



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:53 PM UTC

PDB ID : 6Q0D / pdb_00006q0d
Title : CRYSTAL STRUCTURE OF LDHA IN COMPLEX WITH COMPOUND
NCGC00384414-01 AT 2.05 Å RESOLUTION
Authors : Dranow, D.M.; Davies, D.R.
Deposited on : 2019-08-01
Resolution : 2.05 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

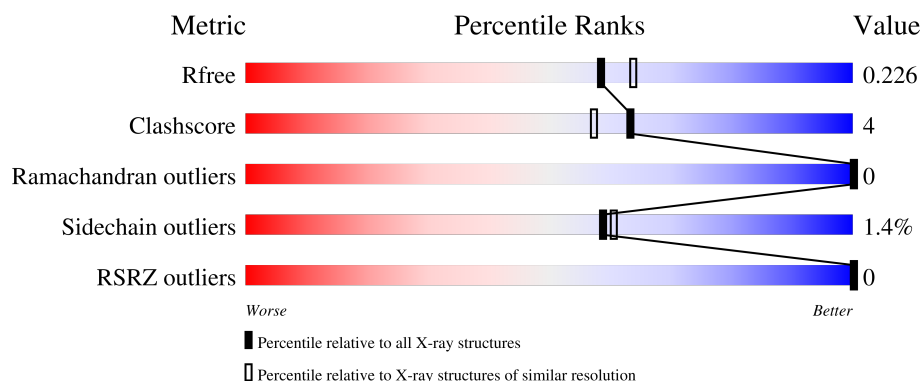
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

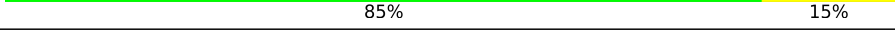
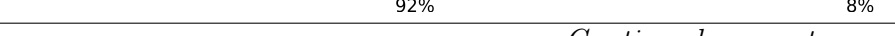
The reported resolution of this entry is 2.05 Å.

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.



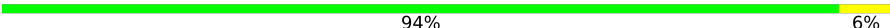
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	332	 89% 11%
1	B	332	 89% 10% .
1	C	332	 90% 9%
1	D	332	 85% 15%
1	E	332	 92% 8%

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Mol	Chain	Length	Quality of chain
1	F	332	 94%6%

2 Entry composition [i](#)

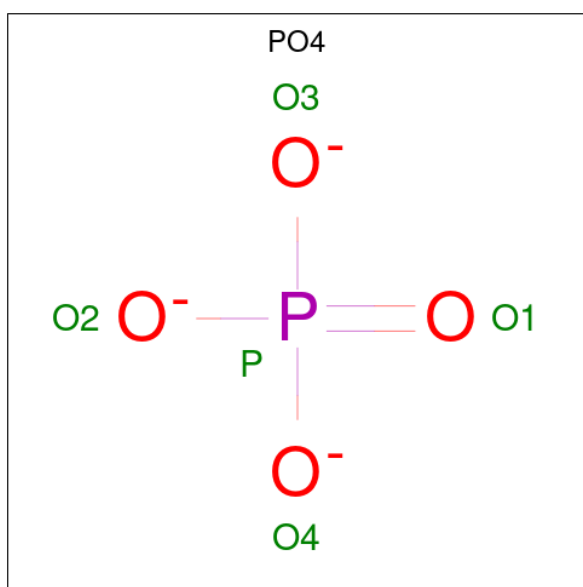
There are 6 unique types of molecules in this entry. The entry contains 16383 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called L-lactate dehydrogenase A chain.

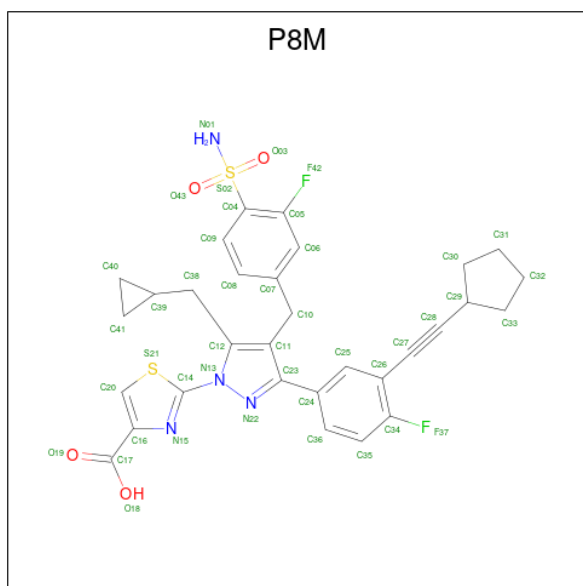
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2488	1589	429	457	13			
1	B	331	Total	C	N	O	S	0	0	0
			2493	1589	425	466	13			
1	C	331	Total	C	N	O	S	0	1	0
			2504	1599	429	463	13			
1	D	331	Total	C	N	O	S	0	0	0
			2468	1577	420	458	13			
1	E	331	Total	C	N	O	S	0	2	0
			2538	1621	432	472	13			
1	F	331	Total	C	N	O	S	0	2	0
			2550	1628	437	472	13			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 2-{3-[3-(cyclopentylethynyl)-4-fluorophenyl]-5-(cyclopropylmethyl)-4-[(3-fluoro-4-sulfamoylphenyl)methyl]-1H-pyrazol-1-yl}-1,3-thiazole-4-carboxylic acid (CCD ID: P8M) (formula: C₃₁H₂₈F₂N₄O₄S₂) (labeled as "Ligand of Interest" by depositor).



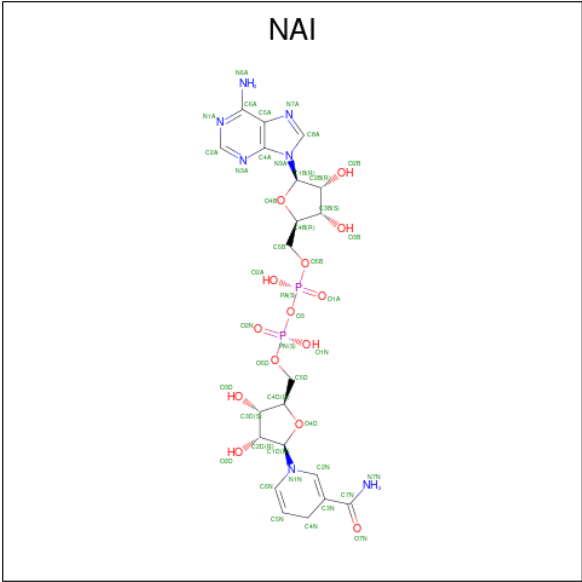
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 43	C 31	F 2	N 4	O 4	S 2	0	0
3	B	1	Total 43	C 31	F 2	N 4	O 4	S 2	0	0
3	C	1	Total 43	C 31	F 2	N 4	O 4	S 2	0	0
3	D	1	Total 43	C 31	F 2	N 4	O 4	S 2	0	0
3	E	1	Total 43	C 31	F 2	N 4	O 4	S 2	0	0

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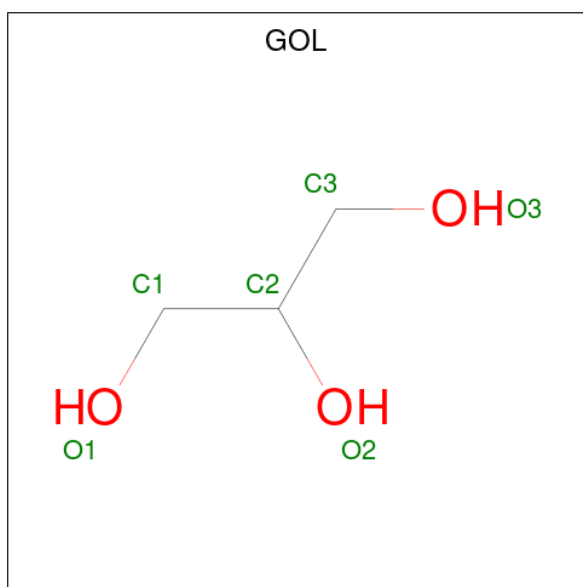
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	F	N	O	S	0
			43	31	2	4	4	2	

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



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		

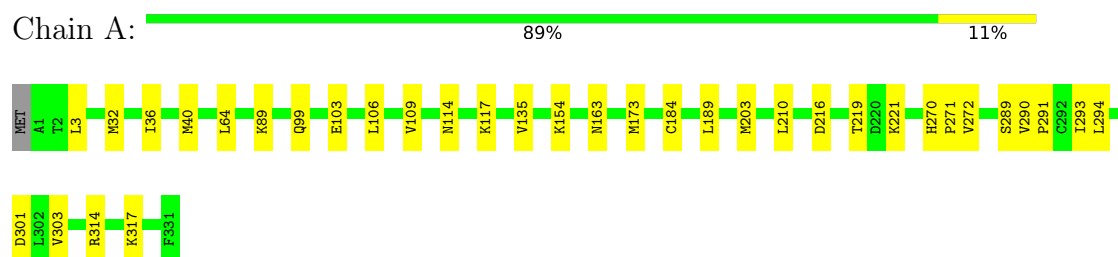
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	118	Total	O	0	0
			118	118		
6	B	121	Total	O	0	0
			121	121		
6	C	83	Total	O	0	0
			83	83		
6	D	86	Total	O	0	0
			86	86		
6	E	164	Total	O	0	0
			164	164		
6	F	182	Total	O	0	0
			182	182		

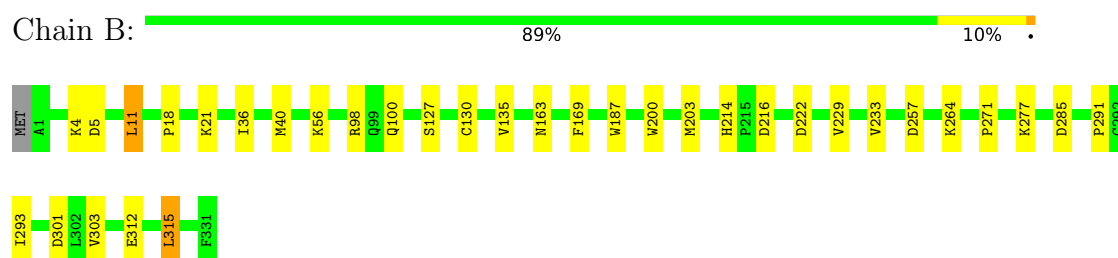
3 Residue-property plots [i](#)

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.

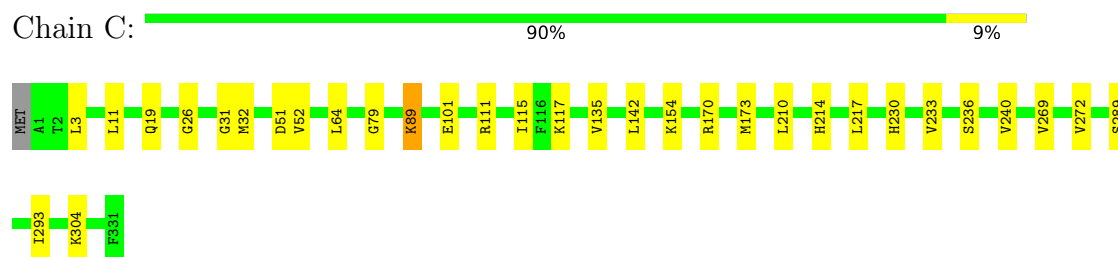
- Molecule 1: L-lactate dehydrogenase A chain



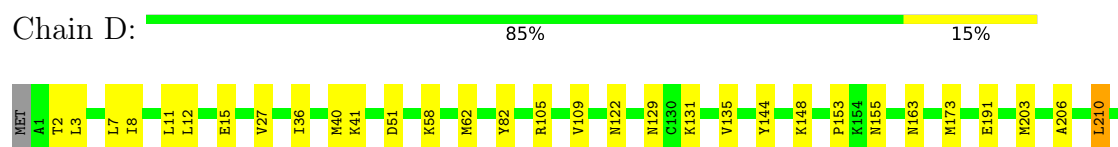
- Molecule 1: L-lactate dehydrogenase A chain

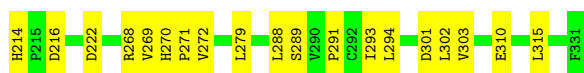


- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain





- Molecule 1: L-lactate dehydrogenase A chain

Chain E: 92% 8%



- Molecule 1: L-lactate dehydrogenase A chain

Chain F: 94% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.04Å 128.07Å 104.14Å 90.00° 119.35° 90.00°	Depositor
Resolution (Å)	46.68 – 2.05 46.68 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.68-2.05) 98.9 (46.68-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.184 , 0.225 0.185 , 0.226	Depositor DCC
R_{free} test set	2014 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.215 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	16383	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, P8M, NAI, GOL

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	0.30	0/2532	0.49	0/3439
1	B	0.29	0/2537	0.48	0/3447
1	C	0.24	0/2548	0.45	0/3460
1	D	0.26	0/2512	0.47	0/3419
1	E	0.33	0/2588	0.54	0/3510
1	F	0.34	0/2600	0.52	0/3522
All	All	0.30	0/15317	0.49	0/20797

