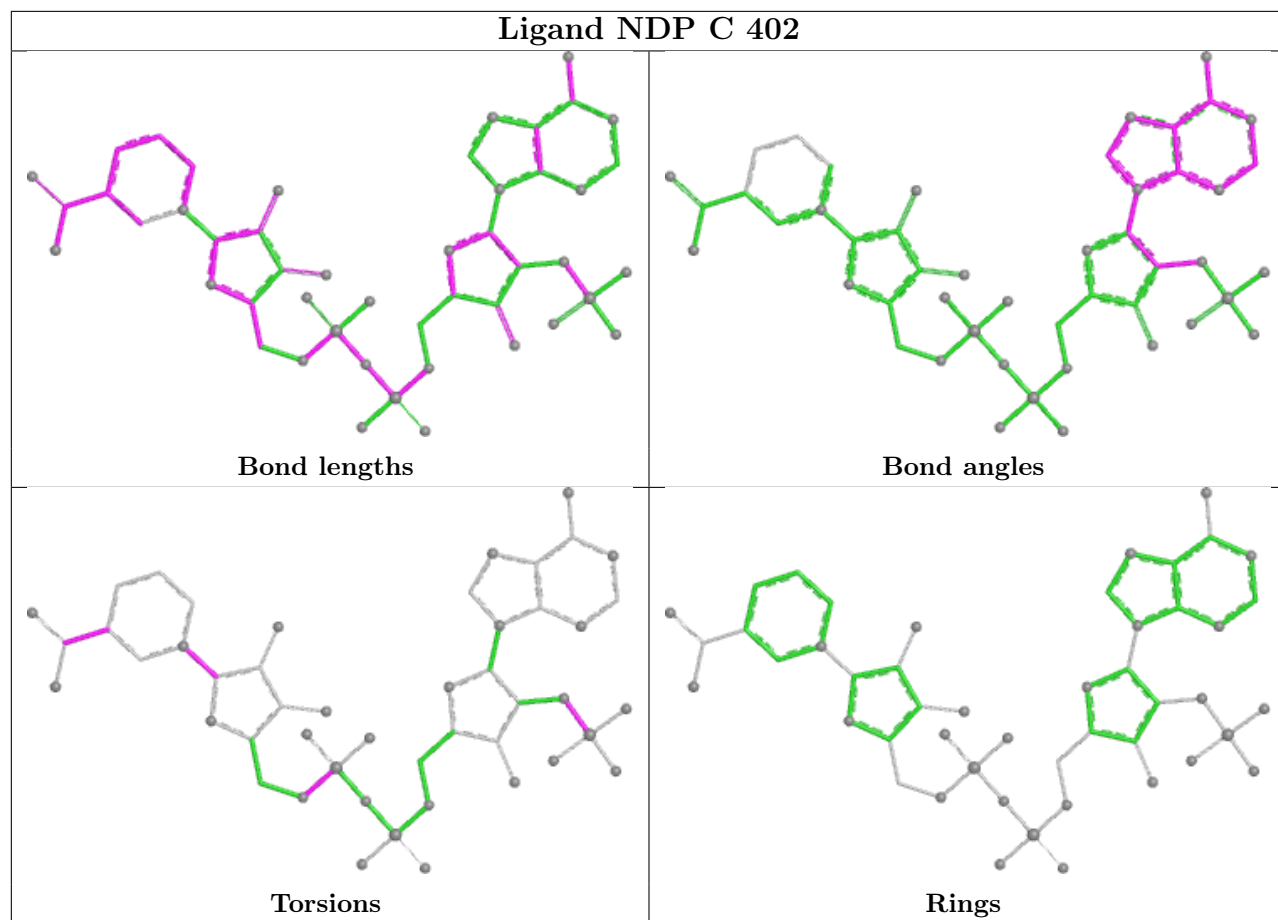
Mol	Chain	Res	Type	Atoms
3	E	402	NDP	C2N-C3N-C7N-N7N
3	F	402	NDP	C2B-O2B-P2B-O1X
3	D	402	NDP	PN-O3-PA-O1A
3	D	402	NDP	PN-O3-PA-O2A
3	B	402	NDP	C2D-C1D-N1N-C2N
2	D	401	GNU	C07-C09-C13-C17
3	D	402	NDP	C3D-C4D-C5D-O5D
2	E	401	GNU	C09-C07-C08-C12
2	E	401	GNU	C11-C07-C08-C10
2	F	401	GNU	C11-C07-C08-C10

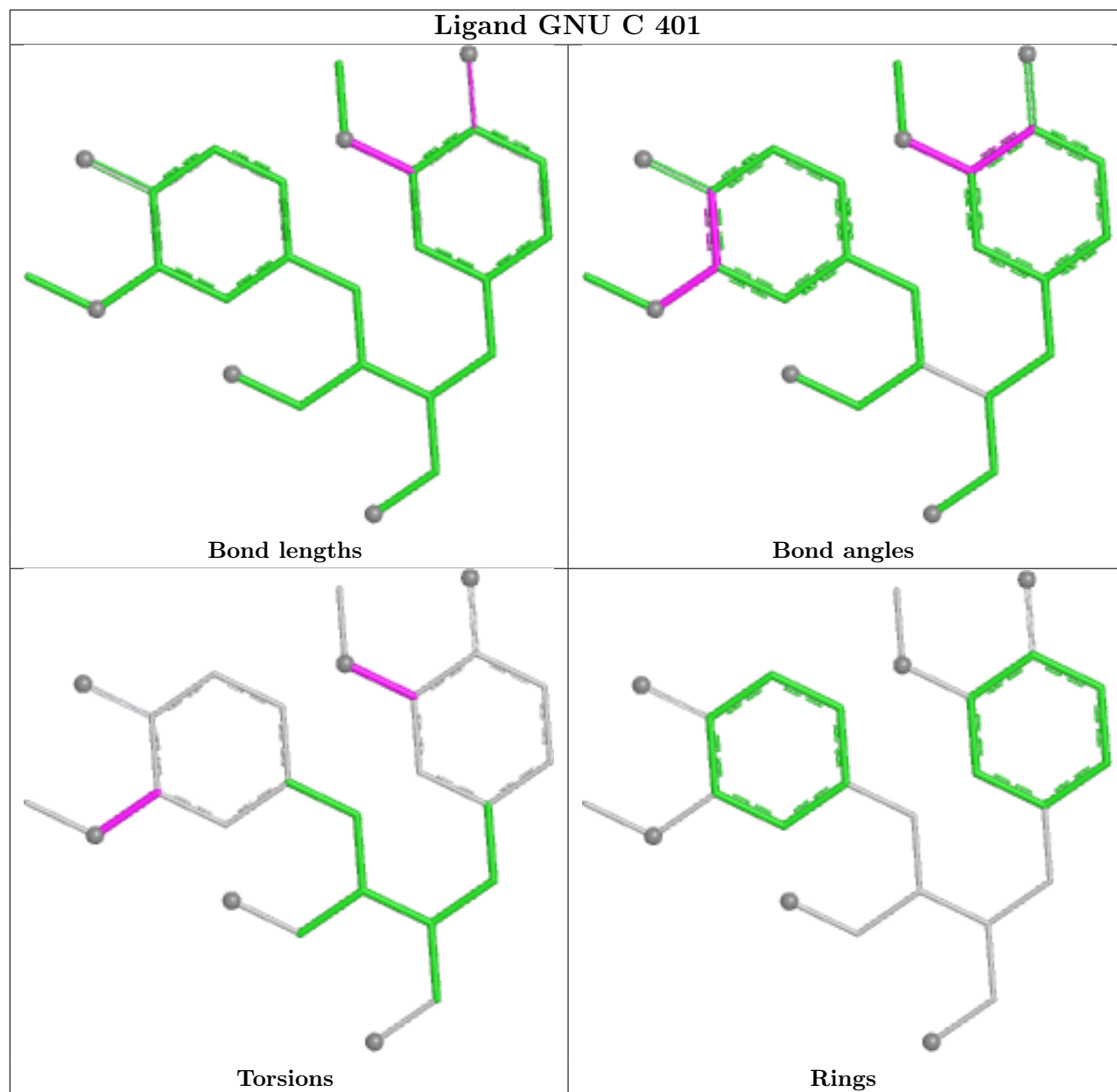
There are no ring outliers.

