



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:20 PM UTC

PDB ID : 8HFK / pdb_00008hfk
Title : Crystal Structure of CbAR mutant (H162F) in complex with NADP⁺ and halogenated aryl ketone
Authors : Hou, X.D.; Yin, D.J.; Rao, Y.J.
Deposited on : 2022-11-10
Resolution : 2.90 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

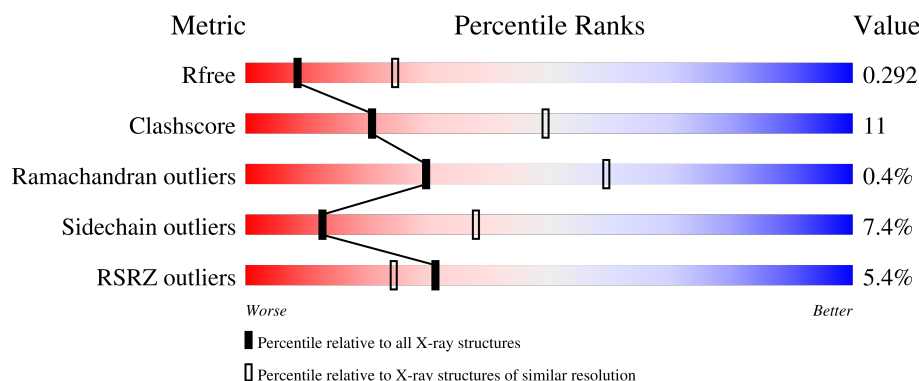
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	279	4% 68% 22% 7%
1	B	279	6% 59% 29% 9%
1	C	279	5% 68% 21% 10%
1	D	279	5% 70% 19% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	L8U	A	302	-	-	X	-
3	L8U	D	302	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7889 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 Versicolorin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1939	1220	344	371	4			
1	B	253	Total	C	N	O	S	0	0	0
			1882	1185	336	358	3			
1	C	251	Total	C	N	O	S	0	0	0
			1876	1183	333	356	4			
1	D	256	Total	C	N	O	S	0	0	0
			1897	1196	337	360	4			

There are 48 discrepancies between the modelled and reference sequences:

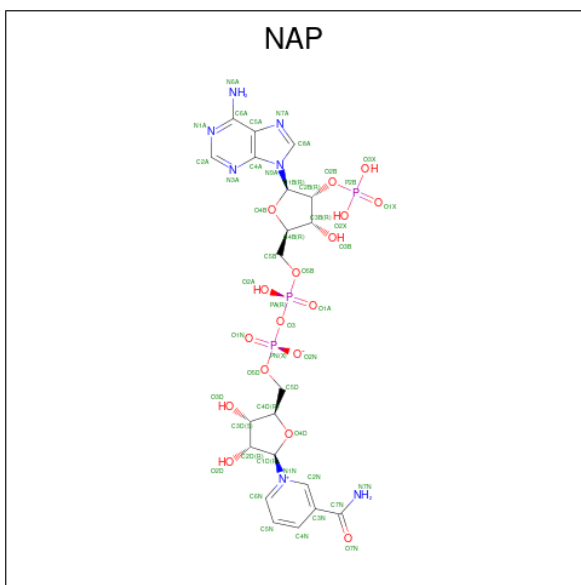
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP A0A2G5I2X5
A	0	ALA	-	expression tag	UNP A0A2G5I2X5
A	162	PHE	HIS	engineered mutation	UNP A0A2G5I2X5
A	269	ALA	-	expression tag	UNP A0A2G5I2X5
A	270	LEU	-	expression tag	UNP A0A2G5I2X5
A	271	GLU	-	expression tag	UNP A0A2G5I2X5
A	272	HIS	-	expression tag	UNP A0A2G5I2X5
A	273	HIS	-	expression tag	UNP A0A2G5I2X5
A	274	HIS	-	expression tag	UNP A0A2G5I2X5
A	275	HIS	-	expression tag	UNP A0A2G5I2X5
A	276	HIS	-	expression tag	UNP A0A2G5I2X5
A	277	HIS	-	expression tag	UNP A0A2G5I2X5
B	-1	MET	-	initiating methionine	UNP A0A2G5I2X5
B	0	ALA	-	expression tag	UNP A0A2G5I2X5
B	162	PHE	HIS	engineered mutation	UNP A0A2G5I2X5
B	269	ALA	-	expression tag	UNP A0A2G5I2X5
B	270	LEU	-	expression tag	UNP A0A2G5I2X5
B	271	GLU	-	expression tag	UNP A0A2G5I2X5
B	272	HIS	-	expression tag	UNP A0A2G5I2X5
B	273	HIS	-	expression tag	UNP A0A2G5I2X5
B	274	HIS	-	expression tag	UNP A0A2G5I2X5