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2488	0	2506	21	0
1	B	2493	0	2489	23	0
1	C	2504	0	2522	18	0
1	D	2468	0	2452	30	0
1	E	2538	0	2587	18	0
1	F	2550	0	2613	12	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	43	0	0	1	0
3	B	43	0	0	2	0
3	C	43	0	0	1	0
3	D	43	0	0	3	0
3	E	43	0	0	1	0
3	F	43	0	0	2	0
4	A	44	0	26	2	0
4	B	44	0	26	4	0
4	C	44	0	27	4	0
4	D	44	0	27	4	0
4	E	44	0	27	2	0
4	F	44	0	27	3	0
5	B	6	0	8	0	0
5	C	6	0	8	1	0
5	E	18	0	24	4	0
5	F	6	0	8	0	0
6	A	118	0	0	2	0
6	B	121	0	0	5	0
6	C	83	0	0	2	0
6	D	86	0	0	3	0
6	E	164	0	0	3	0
6	F	182	0	0	4	0
All	All	16383	0	15377	125	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 4.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:GLY:HA2	5:C:500:GOL:H2	1.60	0.83
1:F:293:ILE:HD12	1:F:301:ASP:HB2	1.61	0.82
1:E:200:TRP:CD1	5:E:401:GOL:H32	2.18	0.78
1:E:293:ILE:HD12	1:E:301:ASP:HB2	1.69	0.74
1:B:5:ASP:O	1:C:304:LYS:NZ	2.22	0.73
1:B:293:ILE:HD13	1:B:301:ASP:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:GLN:NE2	1:E:103:GLU:O	2.23	0.71
3:F:502:P8M:C17	4:F:503:NAI:H42N	2.21	0.70
1:D:41:LYS:NZ	6:D:602:HOH:O	2.25	0.68
1:E:148:LYS:NZ	6:E:502:HOH:O	2.28	0.67
1:F:257:ASP:OD2	6:F:601:HOH:O	2.15	0.64
3:A:502:P8M:C17	4:A:503:NAI:H42N	2.29	0.63
3:B:502:P8M:C17	4:B:503:NAI:H42N	2.29	0.62
3:D:502:P8M:C17	4:D:503:NAI:H42N	2.29	0.62
1:A:314:ARG:NH1	6:A:601:HOH:O	2.33	0.61
1:F:55[B]:ASP:OD2	6:F:602:HOH:O	2.16	0.61
1:A:173:MET:HE2	1:A:203:MET:HE3	1.83	0.59
1:D:58:LYS:NZ	1:D:62:MET:SD	2.75	0.59
1:B:291:PRO:HB2	1:B:303:VAL:HB	1.85	0.59
1:C:3:LEU:HD13	1:D:214:HIS:HB2	1.84	0.58
1:A:203:MET:HE2	1:A:210:LEU:HD22	1.84	0.58
1:F:114:ASN:HA	1:F:117:LYS:HD3	1.86	0.58
1:A:291:PRO:HB2	1:A:303:VAL:HB	1.87	0.57
4:C:503:NAI:O2A	6:C:601:HOH:O	2.18	0.56
1:F:279:LEU:HD13	1:F:302:LEU:HD11	1.86	0.56
1:F:83:ASN:ND2	6:F:610:HOH:O	2.40	0.56
1:B:163:ASN:HA	1:B:271:PRO:HG2	1.89	0.55
1:A:216:ASP:O	1:A:219:THR:HG22	2.06	0.55
1:C:115:ILE:HD12	4:C:503:NAI:N7A	2.22	0.54
1:D:216:ASP:HB3	1:D:222:ASP:HA	1.89	0.54
1:D:269:VAL:HG22	1:D:293:ILE:HG13	1.90	0.53
1:B:56:LYS:NZ	6:B:609:HOH:O	2.41	0.52
1:E:114:ASN:HA	1:E:117:LYS:HD3	1.91	0.52
1:A:135:VAL:O	4:A:503:NAI:H2N	2.09	0.52
1:B:4:LYS:NZ	6:B:610:HOH:O	2.43	0.52
1:B:98:ARG:O	1:B:100:GLN:NE2	2.43	0.52
3:C:502:P8M:C17	4:C:503:NAI:H42N	2.40	0.52
4:B:503:NAI:H6N	6:B:692:HOH:O	2.10	0.52
1:F:270:HIS:CD2	1:F:294:LEU:HD12	2.44	0.51
1:A:189:LEU:HD22	1:A:290:VAL:HA	1.93	0.51
1:D:272:VAL:O	1:D:289:SER:HA	2.09	0.51
3:F:502:P8M:C16	4:F:503:NAI:H42N	2.40	0.51
1:D:288:LEU:HD13	1:D:315:LEU:HD22	1.91	0.51
1:A:99:GLN:NE2	1:A:103:GLU:O	2.44	0.51
1:F:135:VAL:O	4:F:503:NAI:H2N	2.12	0.50
1:D:203:MET:HE2	1:D:210:LEU:HD23	1.93	0.50
1:E:18:PRO:HG3	1:E:46:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ASP:OD2	6:B:601:HOH:O	2.19	0.50
1:C:51:ASP:OD1	1:C:52:VAL:N	2.45	0.49
1:A:106:LEU:O	1:A:109:VAL:HG12	2.11	0.49
1:C:32:MET:HE1	1:C:64:LEU:HD11	1.95	0.49
3:D:502:P8M:C16	4:D:503:NAI:H42N	2.42	0.49
1:C:111:ARG:O	1:C:115:ILE:HG12	2.13	0.49
2:C:501:PO4:O2	6:C:602:HOH:O	2.19	0.49
1:E:32:MET:HE1	1:E:64:LEU:HD11	1.94	0.48
1:E:310:GLU:H	1:E:310:GLU:CD	2.20	0.48
1:A:114:ASN:HA	1:A:117:LYS:HD3	1.95	0.48
1:E:56:LYS:NZ	6:E:510:HOH:O	2.45	0.48
1:E:41:LYS:NZ	5:E:402:GOL:O3	2.33	0.48
3:E:405:P8M:C17	4:E:406:NAI:H42N	2.43	0.48
1:E:200:TRP:HD1	5:E:401:GOL:H32	1.73	0.48
1:C:236:SER:O	1:C:240:VAL:HG23	2.13	0.48
1:A:270:HIS:CD2	1:A:294:LEU:HD12	2.48	0.48
1:B:18:PRO:HB2	1:B:21:LYS:HB2	1.96	0.47
1:C:135:VAL:O	4:C:503:NAI:H2N	2.15	0.47
1:F:101:GLU:H	1:F:101:GLU:CD	2.22	0.47
3:B:502:P8M:C16	4:B:503:NAI:H42N	2.45	0.47
1:C:214:HIS:HB2	1:D:3:LEU:HD13	1.96	0.47
1:D:105:ARG:O	1:D:109:VAL:HG23	2.14	0.46
1:B:127:SER:HB3	1:B:130:CYS:HB3	1.97	0.46
1:C:19:GLN:O	1:C:89:LYS:NZ	2.34	0.46
1:B:169:PHE:HD1	1:B:233:VAL:HG21	1.80	0.46
1:E:200:TRP:NE1	5:E:401:GOL:H32	2.29	0.46
1:D:270:HIS:CD2	1:D:294:LEU:HD12	2.51	0.46
1:C:26:GLY:O	1:C:31:GLY:HA3	2.14	0.46
1:D:27:VAL:HG22	1:D:51:ASP:HB2	1.98	0.45
1:A:3:LEU:HD13	1:B:214:HIS:HB2	1.98	0.45
1:A:173:MET:SD	1:A:184:CYS:HB3	2.57	0.45
1:D:7:LEU:HG	1:D:8:ILE:HG13	2.00	0.44
1:D:173:MET:HE2	1:D:203:MET:HE3	1.99	0.44
1:A:32:MET:HE1	1:A:64:LEU:HD11	2.00	0.44
1:D:291:PRO:HB2	1:D:303:VAL:HB	2.00	0.44
1:D:131:LYS:NZ	6:D:608:HOH:O	2.48	0.44
1:B:135:VAL:O	4:B:503:NAI:H2N	2.17	0.44
1:B:36:ILE:O	1:B:40:MET:HG3	2.17	0.44
1:A:272:VAL:O	1:A:289:SER:HA	2.18	0.43
1:E:304:LYS:HE3	1:F:6:GLN:O	2.18	0.43
1:A:219:THR:HG23	1:A:221:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ILE:HD13	1:A:301:ASP:HB2	2.00	0.43
1:D:163:ASN:HA	1:D:271:PRO:HG2	2.01	0.43
1:E:72:ARG:NH1	6:E:517:HOH:O	2.50	0.43
1:D:51:ASP:OD1	4:D:503:NAI:O2B	2.34	0.43
1:D:144:TYR:CZ	1:D:148:LYS:HG3	2.54	0.43
1:D:191:GLU:OE1	3:D:502:P8M:N01	2.52	0.43
1:A:36:ILE:O	1:A:40:MET:HG3	2.19	0.43
1:D:293:ILE:HD13	1:D:301:ASP:HB2	2.01	0.43
1:B:216:ASP:O	1:B:222:ASP:HB2	2.18	0.42
1:D:135:VAL:O	4:D:503:NAI:H2N	2.19	0.42
1:F:264:LYS:HB3	6:F:663:HOH:O	2.18	0.42
1:A:163:ASN:HA	1:A:271:PRO:HG2	2.00	0.42
1:B:264:LYS:NZ	6:B:615:HOH:O	2.48	0.42
1:C:269:VAL:HG22	1:C:293:ILE:HG13	2.00	0.42
1:B:200:TRP:CE3	1:B:203:MET:SD	3.12	0.42
1:E:55[B]:ASP:OD1	1:E:56:LYS:N	2.53	0.42
1:B:277:LYS:HD2	1:B:285:ASP:OD1	2.20	0.42
1:D:153:PRO:HB2	1:D:155:ASN:OD1	2.20	0.42
1:D:279:LEU:HD13	1:D:302:LEU:HD11	2.02	0.42
1:F:191:GLU:O	1:F:196:SER:HB3	2.20	0.42
1:B:187:TRP:CE2	1:D:206:ALA:HA	2.55	0.41
1:B:11:LEU:HD13	1:C:154:LYS:HD2	2.02	0.41
1:D:129:ASN:OD1	6:D:601:HOH:O	2.21	0.41
1:E:30:VAL:HG21	4:E:406:NAI:H6N	2.03	0.41
1:B:315:LEU:HD23	1:B:315:LEU:HA	1.89	0.41
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.89	0.41
1:C:230:HIS:O	1:C:233:VAL:HB	2.21	0.41
1:D:82:TYR:CG	1:D:122:ASN:HB3	2.56	0.41
1:B:187:TRP:CZ2	1:D:206:ALA:HA	2.56	0.41
1:D:36:ILE:O	1:D:40:MET:HG3	2.21	0.41
1:D:15:GLU:CB	1:E:125:LYS:HG3	2.51	0.41
1:C:170:ARG:HA	1:C:173:MET:HE3	2.03	0.40
1:A:89:LYS:HD3	6:A:688:HOH:O	2.21	0.40
1:B:229:VAL:O	1:B:233:VAL:HG23	2.21	0.40
1:E:200:TRP:CE3	1:E:203:MET:SD	3.15	0.40
1:A:317:LYS:HD2	1:A:317:LYS:HA	1.82	0.40
1:C:272:VAL:O	1:C:289:SER:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/332 (99%)	324 (98%)	5 (2%)	0	100	100
1	B	329/332 (99%)	323 (98%)	6 (2%)	0	100	100
1	C	330/332 (99%)	320 (97%)	10 (3%)	0	100	100
1	D	329/332 (99%)	320 (97%)	9 (3%)	0	100	100
1	E	331/332 (100%)	324 (98%)	7 (2%)	0	100	100
1	F	331/332 (100%)	324 (98%)	7 (2%)	0	100	100
All	All	1979/1992 (99%)	1935 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/288 (92%)	265 (100%)	1 (0%)	84	88
1	B	267/288 (93%)	264 (99%)	3 (1%)	65	68
1	C	269/288 (93%)	263 (98%)	6 (2%)	45	44
1	D	261/288 (91%)	255 (98%)	6 (2%)	44	42
1	E	279/288 (97%)	275 (99%)	4 (1%)	59	60
1	F	281/288 (98%)	279 (99%)	2 (1%)	76	80
All	All	1623/1728 (94%)	1601 (99%)	22 (1%)	59	60

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

Mol	Chain	Res	Type
1	A	154	LYS
1	B	11	LEU
1	B	312	GLU
1	B	315	LEU
1	C	11	LEU
1	C	89	LYS
1	C	101	GLU
1	C	117	LYS
1	C	210	LEU
1	C	217	LEU
1	D	2	THR
1	D	11	LEU
1	D	12	LEU
1	D	210	LEU
1	D	268	ARG
1	D	310	GLU
1	E	11	LEU
1	E	75	LYS
1	E	210	LEU
1	E	315	LEU
1	F	11	LEU
1	F	310	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	10	ASN
1	A	87	ASN
1	B	20	ASN
1	C	20	ASN
1	C	214	HIS
1	C	232	GLN
1	D	20	ASN
1	D	326	GLN
1	E	20	ASN
1	E	225	GLN
1	E	232	GLN
1	E	330	GLN
1	F	20	ASN
1	F	100	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 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	$\# Z > 2$
5	GOL	E	401	-	5,5,5	0.35	0	5,5,5	0.85	0
3	P8M	E	405	-	48,48,48	2.29	9 (18%)	60,71,71	1.31	8 (13%)
2	PO4	D	501	-	4,4,4	0.80	0	6,6,6	0.70	0
2	PO4	F	501	-	4,4,4	0.93	0	6,6,6	0.52	0
3	P8M	F	502	-	48,48,48	2.25	6 (12%)	60,71,71	1.30	8 (13%)
3	P8M	D	502	-	48,48,48	2.32	9 (18%)	60,71,71	1.54	9 (15%)
3	P8M	C	502	-	48,48,48	2.27	9 (18%)	60,71,71	1.41	8 (13%)
5	GOL	E	402	-	5,5,5	0.37	0	5,5,5	0.25	0
5	GOL	E	403	-	5,5,5	0.44	0	5,5,5	0.41	0
3	P8M	B	502	-	48,48,48	2.28	6 (12%)	60,71,71	1.42	8 (13%)
4	NAI	B	503	-	47,48,48	3.84	25 (53%)	64,73,73	2.62	14 (21%)
2	PO4	C	501	-	4,4,4	0.95	0	6,6,6	0.47	0
2	PO4	A	501	-	4,4,4	0.85	0	6,6,6	0.56	0
4	NAI	F	503	-	47,48,48	3.82	26 (55%)	64,73,73	2.65	17 (26%)
5	GOL	B	500	-	5,5,5	0.35	0	5,5,5	0.32	0
3	P8M	A	502	-	48,48,48	2.24	9 (18%)	60,71,71	1.45	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAI	D	503	-	47,48,48	3.90	27 (57%)	64,73,73	2.67	18 (28%)
5	GOL	C	500	-	5,5,5	0.31	0	5,5,5	0.36	0
2	PO4	B	501	-	4,4,4	0.86	0	6,6,6	0.91	0
5	GOL	F	500	-	5,5,5	0.39	0	5,5,5	0.17	0
4	NAI	E	406	-	47,48,48	3.84	25 (53%)	64,73,73	2.57	15 (23%)
4	NAI	C	503	-	47,48,48	3.90	26 (55%)	64,73,73	2.69	16 (25%)
2	PO4	E	404	-	4,4,4	1.05	0	6,6,6	0.51	0
4	NAI	A	503	-	47,48,48	3.85	27 (57%)	64,73,73	2.65	20 (31%)

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
5	GOL	E	401	-	-	2/4/4/4	-
3	P8M	E	405	-	-	3/29/40/40	0/6/6/6
4	NAI	B	503	-	-	6/29/72/72	0/5/5/5
5	GOL	F	500	-	-	2/4/4/4	-
5	GOL	B	500	-	-	2/4/4/4	-
3	P8M	A	502	-	-	2/29/40/40	0/6/6/6
3	P8M	F	502	-	-	2/29/40/40	0/6/6/6
4	NAI	E	406	-	-	4/29/72/72	0/5/5/5
3	P8M	D	502	-	-	1/29/40/40	0/6/6/6
4	NAI	C	503	-	-	5/29/72/72	0/5/5/5
3	P8M	C	502	-	-	4/29/40/40	0/6/6/6
5	GOL	E	402	-	-	3/4/4/4	-
4	NAI	D	503	-	-	4/29/72/72	0/5/5/5
5	GOL	E	403	-	-	4/4/4/4	-
3	P8M	B	502	-	-	1/29/40/40	0/6/6/6
5	GOL	C	500	-	-	4/4/4/4	-
4	NAI	A	503	-	-	10/29/72/72	0/5/5/5
4	NAI	F	503	-	-	5/29/72/72	0/5/5/5