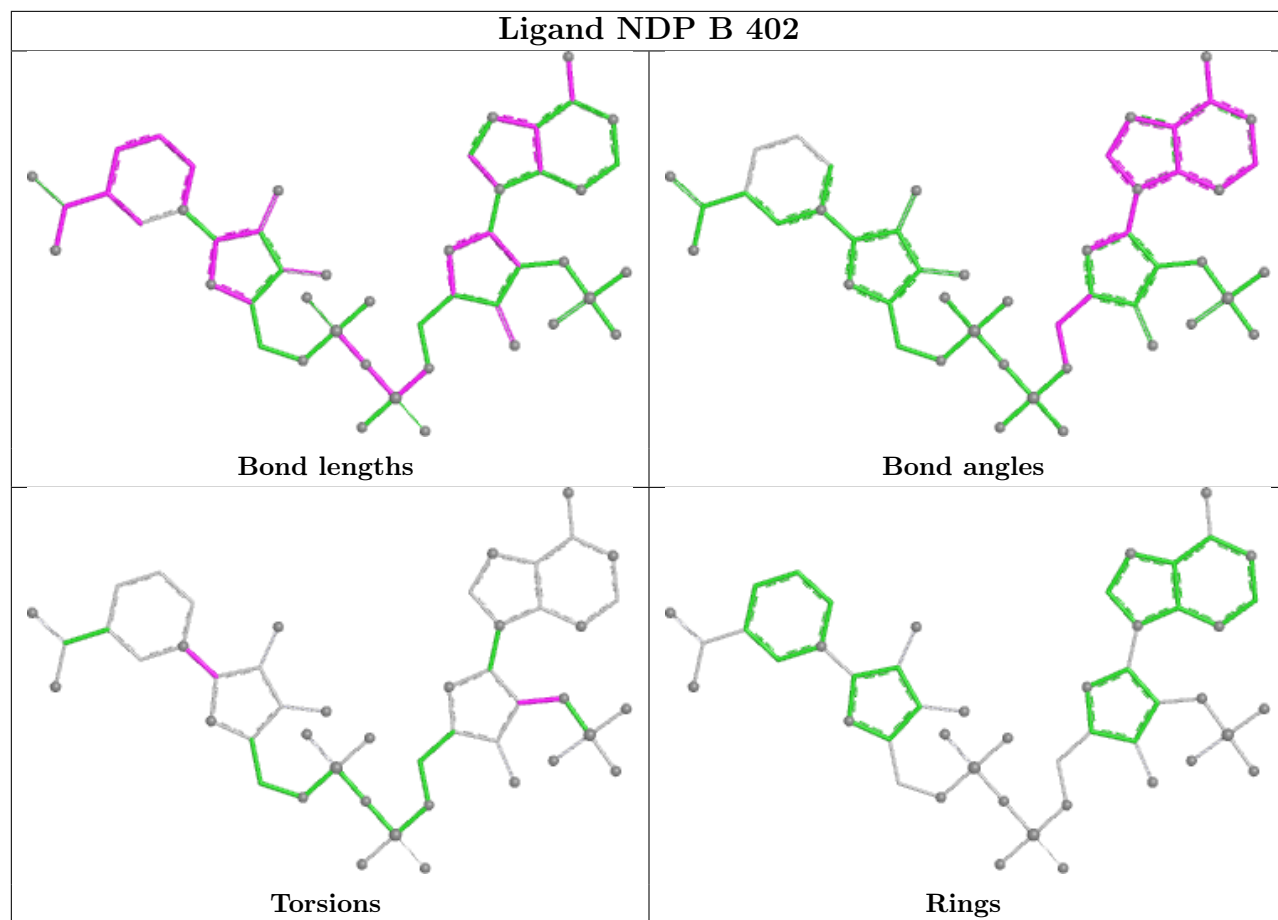
10 monomers are involved in 46 short contacts:

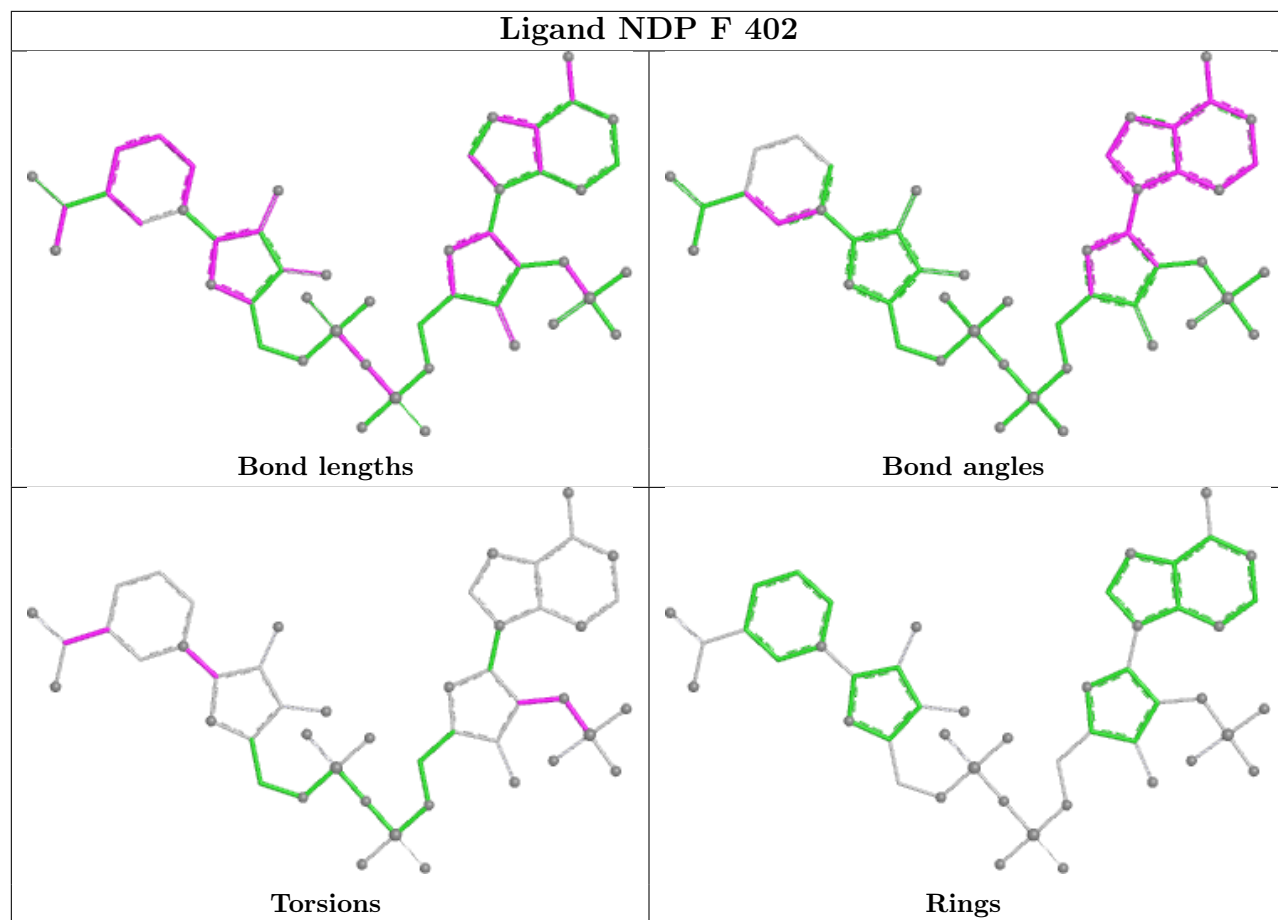
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	NDP	7	0
2	C	401	GNU	1	0
3	B	402	NDP	6	0
3	F	402	NDP	2	0
2	D	401	GNU	2	0
2	E	401	GNU	1	0
3	E	402	NDP	6	0
3	A	402	NDP	9	0
3	D	402	NDP	12	0
2	F	401	GNU	2	0

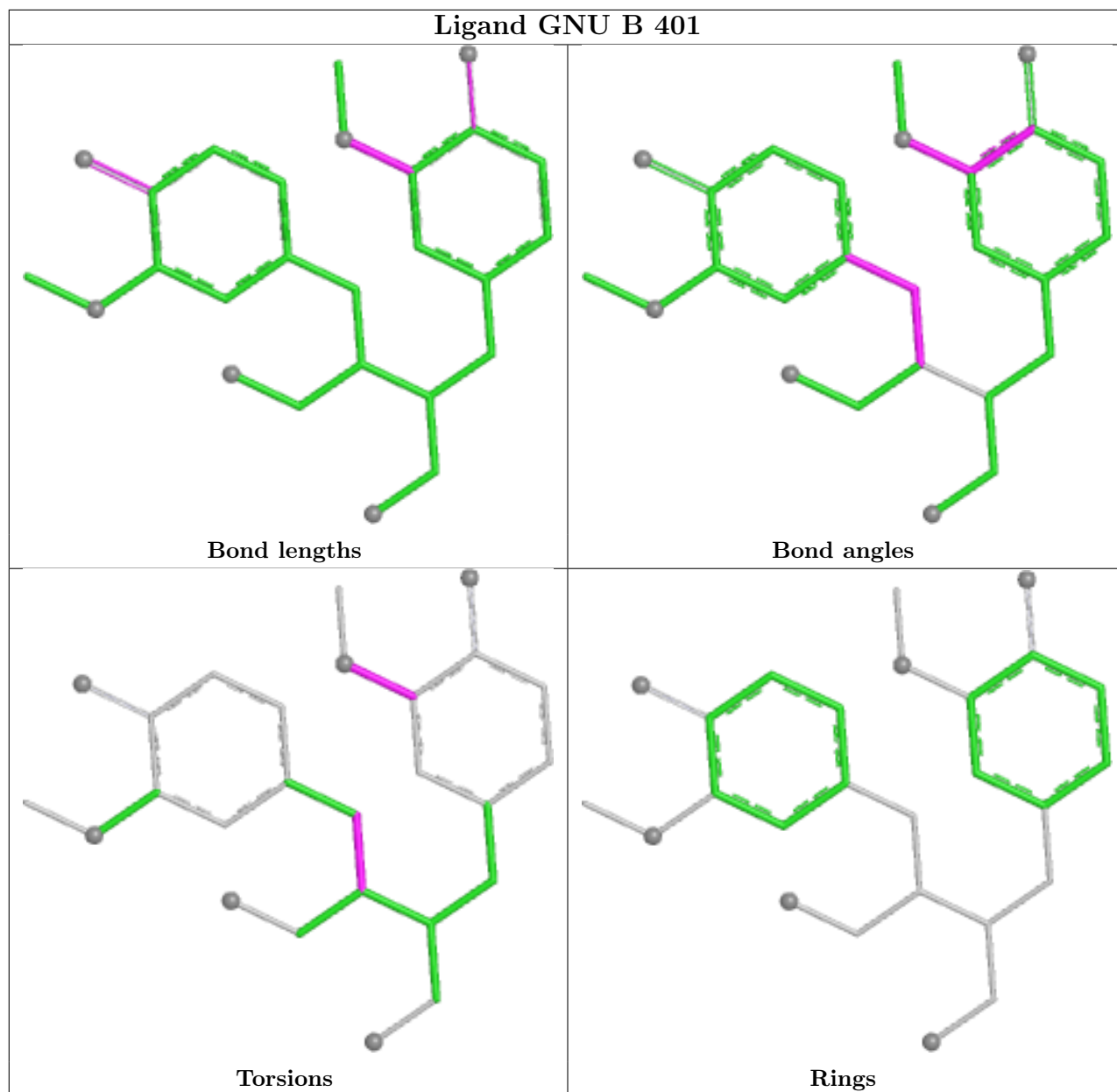
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

