



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:50 PM EDT

PDB ID : 6SBU / pdb_00006sbu
Title : X-ray Structure of Human LDHA with an Allosteric Inhibitor (Compound 3)
Authors : Friberg, A.; Puetter, V.; Nguyen, D.; Rehwinkel, H.
Deposited on : 2019-07-22
Resolution : 2.91 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

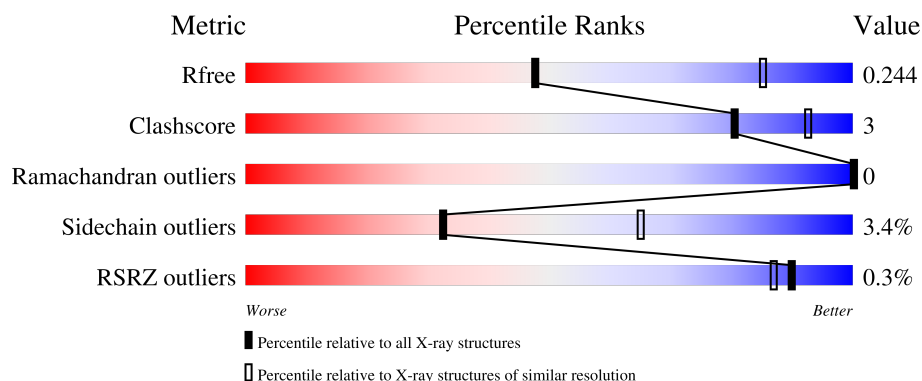
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	% 88% 10% ..
1	B	332	90% 8% .
1	C	332	% 89% 9% ..
1	D	332	90% 8% .
1	E	332	89% 9% .

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Mol	Chain	Length	Quality of chain
1	F	332	91% 8% .
1	G	332	% 91% 8% .
1	H	332	90% 8% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20754 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.

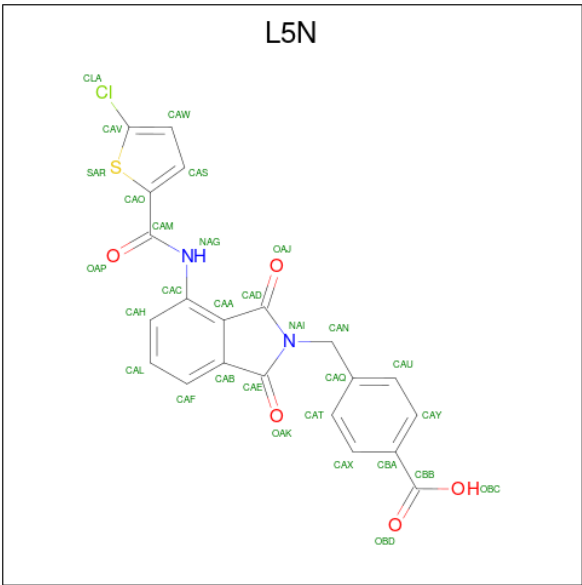
- Molecule 1 is a protein called L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2540	1624	435	468	13			
1	B	328	Total	C	N	O	S	0	1	0
			2546	1628	435	470	13			
1	C	328	Total	C	N	O	S	0	0	0
			2540	1624	435	468	13			
1	D	328	Total	C	N	O	S	0	0	0
			2540	1624	435	468	13			
1	E	328	Total	C	N	O	S	0	1	0
			2548	1629	438	468	13			
1	F	328	Total	C	N	O	S	0	0	0
			2540	1624	435	468	13			
1	G	328	Total	C	N	O	S	0	0	0
			2540	1624	435	468	13			
1	H	328	Total	C	N	O	S	0	0	0
			2540	1624	435	468	13			

There are 8 discrepancies between the modelled and reference sequences:

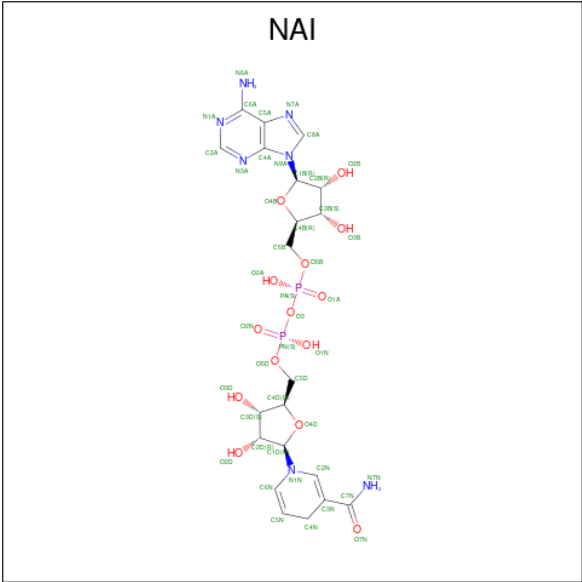
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P00338
B	1	GLY	-	expression tag	UNP P00338
C	1	GLY	-	expression tag	UNP P00338
D	1	GLY	-	expression tag	UNP P00338
E	1	GLY	-	expression tag	UNP P00338
F	1	GLY	-	expression tag	UNP P00338
G	1	GLY	-	expression tag	UNP P00338
H	1	GLY	-	expression tag	UNP P00338

- Molecule 2 is 4-[[4-[(5-chloranylthiophen-2-yl)carbonylamino]-1,3-bis(oxidanylidene)isoindol-2-yl]methyl]benzoic acid (CCD ID: L5N) (formula: C₂₁H₁₃ClN₂O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 30	C 21	Cl 1	N 2	O 5	S 1	0	0
2	B	1	Total 30	C 21	Cl 1	N 2	O 5	S 1	0	0
2	C	1	Total 30	C 21	Cl 1	N 2	O 5	S 1	0	0
2	D	1	Total 30	C 21	Cl 1	N 2	O 5	S 1	0	0
2	E	1	Total 30	C 21	Cl 1	N 2	O 5	S 1	0	0
2	F	1	Total 30	C 21	Cl 1	N 2	O 5	S 1	0	0
2	G	1	Total 30	C 21	Cl 1	N 2	O 5	S 1	0	0
2	H	1	Total 30	C 21	Cl 1	N 2	O 5	S 1	0	0

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



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

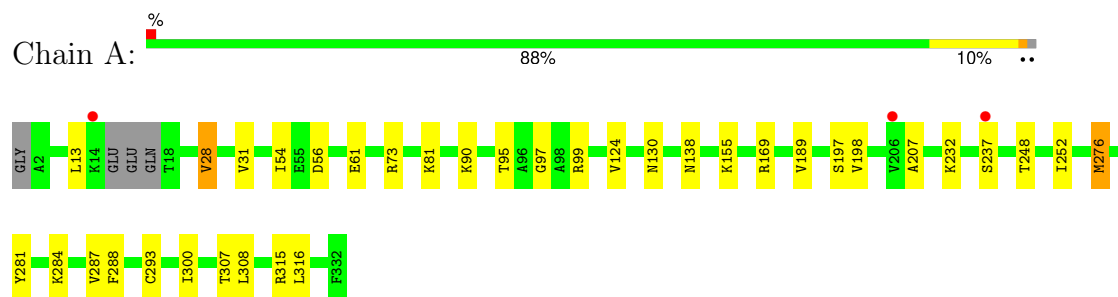
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	15	Total	O	0	0
			15	15		
4	C	14	Total	O	0	0
			14	14		
4	D	9	Total	O	0	0
			9	9		
4	E	17	Total	O	0	0
			17	17		
4	F	4	Total	O	0	0
			4	4		
4	G	11	Total	O	0	0
			11	11		
4	H	12	Total	O	0	0
			12	12		

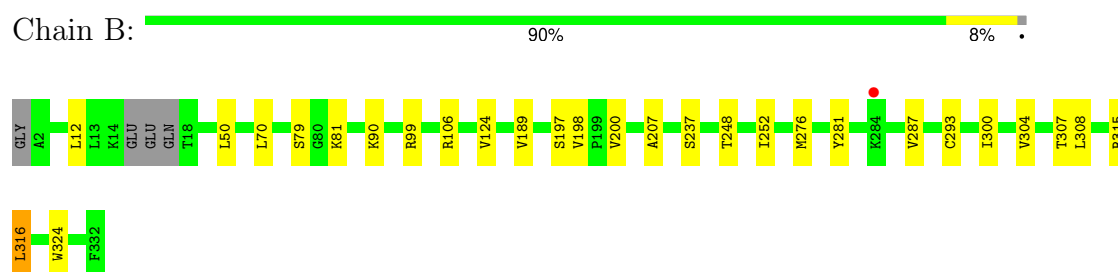
3 Residue-property plots

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.

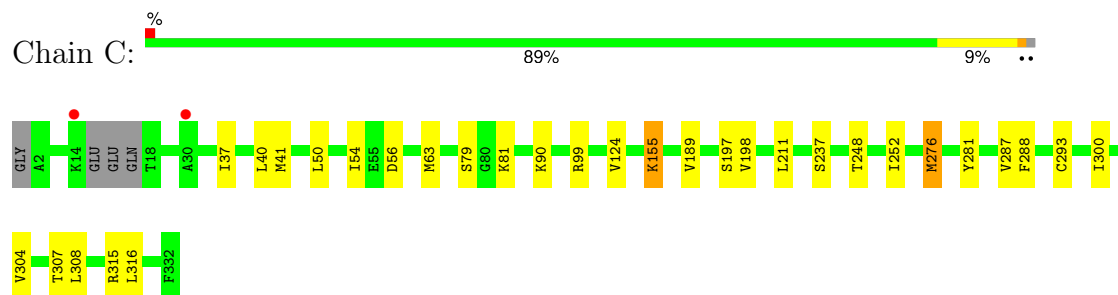
- Molecule 1: L-lactate dehydrogenase A chain



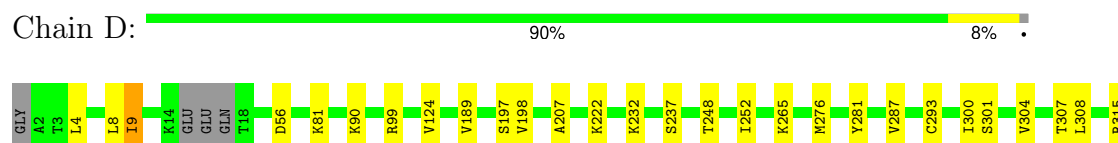
- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain





- Molecule 1: L-lactate dehydrogenase A chain

Chain E: 89% 9%



- Molecule 1: L-lactate dehydrogenase A chain

Chain F: 91% 8%



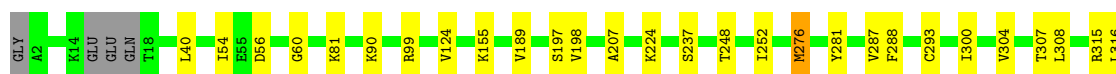
- Molecule 1: L-lactate dehydrogenase A chain

Chain G: 91% 8%



- Molecule 1: L-lactate dehydrogenase A chain

Chain H: 90% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.44Å 143.85Å 311.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.91 48.80 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.80-2.91) 99.0 (48.80-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.207 , 0.244 0.211 , 0.244	Depositor DCC
R_{free} test set	2100 reflections (2.72%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20754	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.32 % 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 1.1649e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L5N, NAI