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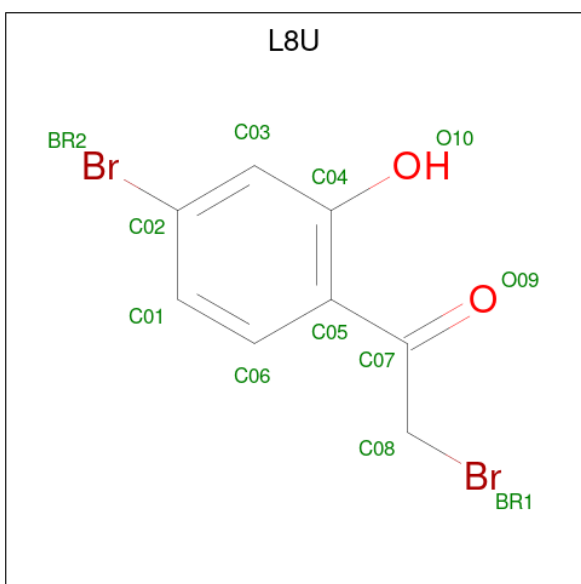
Chain	Residue	Modelled	Actual	Comment	Reference
B	275	HIS	-	expression tag	UNP A0A2G5I2X5
B	276	HIS	-	expression tag	UNP A0A2G5I2X5
B	277	HIS	-	expression tag	UNP A0A2G5I2X5
C	-1	MET	-	initiating methionine	UNP A0A2G5I2X5
C	0	ALA	-	expression tag	UNP A0A2G5I2X5
C	162	PHE	HIS	engineered mutation	UNP A0A2G5I2X5
C	269	ALA	-	expression tag	UNP A0A2G5I2X5
C	270	LEU	-	expression tag	UNP A0A2G5I2X5
C	271	GLU	-	expression tag	UNP A0A2G5I2X5
C	272	HIS	-	expression tag	UNP A0A2G5I2X5
C	273	HIS	-	expression tag	UNP A0A2G5I2X5
C	274	HIS	-	expression tag	UNP A0A2G5I2X5
C	275	HIS	-	expression tag	UNP A0A2G5I2X5
C	276	HIS	-	expression tag	UNP A0A2G5I2X5
C	277	HIS	-	expression tag	UNP A0A2G5I2X5
D	-1	MET	-	initiating methionine	UNP A0A2G5I2X5
D	0	ALA	-	expression tag	UNP A0A2G5I2X5
D	162	PHE	HIS	engineered mutation	UNP A0A2G5I2X5
D	269	ALA	-	expression tag	UNP A0A2G5I2X5
D	270	LEU	-	expression tag	UNP A0A2G5I2X5
D	271	GLU	-	expression tag	UNP A0A2G5I2X5
D	272	HIS	-	expression tag	UNP A0A2G5I2X5
D	273	HIS	-	expression tag	UNP A0A2G5I2X5
D	274	HIS	-	expression tag	UNP A0A2G5I2X5
D	275	HIS	-	expression tag	UNP A0A2G5I2X5
D	276	HIS	-	expression tag	UNP A0A2G5I2X5
D	277	HIS	-	expression tag	UNP A0A2G5I2X5