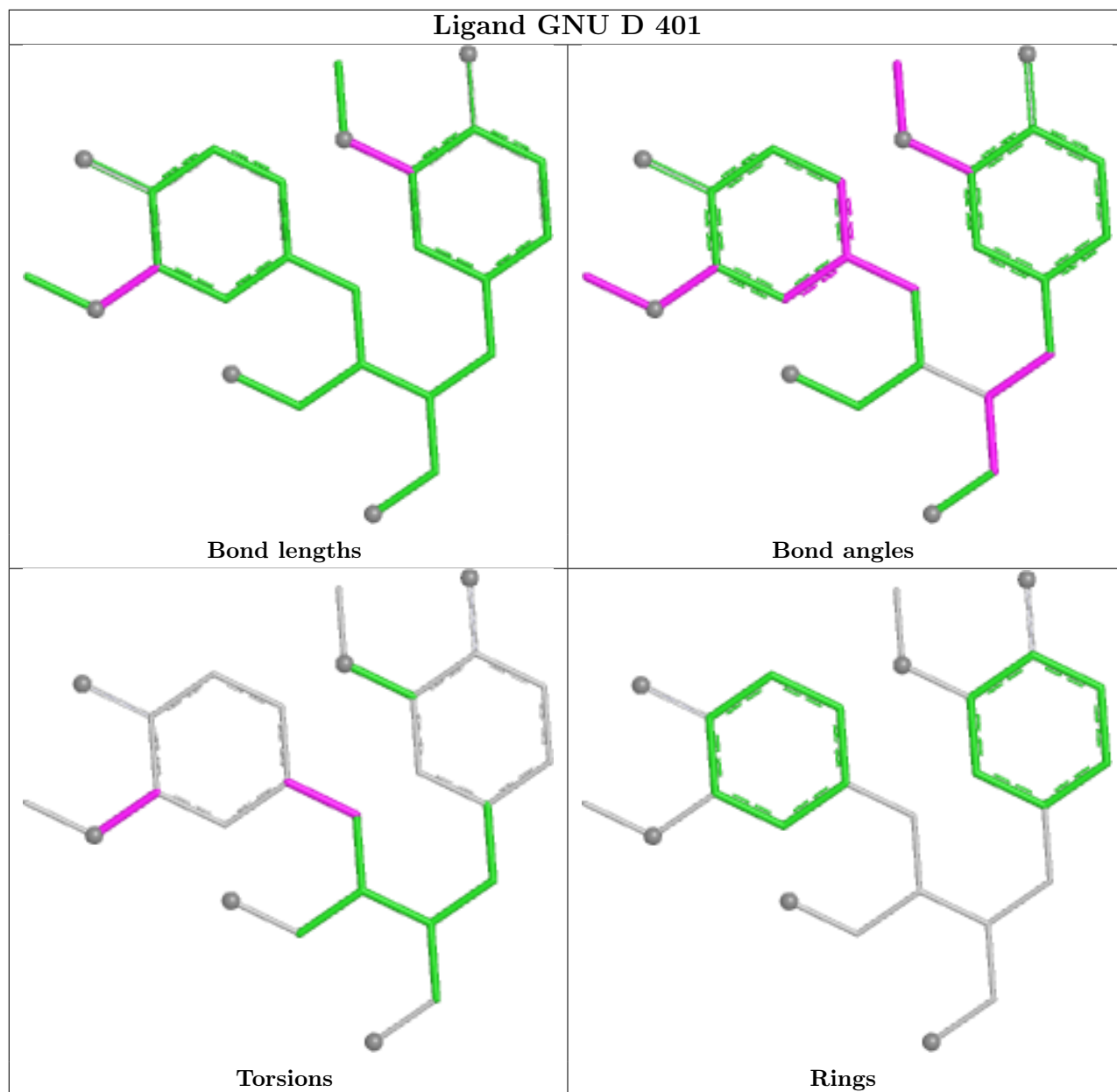


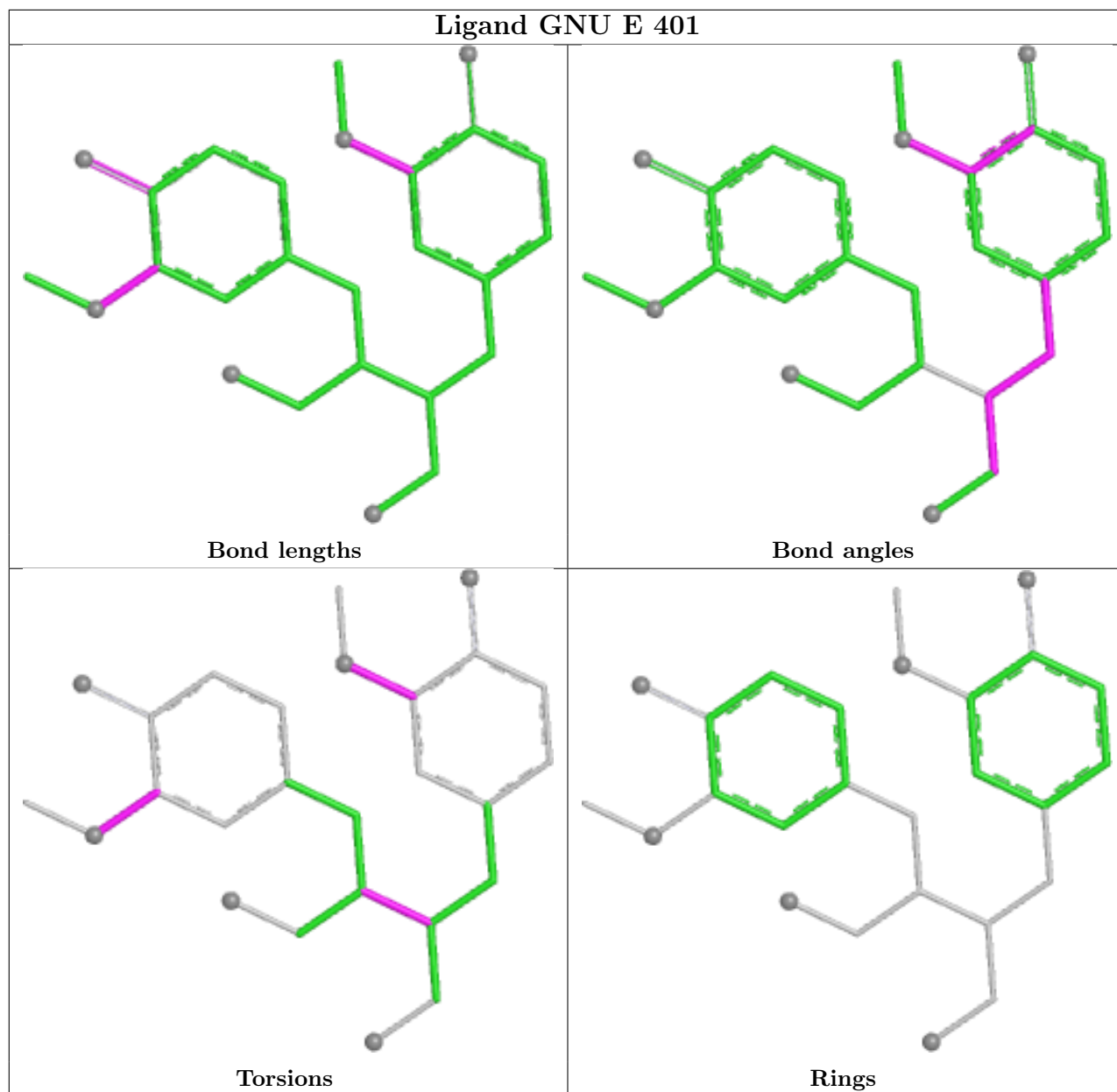


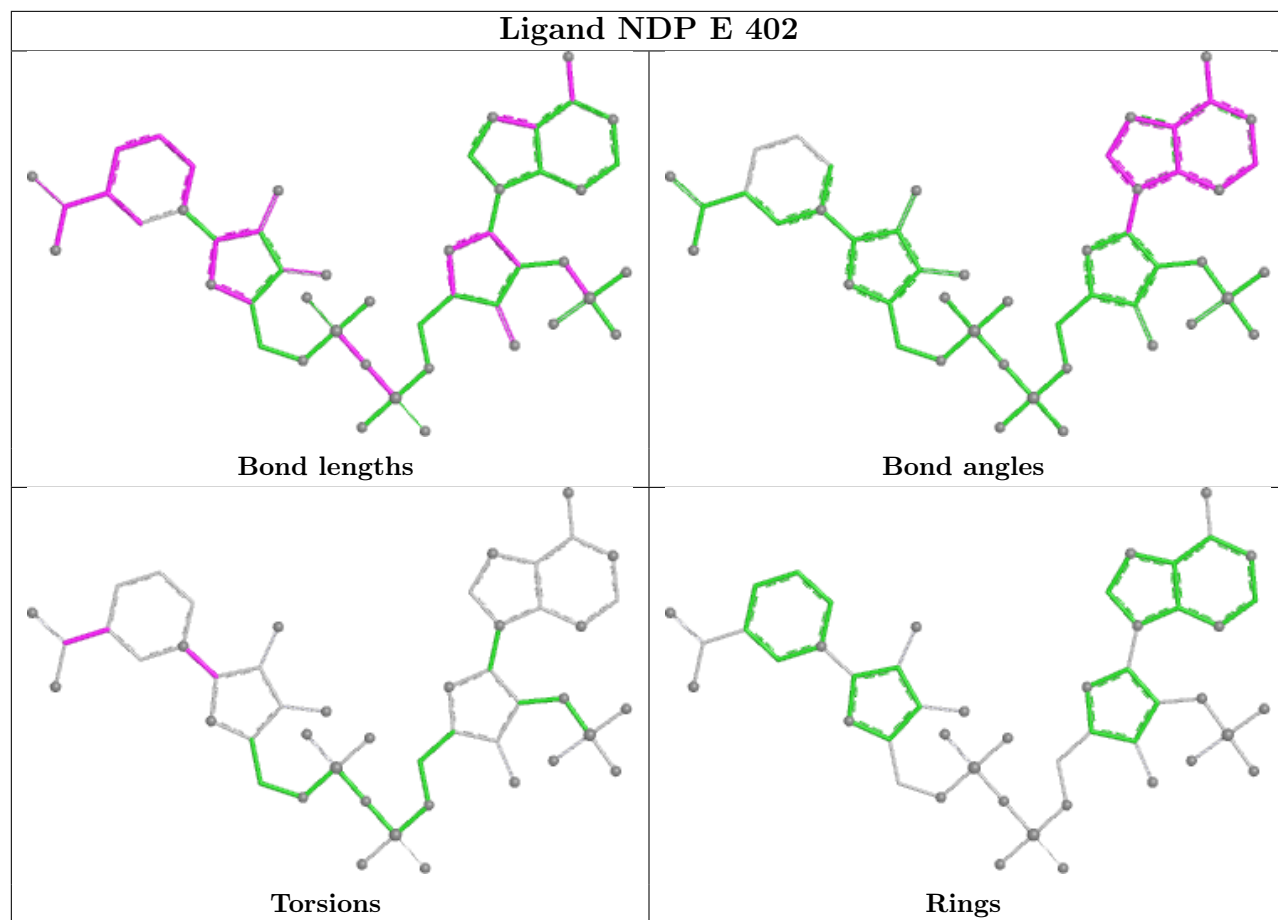


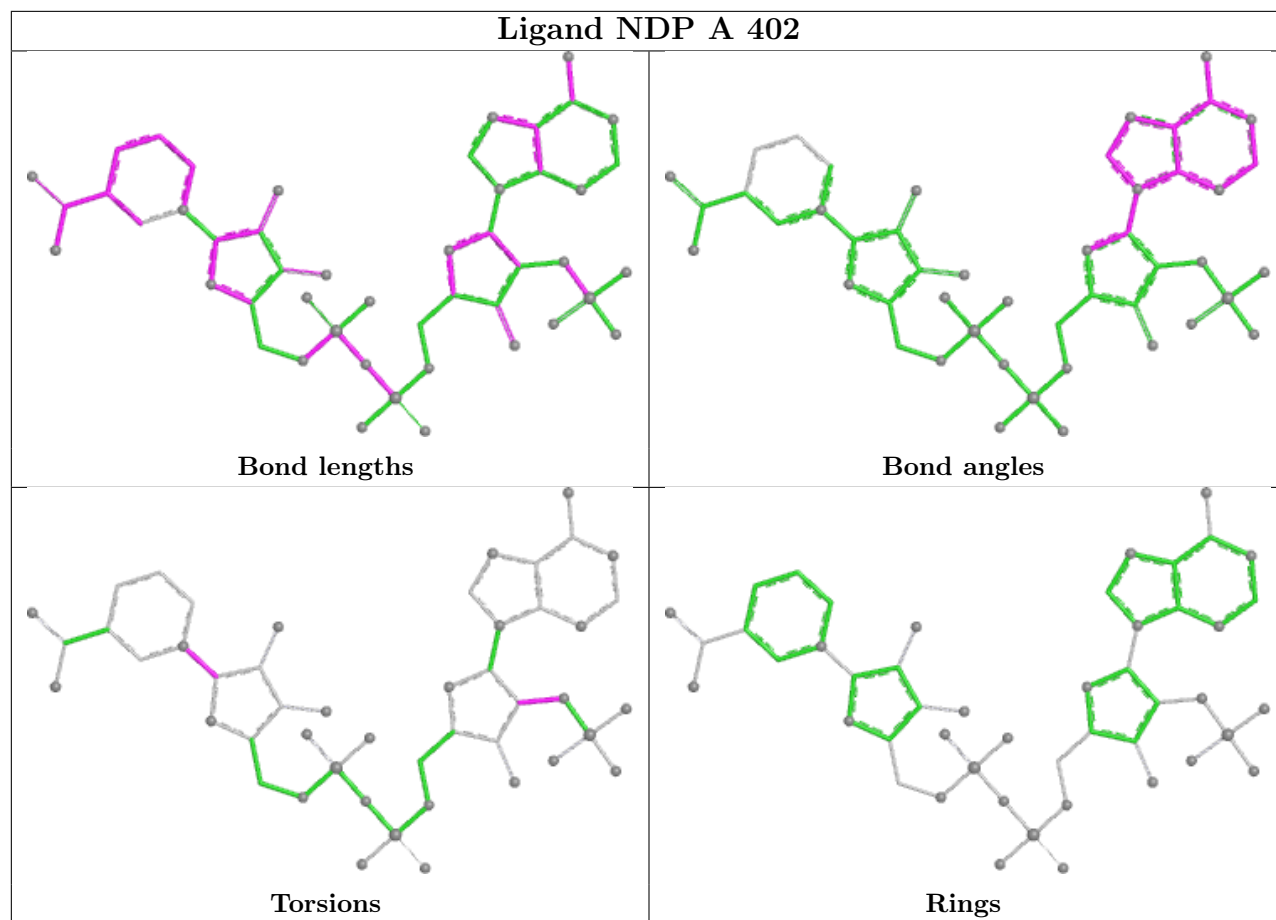


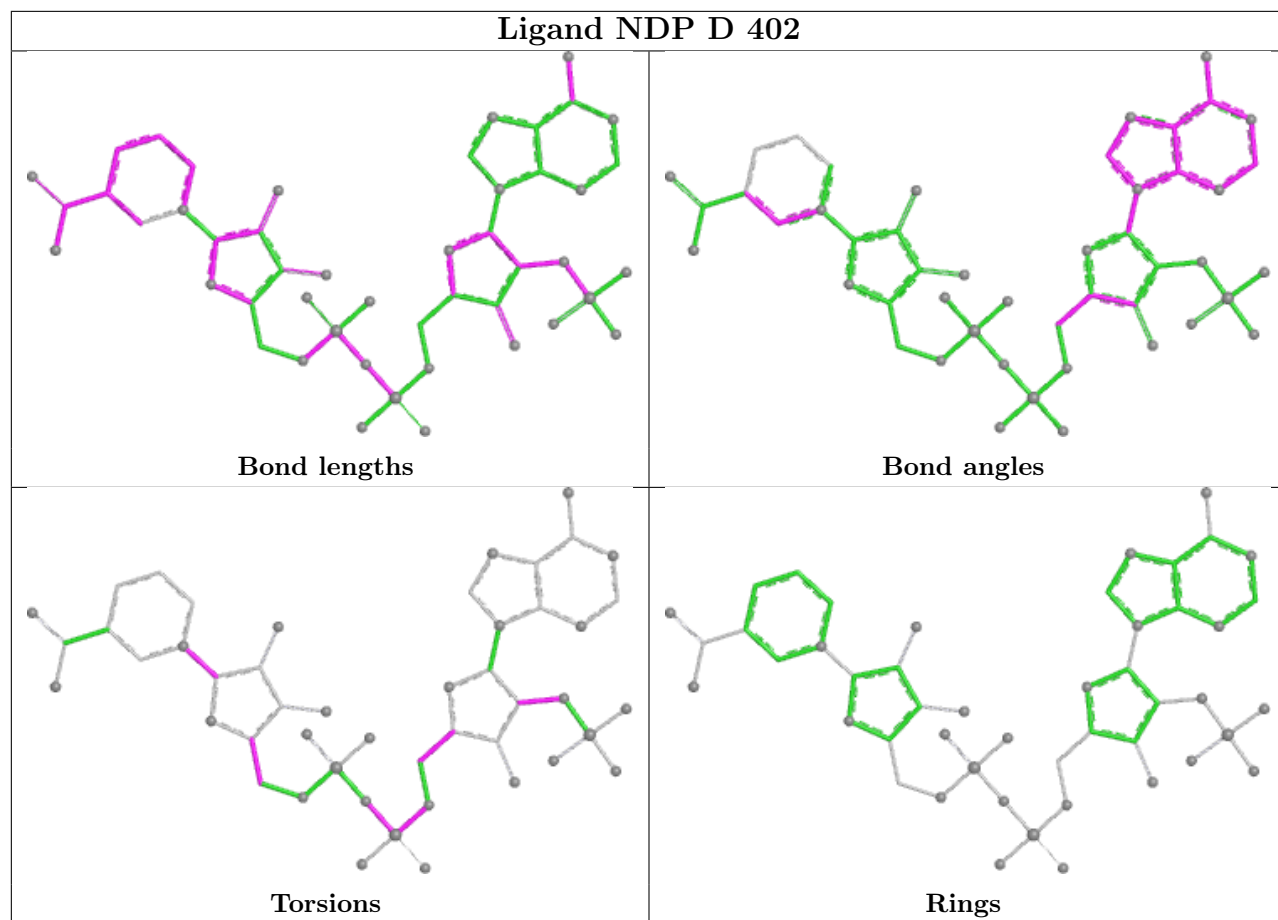


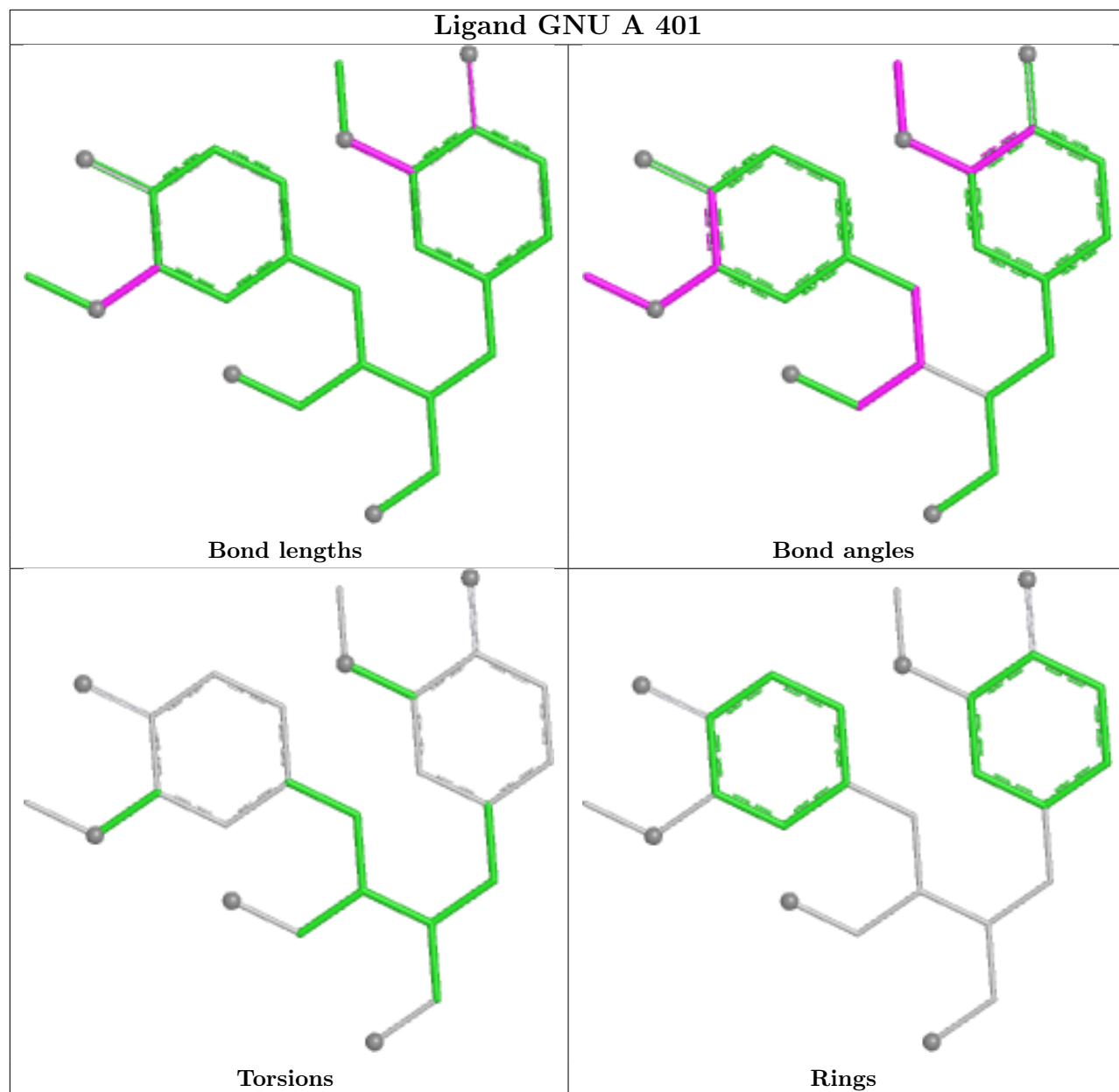


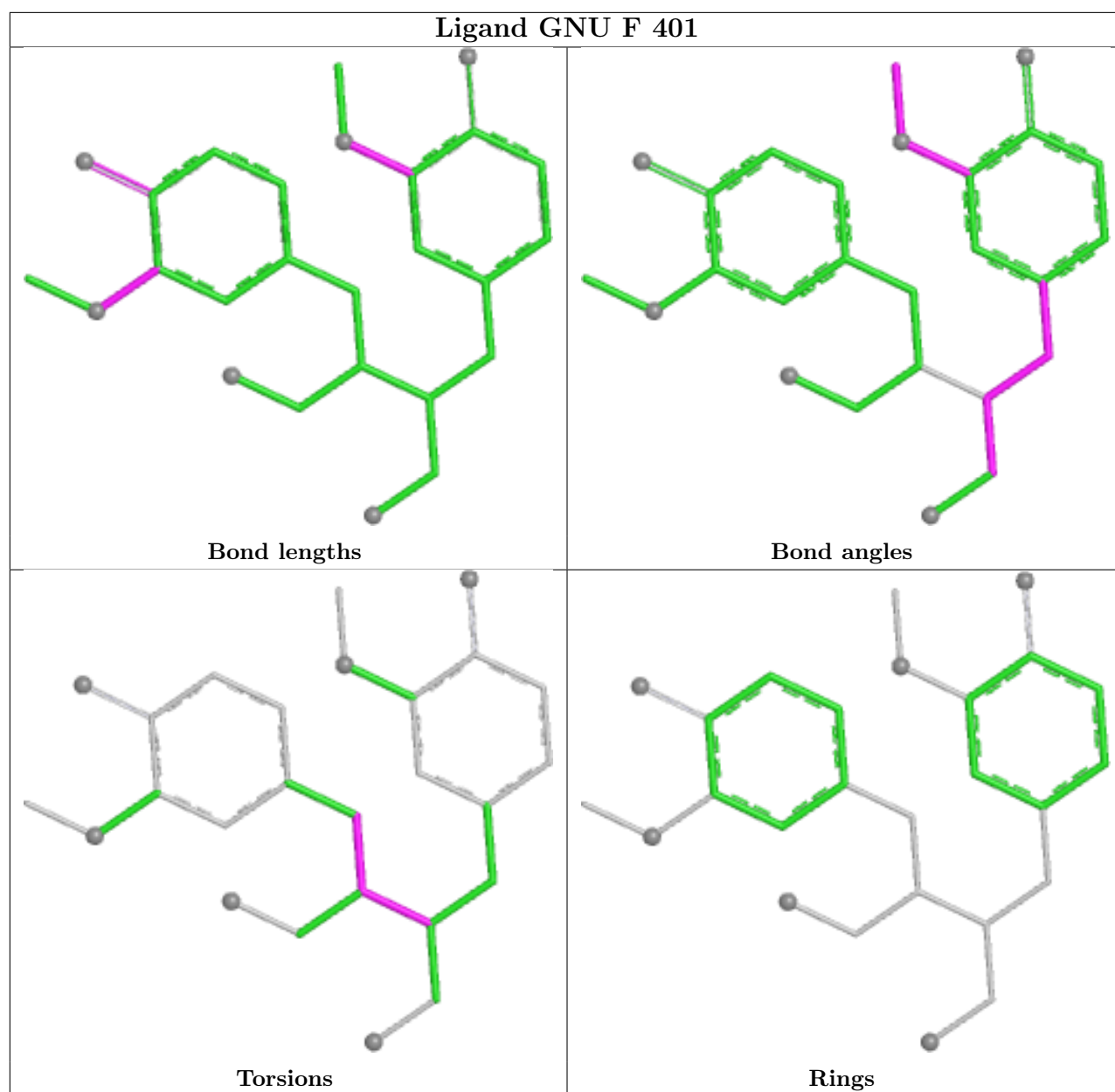












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	285/317 (89%)	-0.21	10 (3%) 47 49	20, 29, 49, 68	0
1	B	287/317 (90%)	0.28	29 (10%) 12 14	20, 32, 66, 88	0
1	C	284/317 (89%)	0.02	9 (3%) 50 52	20, 33, 59, 84	0
1	D	283/317 (89%)	-0.03	10 (3%) 47 49	21, 33, 57, 84	0
1	E	286/317 (90%)	-0.25	11 (3%) 44 46	19, 28, 52, 72	0
1	F	293/317 (92%)	-0.24	10 (3%) 48 50	20, 28, 49, 72	0
All	All	1718/1902 (90%)	-0.07	79 (4%) 37 39	19, 30, 58, 88	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	260	LEU	6.7