All (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	NAI	C3B-C4B	-10.31	1.26	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	NAI	C3B-C4B	-10.28	1.26	1.53
4	A	503	NAI	C3B-C4B	-10.14	1.27	1.53
4	E	406	NAI	C3B-C4B	-10.11	1.27	1.53
4	B	503	NAI	C3B-C4B	-9.83	1.28	1.53
4	F	503	NAI	C3B-C4B	-9.79	1.28	1.53
3	D	502	P8M	O43-S02	8.67	1.59	1.43
3	B	502	P8M	O43-S02	8.60	1.58	1.43
3	B	502	P8M	O03-S02	8.44	1.58	1.43
3	F	502	P8M	O43-S02	8.28	1.58	1.43
3	E	405	P8M	O03-S02	8.25	1.58	1.43
4	B	503	NAI	C2B-C1B	-8.22	1.27	1.53
4	C	503	NAI	C2B-C1B	-8.18	1.27	1.53
4	D	503	NAI	C2B-C1B	-8.13	1.27	1.53
3	F	502	P8M	O03-S02	8.12	1.58	1.43
4	E	406	NAI	C2B-C1B	-8.10	1.28	1.53
3	C	502	P8M	O03-S02	8.04	1.57	1.43
3	A	502	P8M	O43-S02	7.93	1.57	1.43
3	C	502	P8M	O43-S02	7.88	1.57	1.43
4	A	503	NAI	C2B-C1B	-7.87	1.28	1.53
3	D	502	P8M	O03-S02	7.60	1.57	1.43
4	C	503	NAI	C2D-C1D	-7.56	1.29	1.53
4	F	503	NAI	C2B-C1B	-7.55	1.29	1.53
3	A	502	P8M	O03-S02	7.48	1.56	1.43
4	F	503	NAI	C2D-C1D	-7.48	1.30	1.53
3	E	405	P8M	O43-S02	7.47	1.56	1.43
4	A	503	NAI	O4D-C1D	7.47	1.59	1.42
4	A	503	NAI	C2D-C1D	-7.44	1.30	1.53
4	D	503	NAI	O4D-C1D	7.41	1.59	1.42
4	B	503	NAI	C2D-C1D	-7.21	1.30	1.53
4	D	503	NAI	C2D-C1D	-7.21	1.30	1.53
4	E	406	NAI	C2D-C1D	-7.18	1.30	1.53
4	B	503	NAI	O4D-C1D	7.12	1.58	1.42
4	B	503	NAI	C6N-C5N	7.11	1.55	1.33
4	E	406	NAI	O4D-C1D	7.08	1.58	1.42
4	B	503	NAI	C2N-C3N	7.07	1.54	1.35
4	F	503	NAI	C2N-C3N	7.05	1.54	1.35
4	F	503	NAI	O4D-C1D	7.04	1.58	1.42
4	C	503	NAI	C6N-C5N	7.04	1.54	1.33
4	D	503	NAI	C2N-C3N	6.98	1.54	1.35
4	D	503	NAI	C6N-C5N	6.97	1.54	1.33
4	F	503	NAI	C6N-C5N	6.95	1.54	1.33
4	A	503	NAI	C2N-C3N	6.95	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	NAI	C2N-C3N	6.92	1.54	1.35
4	A	503	NAI	C6N-C5N	6.90	1.54	1.33
4	C	503	NAI	O4D-C1D	6.88	1.57	1.42
4	E	406	NAI	C6N-C5N	6.87	1.54	1.33
4	E	406	NAI	C6A-N6A	6.68	1.51	1.34
4	C	503	NAI	C6A-N6A	6.65	1.51	1.34
4	E	406	NAI	C2N-C3N	6.64	1.53	1.35
4	A	503	NAI	C6A-N6A	6.60	1.51	1.34
4	B	503	NAI	C6A-N6A	6.49	1.50	1.34
4	F	503	NAI	C6A-N6A	6.46	1.50	1.34
4	D	503	NAI	C6A-N6A	6.42	1.50	1.34
3	C	502	P8M	C16-C17	6.29	1.54	1.48
4	C	503	NAI	O4D-C4D	-6.05	1.31	1.45
3	F	502	P8M	C16-C17	6.01	1.54	1.48
3	B	502	P8M	C16-C17	5.99	1.54	1.48
4	E	406	NAI	PA-O3	5.99	1.66	1.59
4	A	503	NAI	O4D-C4D	-5.84	1.32	1.45
4	E	406	NAI	O4D-C4D	-5.80	1.32	1.45
4	D	503	NAI	O4D-C4D	-5.74	1.32	1.45
4	F	503	NAI	O4D-C4D	-5.73	1.32	1.45
3	D	502	P8M	C16-C17	5.72	1.53	1.48
4	F	503	NAI	C7N-N7N	5.69	1.49	1.33
3	E	405	P8M	C16-C17	5.67	1.53	1.48
4	C	503	NAI	O4B-C1B	5.59	1.54	1.42
4	B	503	NAI	O4D-C4D	-5.53	1.32	1.45
4	B	503	NAI	C2B-C3B	5.50	1.68	1.53
4	B	503	NAI	O4B-C1B	5.50	1.54	1.42
4	D	503	NAI	O4B-C1B	5.49	1.54	1.42
4	C	503	NAI	C2B-C3B	5.48	1.68	1.53
4	C	503	NAI	O4B-C4B	5.45	1.57	1.45
4	F	503	NAI	C2B-C3B	5.38	1.67	1.53
4	D	503	NAI	C7N-N7N	5.37	1.48	1.33
4	D	503	NAI	O4B-C4B	5.36	1.56	1.45
4	D	503	NAI	C2B-C3B	5.35	1.67	1.53
4	C	503	NAI	C7N-N7N	5.31	1.48	1.33
4	A	503	NAI	C7N-N7N	5.29	1.48	1.33
4	E	406	NAI	O4B-C4B	5.27	1.56	1.45
4	E	406	NAI	C2B-C3B	5.25	1.67	1.53
4	A	503	NAI	C2B-C3B	5.24	1.67	1.53
4	F	503	NAI	PA-O3	5.24	1.65	1.59
4	B	503	NAI	C7N-N7N	5.22	1.48	1.33
4	E	406	NAI	C7N-N7N	5.22	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	NAI	O4B-C4B	5.19	1.56	1.45
4	F	503	NAI	O4B-C4B	5.10	1.56	1.45
4	A	503	NAI	O4B-C4B	5.09	1.56	1.45
4	A	503	NAI	O4B-C1B	5.05	1.53	1.42
4	C	503	NAI	PA-O3	5.03	1.64	1.59
4	E	406	NAI	O4B-C1B	5.01	1.53	1.42
3	A	502	P8M	C16-C17	4.88	1.52	1.48
4	A	503	NAI	PA-O3	4.84	1.64	1.59
4	F	503	NAI	O4B-C1B	4.83	1.53	1.42
4	D	503	NAI	PA-O3	4.64	1.64	1.59
4	B	503	NAI	PA-O3	4.51	1.64	1.59
3	D	502	P8M	S02-N01	4.49	1.69	1.60
3	A	502	P8M	S02-N01	4.44	1.69	1.60
3	A	502	P8M	C05-C04	-4.43	1.36	1.39
3	E	405	P8M	C38-C12	4.37	1.52	1.49
3	B	502	P8M	C20-S21	4.32	1.82	1.71
3	F	502	P8M	C20-S21	4.21	1.82	1.71
3	E	405	P8M	C20-S21	4.17	1.82	1.71
3	D	502	P8M	C20-S21	4.12	1.82	1.71
3	C	502	P8M	C20-S21	4.11	1.82	1.71
3	F	502	P8M	S02-N01	4.07	1.68	1.60
3	C	502	P8M	S02-N01	4.04	1.68	1.60
3	E	405	P8M	S02-N01	3.99	1.68	1.60
4	C	503	NAI	C6N-N1N	3.90	1.46	1.37
4	D	503	NAI	C6N-N1N	3.79	1.46	1.37
4	B	503	NAI	C6N-N1N	3.75	1.46	1.37
4	A	503	NAI	C6N-N1N	3.70	1.46	1.37
3	A	502	P8M	C20-S21	3.68	1.81	1.71
4	F	503	NAI	C6N-N1N	3.58	1.46	1.37
4	F	503	NAI	PN-O3	3.56	1.63	1.59
3	B	502	P8M	S02-N01	3.46	1.67	1.60
4	E	406	NAI	C6N-N1N	3.39	1.45	1.37
3	D	502	P8M	C14-S21	3.37	1.81	1.74
3	D	502	P8M	C05-C04	-3.27	1.36	1.39
4	D	503	NAI	PN-O3	3.27	1.63	1.59
4	D	503	NAI	C7N-C3N	3.15	1.55	1.48
4	B	503	NAI	PN-O3	3.12	1.62	1.59
3	C	502	P8M	C14-S21	3.10	1.80	1.74
4	D	503	NAI	C4N-C5N	3.06	1.57	1.49
4	F	503	NAI	C4N-C5N	3.05	1.56	1.49
4	A	503	NAI	C4N-C5N	2.97	1.56	1.49
3	E	405	P8M	C14-S21	2.97	1.80	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	406	NAI	C4N-C5N	2.95	1.56	1.49
3	B	502	P8M	C14-S21	2.92	1.80	1.74
4	C	503	NAI	PN-O3	2.92	1.62	1.59
3	A	502	P8M	C38-C12	2.92	1.51	1.49
4	B	503	NAI	C4N-C5N	2.90	1.56	1.49
4	E	406	NAI	C5A-C4A	-2.89	1.33	1.39
4	C	503	NAI	O7N-C7N	-2.88	1.17	1.24
4	D	503	NAI	C5A-C4A	-2.86	1.34	1.39
3	D	502	P8M	C14-N15	-2.84	1.25	1.31
4	A	503	NAI	C5A-C4A	-2.83	1.34	1.39
3	A	502	P8M	C14-S21	2.79	1.79	1.74
4	C	503	NAI	C5A-N7A	-2.78	1.34	1.39
4	A	503	NAI	C7N-C3N	2.76	1.54	1.48
4	A	503	NAI	C5A-N7A	-2.75	1.34	1.39
4	E	406	NAI	C8A-N9A	-2.75	1.32	1.37
4	F	503	NAI	O2D-C2D	2.74	1.49	1.43
4	B	503	NAI	C5A-C4A	-2.72	1.34	1.39
4	B	503	NAI	C5A-N7A	-2.71	1.34	1.39
4	C	503	NAI	C5A-C4A	-2.71	1.34	1.39
4	B	503	NAI	O2D-C2D	2.69	1.49	1.43
4	D	503	NAI	C5A-N7A	-2.68	1.34	1.39
4	D	503	NAI	C8A-N9A	-2.65	1.33	1.37
4	C	503	NAI	C4N-C5N	2.61	1.55	1.49
4	F	503	NAI	C5A-N7A	-2.61	1.34	1.39
4	D	503	NAI	O7N-C7N	-2.59	1.18	1.24
4	D	503	NAI	O2D-C2D	2.58	1.49	1.43
4	F	503	NAI	C5A-C4A	-2.57	1.34	1.39
4	E	406	NAI	C7N-C3N	2.55	1.54	1.48
4	A	503	NAI	C4N-C3N	2.54	1.54	1.50
4	E	406	NAI	C5A-N7A	-2.53	1.34	1.39
4	F	503	NAI	C7N-C3N	2.51	1.54	1.48
4	A	503	NAI	C8A-N9A	-2.51	1.33	1.37
4	E	406	NAI	O7N-C7N	-2.47	1.18	1.24
4	A	503	NAI	C2A-N3A	2.44	1.38	1.33
4	A	503	NAI	O2D-C2D	2.44	1.49	1.43
4	B	503	NAI	O7N-C7N	-2.43	1.18	1.24
4	B	503	NAI	C5B-C4B	2.43	1.58	1.51
4	C	503	NAI	O2D-C2D	2.43	1.49	1.43
4	E	406	NAI	O2D-C2D	2.41	1.48	1.43
4	D	503	NAI	C5B-C4B	2.41	1.58	1.51
3	A	502	P8M	C14-N15	-2.41	1.26	1.31
3	E	405	P8M	O18-C17	-2.41	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	406	NAI	C4N-C3N	2.41	1.54	1.50
3	F	502	P8M	C14-S21	2.39	1.79	1.74
4	C	503	NAI	C8A-N9A	-2.39	1.33	1.37
4	C	503	NAI	C7N-C3N	2.38	1.53	1.48
4	B	503	NAI	C8A-N9A	-2.37	1.33	1.37
4	B	503	NAI	C7N-C3N	2.36	1.53	1.48
4	B	503	NAI	O3B-C3B	2.36	1.48	1.43
4	A	503	NAI	C5B-C4B	2.35	1.58	1.51
3	E	405	P8M	C14-N15	-2.33	1.26	1.31
4	D	503	NAI	PN-O5D	2.33	1.68	1.59
4	A	503	NAI	O7N-C7N	-2.30	1.19	1.24
4	C	503	NAI	C5B-C4B	2.30	1.58	1.51
4	F	503	NAI	C8A-N9A	-2.29	1.33	1.37
4	A	503	NAI	PN-O5D	2.26	1.68	1.59
3	C	502	P8M	C14-N15	-2.25	1.26	1.31
4	C	503	NAI	O3D-C3D	-2.25	1.37	1.43
4	D	503	NAI	C2A-N3A	2.24	1.37	1.33
4	F	503	NAI	C2A-N3A	2.22	1.37	1.33
4	E	406	NAI	C2A-N3A	2.21	1.37	1.33
4	F	503	NAI	C5B-C4B	2.20	1.58	1.51
4	E	406	NAI	PN-O3	2.19	1.61	1.59
4	D	503	NAI	O3D-C3D	-2.18	1.37	1.43
4	F	503	NAI	C4N-C3N	2.17	1.54	1.50
4	B	503	NAI	C2A-N3A	2.16	1.37	1.33
4	A	503	NAI	O3B-C3B	2.13	1.48	1.43
3	D	502	P8M	C38-C12	2.10	1.50	1.49
3	C	502	P8M	O18-C17	-2.10	1.24	1.30
4	D	503	NAI	C4N-C3N	2.09	1.54	1.50
4	C	503	NAI	C2A-N3A	2.08	1.37	1.33
4	F	503	NAI	PN-O5D	2.05	1.67	1.59
3	C	502	P8M	C05-C04	-2.05	1.37	1.39
4	F	503	NAI	O3D-C3D	-2.05	1.37	1.43
4	C	503	NAI	O3B-C3B	2.02	1.48	1.43
4	E	406	NAI	C2A-N1A	2.01	1.37	1.33
4	A	503	NAI	O3D-C3D	-2.00	1.38	1.43