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	1.00	0/2583	1.45	3/3493 (0.1%)
1	B	0.99	0/2592	1.44	6/3505 (0.2%)
1	C	1.00	0/2583	1.44	3/3493 (0.1%)
1	D	0.99	0/2583	1.44	3/3493 (0.1%)
1	E	0.99	0/2594	1.44	3/3507 (0.1%)
1	F	0.99	0/2583	1.44	4/3493 (0.1%)
1	G	0.99	0/2583	1.43	3/3493 (0.1%)
1	H	0.99	0/2583	1.44	6/3493 (0.2%)
All	All	0.99	0/20684	1.44	31/27970 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	56	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	56	ASP	CA-CB-CG	5.87	118.47	112.60
1	E	56	ASP	CA-CB-CG	5.80	118.40	112.60
1	C	56	ASP	CA-CB-CG	5.76	118.36	112.60
1	D	56	ASP	CA-CB-CG	5.75	118.35	112.60
1	H	56	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	324	TRP	CA-C-N	5.58	126.28	120.03
1	B	324	TRP	C-N-CA	5.58	126.28	120.03
1	B	124	VAL	CA-C-N	5.57	127.58	120.56
1	B	124	VAL	C-N-CA	5.57	127.58	120.56
1	F	324	TRP	CA-C-N	5.51	126.20	120.03
1	F	324	TRP	C-N-CA	5.51	126.20	120.03
1	F	124	VAL	CA-C-N	5.48	127.47	120.56
1	F	124	VAL	C-N-CA	5.48	127.47	120.56
1	D	124	VAL	CA-C-N	5.44	127.41	120.56
1	D	124	VAL	C-N-CA	5.44	127.41	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	124	VAL	CA-C-N	5.41	127.48	120.56
1	H	124	VAL	C-N-CA	5.41	127.48	120.56
1	C	124	VAL	CA-C-N	5.33	127.27	120.56
1	C	124	VAL	C-N-CA	5.33	127.27	120.56
1	H	99	ARG	CB-CG-CD	5.30	123.49	111.30
1	G	124	VAL	CA-C-N	5.28	127.22	120.56
1	G	124	VAL	C-N-CA	5.28	127.22	120.56
1	H	324	TRP	CA-C-N	5.20	125.85	120.03
1	H	324	TRP	C-N-CA	5.20	125.85	120.03
1	A	124	VAL	CA-C-N	5.14	127.14	120.56
1	A	124	VAL	C-N-CA	5.14	127.14	120.56
1	E	124	VAL	CA-C-N	5.14	127.14	120.56
1	E	124	VAL	C-N-CA	5.14	127.14	120.56
1	B	200	VAL	CA-C-N	5.07	127.08	120.28
1	B	200	VAL	C-N-CA	5.07	127.08	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2540	0	2632	22	0
1	B	2546	0	2638	12	0
1	C	2540	0	2632	14	0
1	D	2540	0	2632	13	0
1	E	2548	0	2645	20	0
1	F	2540	0	2632	11	0
1	G	2540	0	2632	10	0
1	H	2540	0	2632	12	0
2	A	30	0	0	0	0
2	B	30	0	0	3	0
2	C	30	0	0	1	0
2	D	30	0	0	0	0
2	E	30	0	0	2	0
2	F	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	30	0	0	1	0
2	H	30	0	0	0	0
3	A	44	0	27	7	0
3	E	44	0	27	8	0
4	A	10	0	0	1	0
4	B	15	0	0	0	0
4	C	14	0	0	1	0
4	D	9	0	0	0	0
4	E	17	0	0	0	0
4	F	4	0	0	0	0
4	G	11	0	0	0	0
4	H	12	0	0	1	0
All	All	20754	0	21129	108	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 3.

All (108) 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:E:95:THR:O	3:E:1002:NAI:H51N	1.87	0.74
1:A:95:THR:O	3:A:1002:NAI:H4D	1.90	0.71
1:E:198:VAL:HG22	1:E:315:ARG:HD2	1.78	0.66
1:E:252:ILE:HD11	3:E:1002:NAI:H4N	1.80	0.63
1:A:252:ILE:HD11	3:A:1002:NAI:H4N	1.82	0.61
1:F:198:VAL:HG22	1:F:315:ARG:HD2	1.83	0.60
1:E:95:THR:O	3:E:1002:NAI:H4D	2.02	0.59
1:A:28:VAL:CG1	1:A:28:VAL:O	2.51	0.58
1:A:248:THR:HG23	1:A:252:ILE:HD11	1.87	0.57
1:G:198:VAL:HG22	1:G:315:ARG:HD2	1.85	0.56
1:H:198:VAL:HG22	1:H:315:ARG:HD2	1.87	0.56
1:E:95:THR:O	3:E:1002:NAI:C5D	2.54	0.56
1:H:248:THR:HG23	1:H:252:ILE:HD11	1.88	0.56
1:D:248:THR:HG23	1:D:252:ILE:HD11	1.88	0.55
1:E:248:THR:HG23	1:E:252:ILE:HD11	1.88	0.55
1:C:248:THR:HG23	1:C:252:ILE:HD11	1.88	0.55
1:F:248:THR:HG23	1:F:252:ILE:HD11	1.88	0.55
1:G:248:THR:HG23	1:G:252:ILE:HD11	1.87	0.55
1:B:198:VAL:HG22	1:B:315:ARG:HD2	1.88	0.54
1:B:248:THR:HG23	1:B:252:ILE:HD11	1.89	0.54
1:A:28:VAL:O	1:A:28:VAL:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:VAL:HG22	1:C:315:ARG:HD2	1.92	0.51
1:C:281:TYR:CE1	1:C:308:LEU:HD12	2.46	0.51
1:A:281:TYR:CE1	1:A:308:LEU:HD12	2.46	0.50
1:D:8:LEU:HD23	1:D:9:ILE:HD12	1.94	0.50
1:E:281:TYR:CE1	1:E:308:LEU:HD12	2.46	0.50
1:G:281:TYR:CE1	1:G:308:LEU:HD12	2.45	0.50
1:E:66:GLN:HE22	2:E:1001:L5N:CAT	2.25	0.50
1:A:198:VAL:HG22	1:A:315:ARG:HD2	1.94	0.49
1:H:281:TYR:CE1	1:H:308:LEU:HD12	2.48	0.49
1:A:130:ASN:ND2	4:A:1101:HOH:O	2.46	0.49
1:D:281:TYR:CE1	1:D:308:LEU:HD12	2.49	0.48
1:E:138:ASN:HD21	3:E:1002:NAI:C3N	2.27	0.48
1:A:138:ASN:ND2	3:A:1002:NAI:C3N	2.77	0.48
1:D:189:VAL:CG1	1:D:197:SER:HB2	2.44	0.48
1:B:189:VAL:CG1	1:B:197:SER:HB2	2.44	0.47
1:F:281:TYR:CE1	1:F:308:LEU:HD12	2.49	0.47
2:F:1001:L5N:OAP	2:F:1001:L5N:CAH	2.60	0.47
1:D:293:CYS:HB3	1:D:300:ILE:HG23	1.95	0.47
1:E:293:CYS:HB3	1:E:300:ILE:HG23	1.96	0.47
1:F:293:CYS:HB3	1:F:300:ILE:HG23	1.96	0.47
1:G:293:CYS:HB3	1:G:300:ILE:HG23	1.97	0.47
1:H:293:CYS:HB3	1:H:300:ILE:HG23	1.96	0.47
2:B:1001:L5N:OAP	2:B:1001:L5N:CAH	2.58	0.47
1:C:63:MET:HE3	4:C:1112:HOH:O	2.13	0.47
1:B:281:TYR:CE1	1:B:308:LEU:HD12	2.50	0.47
1:F:207:ALA:HB3	1:H:304:VAL:HG11	1.97	0.47
1:B:293:CYS:HB3	1:B:300:ILE:HG23	1.96	0.47
1:A:207:ALA:HB3	1:C:304:VAL:HG11	1.97	0.46
1:D:8:LEU:HD23	1:D:9:ILE:CD1	2.45	0.46
1:E:189:VAL:CG1	1:E:197:SER:HB2	2.45	0.46
1:A:189:VAL:CG1	1:A:197:SER:HB2	2.46	0.46
1:C:211:LEU:HG	1:D:4:LEU:HD21	1.96	0.46
1:A:28:VAL:HG13	1:A:61:GLU:HG3	1.98	0.46
1:F:189:VAL:CG1	1:F:197:SER:HB2	2.45	0.46
1:A:293:CYS:HB3	1:A:300:ILE:HG23	1.97	0.46
1:G:189:VAL:CG1	1:G:197:SER:HB2	2.46	0.46
1:C:189:VAL:CG1	1:C:197:SER:HB2	2.46	0.45
1:C:293:CYS:HB3	1:C:300:ILE:HG23	1.97	0.45
1:E:138:ASN:ND2	3:E:1002:NAI:C2N	2.79	0.45
1:H:224:LYS:NZ	4:H:1102:HOH:O	2.50	0.45
1:H:189:VAL:CG1	1:H:197:SER:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:LEU:HD21	1:F:211:LEU:HG	1.99	0.45
1:E:138:ASN:ND2	3:E:1002:NAI:C3N	2.80	0.44
1:B:198:VAL:HG21	1:B:316:LEU:HD12	1.99	0.43
2:C:1001:L5N:OAP	2:C:1001:L5N:CAH	2.64	0.43
1:A:13:LEU:HD12	1:D:301:SER:HA	1.99	0.43
1:F:304:VAL:HG11	1:H:207:ALA:HB3	1.99	0.43
1:A:73:ARG:NH2	1:D:265:LYS:HD3	2.34	0.43
1:F:37:ILE:O	1:F:41:MET:HG3	2.19	0.43
1:E:138:ASN:HB2	3:E:1002:NAI:O2D	2.18	0.43
1:A:169:ARG:HB3	2:B:1001:L5N:CLA	2.56	0.42
1:B:207:ALA:HB3	1:D:304:VAL:HG11	2.00	0.42
1:C:276:MET:HG2	1:C:288:PHE:CE1	2.54	0.42
1:A:31:VAL:HG23	3:A:1002:NAI:O1N	2.20	0.42
1:A:252:ILE:CD1	3:A:1002:NAI:H4N	2.47	0.42
1:C:40:LEU:HD23	1:C:40:LEU:HA	1.84	0.42
1:F:281:TYR:CD1	1:F:308:LEU:HD12	2.55	0.42
1:D:198:VAL:HG22	1:D:315:ARG:HD2	2.01	0.42
1:B:12:LEU:HD21	1:C:155:LYS:HE2	2.02	0.42
1:G:40:LEU:HD23	1:G:40:LEU:HA	1.85	0.42
1:G:281:TYR:CD1	1:G:308:LEU:HD12	2.55	0.42
1:A:28:VAL:CG1	1:A:61:GLU:HG3	2.50	0.42
1:B:304:VAL:HG11	1:D:207:ALA:HB3	2.01	0.41
1:C:281:TYR:CD1	1:C:308:LEU:HD12	2.55	0.41
1:A:276:MET:HG2	1:A:288:PHE:CE1	2.55	0.41
2:G:1001:L5N:OAP	2:G:1001:L5N:CAH	2.68	0.41
1:A:97:GLY:HA3	3:A:1002:NAI:O3D	2.19	0.41
1:E:40:LEU:HD23	1:E:40:LEU:HA	1.85	0.41
1:E:41:MET:HE2	1:E:41:MET:HB3	1.99	0.41
1:H:40:LEU:HD23	1:H:40:LEU:HA	1.84	0.41
1:D:281:TYR:CD1	1:D:308:LEU:HD12	2.55	0.41
1:E:281:TYR:CD1	1:E:308:LEU:HD12	2.56	0.41
1:A:138:ASN:HD21	3:A:1002:NAI:C3N	2.33	0.41
1:B:50:LEU:O	1:B:79:SER:HA	2.21	0.41
1:B:281:TYR:CD1	1:B:308:LEU:HD12	2.55	0.41
1:H:281:TYR:CD1	1:H:308:LEU:HD12	2.55	0.41
1:C:37:ILE:O	1:C:41:MET:HG3	2.21	0.41
1:F:50:LEU:O	1:F:79:SER:HA	2.21	0.41
2:E:1001:L5N:OAP	2:E:1001:L5N:CAH	2.68	0.41
1:B:70:LEU:HD21	2:B:1001:L5N:OAP	2.21	0.40
1:G:276:MET:HG2	1:G:288:PHE:CE1	2.56	0.40
1:E:50:LEU:O	1:E:79:SER:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:LEU:O	1:C:79:SER:HA	2.21	0.40
1:G:50:LEU:O	1:G:79:SER:HA	2.21	0.40
1:H:276:MET:HG2	1:H:288:PHE:CE1	2.57	0.40
1:E:156:ASN:ND2	1:E:157[B]:ARG:HG3	2.36	0.40
1:G:245:LYS:HB2	1:H:60:GLY:HA3	2.03	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	324/332 (98%)	308 (95%)	16 (5%)	0	100	100
1	B	325/332 (98%)	309 (95%)	16 (5%)	0	100	100
1	C	324/332 (98%)	309 (95%)	15 (5%)	0	100	100
1	D	324/332 (98%)	307 (95%)	17 (5%)	0	100	100
1	E	325/332 (98%)	309 (95%)	16 (5%)	0	100	100
1	F	324/332 (98%)	307 (95%)	17 (5%)	0	100	100
1	G	324/332 (98%)	308 (95%)	16 (5%)	0	100	100
1	H	324/332 (98%)	308 (95%)	16 (5%)	0	100	100
All	All	2594/2656 (98%)	2465 (95%)	129 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/287 (99%)	271 (95%)	13 (5%)	24	56
1	B	285/287 (99%)	276 (97%)	9 (3%)	34	66
1	C	284/287 (99%)	274 (96%)	10 (4%)	32	64
1	D	284/287 (99%)	273 (96%)	11 (4%)	28	61
1	E	285/287 (99%)	276 (97%)	9 (3%)	34	66
1	F	284/287 (99%)	276 (97%)	8 (3%)	38	70
1	G	284/287 (99%)	275 (97%)	9 (3%)	34	66
1	H	284/287 (99%)	275 (97%)	9 (3%)	34	66
All	All	2274/2296 (99%)	2196 (97%)	78 (3%)	32	65