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is 2-bromanyl-1-(4-bromanyl-2-oxidanyl-phenyl)ethanone (CCD ID: L8U) (formula: $\text{C}_8\text{H}_6\text{Br}_2\text{O}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	Br	C	O	0	0
			12	2	8	2		
3	B	1	Total	Br	C	O	0	0
			12	2	8	2		
3	C	1	Total	Br	C	O	0	0
			12	2	8	2		
3	D	1	Total	Br	C	O	0	0
			12	2	8	2		

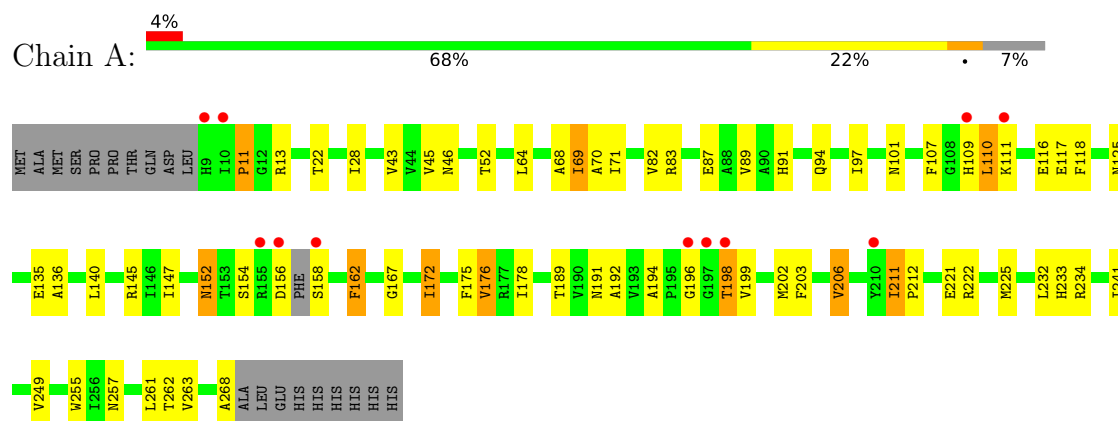
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	10	Total	O	0	0
			10	10		
4	C	16	Total	O	0	0
			16	16		
4	D	17	Total	O	0	0
			17	17		

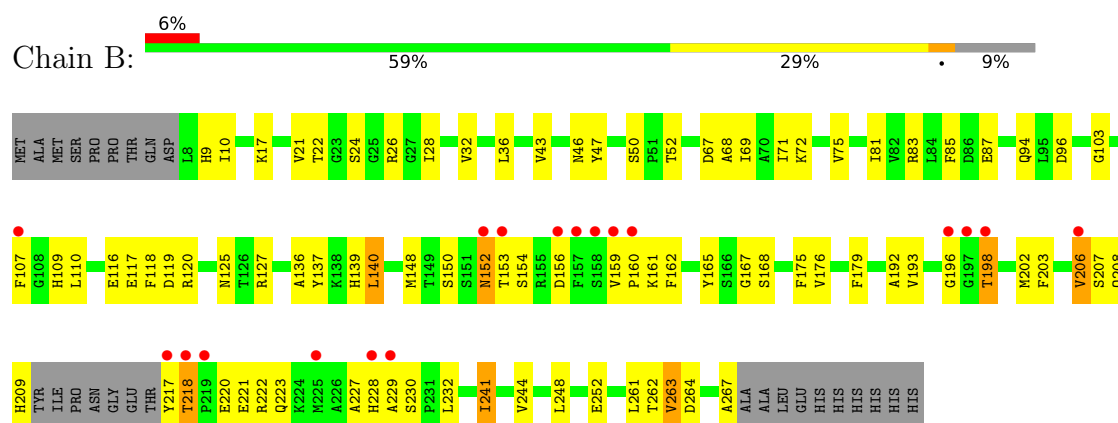
3 Residue-property plots

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.