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	NAI	N6A-C6A-N1A	-9.98	96.14	118.38
4	C	503	NAI	N6A-C6A-N1A	-9.96	96.18	118.38
4	B	503	NAI	N6A-C6A-N1A	-9.91	96.30	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	503	NAI	N6A-C6A-N1A	-9.79	96.56	118.38
4	A	503	NAI	N6A-C6A-N1A	-9.70	96.77	118.38
4	E	406	NAI	N6A-C6A-N1A	-9.16	97.97	118.38
4	C	503	NAI	C5A-C6A-N6A	8.35	143.95	123.29
4	B	503	NAI	C5A-C6A-N6A	8.24	143.68	123.29
4	D	503	NAI	C5A-C6A-N6A	8.14	143.44	123.29
4	F	503	NAI	C5A-C6A-N6A	7.93	142.92	123.29
4	A	503	NAI	C5A-C6A-N6A	7.91	142.87	123.29
4	E	406	NAI	C5A-C6A-N6A	7.76	142.51	123.29
4	D	503	NAI	C4A-N9A-C1B	-6.77	110.80	126.63
4	C	503	NAI	C4A-N9A-C1B	-6.75	110.86	126.63
4	B	503	NAI	C4A-N9A-C1B	-6.41	111.64	126.63
4	E	406	NAI	C4A-N9A-C1B	-6.29	111.92	126.63
3	D	502	P8M	O19-C17-C16	-6.28	112.10	122.02
4	F	503	NAI	N3A-C2A-N1A	-6.10	119.35	128.58
4	A	503	NAI	C4A-N9A-C1B	-5.97	112.67	126.63
4	D	503	NAI	N3A-C2A-N1A	-5.88	119.68	128.58
4	A	503	NAI	N3A-C2A-N1A	-5.81	119.79	128.58
4	F	503	NAI	C5A-C4A-N3A	-5.59	119.02	126.72
4	C	503	NAI	N3A-C2A-N1A	-5.53	120.22	128.58
4	C	503	NAI	C1B-N9A-C8A	5.50	139.31	127.09
4	D	503	NAI	C1B-N9A-C8A	5.50	139.29	127.09
4	E	406	NAI	N3A-C2A-N1A	-5.45	120.34	128.58
3	B	502	P8M	O19-C17-C16	-5.40	113.50	122.02
4	B	503	NAI	N3A-C2A-N1A	-5.40	120.41	128.58
4	F	503	NAI	C4A-N9A-C1B	-5.36	114.10	126.63
3	A	502	P8M	O19-C17-C16	-5.29	113.66	122.02
4	A	503	NAI	C5A-C4A-N3A	-5.25	119.49	126.72
4	B	503	NAI	C1B-N9A-C8A	5.19	138.60	127.09
4	C	503	NAI	N9A-C8A-N7A	-5.17	106.60	113.94
4	B	503	NAI	C5A-C4A-N3A	-5.01	119.82	126.72
3	F	502	P8M	O19-C17-C16	-4.98	114.16	122.02
4	F	503	NAI	N3A-C4A-N9A	4.97	135.61	127.17
4	B	503	NAI	N9A-C8A-N7A	-4.94	106.93	113.94
4	D	503	NAI	N9A-C8A-N7A	-4.89	107.00	113.94
3	E	405	P8M	O19-C17-C16	-4.88	114.31	122.02
4	A	503	NAI	N9A-C8A-N7A	-4.87	107.03	113.94
4	E	406	NAI	N9A-C8A-N7A	-4.87	107.03	113.94
4	C	503	NAI	C5A-C4A-N3A	-4.87	120.01	126.72
4	F	503	NAI	N9A-C8A-N7A	-4.82	107.10	113.94
3	C	502	P8M	O19-C17-C16	-4.81	114.42	122.02
4	D	503	NAI	C5A-C4A-N3A	-4.80	120.11	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	406	NAI	C1B-N9A-C8A	4.73	137.60	127.09
4	A	503	NAI	C1B-N9A-C8A	4.71	137.55	127.09
4	A	503	NAI	N3A-C4A-N9A	4.58	134.95	127.17
4	E	406	NAI	C4A-N9A-C8A	4.50	110.47	105.74
4	E	406	NAI	C5A-C4A-N3A	-4.48	120.55	126.72
4	E	406	NAI	N3A-C4A-N9A	4.37	134.61	127.17
4	B	503	NAI	N3A-C4A-N9A	4.20	134.31	127.17
4	D	503	NAI	N3A-C4A-N9A	4.15	134.23	127.17
4	C	503	NAI	N3A-C4A-N9A	4.09	134.12	127.17
4	F	503	NAI	C1B-N9A-C8A	4.07	136.13	127.09
4	D	503	NAI	C4A-N9A-C8A	3.95	109.88	105.74
4	C	503	NAI	C4A-N9A-C8A	3.90	109.83	105.74
4	B	503	NAI	C4B-O4B-C1B	-3.82	101.03	109.47
3	C	502	P8M	O43-S02-C04	3.82	112.81	107.26
4	B	503	NAI	C4A-N9A-C8A	3.77	109.70	105.74
4	A	503	NAI	C4A-N9A-C8A	3.76	109.68	105.74
4	F	503	NAI	C4A-N9A-C8A	3.74	109.67	105.74
4	C	503	NAI	C4B-O4B-C1B	-3.71	101.27	109.47
4	E	406	NAI	C4B-O4B-C1B	-3.64	101.44	109.47
3	D	502	P8M	C06-C05-C04	-3.59	120.98	122.66
3	A	502	P8M	O43-S02-C04	3.59	112.47	107.26
3	E	405	P8M	C09-C04-C05	3.58	120.86	118.53
4	F	503	NAI	C2A-N3A-C4A	3.58	120.56	111.83
4	F	503	NAI	C4B-O4B-C1B	-3.57	101.57	109.47
3	A	502	P8M	C09-C04-C05	3.55	120.84	118.53
3	D	502	P8M	C09-C04-C05	3.54	120.83	118.53
4	D	503	NAI	C4B-O4B-C1B	-3.52	101.69	109.47
3	C	502	P8M	C06-C05-C04	-3.51	121.02	122.66
3	B	502	P8M	O03-S02-C04	-3.46	102.23	107.26
4	C	503	NAI	C5A-N7A-C8A	3.46	108.89	103.45
4	D	503	NAI	C2B-C1B-N9A	-3.45	104.73	113.30
3	B	502	P8M	C06-C05-C04	-3.45	121.05	122.66
4	E	406	NAI	C2B-C1B-N9A	-3.34	105.01	113.30
3	A	502	P8M	O18-C17-O19	3.33	131.83	123.90
3	D	502	P8M	O43-S02-C04	3.27	112.01	107.26
3	D	502	P8M	O18-C17-O19	3.25	131.63	123.90
3	B	502	P8M	O18-C17-O19	3.23	131.60	123.90
3	B	502	P8M	O43-S02-C04	3.21	111.92	107.26
4	F	503	NAI	O4B-C1B-C2B	-3.20	99.77	106.62
3	F	502	P8M	C06-C05-C04	-3.19	121.17	122.66
4	D	503	NAI	C2A-N3A-C4A	3.18	119.60	111.83
3	D	502	P8M	C14-N15-C16	3.18	114.38	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	P8M	C09-C04-C05	3.18	120.60	118.53
4	A	503	NAI	C2A-N3A-C4A	3.13	119.47	111.83
4	B	503	NAI	C5A-N7A-C8A	3.13	108.36	103.45
4	F	503	NAI	C5A-N7A-C8A	3.08	108.30	103.45
4	B	503	NAI	C2B-C1B-N9A	-3.06	105.70	113.30
4	A	503	NAI	C5A-N7A-C8A	3.04	108.22	103.45
4	D	503	NAI	C5A-N7A-C8A	3.03	108.21	103.45
4	C	503	NAI	C2A-N3A-C4A	3.02	119.21	111.83
4	A	503	NAI	C4B-O4B-C1B	-3.01	102.82	109.47
4	B	503	NAI	C2A-N3A-C4A	3.00	119.17	111.83
3	E	405	P8M	O18-C17-O19	2.97	130.97	123.90
3	A	502	P8M	C06-C05-C04	-2.97	121.27	122.66
3	C	502	P8M	O18-C17-O19	2.90	130.81	123.90
3	F	502	P8M	O18-C17-O19	2.90	130.81	123.90
4	A	503	NAI	C2B-C1B-N9A	-2.87	106.16	113.30
3	A	502	P8M	C14-N15-C16	2.84	113.58	106.79
3	E	405	P8M	C14-N15-C16	2.83	113.56	106.79
4	F	503	NAI	C2B-C1B-N9A	-2.83	106.28	113.30
4	E	406	NAI	C6A-C5A-C4A	2.81	121.01	117.18
3	D	502	P8M	C04-S02-N01	-2.81	103.23	108.28
4	E	406	NAI	C5A-N7A-C8A	2.81	107.86	103.45
3	C	502	P8M	C14-N15-C16	2.80	113.48	106.79
3	B	502	P8M	C09-C04-C05	2.73	120.31	118.53
4	A	503	NAI	C6A-C5A-C4A	2.73	120.90	117.18
3	F	502	P8M	C14-N15-C16	2.72	113.28	106.79
4	E	406	NAI	O4D-C1D-C2D	-2.70	100.83	106.62
4	E	406	NAI	C2A-N3A-C4A	2.63	118.26	111.83
4	B	503	NAI	C6A-C5A-C4A	2.62	120.76	117.18
3	B	502	P8M	C14-N15-C16	2.60	113.00	106.79
3	F	502	P8M	O43-S02-C04	2.59	111.03	107.26
3	F	502	P8M	C09-C04-C05	2.59	120.22	118.53
4	A	503	NAI	O4B-C1B-C2B	-2.57	101.13	106.62
4	A	503	NAI	O1N-PN-O3	2.55	114.16	107.27
3	C	502	P8M	O03-S02-C04	-2.53	103.58	107.26
4	C	503	NAI	C6A-C5A-C4A	2.53	120.63	117.18
4	F	503	NAI	C6A-C5A-C4A	2.51	120.60	117.18
3	B	502	P8M	C20-S21-C14	-2.48	85.20	89.41
4	F	503	NAI	O1N-PN-O3	2.47	113.96	107.27
3	E	405	P8M	C06-C05-C04	-2.46	121.51	122.66
3	D	502	P8M	C05-C04-S02	-2.39	119.67	121.21
4	A	503	NAI	O4B-C1B-N9A	2.37	112.64	108.09
3	C	502	P8M	C20-S21-C14	-2.37	85.39	89.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	P8M	O03-S02-C04	-2.35	103.84	107.26
3	E	405	P8M	O43-S02-C04	2.35	110.67	107.26
3	E	405	P8M	C20-S21-C14	-2.29	85.52	89.41
4	D	503	NAI	C3B-C2B-C1B	2.27	105.75	101.46
4	A	503	NAI	C3B-C2B-C1B	2.23	105.67	101.46
4	C	503	NAI	O4D-C1D-N1N	2.19	112.27	108.08
4	A	503	NAI	C1D-N1N-C2N	-2.19	117.53	121.14
3	F	502	P8M	C20-S21-C14	-2.18	85.71	89.41
3	F	502	P8M	O03-S02-C04	-2.18	104.09	107.26
4	C	503	NAI	C4D-O4D-C1D	-2.17	104.68	109.47
4	D	503	NAI	C6A-C5A-C4A	2.15	120.11	117.18
4	D	503	NAI	C2B-C3B-C4B	2.12	106.71	102.61
4	D	503	NAI	C1D-N1N-C2N	-2.12	117.65	121.14
3	D	502	P8M	C20-S21-C14	-2.12	85.81	89.41
4	C	503	NAI	C3N-C2N-N1N	-2.11	120.11	123.20
3	A	502	P8M	O03-S02-N01	2.09	110.37	107.35
4	D	503	NAI	C4D-O4D-C1D	-2.06	104.91	109.47
3	E	405	P8M	C04-S02-N01	-2.04	104.61	108.28
4	F	503	NAI	C4D-O4D-C1D	-2.03	104.98	109.47
4	A	503	NAI	O4B-C4B-C5B	-2.02	102.86	109.33

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	P8M	C26-C27-C28-C29
5	B	500	GOL	O1-C1-C2-O2
5	B	500	GOL	O1-C1-C2-C3
5	C	500	GOL	C1-C2-C3-O3
5	E	403	GOL	O1-C1-C2-C3
5	E	403	GOL	C1-C2-C3-O3
5	F	500	GOL	O1-C1-C2-C3
5	C	500	GOL	O1-C1-C2-O2
5	E	402	GOL	O1-C1-C2-O2
5	C	500	GOL	O1-C1-C2-C3
5	E	401	GOL	O1-C1-C2-C3
5	E	402	GOL	O1-C1-C2-C3
5	E	403	GOL	O2-C2-C3-O3
3	C	502	P8M	C34-C26-C27-C28
3	E	405	P8M	C34-C26-C27-C28
5	E	403	GOL	O1-C1-C2-O2
5	F	500	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	503	NAI	C2D-C1D-N1N-C2N
4	A	503	NAI	C2D-C1D-N1N-C6N
3	C	502	P8M	C25-C26-C27-C28
3	E	405	P8M	C25-C26-C27-C28
4	C	503	NAI	C2B-C1B-N9A-C8A
4	E	406	NAI	C2B-C1B-N9A-C8A
3	C	502	P8M	C26-C27-C28-C29
3	D	502	P8M	C26-C27-C28-C29
3	F	502	P8M	C26-C27-C28-C29
4	B	503	NAI	C2D-C1D-N1N-C2N
4	F	503	NAI	C2D-C1D-N1N-C2N
3	B	502	P8M	N15-C14-N13-N22
4	A	503	NAI	C5B-O5B-PA-O2A
4	A	503	NAI	O4D-C1D-N1N-C6N
4	A	503	NAI	O4D-C1D-N1N-C2N
4	A	503	NAI	C2B-C1B-N9A-C8A
4	B	503	NAI	C2B-C1B-N9A-C8A
4	F	503	NAI	C2B-C1B-N9A-C8A
4	C	503	NAI	C2D-C1D-N1N-C2N
4	B	503	NAI	O4D-C1D-N1N-C2N
4	F	503	NAI	O4D-C1D-N1N-C2N
4	D	503	NAI	O4D-C1D-N1N-C2N
4	E	406	NAI	O4D-C1D-N1N-C2N
4	D	503	NAI	C2D-C1D-N1N-C2N
5	C	500	GOL	O2-C2-C3-O3
5	E	401	GOL	O1-C1-C2-O2
4	A	503	NAI	C2N-C3N-C7N-N7N
4	B	503	NAI	C2N-C3N-C7N-N7N
4	C	503	NAI	O4D-C1D-N1N-C2N
4	C	503	NAI	C2N-C3N-C7N-N7N
4	B	503	NAI	C2D-C1D-N1N-C6N
4	F	503	NAI	C2D-C1D-N1N-C6N
4	A	503	NAI	PA-O3-PN-O1N
4	E	406	NAI	C2D-C1D-N1N-C2N
5	E	402	GOL	C1-C2-C3-O3
4	C	503	NAI	C2D-C1D-N1N-C6N
4	A	503	NAI	O4B-C4B-C5B-O5B
4	D	503	NAI	O4B-C4B-C5B-O5B
4	D	503	NAI	C2B-C1B-N9A-C8A
4	A	503	NAI	C3B-C4B-C5B-O5B
4	F	503	NAI	O4D-C1D-N1N-C6N
4	B	503	NAI	O4D-C1D-N1N-C6N

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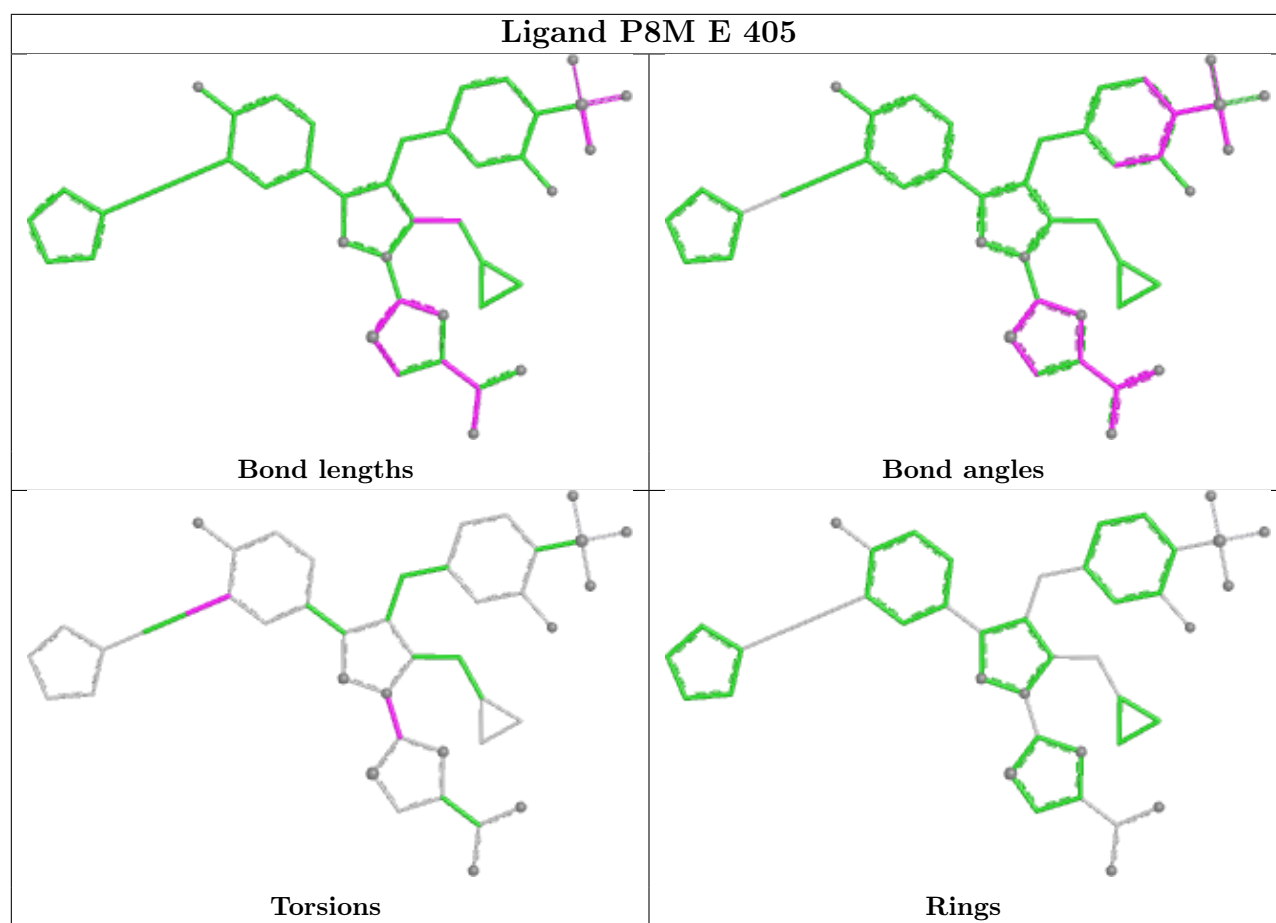
Mol	Chain	Res	Type	Atoms
3	A	502	P8M	N15-C14-N13-N22
3	C	502	P8M	N15-C14-N13-N22
3	E	405	P8M	N15-C14-N13-N22
3	F	502	P8M	N15-C14-N13-N22
4	E	406	NAI	O4B-C4B-C5B-O5B