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	54	ILE
1	A	81	LYS
1	A	90	LYS
1	A	99	ARG
1	A	155	LYS
1	A	232	LYS
1	A	237	SER
1	A	276	MET
1	A	284	LYS
1	A	287	VAL
1	A	307	THR
1	A	316	LEU
1	B	81	LYS
1	B	90	LYS
1	B	99	ARG
1	B	106	ARG
1	B	237	SER
1	B	276	MET
1	B	287	VAL
1	B	307	THR
1	B	316	LEU
1	C	54	ILE
1	C	81	LYS

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Mol	Chain	Res	Type
1	C	90	LYS
1	C	99	ARG
1	C	155	LYS
1	C	237	SER
1	C	276	MET
1	C	287	VAL
1	C	307	THR
1	C	316	LEU
1	D	9	ILE
1	D	81	LYS
1	D	90	LYS
1	D	99	ARG
1	D	222	LYS
1	D	232	LYS
1	D	237	SER
1	D	276	MET
1	D	287	VAL
1	D	307	THR
1	D	316	LEU
1	E	81	LYS
1	E	90	LYS
1	E	149	LYS
1	E	155	LYS
1	E	232	LYS
1	E	237	SER
1	E	287	VAL
1	E	307	THR
1	E	316	LEU
1	F	81	LYS
1	F	90	LYS
1	F	155	LYS
1	F	237	SER
1	F	276	MET
1	F	287	VAL
1	F	307	THR
1	F	316	LEU
1	G	54	ILE
1	G	81	LYS
1	G	90	LYS
1	G	155	LYS
1	G	237	SER
1	G	276	MET

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Mol	Chain	Res	Type
1	G	287	VAL
1	G	307	THR
1	G	316	LEU
1	H	54	ILE
1	H	81	LYS
1	H	90	LYS
1	H	155	LYS
1	H	237	SER
1	H	276	MET
1	H	287	VAL
1	H	307	THR
1	H	316	LEU

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

Mol	Chain	Res	Type
1	A	138	ASN
1	A	193	HIS
1	B	66	GLN
1	B	101	GLN
1	B	138	ASN
1	B	156	ASN
1	C	101	GLN
1	C	138	ASN
1	C	156	ASN
1	C	193	HIS
1	C	231	HIS
1	D	66	GLN
1	D	138	ASN
1	E	66	GLN
1	E	101	GLN
1	E	138	ASN
1	E	156	ASN
1	E	193	HIS
1	E	231	HIS
1	F	101	GLN
1	F	138	ASN
1	F	193	HIS
1	F	231	HIS
1	G	101	GLN
1	G	138	ASN
1	G	193	HIS

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Mol	Chain	Res	Type
1	H	66	GLN
1	H	101	GLN
1	H	138	ASN
1	H	156	ASN
1	H	193	HIS

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](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	L5N	E	1001	-	33,33,33	2.47	9 (27%)	48,48,48	2.55	16 (33%)
3	NAI	E	1002	-	47,48,48	1.67	10 (21%)	64,73,73	2.08	18 (28%)
2	L5N	C	1001	-	33,33,33	2.59	8 (24%)	48,48,48	2.03	15 (31%)
2	L5N	H	1001	-	33,33,33	2.36	8 (24%)	48,48,48	2.40	15 (31%)
2	L5N	D	1001	-	33,33,33	2.54	8 (24%)	48,48,48	2.36	16 (33%)
2	L5N	B	1001	-	33,33,33	2.74	9 (27%)	48,48,48	2.85	16 (33%)
2	L5N	F	1001	-	33,33,33	2.59	10 (30%)	48,48,48	2.79	14 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	L5N	A	1001	-	33,33,33	2.31	7 (21%)	48,48,48	2.48	17 (35%)
2	L5N	G	1001	-	33,33,33	2.36	9 (27%)	48,48,48	2.37	15 (31%)
3	NAI	A	1002	-	47,48,48	1.53	7 (14%)	64,73,73	2.17	17 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	L5N	E	1001	-	-	4/16/32/32	0/4/4/4
3	NAI	E	1002	-	-	10/29/72/72	0/5/5/5
2	L5N	C	1001	-	-	0/16/32/32	0/4/4/4
2	L5N	H	1001	-	-	0/16/32/32	0/4/4/4
2	L5N	D	1001	-	-	4/16/32/32	0/4/4/4
2	L5N	B	1001	-	-	0/16/32/32	0/4/4/4
2	L5N	F	1001	-	-	4/16/32/32	0/4/4/4
2	L5N	A	1001	-	-	4/16/32/32	0/4/4/4
2	L5N	G	1001	-	-	0/16/32/32	0/4/4/4
3	NAI	A	1002	-	-	11/29/72/72	0/5/5/5

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	L5N	CAA-CAD	-7.12	1.36	1.49
2	B	1001	L5N	CAA-CAD	-7.09	1.36	1.49
2	F	1001	L5N	CAA-CAD	-7.05	1.36	1.49
2	B	1001	L5N	CAB-CAE	-6.79	1.37	1.48
2	F	1001	L5N	CAB-CAE	-6.69	1.38	1.48
2	C	1001	L5N	CAA-CAD	-6.65	1.37	1.49
2	G	1001	L5N	CAB-CAE	-6.30	1.38	1.48
2	H	1001	L5N	CAB-CAE	-6.26	1.38	1.48
2	D	1001	L5N	CAD-NAI	-6.24	1.32	1.39
2	D	1001	L5N	CAA-CAD	-6.19	1.38	1.49
2	G	1001	L5N	CAA-CAD	-6.14	1.38	1.49
2	C	1001	L5N	CAD-NAI	-6.12	1.32	1.39
2	D	1001	L5N	CAE-NAI	-6.08	1.32	1.39
2	C	1001	L5N	CAB-CAE	-6.00	1.39	1.48
2	H	1001	L5N	CAE-NAI	-5.96	1.32	1.39
2	E	1001	L5N	CAO-SAR	-5.95	1.61	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1001	L5N	CAB-CAE	-5.87	1.39	1.48
2	B	1001	L5N	CAD-NAI	-5.80	1.32	1.39
2	H	1001	L5N	CAD-NAI	-5.79	1.32	1.39
2	E	1001	L5N	CAA-CAD	-5.76	1.39	1.49
2	A	1001	L5N	CAB-CAE	-5.63	1.39	1.48
2	E	1001	L5N	CAC-NAG	-5.56	1.30	1.41
2	G	1001	L5N	CAE-NAI	-5.54	1.33	1.39
2	H	1001	L5N	CAA-CAD	-5.53	1.39	1.49
2	D	1001	L5N	CAB-CAE	-5.27	1.40	1.48
2	C	1001	L5N	CAE-NAI	-5.18	1.33	1.39
2	D	1001	L5N	CAO-SAR	-4.98	1.63	1.73
2	A	1001	L5N	CAD-NAI	-4.98	1.33	1.39
2	E	1001	L5N	CAD-NAI	-4.95	1.33	1.39
3	E	1002	NAI	PA-O3	4.81	1.64	1.59
3	A	1002	NAI	C5A-C4A	4.80	1.47	1.39
2	F	1001	L5N	CAD-NAI	-4.78	1.33	1.39
2	B	1001	L5N	CAV-SAR	-4.77	1.62	1.71
3	E	1002	NAI	C5A-C4A	4.75	1.47	1.39
2	F	1001	L5N	CAE-NAI	-4.75	1.33	1.39
3	E	1002	NAI	PN-O3	4.64	1.64	1.59
2	C	1001	L5N	CAC-NAG	-4.63	1.32	1.41
2	F	1001	L5N	CAC-NAG	-4.57	1.32	1.41
2	G	1001	L5N	CAC-NAG	-4.55	1.32	1.41
2	B	1001	L5N	CAC-NAG	-4.53	1.32	1.41
2	A	1001	L5N	CAE-NAI	-4.46	1.34	1.39
2	A	1001	L5N	CAC-NAG	-4.36	1.33	1.41
2	F	1001	L5N	CAV-SAR	-4.30	1.63	1.71
2	B	1001	L5N	CAE-NAI	-4.20	1.34	1.39
2	D	1001	L5N	CAC-NAG	-4.15	1.33	1.41
3	A	1002	NAI	PN-O3	3.99	1.63	1.59
2	G	1001	L5N	CAD-NAI	-3.90	1.35	1.39
2	C	1001	L5N	CAV-SAR	-3.72	1.64	1.71
2	C	1001	L5N	CAO-SAR	-3.69	1.65	1.73
2	B	1001	L5N	CAO-SAR	-3.69	1.65	1.73
3	A	1002	NAI	C5A-C6A	3.64	1.51	1.41
2	H	1001	L5N	CAC-NAG	-3.59	1.34	1.41
3	A	1002	NAI	PA-O3	3.30	1.63	1.59
2	G	1001	L5N	CAO-SAR	-3.17	1.67	1.73
3	E	1002	NAI	C5A-C6A	3.11	1.49	1.41
2	F	1001	L5N	CAO-SAR	-3.10	1.67	1.73
3	A	1002	NAI	C8A-N7A	2.86	1.37	1.31
2	E	1001	L5N	CAV-SAR	-2.84	1.66	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	L5N	CAO-SAR	-2.77	1.67	1.73
2	A	1001	L5N	CAA-CAC	-2.61	1.36	1.41
2	B	1001	L5N	CAA-CAC	-2.55	1.36	1.41
2	F	1001	L5N	CAM-CAO	2.48	1.53	1.48
3	E	1002	NAI	C7N-C3N	2.48	1.54	1.48
2	E	1001	L5N	CAE-NAI	-2.43	1.36	1.39
2	E	1001	L5N	CAM-NAG	-2.43	1.30	1.35
2	H	1001	L5N	CAM-CAO	2.41	1.53	1.48
2	B	1001	L5N	CAM-CAO	2.40	1.53	1.48
2	C	1001	L5N	CAM-CAO	2.38	1.53	1.48
2	H	1001	L5N	CAO-SAR	-2.35	1.68	1.73
3	E	1002	NAI	C6N-C5N	2.31	1.40	1.33
3	A	1002	NAI	C4A-N3A	2.27	1.38	1.34
2	G	1001	L5N	CAV-SAR	-2.26	1.67	1.71
2	E	1001	L5N	CAA-CAC	-2.20	1.37	1.41
2	D	1001	L5N	OBC-CBB	-2.20	1.24	1.30
3	E	1002	NAI	C8A-N7A	2.19	1.35	1.31
2	F	1001	L5N	CAA-CAC	-2.19	1.37	1.41
3	A	1002	NAI	C6N-C5N	2.18	1.39	1.33
3	E	1002	NAI	C4A-N3A	2.12	1.38	1.34
3	E	1002	NAI	C4N-C3N	2.10	1.54	1.50
2	D	1001	L5N	CAN-CAQ	2.09	1.55	1.51
2	H	1001	L5N	CAV-SAR	-2.08	1.67	1.71
2	F	1001	L5N	CAN-CAQ	2.07	1.55	1.51
3	E	1002	NAI	C2N-C3N	2.01	1.40	1.35
2	G	1001	L5N	OBC-CBB	-2.00	1.24	1.30
2	G	1001	L5N	CAM-CAO	2.00	1.52	1.48