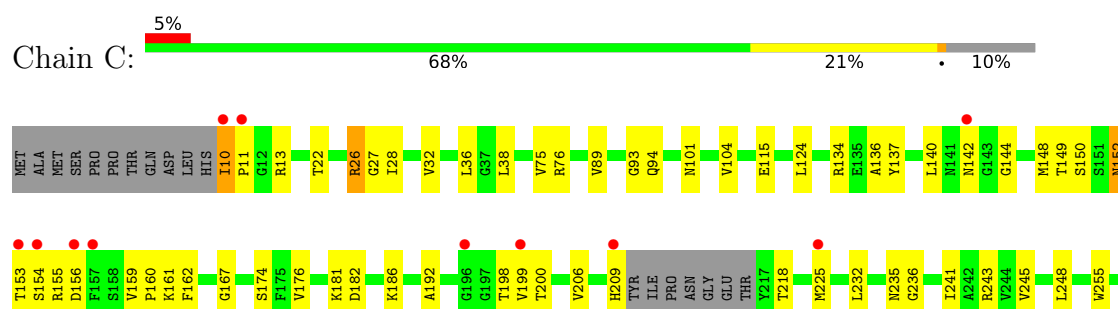
• Molecule 1: Versicolorin reductase

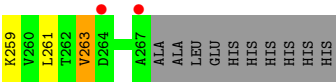


• Molecule 1: Versicolorin reductase

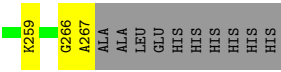
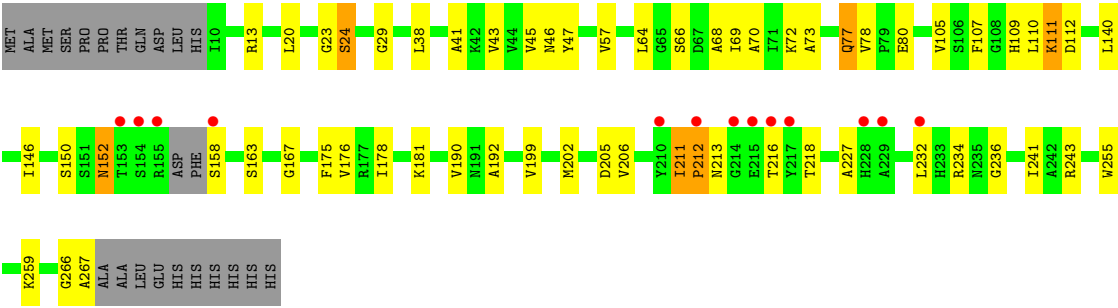


• Molecule 1: Versicolorin reductase





● Molecule 1: Versicolorin reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.87Å 124.87Å 133.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.05 – 2.90 24.05 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.05-2.90) 99.7 (24.05-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.202 , 0.289 0.217 , 0.292	Depositor DCC
R_{free} test set	1041 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7889	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: NAP, L8U

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	1.05	0/1976	1.51	2/2676 (0.1%)
1	B	1.08	1/1917 (0.1%)	1.48	4/2597 (0.2%)
1	C	1.04	0/1911	1.54	5/2586 (0.2%)
1	D	1.06	0/1931	1.52	5/2614 (0.2%)
All	All	1.06	1/7735 (0.0%)	1.51	16/10473 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	10	ILE	N-CA	5.29	1.50	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	ARG	N-CA-C	-6.91	104.49	113.12
1	D	77	GLN	CA-C-N	6.71	124.47	120.24
1	D	77	GLN	C-N-CA	6.71	124.47	120.24
1	A	257	ASN	CB-CA-C	5.88	119.20	110.14
1	D	232	LEU	N-CA-C	-5.79	106.17	113.18
1	B	241	ILE	N-CA-C	-5.71	105.53	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	227	ALA	CA-C-N	5.36	127.46	120.28
1	D	227	ALA	C-N-CA	5.36	127.46	120.28
1	C	232	LEU	N-CA-C	-5.35	106.76	113.28
1	B	267	ALA	CA-C-O	-5.28	111.83	120.80
1	C	144	GLY	CA-C-O	-5.19	117.09	122.28
1	A	116	GLU	CB-CG-CD	5.12	121.30	112.60
1	C	245	VAL	CA-C-N	5.11	125.65	119.98
1	C	245	VAL	C-N-CA	5.11	125.65	119.98
1	B	116	GLU	N-CA-C	-5.05	105.77	111.28
1	B	67	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain
1	A	222	ARG	Sidechain
1	A	234	ARG	Sidechain
1	D	234	ARG	Sidechain