1	E	44	THR	6.6
1	C	6	SER	5.8
1	D	6	SER	5.8
1	F	268	ILE	5.8
1	E	260	LEU	5.7
1	C	260	LEU	5.7
1	D	260	LEU	5.6
1	D	7	GLY	5.3
1	A	46	VAL	5.2
1	C	7	GLY	5.2
1	B	92	VAL	4.8
1	A	260	LEU	4.7
1	E	272	ALA	4.7
1	B	7	GLY	4.6
1	B	278	TYR	4.6
1	B	6	SER	4.5
1	E	6	SER	4.5
1	A	45	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	6	SER	4.3
1	B	94	PHE	4.3
1	B	277	PHE	3.8
1	B	254	ILE	3.8
1	B	257	ASN	3.8
1	B	249	LEU	3.6
1	F	272	ALA	3.5
1	A	97	HIS	3.5
1	B	252	THR	3.5
1	B	259	PHE	3.5
1	A	43	GLU	3.3
1	B	282	TYR	3.2
1	B	189	ILE	3.2
1	B	256	ALA	3.1
1	D	44	THR	3.1
1	B	190	TYR	3.1
1	E	130	MET	3.0
1	F	271	GLN	3.0
1	D	259	PHE	2.9
1	F	260	LEU	2.9
1	B	44	THR	2.9
1	F	6	SER	2.8
1	F	125	MET	2.8
1	A	272	ALA	2.8
1	E	90	SER	2.7