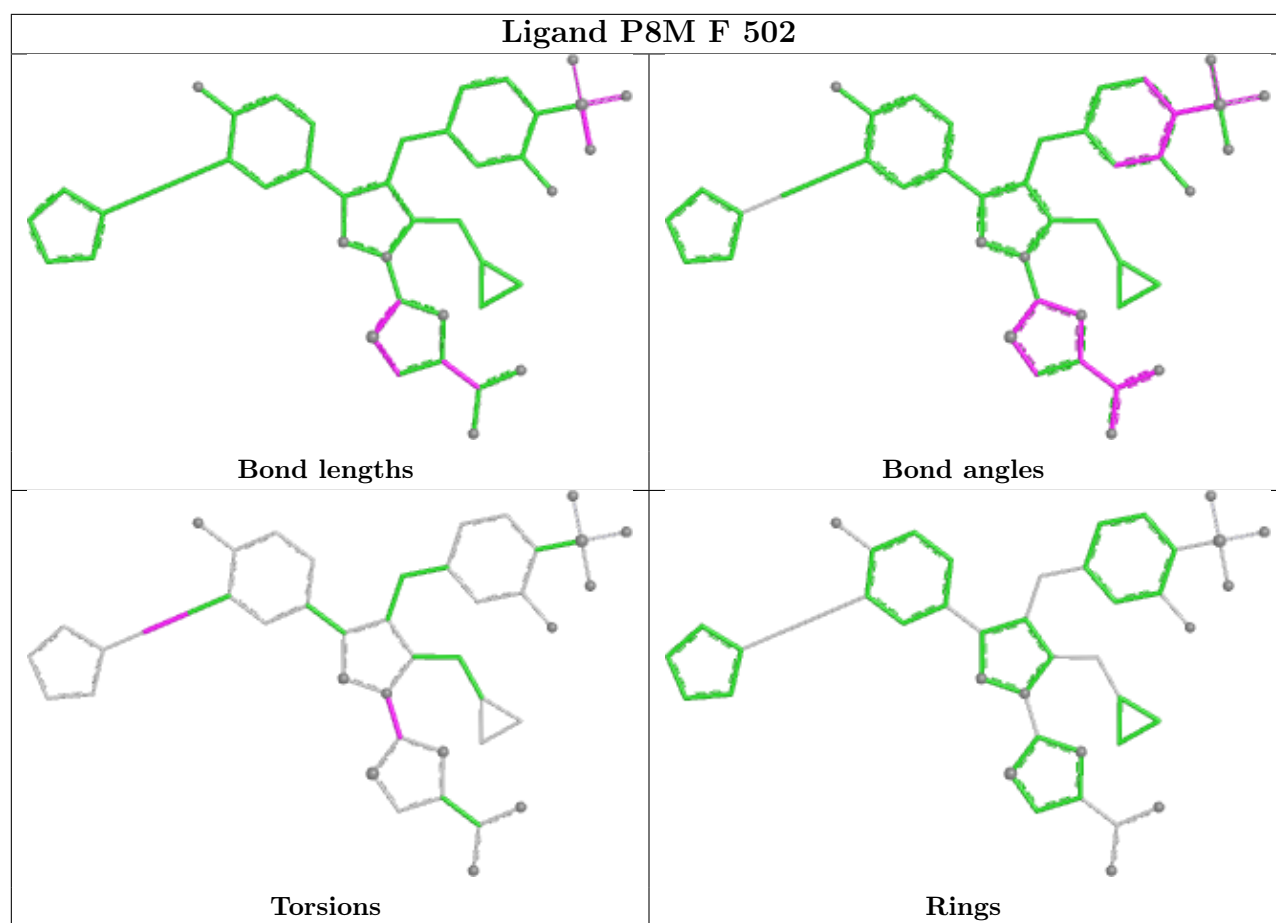
There are no ring outliers.

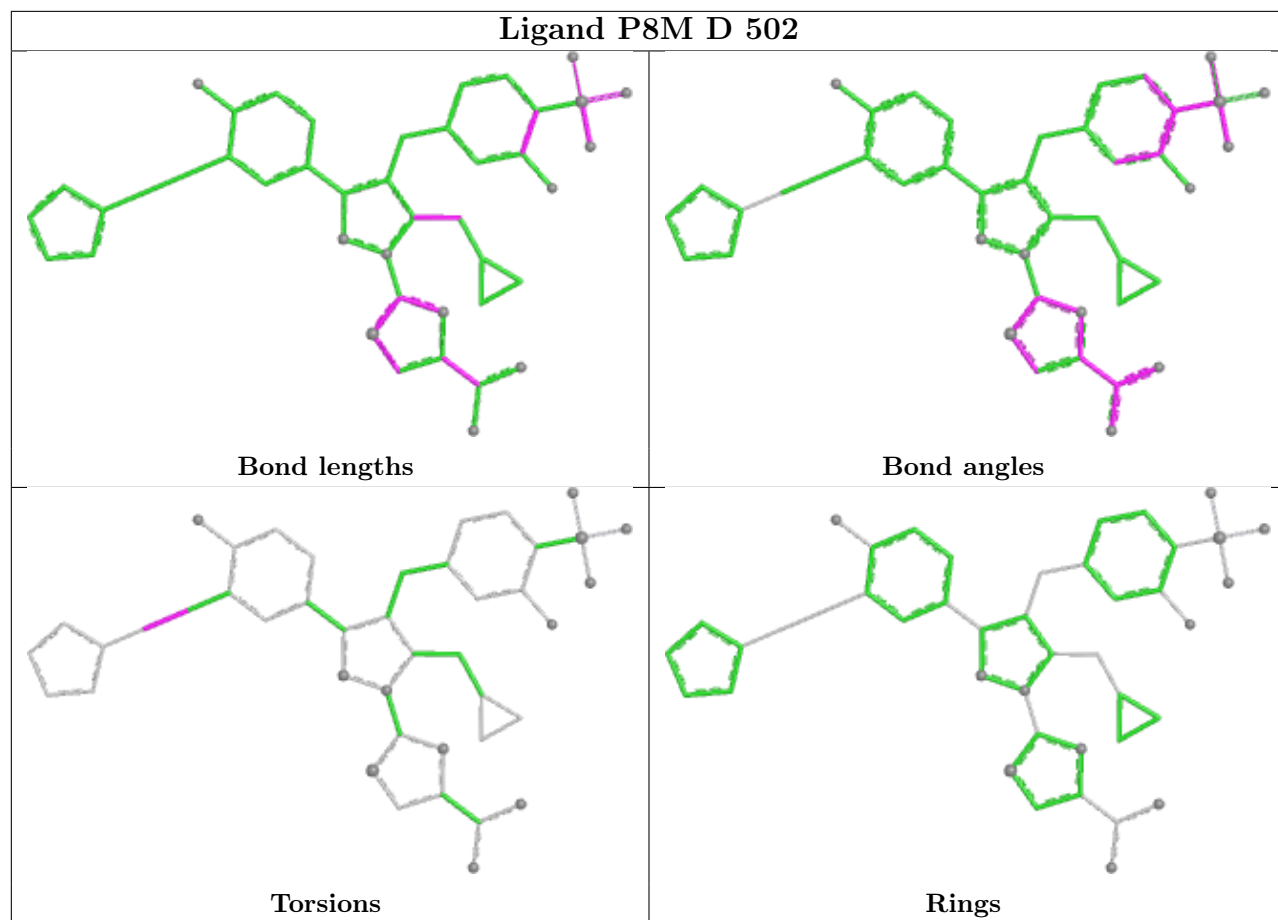
16 monomers are involved in 26 short contacts:

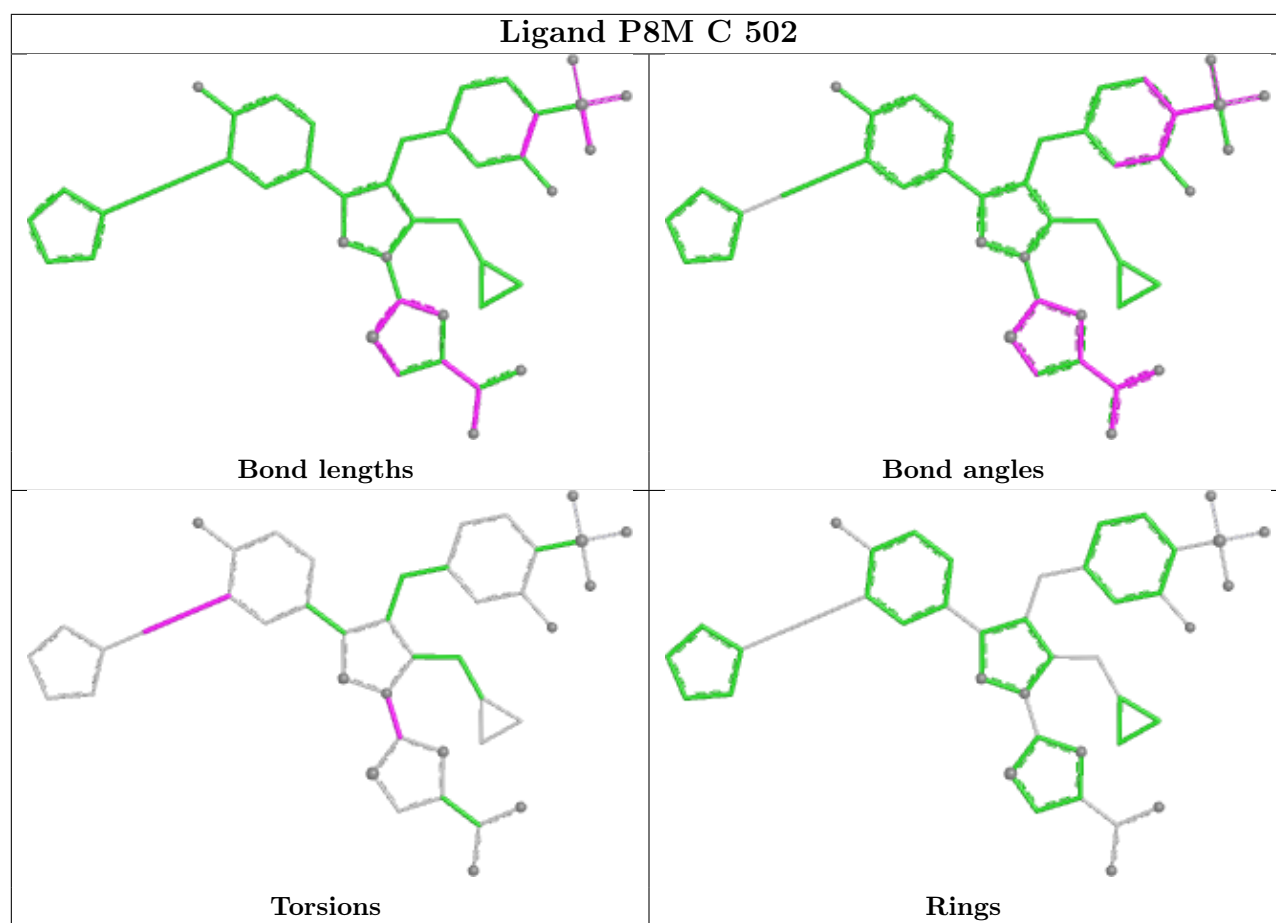
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	401	GOL	3	0
3	E	405	P8M	1	0
3	F	502	P8M	2	0
3	D	502	P8M	3	0
3	C	502	P8M	1	0
5	E	402	GOL	1	0
3	B	502	P8M	2	0
4	B	503	NAI	4	0
2	C	501	PO4	1	0
4	F	503	NAI	3	0
3	A	502	P8M	1	0
4	D	503	NAI	4	0
5	C	500	GOL	1	0
4	E	406	NAI	2	0
4	C	503	NAI	4	0
4	A	503	NAI	2	0

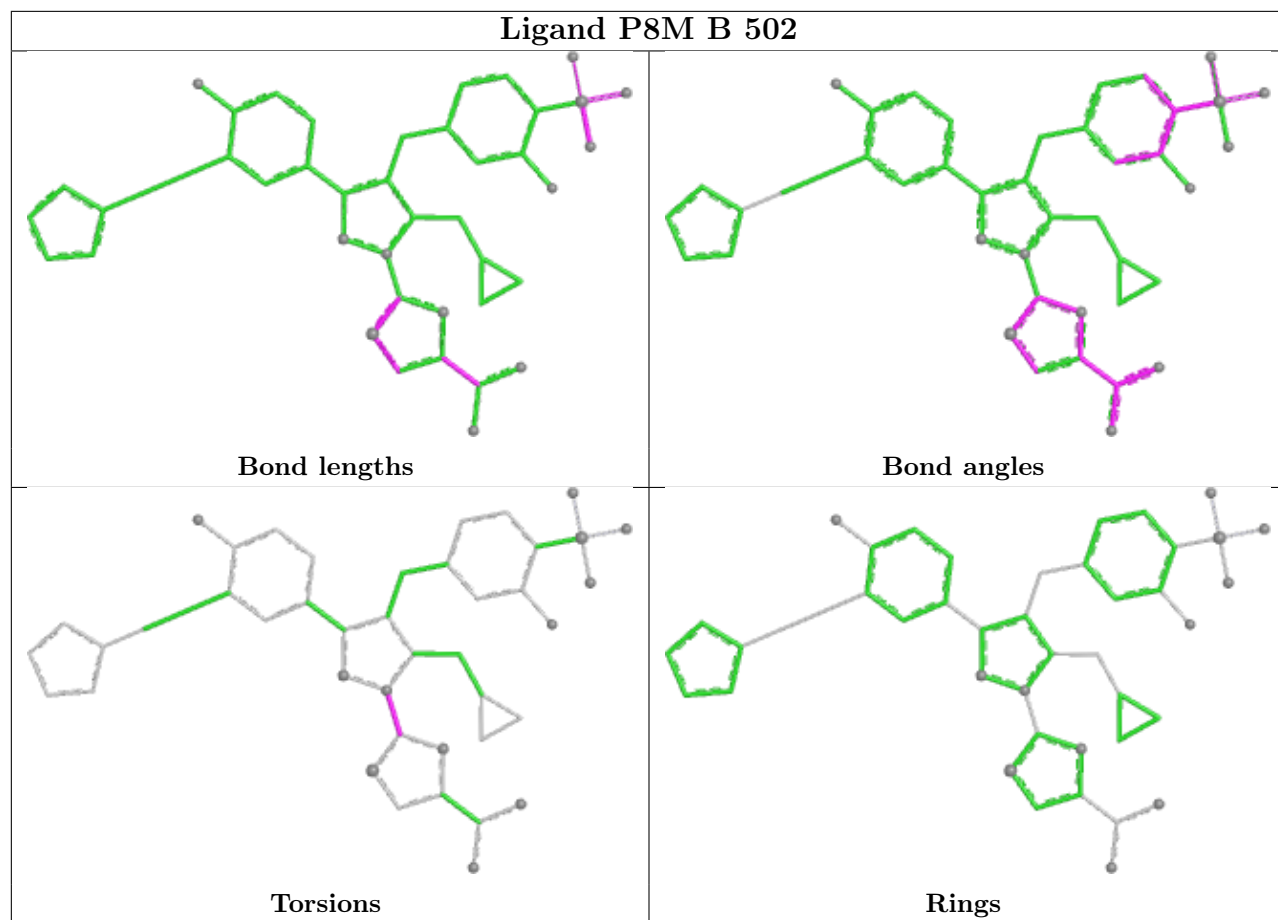
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