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1001	L5N	CAA-CAD-NAI	11.25	111.31	105.58
2	B	1001	L5N	CAA-CAD-NAI	9.53	110.43	105.58
2	D	1001	L5N	CAA-CAD-NAI	8.96	110.14	105.58
2	H	1001	L5N	CAA-CAD-NAI	8.83	110.08	105.58
2	C	1001	L5N	CAA-CAD-NAI	8.29	109.80	105.58
2	A	1001	L5N	CAA-CAD-NAI	8.23	109.77	105.58
2	G	1001	L5N	CAA-CAD-NAI	7.72	109.51	105.58
2	E	1001	L5N	CAA-CAD-NAI	7.61	109.45	105.58
2	B	1001	L5N	CAB-CAE-NAI	7.33	111.30	105.88
2	F	1001	L5N	CAD-NAI-CAE	-7.30	105.80	112.02
2	B	1001	L5N	CAD-NAI-CAE	-7.18	105.89	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	NAI	C5A-C4A-N3A	-6.85	117.29	126.72
2	F	1001	L5N	OAJ-CAD-CAA	-6.41	119.41	129.15
2	H	1001	L5N	CAB-CAE-NAI	6.38	110.60	105.88
2	F	1001	L5N	CAB-CAE-NAI	6.14	110.42	105.88
3	E	1002	NAI	C5A-C4A-N3A	-6.08	118.34	126.72
2	E	1001	L5N	CAB-CAE-NAI	5.97	110.29	105.88
2	E	1001	L5N	CAD-NAI-CAE	-5.72	107.14	112.02
3	A	1002	NAI	N3A-C4A-N9A	5.47	136.47	127.17
3	E	1002	NAI	O4B-C1B-N9A	5.44	118.54	108.09
3	E	1002	NAI	N3A-C4A-N9A	5.42	136.39	127.17
3	A	1002	NAI	O4B-C1B-N9A	5.28	118.22	108.09
2	A	1001	L5N	OAJ-CAD-CAA	-5.27	121.13	129.15
2	B	1001	L5N	OAJ-CAD-CAA	-5.26	121.15	129.15
2	G	1001	L5N	OAJ-CAD-CAA	-5.21	121.23	129.15
2	D	1001	L5N	CAW-CAV-CLA	-5.09	121.51	126.83
2	G	1001	L5N	CAB-CAE-NAI	4.89	109.49	105.88
2	E	1001	L5N	CAA-CAC-NAG	-4.88	112.31	118.46
2	H	1001	L5N	CAD-NAI-CAE	-4.88	107.86	112.02
3	A	1002	NAI	C2A-N3A-C4A	4.84	123.64	111.83
2	G	1001	L5N	CAD-NAI-CAE	-4.82	107.91	112.02
2	A	1001	L5N	CAW-CAV-CLA	-4.75	121.86	126.83
3	E	1002	NAI	O4D-C1D-N1N	4.63	116.91	108.08
2	B	1001	L5N	CAV-SAR-CAO	4.54	93.80	90.76
3	E	1002	NAI	C2A-N3A-C4A	4.51	122.84	111.83
3	E	1002	NAI	N3A-C2A-N1A	-4.49	121.79	128.58
2	H	1001	L5N	CAC-CAA-CAD	4.46	134.35	129.42
2	D	1001	L5N	CAB-CAE-NAI	4.45	109.17	105.88
2	F	1001	L5N	OAJ-CAD-NAI	4.44	129.28	124.79
2	A	1001	L5N	CAD-NAI-CAE	-4.41	108.26	112.02
2	G	1001	L5N	OAJ-CAD-NAI	4.41	129.25	124.79
2	A	1001	L5N	OAJ-CAD-NAI	4.25	129.09	124.79
2	A	1001	L5N	CAV-SAR-CAO	-4.18	87.96	90.76
3	A	1002	NAI	C4A-C5A-N7A	-4.15	105.84	110.58
2	B	1001	L5N	CAA-CAB-CAE	-4.05	104.46	108.19
3	A	1002	NAI	N3A-C2A-N1A	-4.01	122.51	128.58
2	E	1001	L5N	CAN-NAI-CAE	3.98	128.71	123.66
2	H	1001	L5N	CAB-CAA-CAC	-3.98	119.82	121.88
2	B	1001	L5N	CAA-CAC-NAG	-3.95	113.47	118.46
2	E	1001	L5N	OAK-CAE-CAB	-3.88	121.14	128.66
2	E	1001	L5N	OAK-CAE-NAI	3.73	128.56	124.79
2	A	1001	L5N	CAB-CAE-NAI	3.72	108.63	105.88
2	D	1001	L5N	CAD-NAI-CAE	-3.72	108.84	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1001	L5N	CAB-CAA-CAC	-3.65	119.99	121.88
2	C	1001	L5N	CAM-CAO-SAR	3.63	126.69	117.18
3	E	1002	NAI	C1D-N1N-C2N	-3.63	115.16	121.14
2	B	1001	L5N	OAK-CAE-CAB	-3.61	121.66	128.66
2	B	1001	L5N	CAF-CAB-CAE	3.59	135.62	129.59
2	B	1001	L5N	CAN-NAI-CAE	3.58	128.20	123.66
2	B	1001	L5N	OAJ-CAD-NAI	3.58	128.41	124.79
2	A	1001	L5N	CAF-CAB-CAE	3.58	135.59	129.59
3	A	1002	NAI	C1D-N1N-C2N	-3.57	115.26	121.14
2	E	1001	L5N	CAA-CAB-CAE	-3.51	104.95	108.19
2	F	1001	L5N	OAK-CAE-CAB	-3.51	121.86	128.66
2	D	1001	L5N	CAC-CAA-CAD	3.48	133.27	129.42
2	D	1001	L5N	CAN-NAI-CAD	3.47	128.06	123.66
3	A	1002	NAI	C5A-N7A-C8A	3.47	108.90	103.45
3	A	1002	NAI	O4D-C4D-C3D	3.44	111.98	105.15
2	A	1001	L5N	CAA-CAC-NAG	-3.39	114.18	118.46
2	A	1001	L5N	OBD-CBB-CBA	-3.38	112.59	121.46
2	C	1001	L5N	OAJ-CAD-CAA	-3.37	124.03	129.15
2	G	1001	L5N	CAN-NAI-CAD	3.36	127.92	123.66
2	E	1001	L5N	OAJ-CAD-CAA	-3.36	124.05	129.15
2	G	1001	L5N	CAF-CAB-CAE	3.33	135.17	129.59
2	D	1001	L5N	CAF-CAB-CAE	3.30	135.13	129.59
2	E	1001	L5N	CAU-CAY-CBA	-3.29	117.28	120.80
2	E	1001	L5N	CAF-CAB-CAE	3.29	135.11	129.59
2	H	1001	L5N	CAW-CAV-SAR	-3.26	110.33	113.30
3	A	1002	NAI	C4A-N9A-C8A	3.23	109.13	105.74
3	A	1002	NAI	C6A-C5A-N7A	3.19	138.24	132.09
2	D	1001	L5N	OAJ-CAD-CAA	-3.18	124.31	129.15
2	G	1001	L5N	CAM-CAO-SAR	3.12	125.33	117.18
2	G	1001	L5N	CAW-CAV-CLA	-3.07	123.61	126.83
2	C	1001	L5N	CAD-NAI-CAE	-3.07	109.40	112.02
2	D	1001	L5N	CLA-CAV-SAR	3.05	124.53	119.72
2	C	1001	L5N	CAF-CAB-CAE	3.04	134.69	129.59
2	D	1001	L5N	CAA-CAC-NAG	-3.04	114.63	118.46
2	A	1001	L5N	CLA-CAV-SAR	3.04	124.51	119.72
3	A	1002	NAI	C6N-N1N-C2N	3.02	122.55	119.32
2	F	1001	L5N	CAN-NAI-CAD	3.00	127.47	123.66
2	H	1001	L5N	CAM-CAO-SAR	2.99	125.00	117.18
2	B	1001	L5N	CAW-CAV-CLA	2.99	129.94	126.83
3	E	1002	NAI	C4A-N9A-C8A	2.91	108.79	105.74
2	C	1001	L5N	CAN-NAI-CAE	2.90	127.34	123.66
3	A	1002	NAI	C4B-O4B-C1B	-2.90	103.06	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1001	L5N	OAK-CAE-NAI	2.90	127.72	124.79
3	A	1002	NAI	N9A-C8A-N7A	-2.86	109.88	113.94
3	E	1002	NAI	O4B-C1B-C2B	-2.82	100.58	106.62
2	H	1001	L5N	CLA-CAV-SAR	2.79	124.12	119.72
2	H	1001	L5N	CAA-CAB-CAE	-2.79	105.62	108.19
2	G	1001	L5N	CAA-CAC-NAG	-2.77	114.97	118.46
2	H	1001	L5N	CAN-NAI-CAD	2.76	127.16	123.66
2	F	1001	L5N	CAF-CAB-CAE	2.74	134.19	129.59
2	C	1001	L5N	CAW-CAV-CLA	-2.72	123.98	126.83
2	D	1001	L5N	CAV-SAR-CAO	-2.68	88.97	90.76
2	F	1001	L5N	CAT-CAX-CBA	-2.68	117.94	120.80
3	E	1002	NAI	C4A-C5A-N7A	-2.67	107.53	110.58
2	C	1001	L5N	CAB-CAE-NAI	2.67	107.86	105.88
2	D	1001	L5N	CAA-CAB-CAE	-2.64	105.76	108.19
2	G	1001	L5N	CAY-CBA-CAX	2.60	121.88	118.57
2	B	1001	L5N	CAC-NAG-CAM	-2.56	119.72	126.84
2	C	1001	L5N	CLA-CAV-SAR	2.55	123.74	119.72
2	B	1001	L5N	CAW-CAV-SAR	-2.54	110.98	113.30
2	A	1001	L5N	CAS-CAO-SAR	2.53	114.18	110.49
3	E	1002	NAI	C5A-N7A-C8A	2.52	107.41	103.45
3	A	1002	NAI	O4D-C1D-N1N	2.49	112.84	108.08
2	H	1001	L5N	CAB-CAA-CAD	-2.44	105.83	108.14
3	E	1002	NAI	C3D-C2D-C1D	2.42	106.04	101.46
2	F	1001	L5N	CAN-NAI-CAE	2.41	126.71	123.66
2	G	1001	L5N	CAT-CAX-CBA	-2.39	118.25	120.80
2	G	1001	L5N	CAF-CAB-CAA	-2.38	117.93	121.60
2	D	1001	L5N	CAB-CAA-CAC	-2.36	120.66	121.88
2	A	1001	L5N	OBC-CBB-CBA	2.35	120.88	114.84
3	E	1002	NAI	O5D-C5D-C4D	2.34	116.96	108.99
2	A	1001	L5N	CAH-CAC-NAG	2.34	127.24	121.82
2	H	1001	L5N	CAV-SAR-CAO	2.34	92.33	90.76
2	C	1001	L5N	CAB-CAA-CAD	-2.32	105.95	108.14
2	C	1001	L5N	CAV-SAR-CAO	2.28	92.29	90.76
3	E	1002	NAI	C5A-C6A-N6A	-2.28	117.65	123.29
2	A	1001	L5N	CAA-CAB-CAE	-2.27	106.09	108.19
2	E	1001	L5N	CAW-CAV-CLA	-2.24	124.49	126.83
2	B	1001	L5N	OAK-CAE-NAI	2.22	127.04	124.79
3	E	1002	NAI	N6A-C6A-N1A	2.21	123.30	118.38
2	E	1001	L5N	CAC-CAA-CAD	2.21	131.86	129.42
2	G	1001	L5N	CAC-CAA-CAD	2.20	131.85	129.42
2	D	1001	L5N	CAB-CAA-CAD	-2.19	106.08	108.14
3	A	1002	NAI	C3D-C2D-C1D	2.19	105.60	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	L5N	CAB-CAA-CAC	2.14	122.99	121.88
2	D	1001	L5N	CAM-CAO-SAR	2.14	122.77	117.18
2	F	1001	L5N	CAB-CAA-CAD	-2.12	106.14	108.14
2	A	1001	L5N	CAF-CAB-CAA	-2.12	118.32	121.60
2	C	1001	L5N	CAF-CAB-CAA	-2.12	118.32	121.60
2	H	1001	L5N	OAJ-CAD-CAA	-2.12	125.93	129.15
2	E	1001	L5N	CLA-CAV-SAR	2.11	123.05	119.72
2	C	1001	L5N	CAC-CAA-CAD	2.10	131.74	129.42
2	D	1001	L5N	CAT-CAX-CBA	-2.09	118.56	120.80
3	E	1002	NAI	N9A-C8A-N7A	-2.07	111.00	113.94
2	C	1001	L5N	CAY-CBA-CAX	2.07	121.19	118.57
2	H	1001	L5N	CAF-CAB-CAE	2.07	133.05	129.59
2	E	1001	L5N	CAX-CAT-CAQ	-2.06	118.28	121.00
2	G	1001	L5N	CAB-CAA-CAD	-2.06	106.19	108.14
3	E	1002	NAI	C6A-C5A-N7A	2.06	136.06	132.09
2	C	1001	L5N	CAT-CAX-CBA	-2.04	118.61	120.80
2	F	1001	L5N	CAC-CAA-CAD	2.03	131.67	129.42
2	H	1001	L5N	OAK-CAE-CAB	-2.01	124.77	128.66
3	E	1002	NAI	O4D-C4D-C3D	2.01	109.14	105.15
2	F	1001	L5N	CAA-CAB-CAE	-2.00	106.34	108.19
3	A	1002	NAI	O2B-C2B-C1B	2.00	117.00	110.10
2	B	1001	L5N	CAN-CAQ-CAU	-2.00	117.06	120.75