1	E	97	HIS	2.7
1	A	90	SER	2.6
1	B	238	VAL	2.6
1	C	45	ARG	2.6
1	B	195	VAL	2.6
1	B	272	ALA	2.6
1	D	271	GLN	2.5
1	F	273	GLY	2.5
1	C	98	SER	2.5
1	E	8	GLU	2.5
1	A	91	GLY	2.5
1	B	45	ARG	2.4
1	D	45	ARG	2.4
1	E	43	GLU	2.4
1	B	185	LYS	2.4
1	B	192	ASP	2.4
1	E	142	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	91	GLY	2.3
1	D	257	ASN	2.3
1	F	44	THR	2.3
1	D	272	ALA	2.3
1	F	95	ARG	2.2
1	B	251	LYS	2.2
1	D	129	ARG	2.2
1	C	289	HIS	2.2
1	B	274	LEU	2.2
1	A	271	GLN	2.2
1	B	276	HIS	2.1
1	C	276	HIS	2.1
1	B	188	ASN	2.1
1	C	43	GLU	2.1
1	E	271	GLN	2.1
1	F	270	HIS	2.1
1	B	273	GLY	2.0
1	C	186	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.

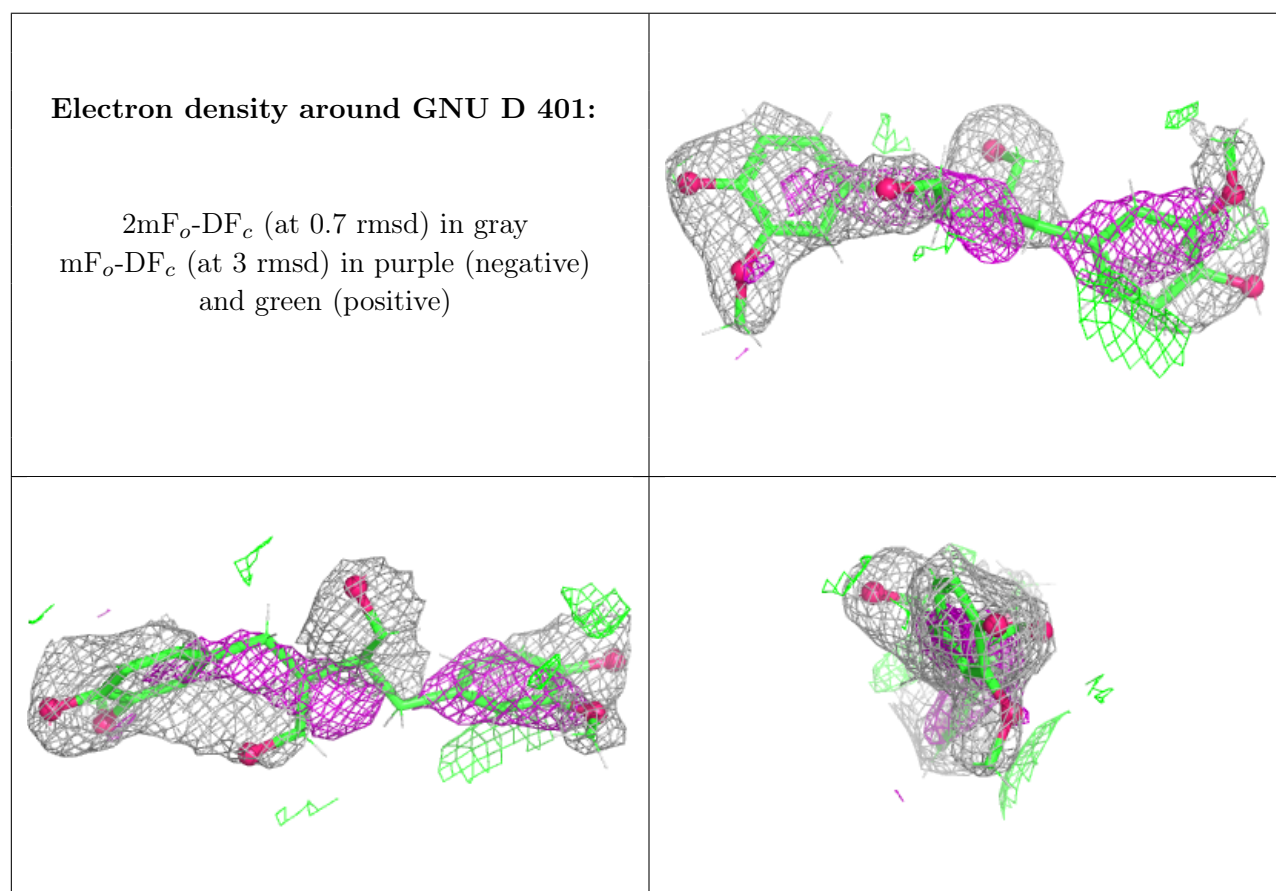
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GNU	D	401	26/26	0.62	0.17	48,59,71,75	0