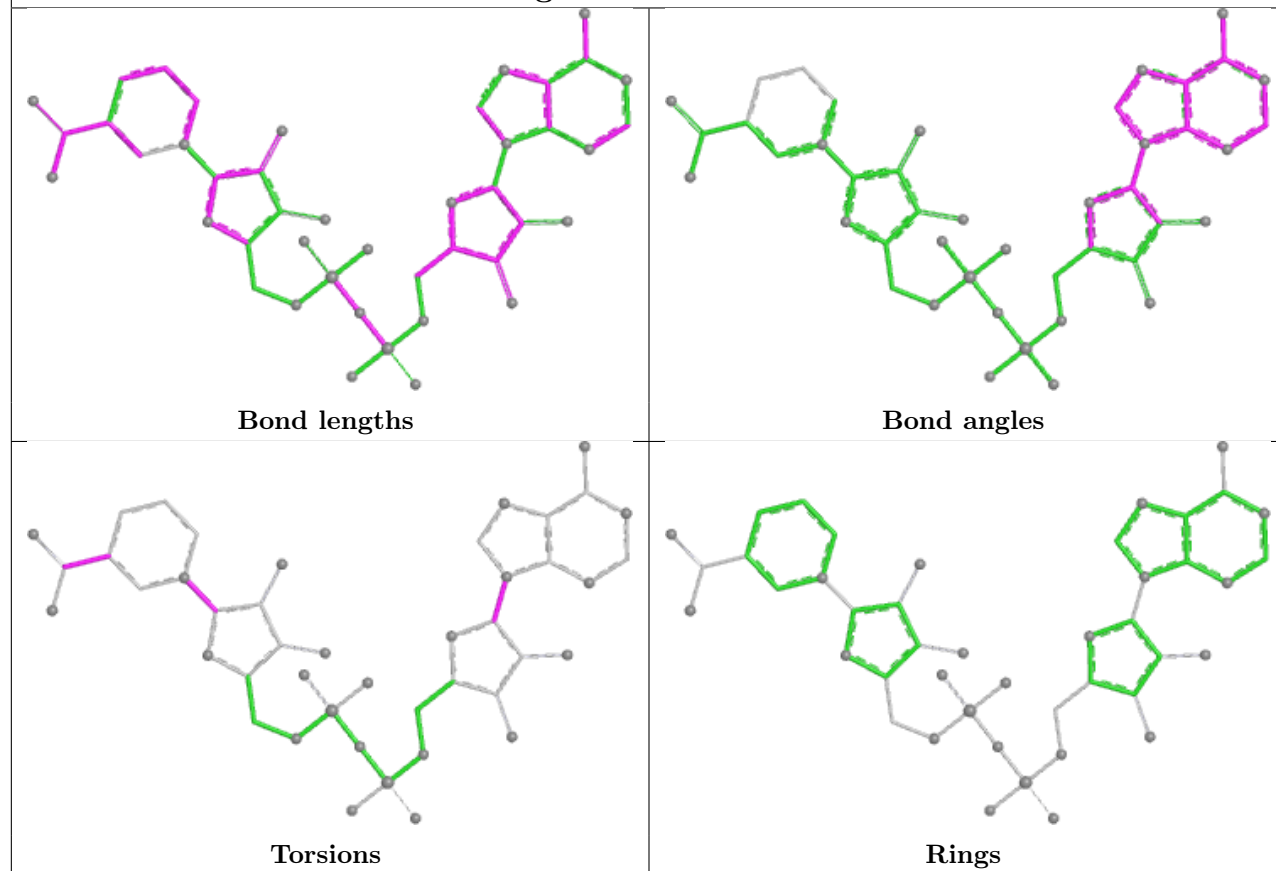




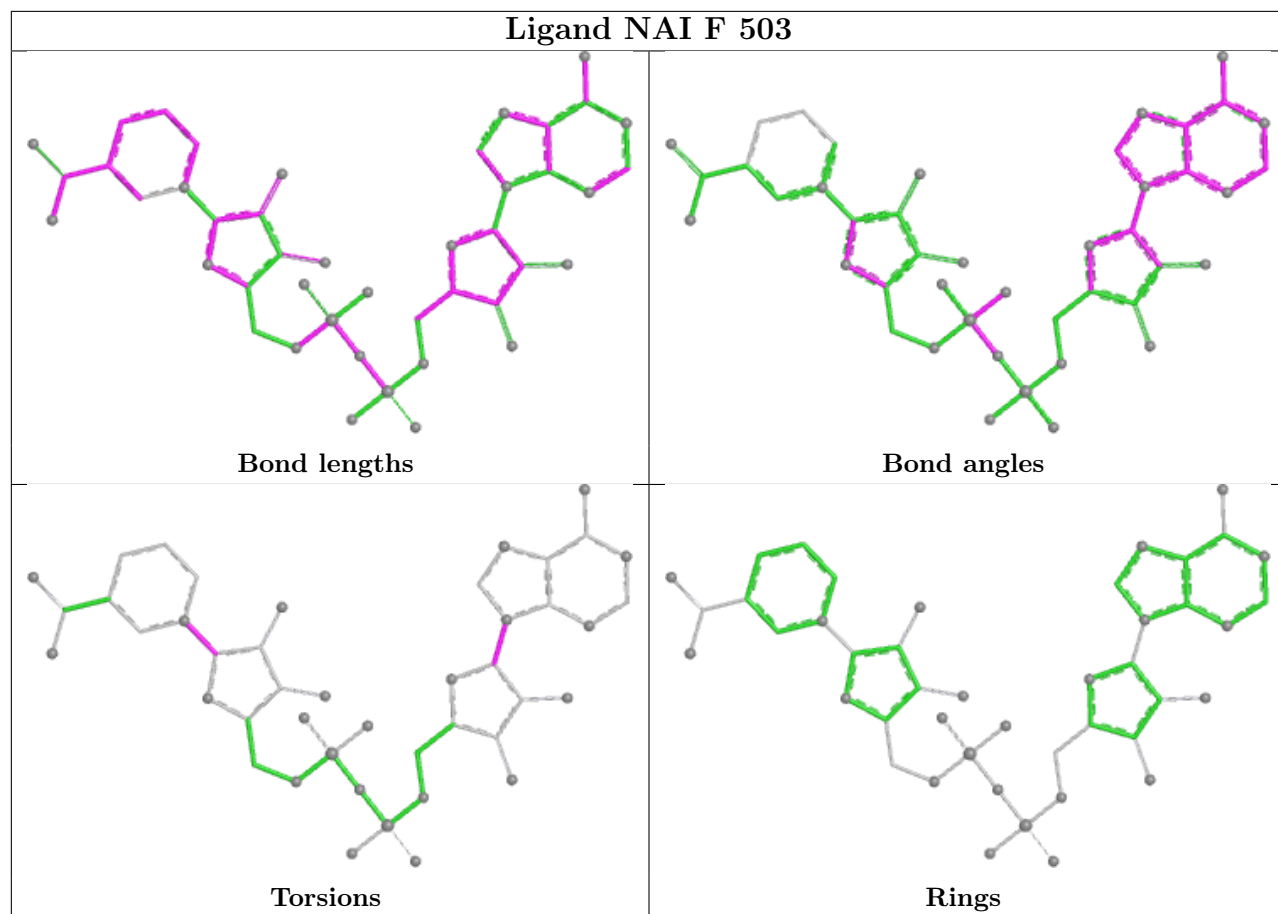


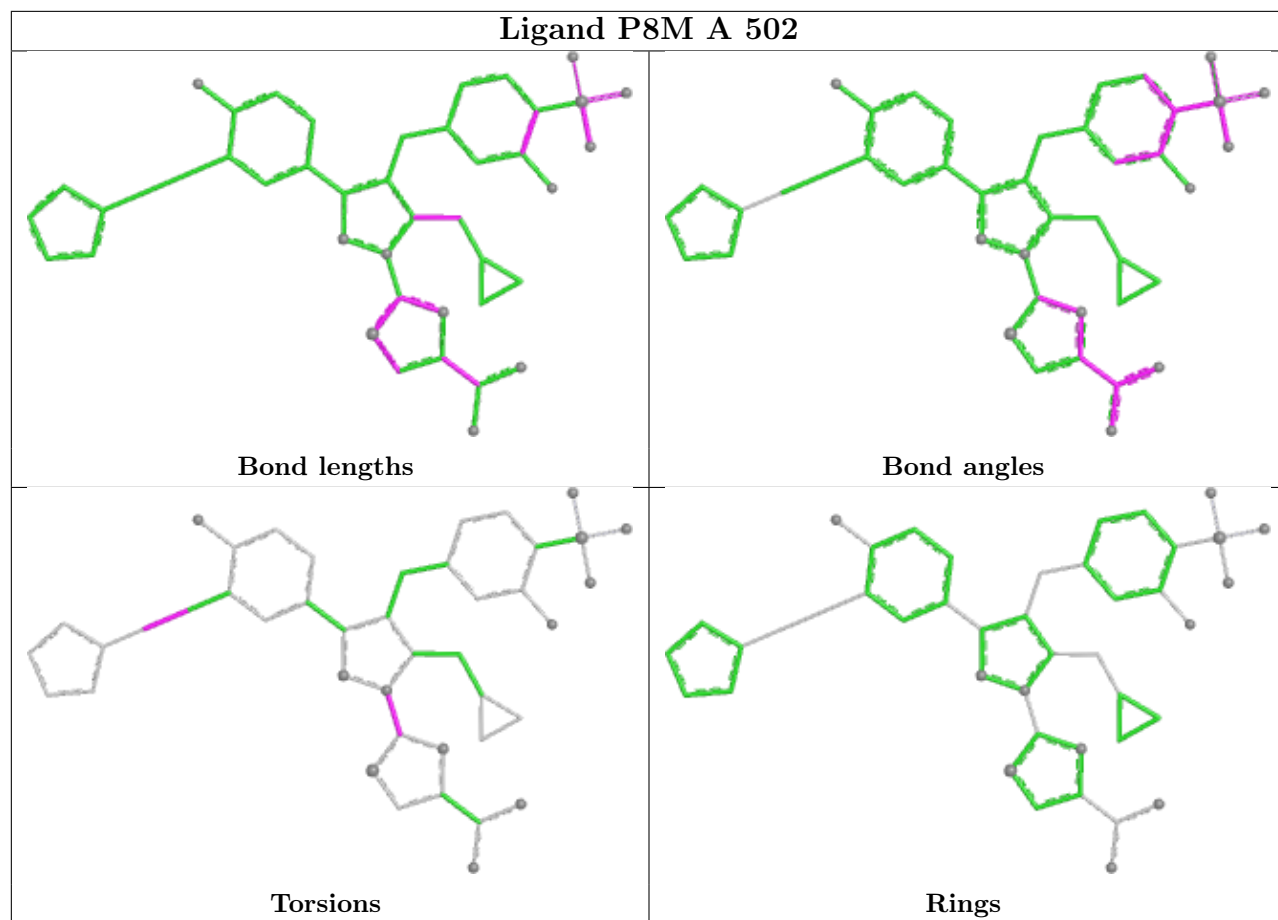


Ligand NAI B 503

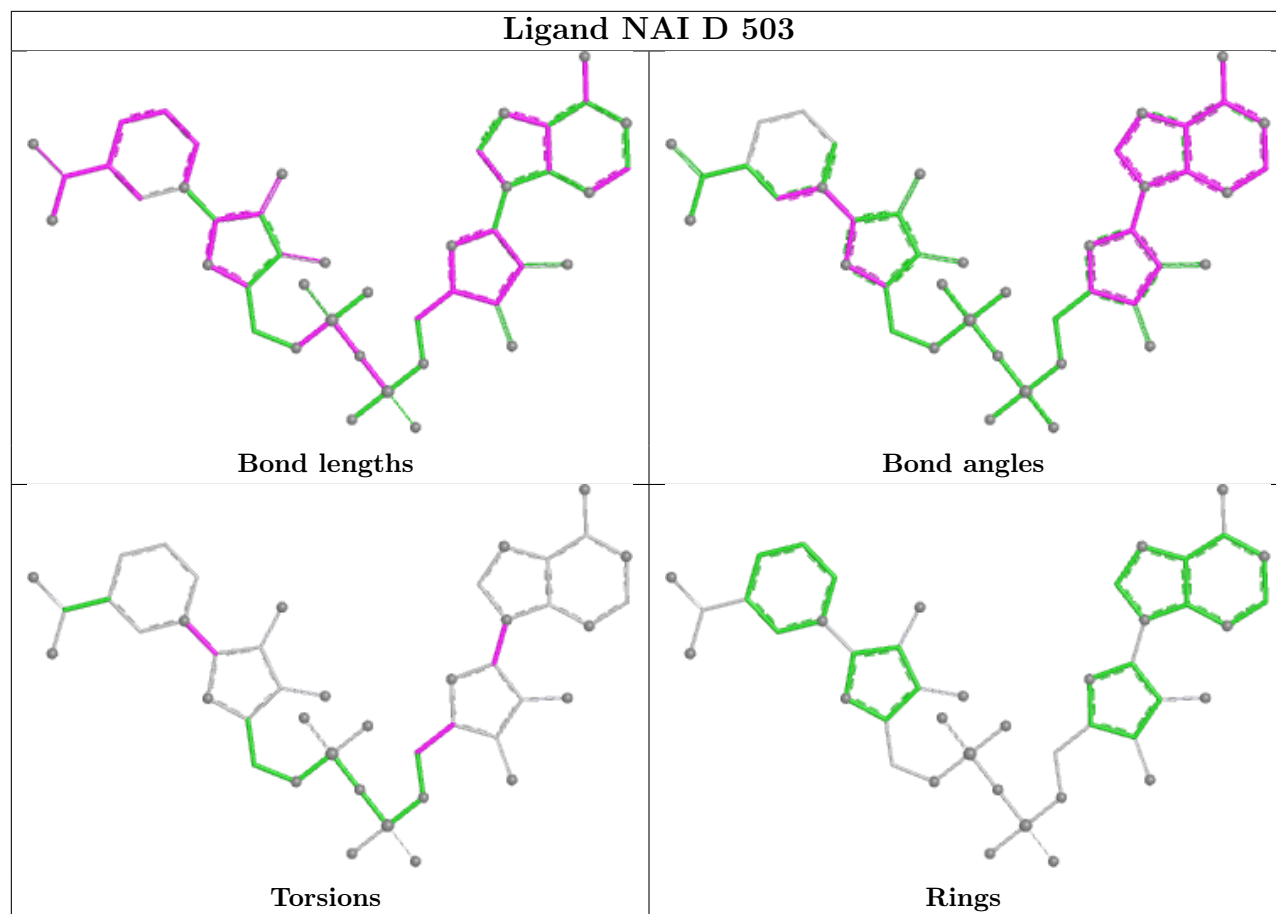


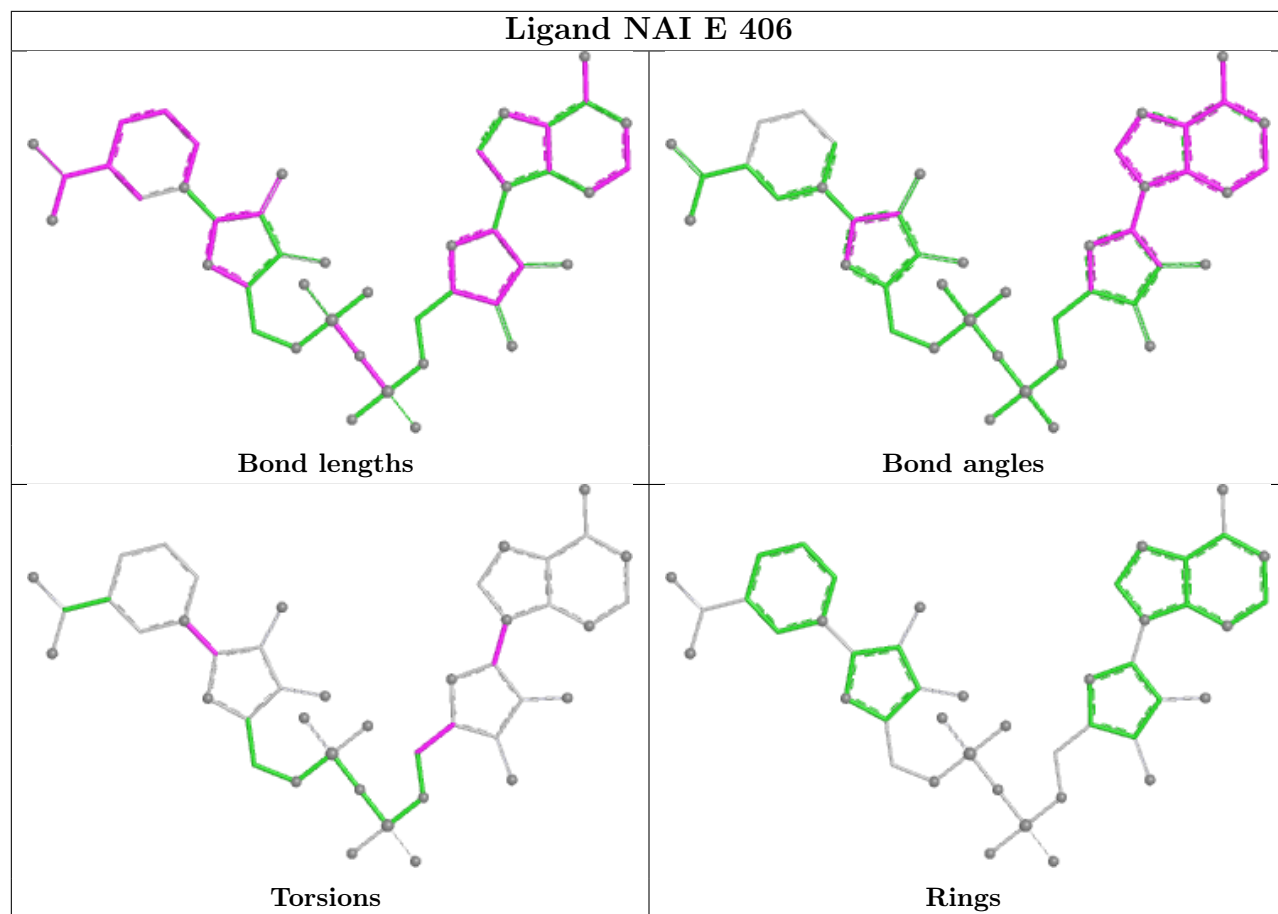
Ligand NAI F 503



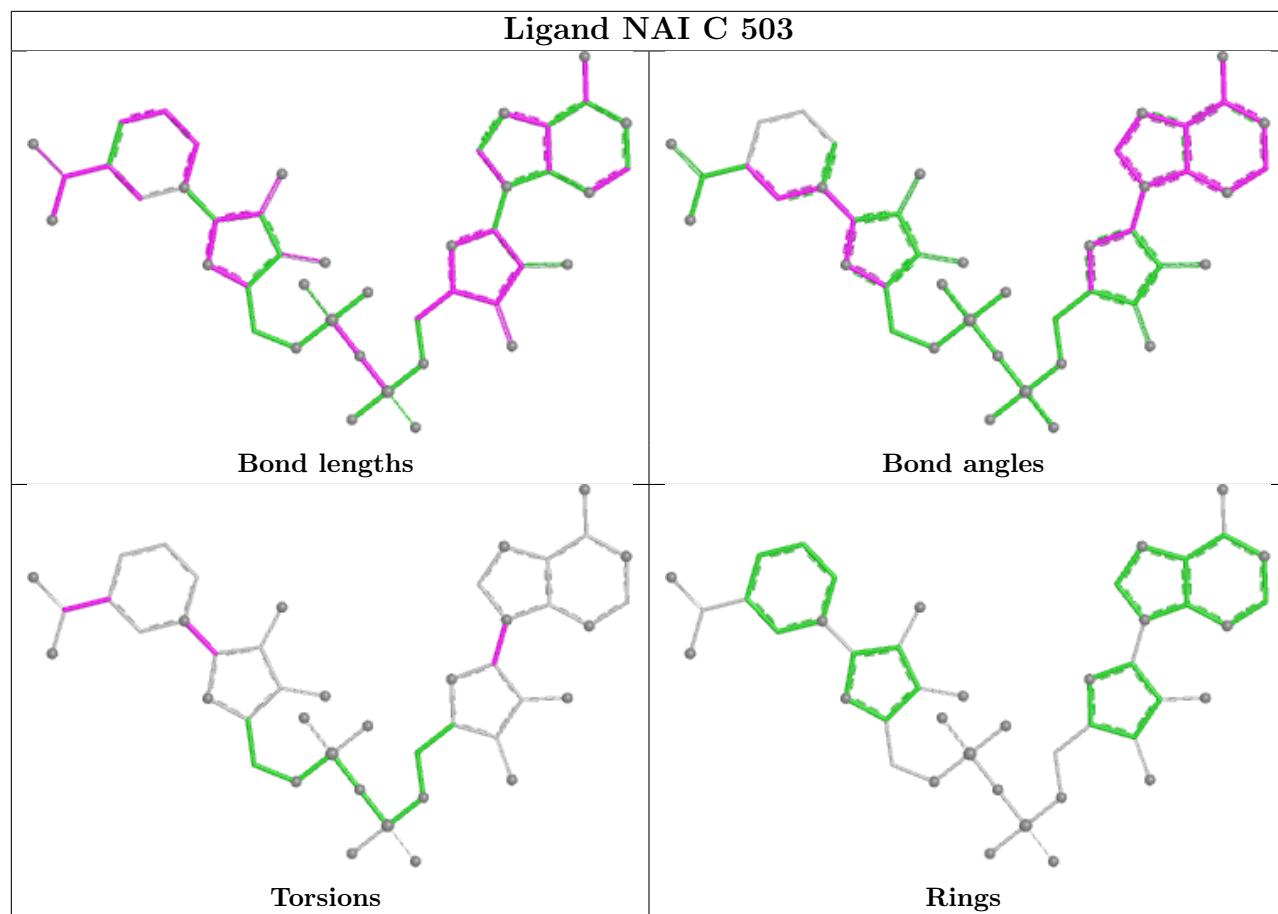


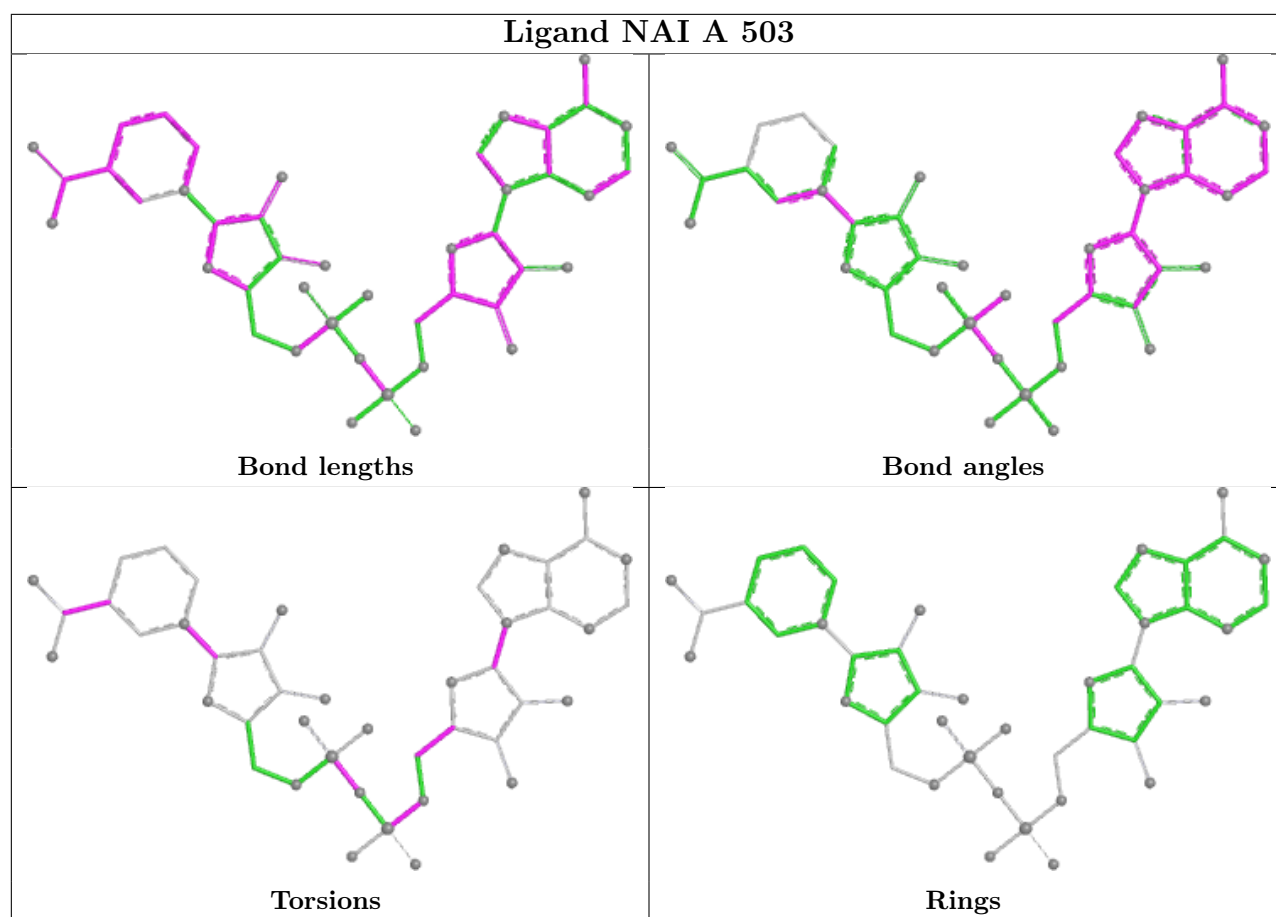
Ligand NAI D 503





Ligand NAI C 503





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	331/332 (99%)	-1.46	0 100 100	22, 35, 61, 87	0
1	B	331/332 (99%)	-1.43	0 100 100	24, 36, 62, 107	0
1	C	331/332 (99%)	-1.35	0 100 100	19, 43, 65, 104	1 (0%)
1	D	331/332 (99%)	-1.39	0 100 100	25, 38, 69, 115	0
1	E	331/332 (99%)	-1.52	0 100 100	17, 28, 55, 90	2 (0%)
1	F	331/332 (99%)	-1.55	0 100 100	15, 28, 52, 73	2 (0%)
All	All	1986/1992 (99%)	-1.45	0 100 100	15, 36, 63, 115	5 (0%)

There are no RSRZ outliers to report.

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
5	GOL	E	402	6/6	0.94	0.08	60,66,75,78	0

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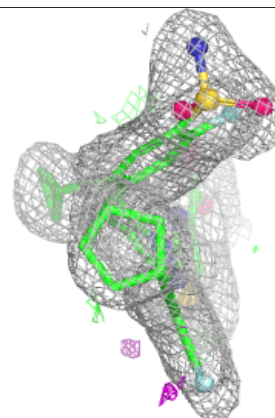
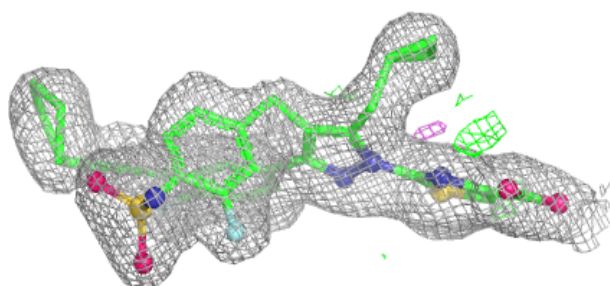
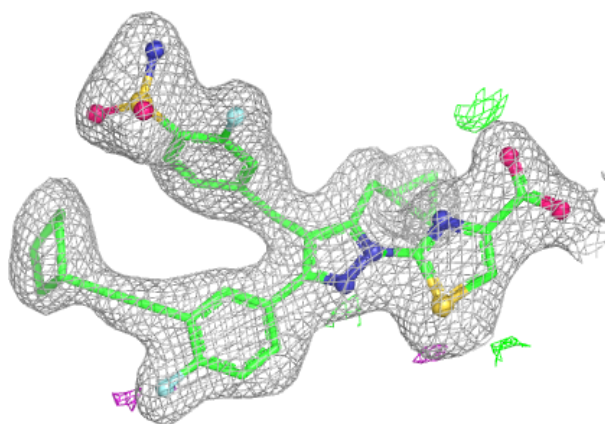