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	1939	0	1898	53	0
1	B	1882	0	1837	57	0
1	C	1876	0	1842	42	0
1	D	1897	0	1869	45	0
2	A	48	0	25	3	0
2	B	48	0	25	2	0
2	C	48	0	25	4	0
2	D	48	0	25	1	0
3	A	12	0	0	5	0
3	B	12	0	0	0	0
3	C	12	0	0	2	0
3	D	12	0	0	4	0
4	A	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	0	0	0
4	C	16	0	0	2	0
4	D	17	0	0	0	0
All	All	7889	0	7546	170	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (170) 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:D:202:MET:SD	3:D:302:L8U:BR1	2.87	0.88
1:D:152:ASN:HD22	1:D:152:ASN:H	1.26	0.83
1:A:11:PRO:HD2	1:C:11:PRO:HG2	1.60	0.82
1:A:28:ILE:HD12	2:A:301:NAP:H51N	1.62	0.81
1:B:136:ALA:O	1:B:140:LEU:HB2	1.82	0.79
1:D:107:PHE:HZ	1:D:206:VAL:HG22	1.47	0.79
1:C:22:THR:O	1:C:101:ASN:HB3	1.83	0.78
1:A:152:ASN:HD21	3:A:302:L8U:C03	1.99	0.75
1:B:153:THR:HG21	1:B:162:PHE:HE2	1.54	0.72
1:D:107:PHE:CZ	1:D:206:VAL:HG22	2.27	0.69
1:A:196:GLY:O	2:A:301:NAP:H4N	1.93	0.68
1:C:174:SER:HB2	1:D:167:GLY:HA2	1.76	0.67
1:A:202:MET:SD	3:A:302:L8U:BR1	3.08	0.67
1:B:176:VAL:HG11	1:B:192:ALA:HB2	1.76	0.67
1:A:202:MET:O	1:A:206:VAL:HG13	1.96	0.66
1:A:152:ASN:O	1:A:156:ASP:HB2	1.96	0.66
1:B:208:GLN:HG3	1:B:222:ARG:CZ	2.27	0.65
1:A:176:VAL:HG11	1:A:192:ALA:HB2	1.79	0.64
1:B:202:MET:O	1:B:206:VAL:HG13	1.99	0.63
1:D:152:ASN:HD22	1:D:152:ASN:N	1.95	0.62
1:B:208:GLN:HG3	1:B:222:ARG:NH1	2.14	0.62
1:C:243:ARG:CZ	4:C:402:HOH:O	2.49	0.61
1:C:104:VAL:HG13	1:C:124:LEU:HD23	1.83	0.60
1:D:150:SER:O	2:D:301:NAP:H6N	2.02	0.60
1:A:178:ILE:HG23	1:B:160:PRO:HA	1.84	0.60
1:B:153:THR:HG21	1:B:162:PHE:CE2	2.37	0.58
1:C:32:VAL:O	1:C:36:LEU:HG	2.03	0.58
1:D:152:ASN:HD21	3:D:302:L8U:C03	2.16	0.58
1:A:136:ALA:O	1:A:140:LEU:HB2	2.05	0.57
1:D:202:MET:HG2	3:D:302:L8U:BR1	2.60	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:VAL:O	1:B:36:LEU:HG	2.05	0.56
1:D:202:MET:O	1:D:206:VAL:HG23	2.05	0.56
1:A:167:GLY:HA3	1:B:175:PHE:CE1	2.41	0.56