2	GNU	C	401	26/26	0.66	0.17	49,61,73,81	0
2	GNU	A	401	26/26	0.68	0.16	38,56,68,79	0
2	GNU	B	401	26/26	0.75	0.14	42,55,68,74	0
2	GNU	E	401	26/26	0.81	0.12	38,49,64,76	0

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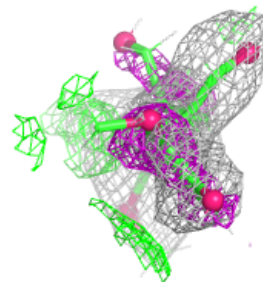
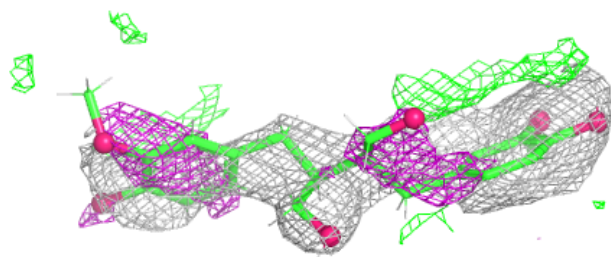
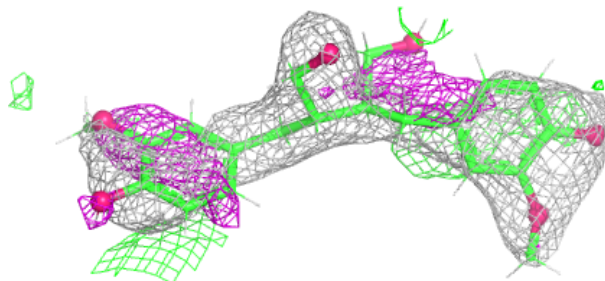
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NDP	A	402	48/48	0.84	0.12	35,50,61,63	0
3	NDP	C	402	48/48	0.84	0.12	37,53,64,80	0
3	NDP	D	402	48/48	0.84	0.12	40,50,59,64	0
2	GNU	F	401	26/26	0.89	0.09	26,33,40,53	0
3	NDP	E	402	48/48	0.91	0.09	30,43,52,56	0
3	NDP	B	402	48/48	0.95	0.07	30,38,49,50	0
3	NDP	F	402	48/48	0.97	0.06	23,31,42,47	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.