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	E	401	6/6	0.97	0.07	48,57,61,68	0
5	GOL	B	500	6/6	0.97	0.05	58,65,66,68	0
5	GOL	F	500	6/6	0.97	0.06	67,75,78,79	0
5	GOL	E	403	6/6	0.98	0.05	40,45,47,54	0
5	GOL	C	500	6/6	0.98	0.06	65,68,68,70	0
2	PO4	A	501	5/5	0.99	0.04	34,35,47,48	0
3	P8M	C	502	43/43	0.99	0.03	30,39,44,47	0
4	NAI	C	503	44/44	0.99	0.03	25,37,48,51	0
3	P8M	D	502	43/43	1.00	0.03	33,39,53,56	0
3	P8M	E	405	43/43	1.00	0.03	20,28,34,37	0
3	P8M	F	502	43/43	1.00	0.03	23,29,37,46	0
4	NAI	A	503	44/44	1.00	0.02	22,29,39,44	0
4	NAI	B	503	44/44	1.00	0.02	24,33,41,50	0
2	PO4	C	501	5/5	1.00	0.02	34,41,43,45	0
4	NAI	D	503	44/44	1.00	0.02	33,37,43,52	0
4	NAI	E	406	44/44	1.00	0.02	15,27,32,36	0
4	NAI	F	503	44/44	1.00	0.03	19,27,32,39	0
2	PO4	D	501	5/5	1.00	0.04	30,35,36,36	0
2	PO4	E	404	5/5	1.00	0.01	29,29,33,33	0
2	PO4	F	501	5/5	1.00	0.04	23,28,32,33	0
3	P8M	A	502	43/43	1.00	0.03	27,35,55,57	0
3	P8M	B	502	43/43	1.00	0.03	24,32,49,52	0
2	PO4	B	501	5/5	1.00	0.04	32,38,41,44	0

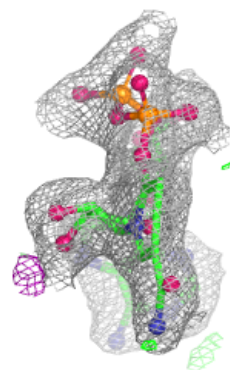
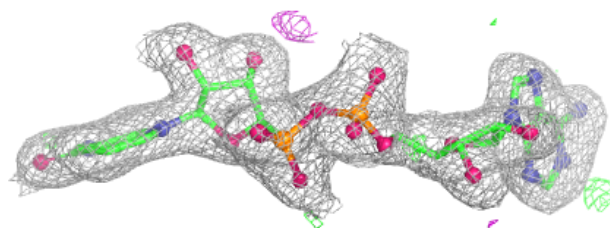
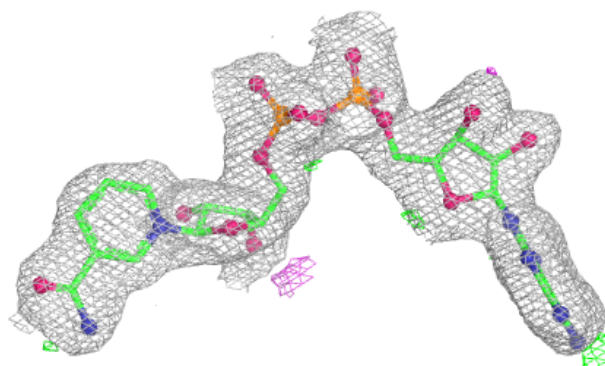
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P8M C 502:

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

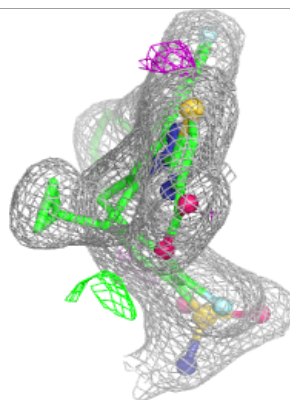
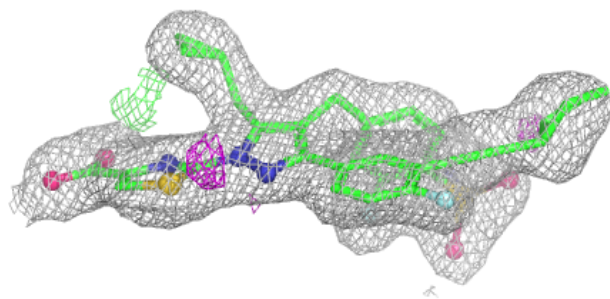
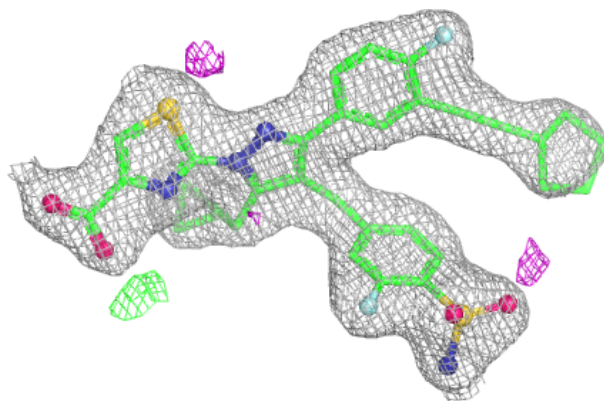
**Electron density around NAI C 503:**

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

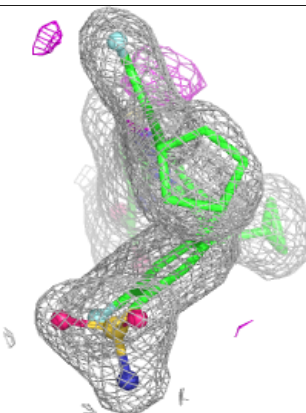
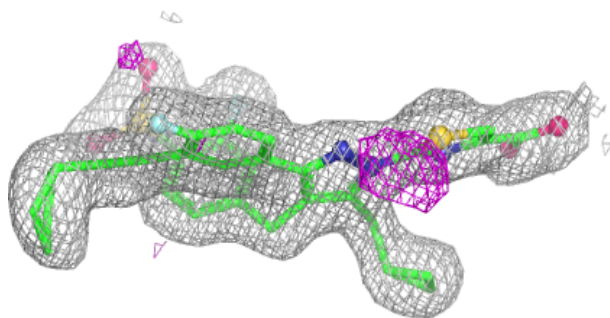
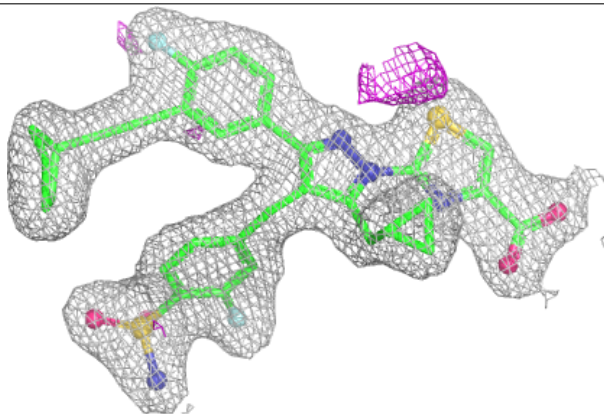


Electron density around P8M D 502:

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

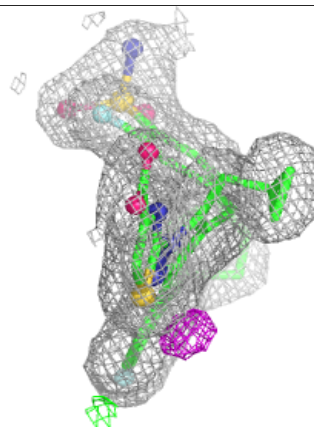
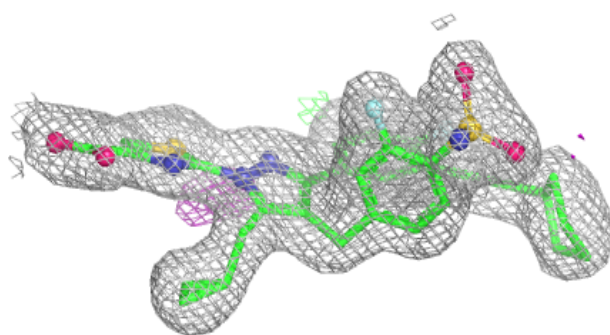
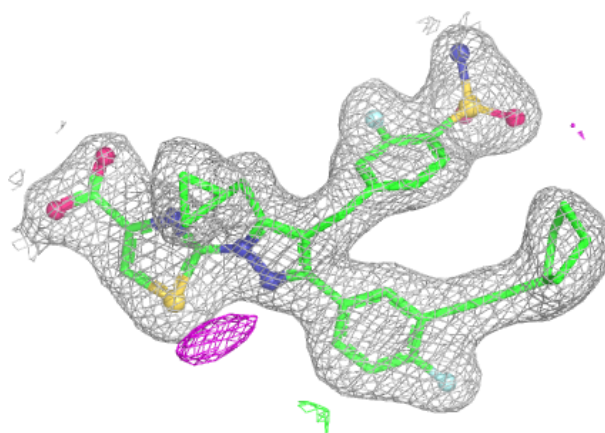
**Electron density around P8M E 405:**

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

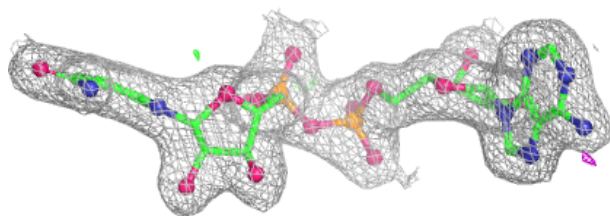
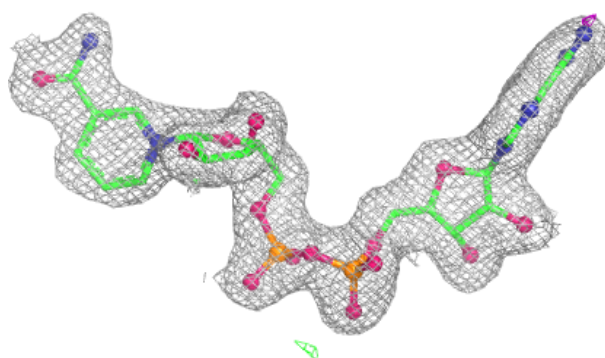


Electron density around P8M F 502:

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

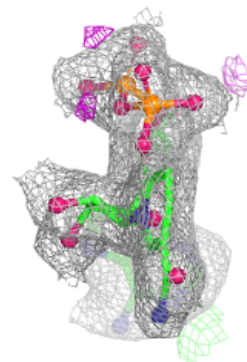
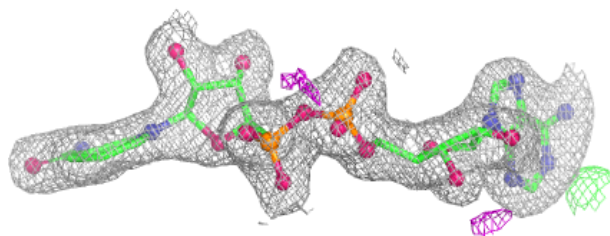
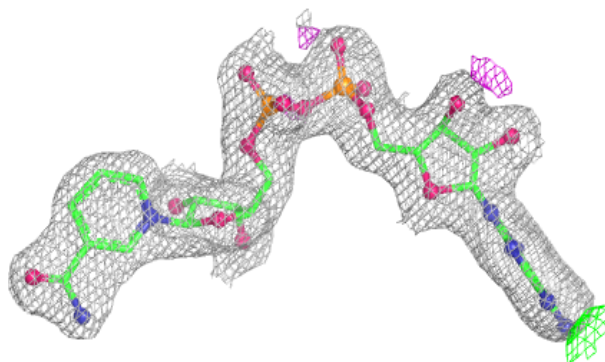
**Electron density around NAI A 503:**

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and green (positive)

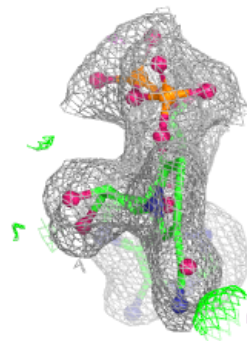
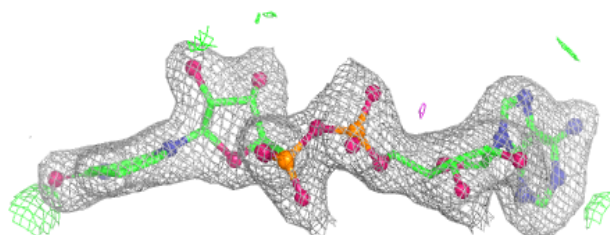
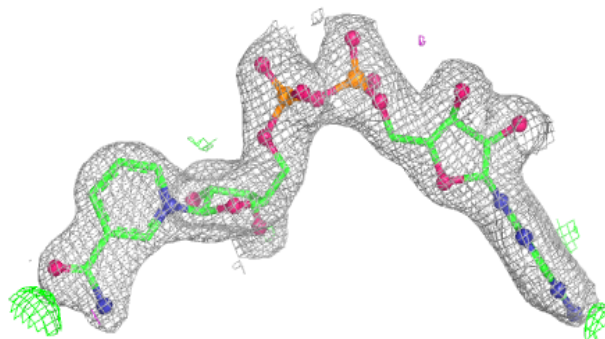


Electron density around NAI B 503:

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

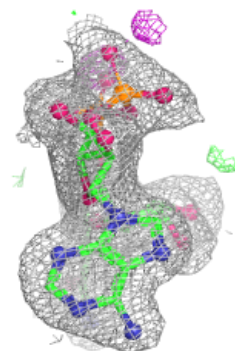
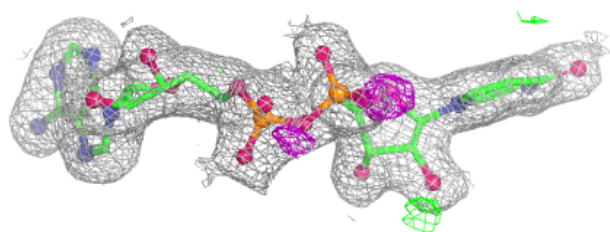
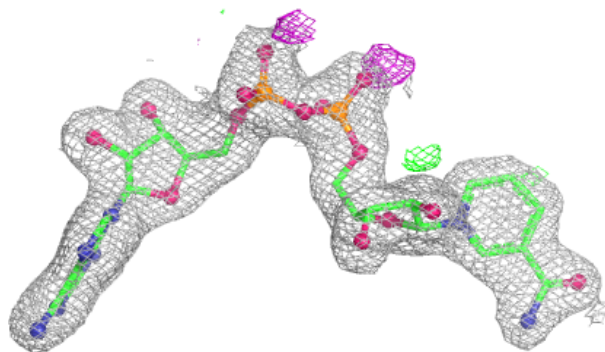
**Electron density around NAI D 503:**

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

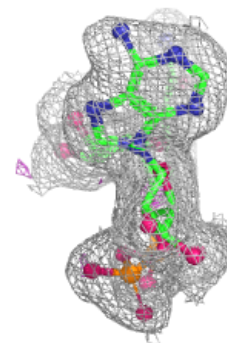
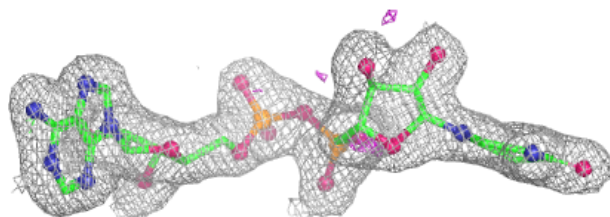
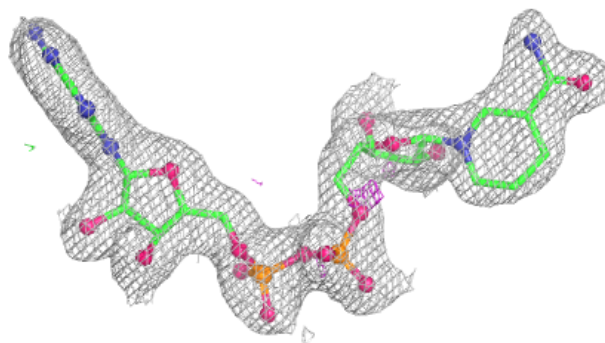


Electron density around NAI E 406:

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

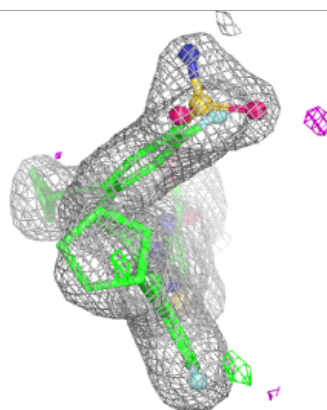
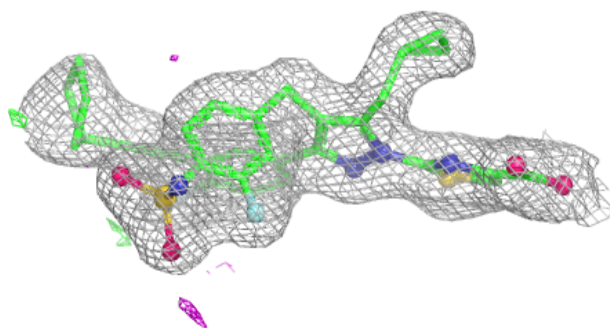
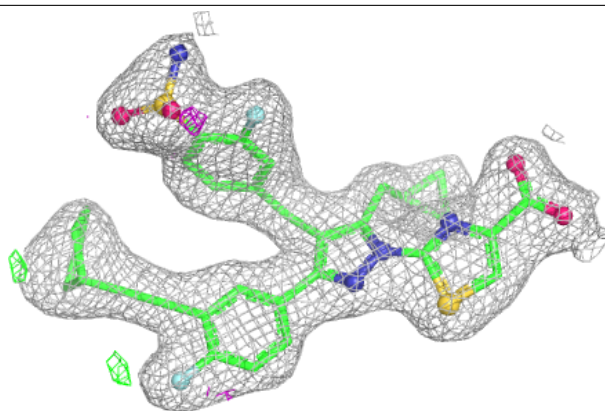
**Electron density around NAI F 503:**

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

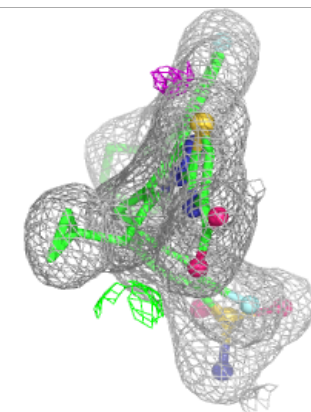
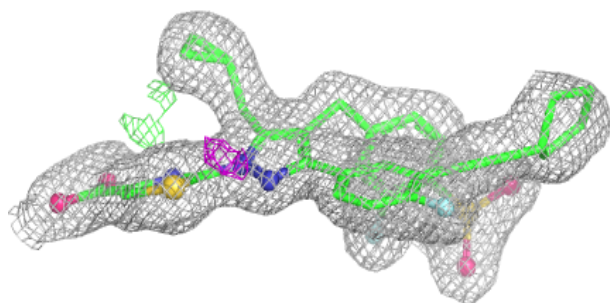
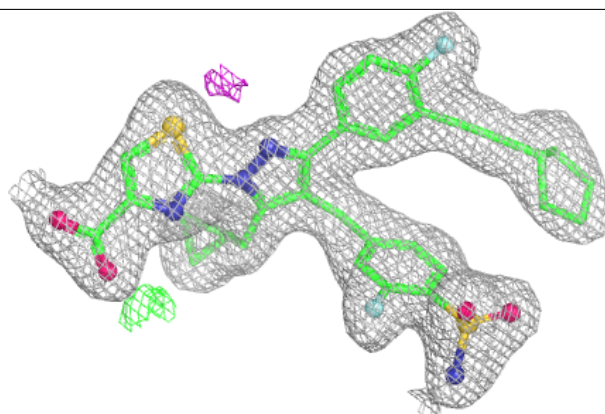


Electron density around P8M A 502:

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

**Electron density around P8M B 502:**

$2mF_o-DF_c$ (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.