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	NAI	C5B-O5B-PA-O1A
3	A	1002	NAI	C5B-O5B-PA-O3
3	A	1002	NAI	PN-O3-PA-O5B
3	A	1002	NAI	C5D-O5D-PN-O3
3	A	1002	NAI	C5D-O5D-PN-O2N
3	E	1002	NAI	C5D-O5D-PN-O3
3	E	1002	NAI	C5D-O5D-PN-O1N
3	E	1002	NAI	O4D-C4D-C5D-O5D
2	E	1001	L5N	CAX-CBA-CBB-OBC
2	E	1001	L5N	CAX-CBA-CBB-OB
2	E	1001	L5N	CAY-CBA-CBB-OB
2	E	1001	L5N	CAY-CBA-CBB-OBC
2	F	1001	L5N	CAX-CBA-CBB-OBC
2	F	1001	L5N	CAX-CBA-CBB-OB
2	F	1001	L5N	CAY-CBA-CBB-OBC

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Mol	Chain	Res	Type	Atoms
2	F	1001	L5N	CAY-CBA-CBB-OB
3	E	1002	NAI	C3D-C4D-C5D-O5D
3	A	1002	NAI	O4B-C4B-C5B-O5B
3	E	1002	NAI	C4D-C5D-O5D-PN
3	A	1002	NAI	C5B-O5B-PA-O2A
3	A	1002	NAI	C5D-O5D-PN-O1N
3	E	1002	NAI	C5D-O5D-PN-O2N
3	E	1002	NAI	O4D-C1D-N1N-C6N
3	E	1002	NAI	O4D-C1D-N1N-C2N
3	E	1002	NAI	C2D-C1D-N1N-C6N
2	D	1001	L5N	CAX-CBA-CBB-OB
3	E	1002	NAI	C2D-C1D-N1N-C2N
3	A	1002	NAI	O4D-C1D-N1N-C2N
2	A	1001	L5N	CAX-CBA-CBB-OB
2	A	1001	L5N	CAY-CBA-CBB-OB
2	D	1001	L5N	CAX-CBA-CBB-OB
2	D	1001	L5N	CAY-CBA-CBB-OB
2	A	1001	L5N	CAY-CBA-CBB-OB
2	A	1001	L5N	CAX-CBA-CBB-OB
3	A	1002	NAI	C2D-C1D-N1N-C2N
2	D	1001	L5N	CAY-CBA-CBB-OB
3	A	1002	NAI	O4D-C1D-N1N-C6N

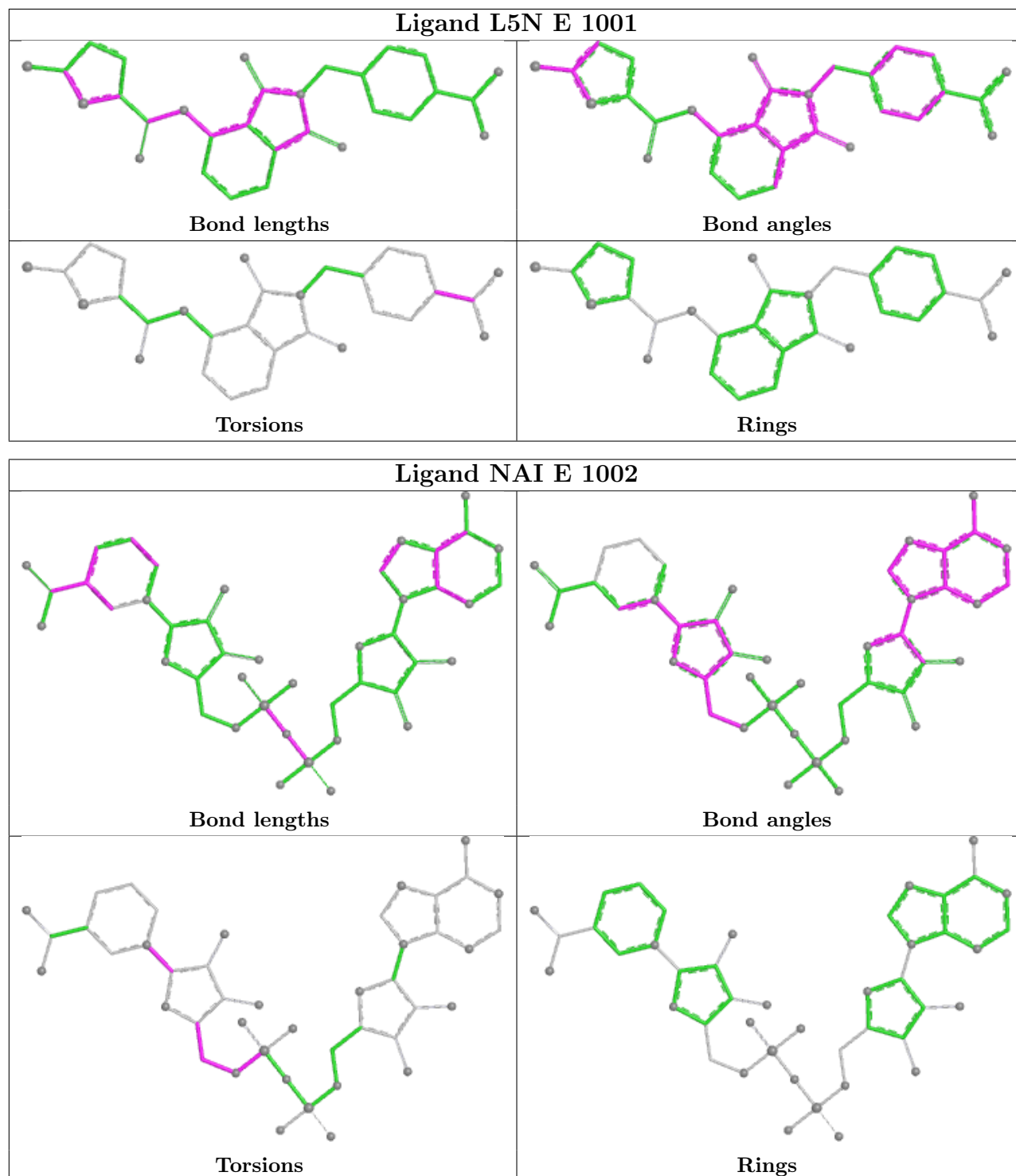
There are no ring outliers.