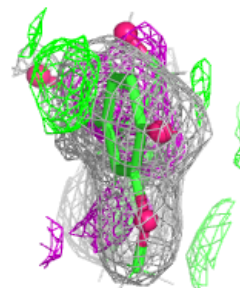
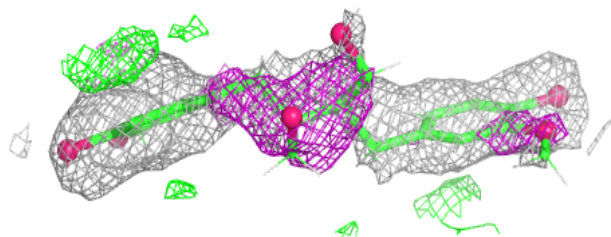
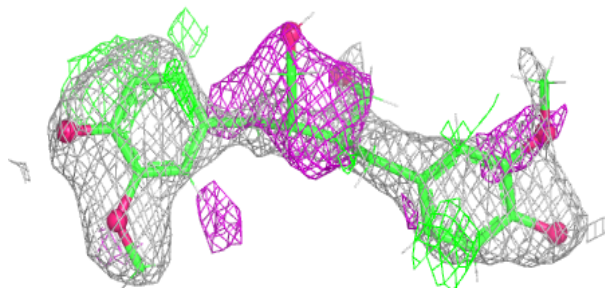


Electron density around GNU C 401:

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

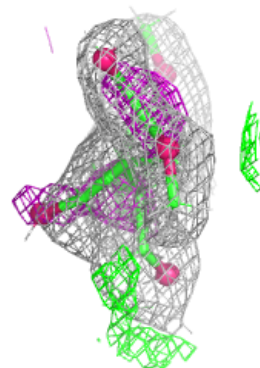
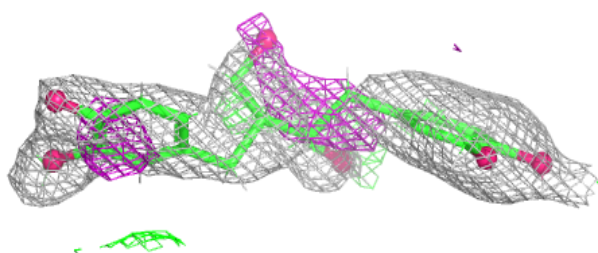
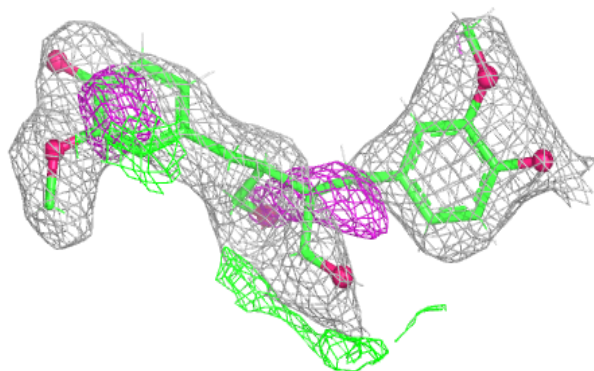
**Electron density around GNU A 401:**

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

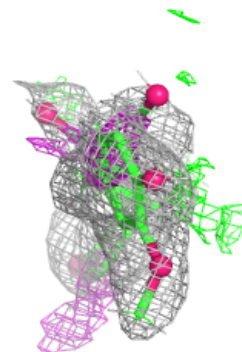
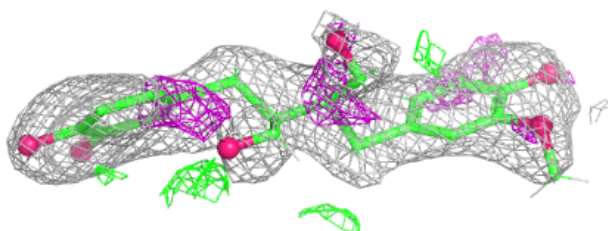
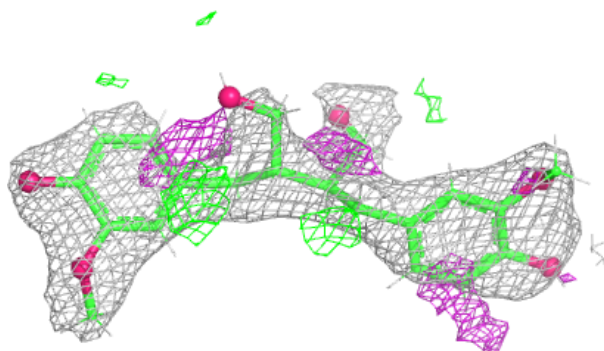


Electron density around GNU B 401:

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

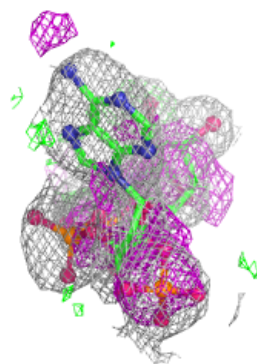
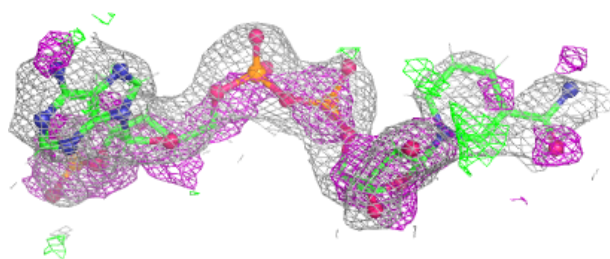
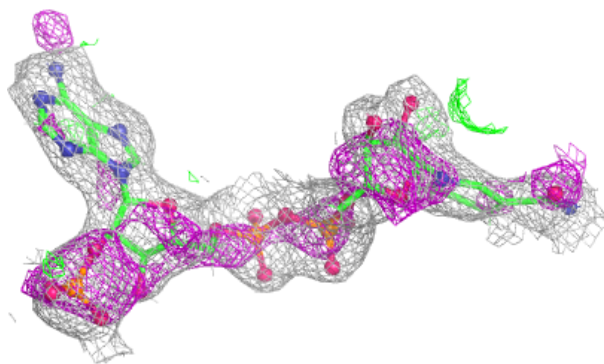
**Electron density around GNU E 401:**

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

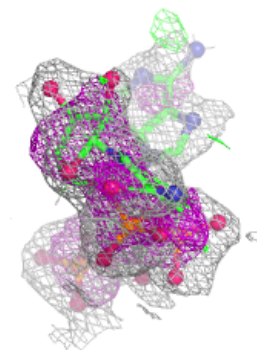
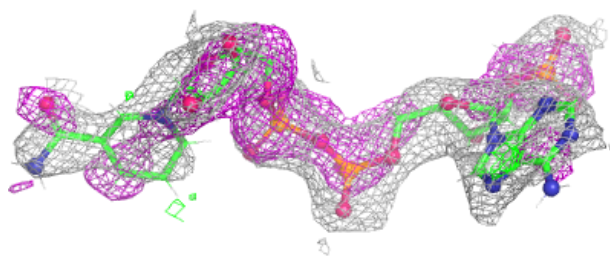
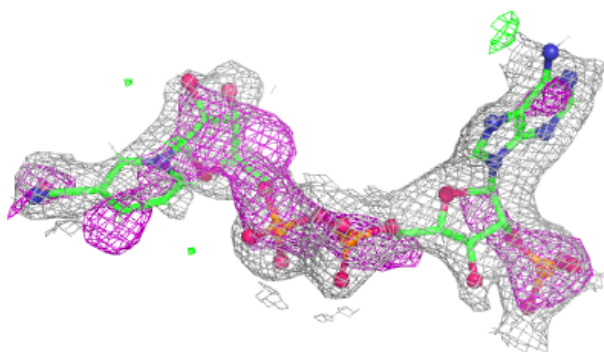


Electron density around NDP A 402:

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

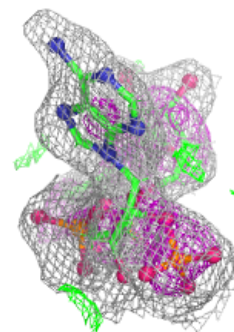
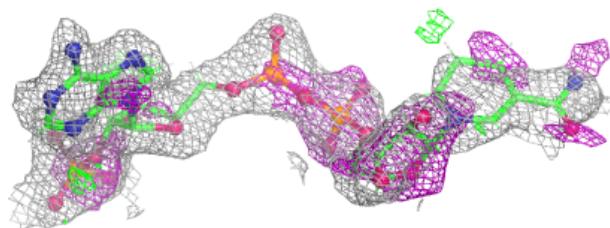
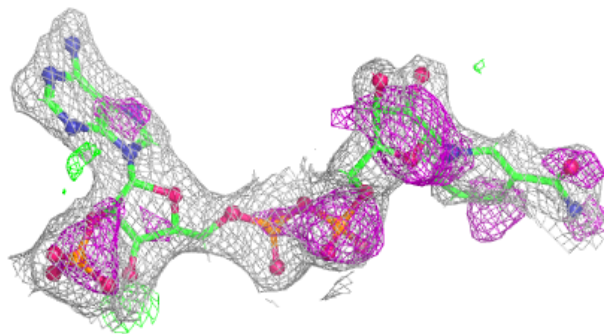
**Electron density around NDP C 402:**