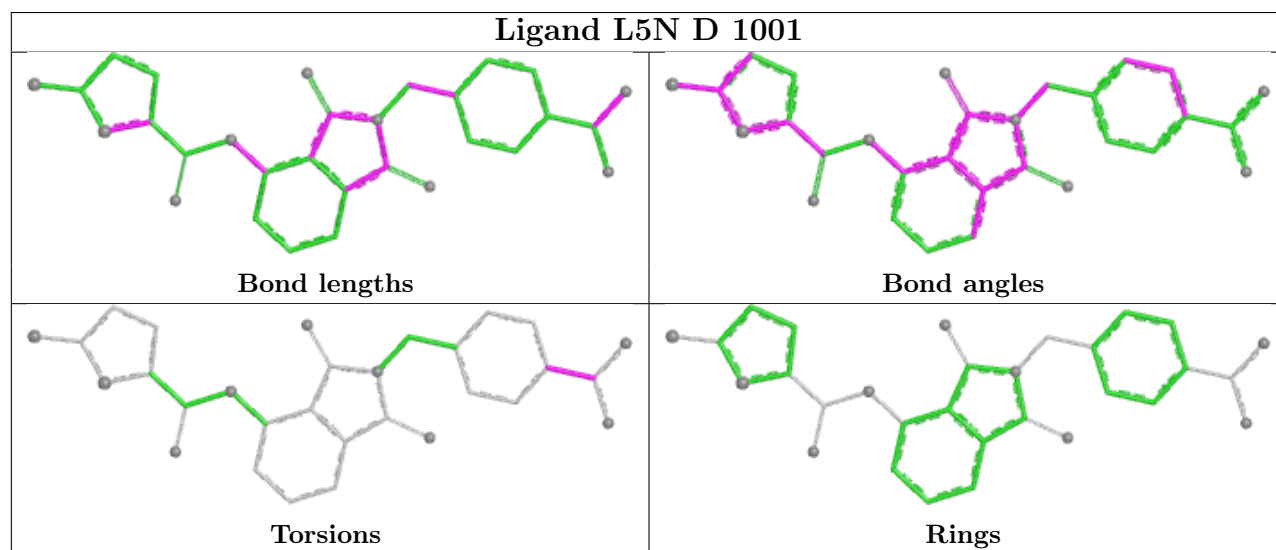
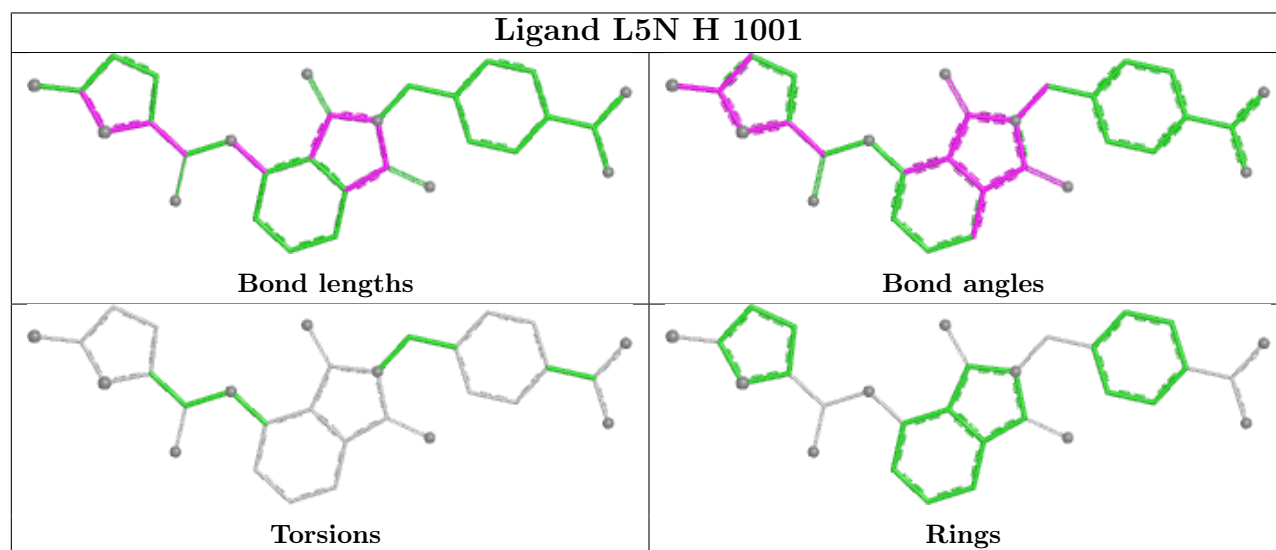
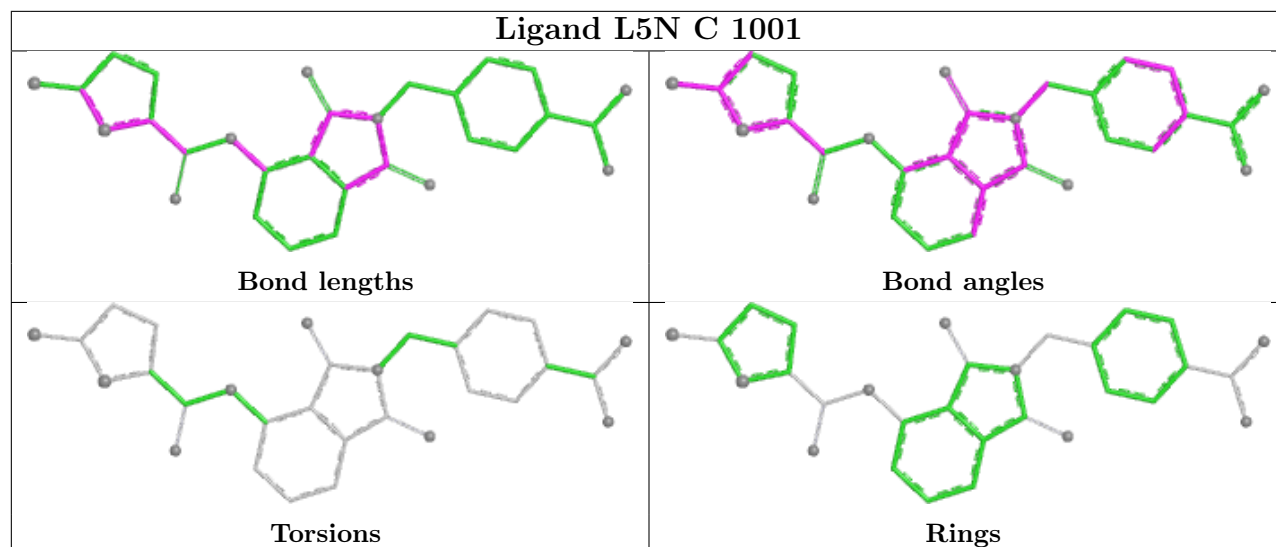
7 monomers are involved in 23 short contacts:

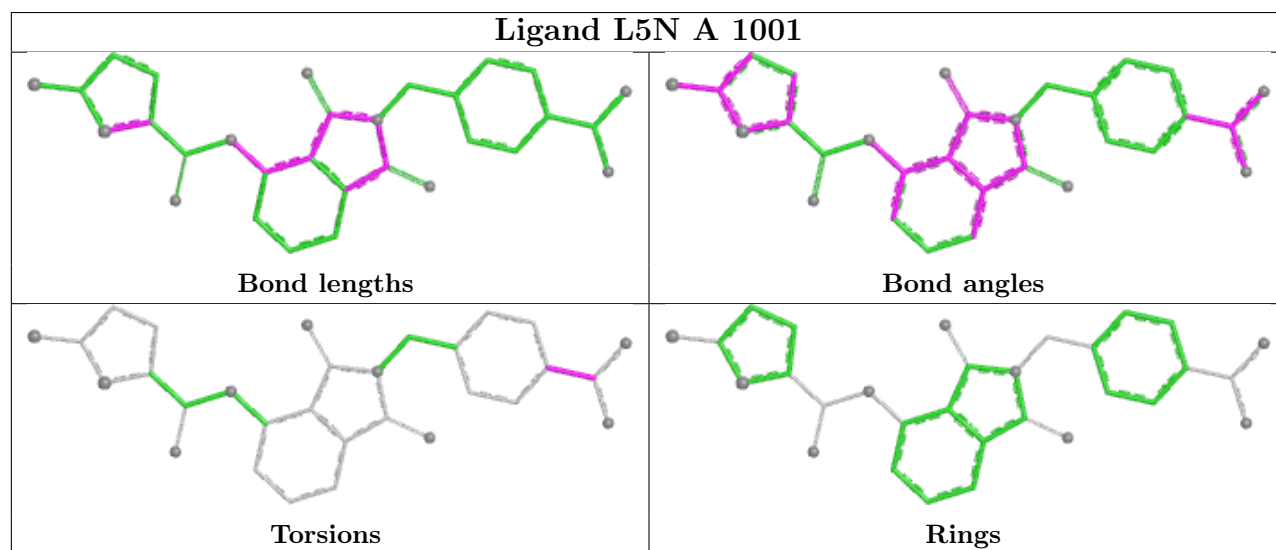
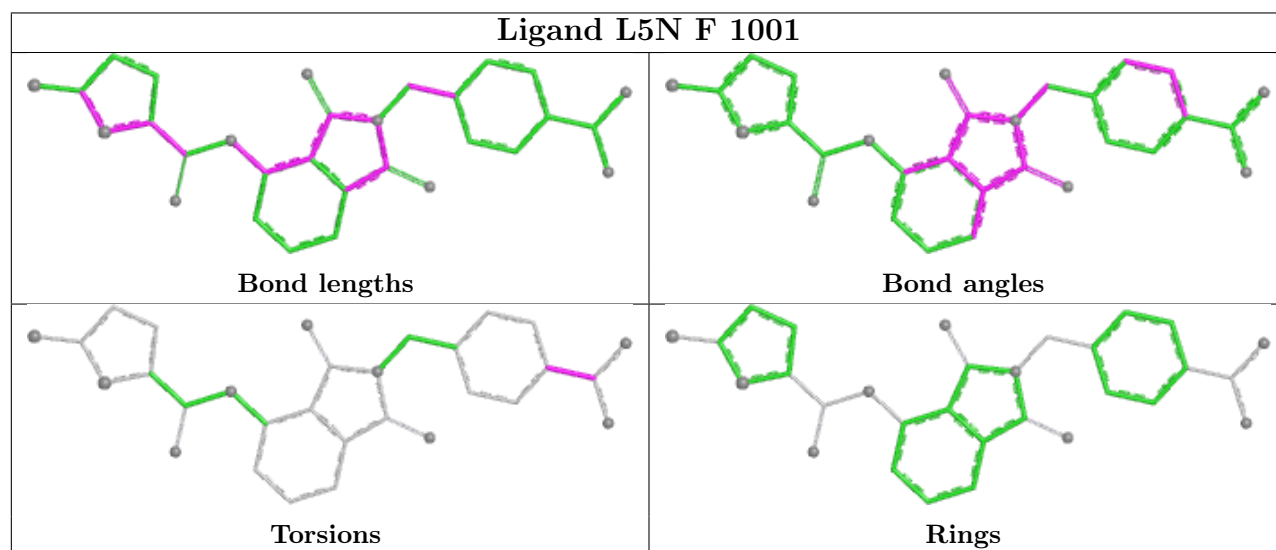
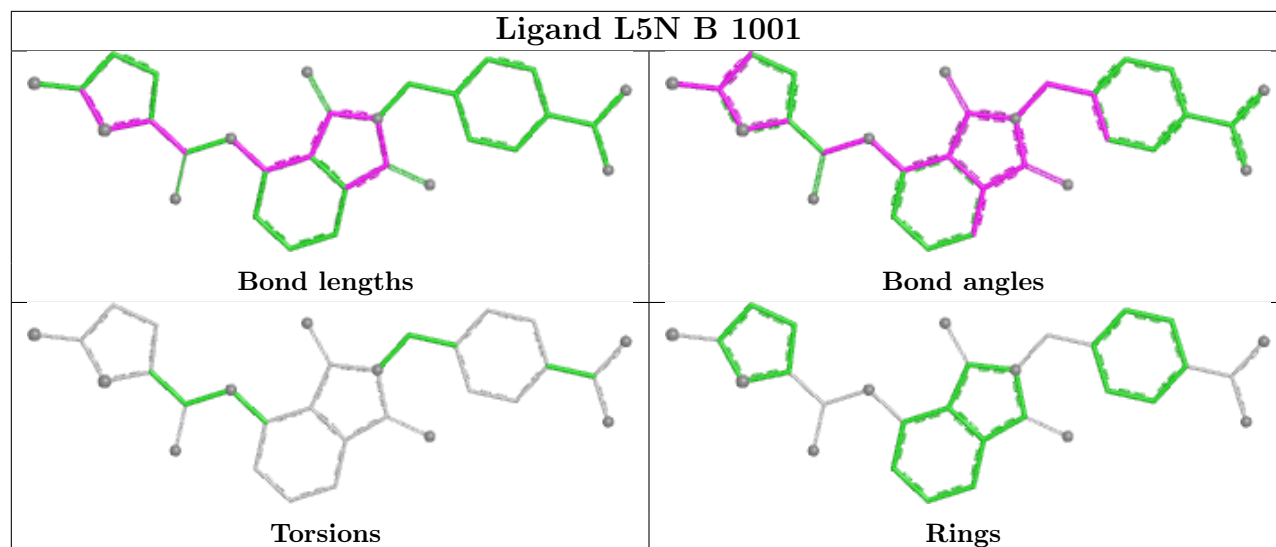
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1001	L5N	2	0
3	E	1002	NAI	8	0
2	C	1001	L5N	1	0
2	B	1001	L5N	3	0
2	F	1001	L5N	1	0
2	G	1001	L5N	1	0
3	A	1002	NAI	7	0

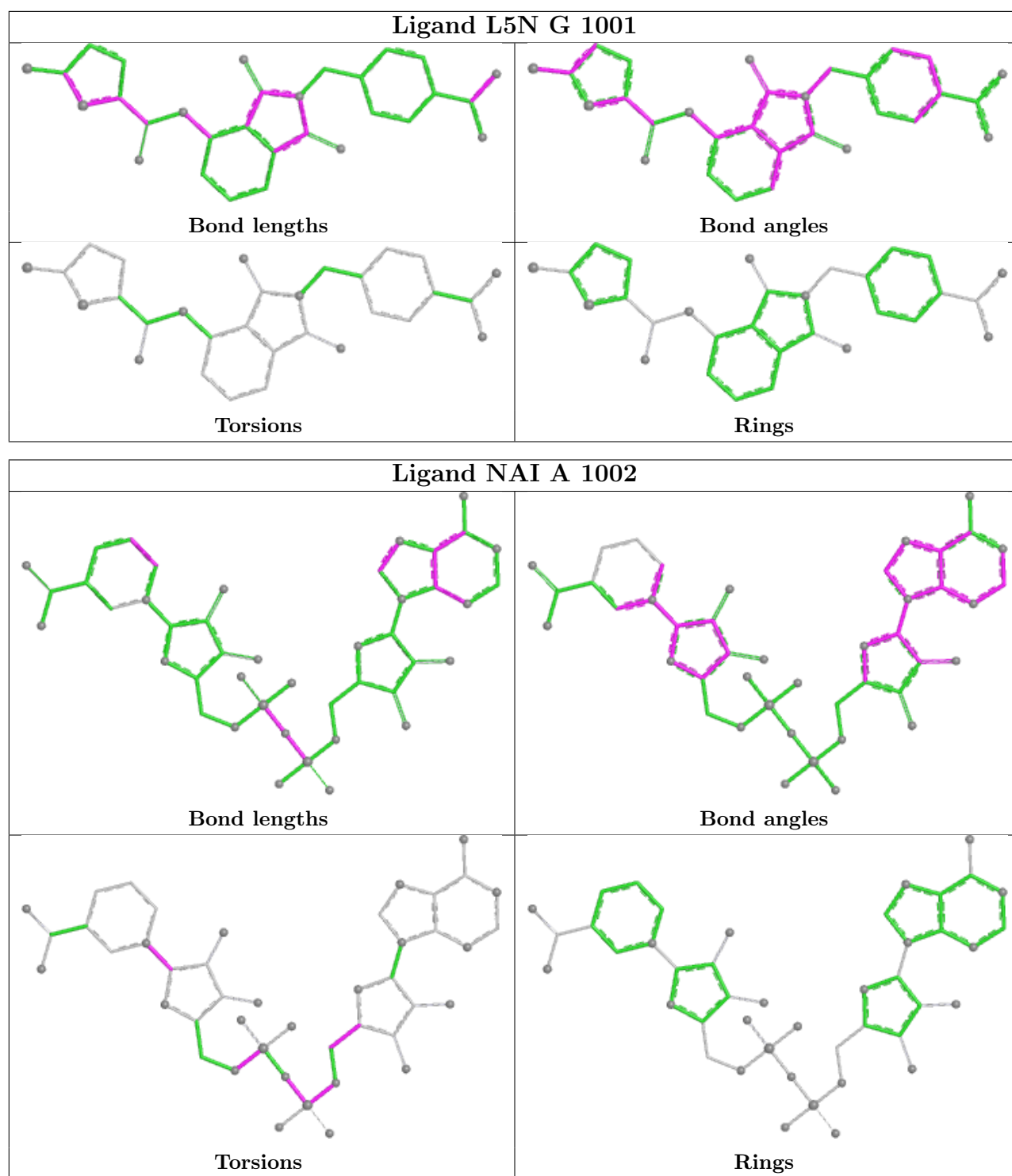
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	328/332 (98%)	0.00	3 (0%) 81 74	41, 61, 93, 122	0
1	B	328/332 (98%)	-0.11	1 (0%) 90 87	37, 60, 88, 109	1 (0%)
1	C	328/332 (98%)	0.02	2 (0%) 85 81	42, 63, 92, 107	0
1	D	328/332 (98%)	-0.26	0 100 100	41, 57, 88, 111	0
1	E	328/332 (98%)	0.19	0 100 100	34, 73, 106, 128	1 (0%)
1	F	328/332 (98%)	-0.12	1 (0%) 90 87	43, 67, 95, 108	0
1	G	328/332 (98%)	-0.06	2 (0%) 85 81	47, 68, 100, 115	0
1	H	328/332 (98%)	-0.12	0 100 100	45, 65, 95, 115	0
All	All	2624/2656 (98%)	-0.06	9 (0%) 90 87	34, 65, 96, 128	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	30	ALA	2.6
1	G	2	ALA	2.6
1	C	14	LYS	2.4
1	A	14	LYS	2.2
1	F	14	LYS	2.1
1	A	237	SER	2.1
1	B	284	LYS	2.0
1	G	14	LYS	2.0
1	A	206	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

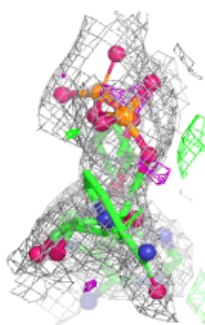
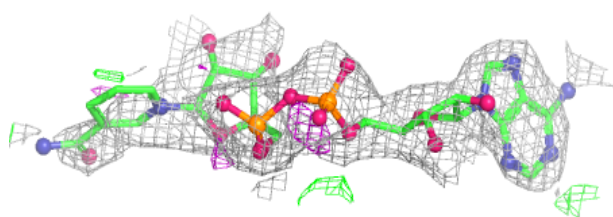
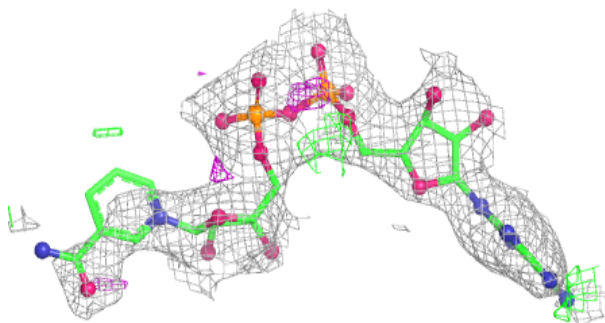
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAI	E	1002	44/44	0.82	0.14	80,115,128,136	0
3	NAI	A	1002	44/44	0.83	0.14	79,107,118,129	0
2	L5N	B	1001	30/30	0.92	0.09	48,64,79,106	0
2	L5N	E	1001	30/30	0.93	0.09	41,64,86,112	0
2	L5N	F	1001	30/30	0.94	0.08	60,72,85,147	0
2	L5N	G	1001	30/30	0.94	0.08	49,58,76,121	0
2	L5N	D	1001	30/30	0.95	0.07	50,59,69,105	0
2	L5N	H	1001	30/30	0.95	0.08	58,66,80,121	0
2	L5N	A	1001	30/30	0.95	0.07	42,52,67,100	0
2	L5N	C	1001	30/30	0.95	0.08	53,59,73,118	0

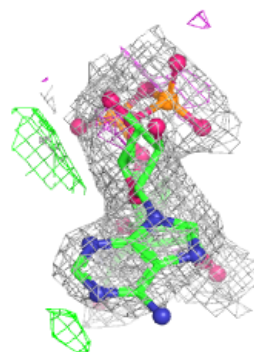
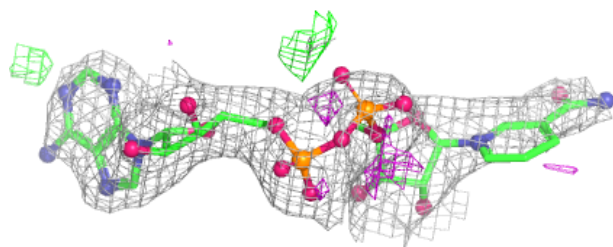
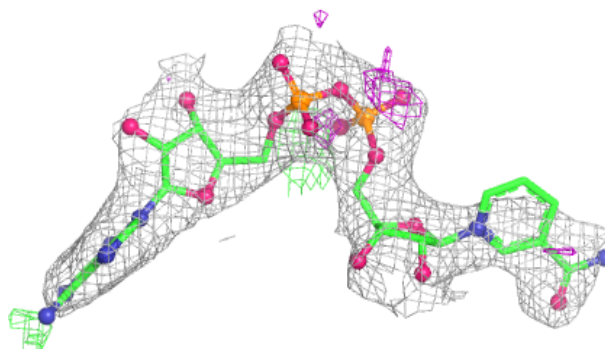
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI E 1002:

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

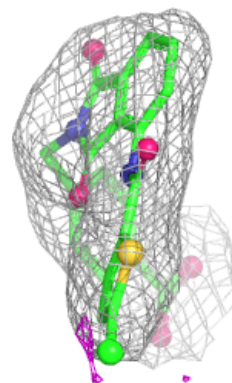
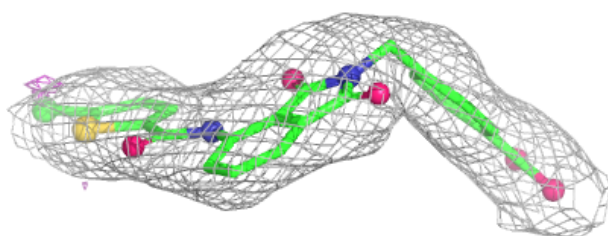
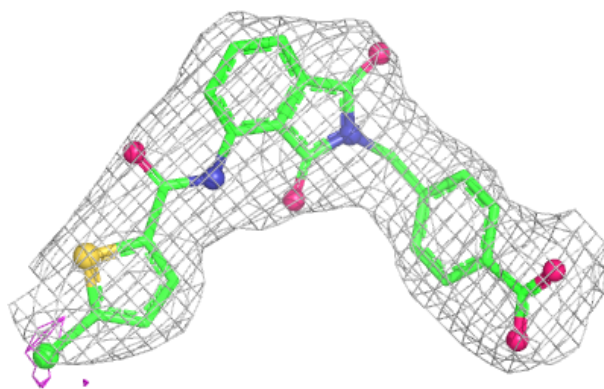
**Electron density around NAI A 1002:**

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



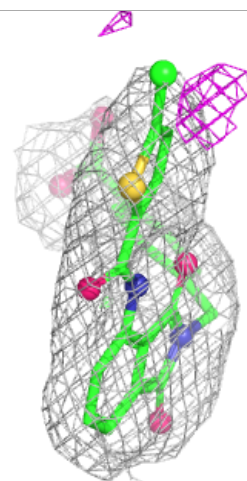
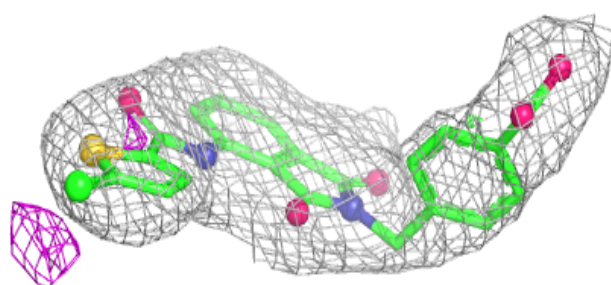
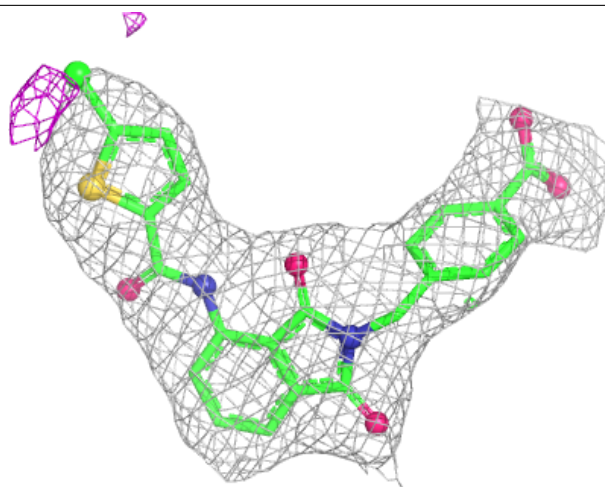
Electron density around L5N B 1001:

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



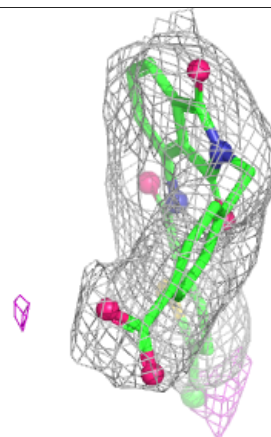
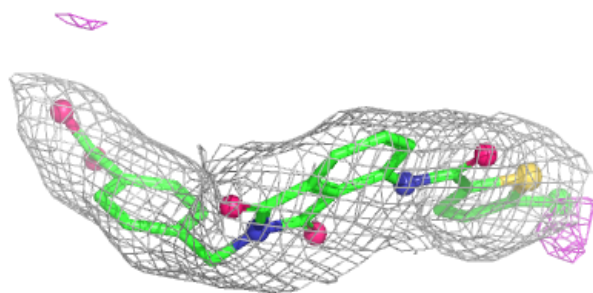
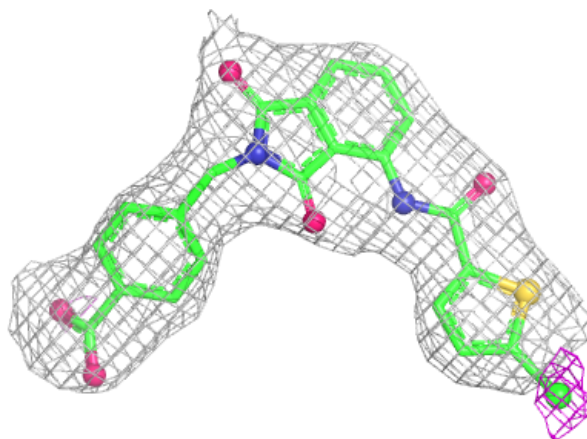
Electron density around L5N E 1001:

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



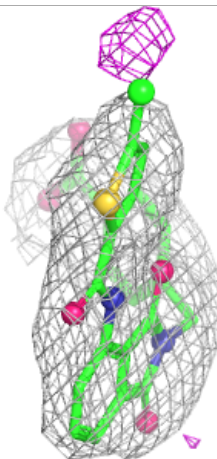
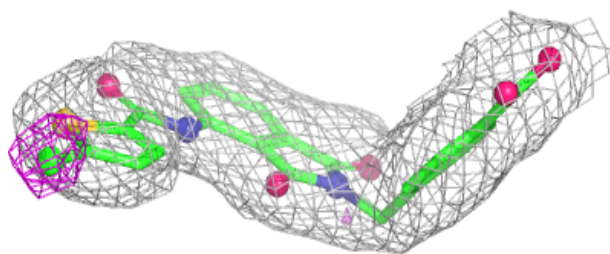
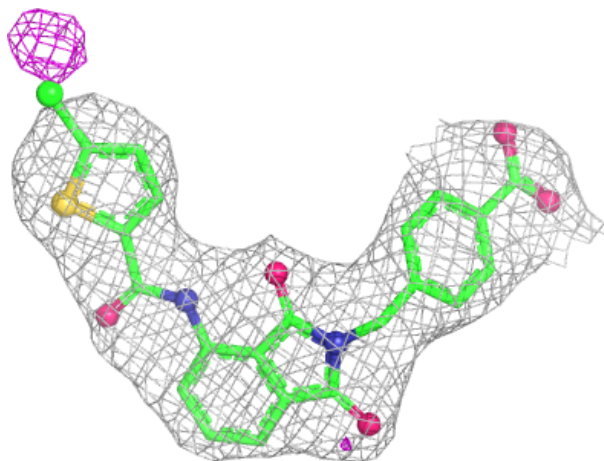
Electron density around L5N F 1001:

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



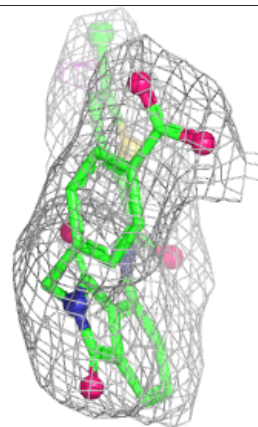
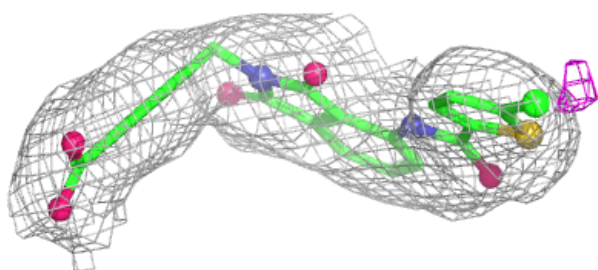
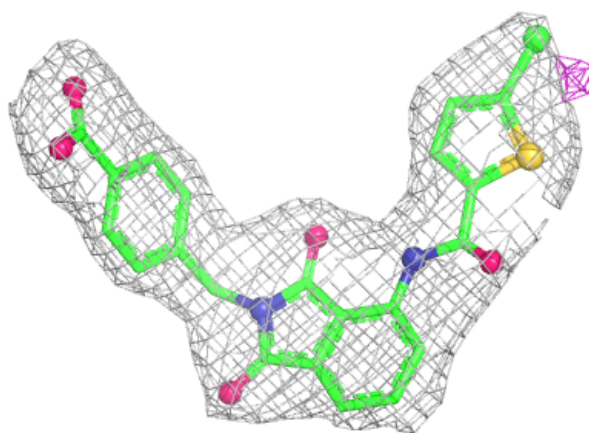
Electron density around L5N G 1001:

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

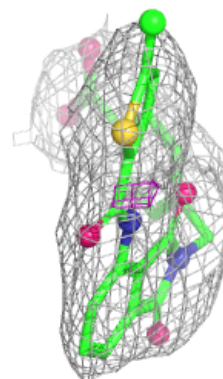
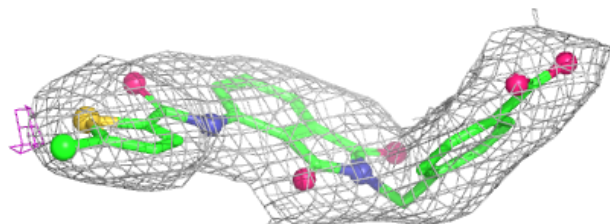
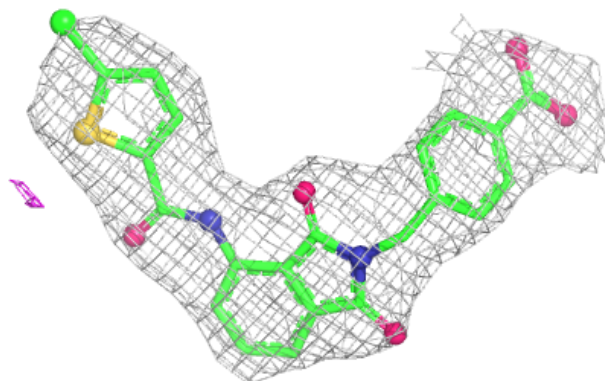


Electron density around L5N D 1001:

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

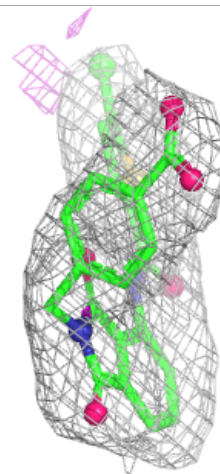
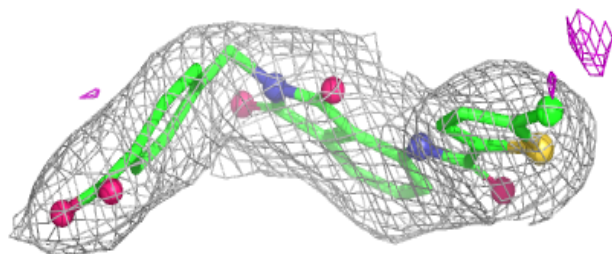
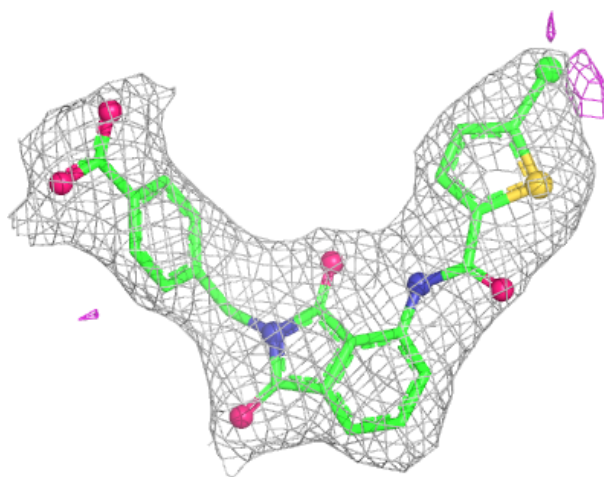
**Electron density around L5N H 1001:**

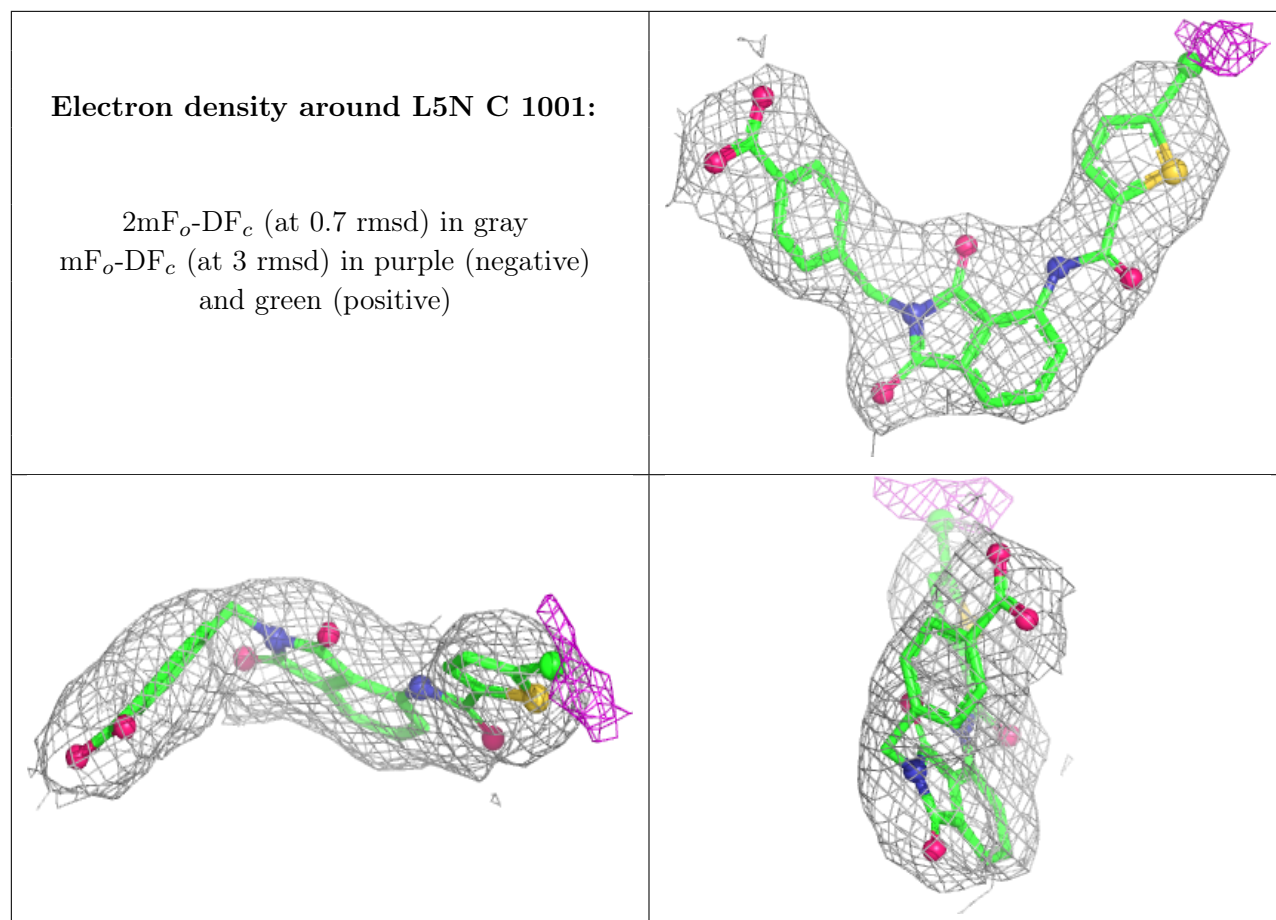
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around L5N A 1001:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.