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

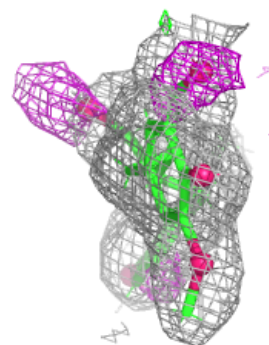
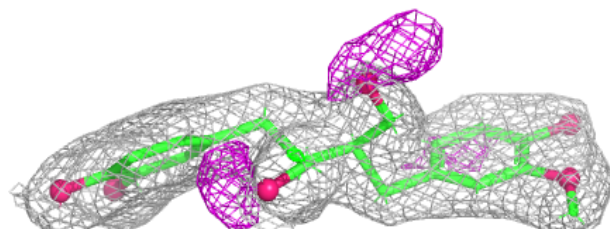
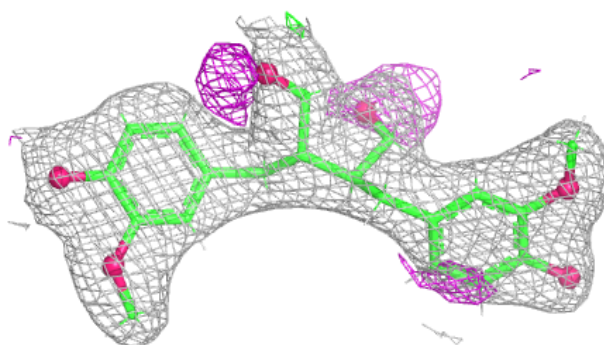


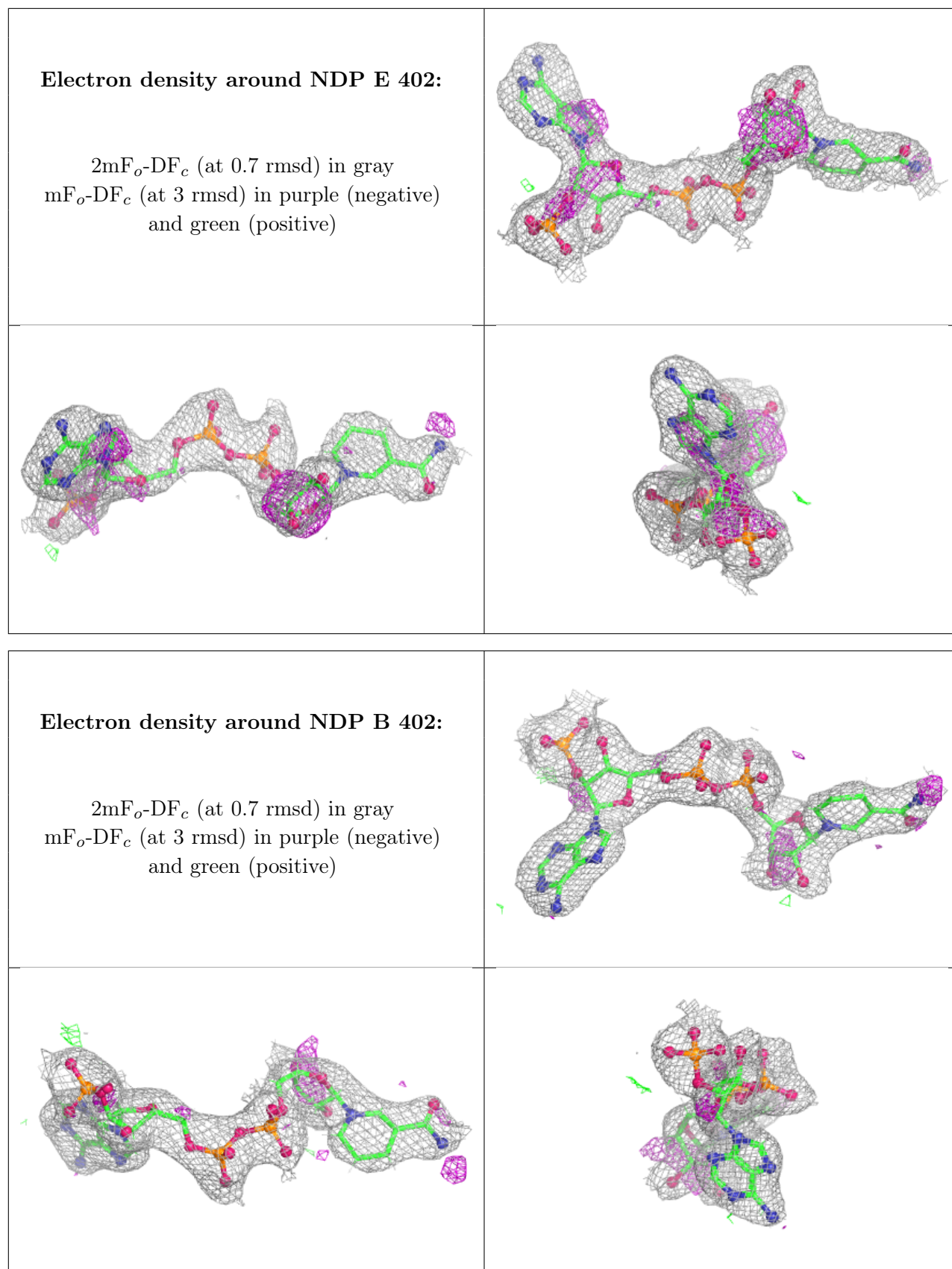
Electron density around NDP D 402:

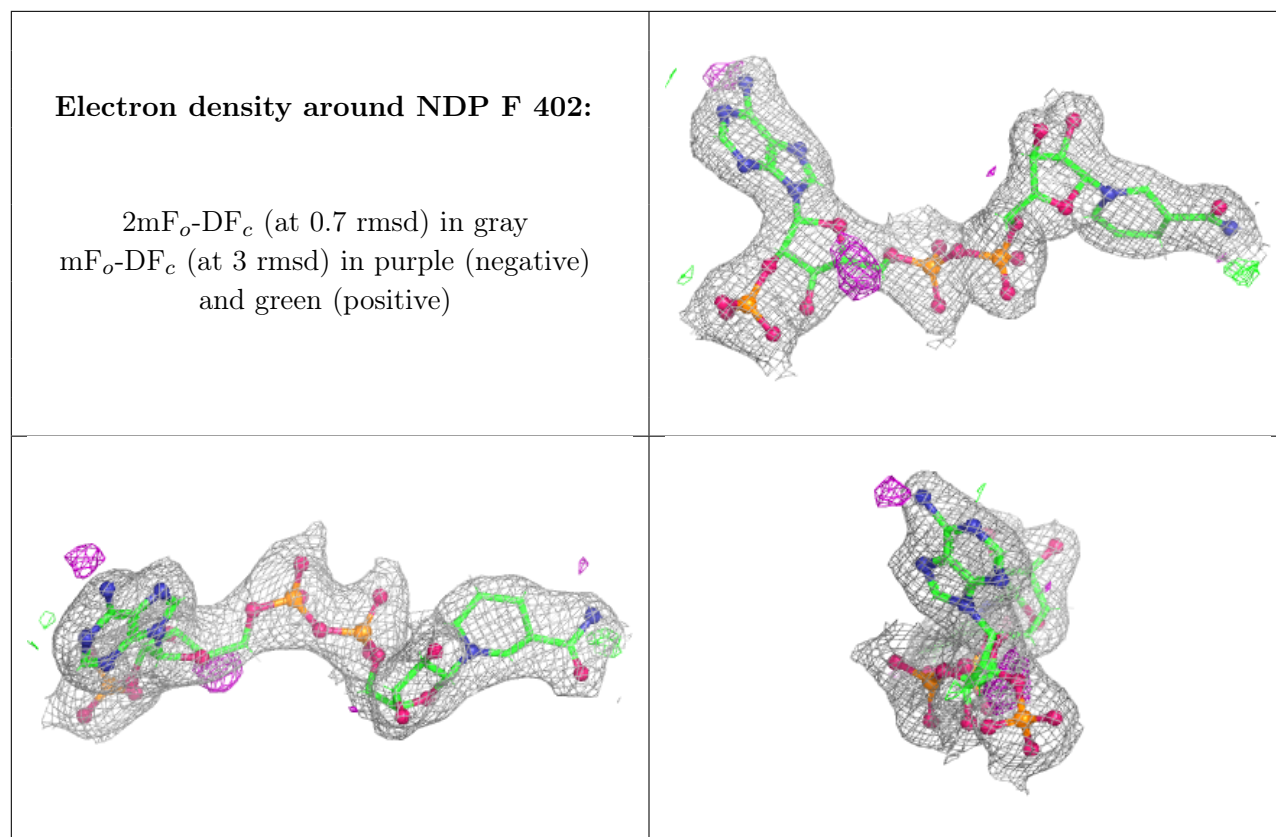
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GNU 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)







6.5 Other polymers [i](#)

There are no such residues in this entry.