1:D:41:ALA:O	1:D:66:SER:OG	2.20	0.55
1:D:211:ILE:O	1:D:213:ASN:N	2.39	0.55
1:C:199:VAL:HG13	1:C:236:GLY:O	2.06	0.55
1:A:263:VAL:HG12	1:C:255:TRP:CD1	2.42	0.54
1:C:199:VAL:O	1:C:200:THR:HG23	2.08	0.54
1:B:160:PRO:O	1:B:161:LYS:C	2.50	0.54
1:B:196:GLY:O	2:B:301:NAP:H4N	2.07	0.54
1:A:263:VAL:HG12	1:C:255:TRP:HD1	1.73	0.53
1:A:111:LYS:HD3	1:B:137:TYR:HE2	1.72	0.53
1:A:69:ILE:HD12	1:A:71:ILE:HG13	1.92	0.52
1:C:153:THR:O	1:C:154:SER:C	2.52	0.52
1:D:20:LEU:C	1:D:20:LEU:HD23	2.35	0.52
1:B:152:ASN:HD22	1:B:152:ASN:N	2.08	0.51
1:B:207:SER:C	1:B:209:HIS:H	2.18	0.51
1:C:243:ARG:NE	4:C:402:HOH:O	2.44	0.51
1:A:109:HIS:ND1	1:A:111:LYS:HG2	2.26	0.51
1:B:264:ASP:OD1	1:D:259:LYS:NZ	2.44	0.51
1:B:9:HIS:O	1:D:13:ARG:NH1	2.44	0.51
1:A:109:HIS:O	1:A:110:LEU:C	2.53	0.51
1:B:198:THR:O	1:B:203:PHE:HB2	2.11	0.51
1:A:147:ILE:HA	1:A:191:ASN:O	2.11	0.50
1:A:262:THR:HB	1:C:259:LYS:HE2	1.92	0.50
1:B:227:ALA:C	1:B:229:ALA:H	2.20	0.50
1:A:203:PHE:O	1:A:206:VAL:HG22	2.12	0.50
1:B:160:PRO:C	1:B:162:PHE:N	2.69	0.50
1:D:152:ASN:H	1:D:152:ASN:ND2	2.03	0.50
1:A:255:TRP:HB3	1:C:263:VAL:HG12	1.94	0.50
1:A:110:LEU:HG	1:B:179:PHE:CE1	2.47	0.50
1:D:107:PHE:CZ	1:D:206:VAL:HA	2.47	0.50
1:B:28:ILE:HD11	1:B:198:THR:OG1	2.12	0.49
1:A:107:PHE:CZ	1:A:206:VAL:HG12	2.46	0.49
1:B:22:THR:HA	1:B:46:ASN:HB3	1.94	0.49
1:A:82:VAL:HG22	1:A:135:GLU:CD	2.38	0.49
1:A:263:VAL:HG12	1:C:255:TRP:HB3	1.94	0.49
1:C:167:GLY:HA3	1:D:175:PHE:CE1	2.47	0.49
1:D:266:GLY:O	1:D:267:ALA:C	2.55	0.49
1:D:77:GLN:HB2	1:D:80:GLU:HB2	1.95	0.49
1:D:105:VAL:HG21	1:D:206:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:HIS:HB2	1:B:161:LYS:HE2	1.95	0.48
1:C:181:LYS:NZ	1:D:158:SER:O	2.36	0.48
1:D:178:ILE:O	1:D:181:LYS:N	2.46	0.48
1:B:263:VAL:HG12	1:D:255:TRP:HB3	1.95	0.48
1:C:198:THR:CG2	1:C:241:ILE:HD13	2.44	0.48
1:B:153:THR:O	1:B:154:SER:C	2.57	0.48
1:B:218:THR:OG1	1:B:221:GLU:HG3	2.14	0.48
1:B:75:VAL:O	1:B:81:ILE:HD11	2.13	0.47
1:D:38:LEU:HA	1:D:64:LEU:HD13	1.95	0.47
1:D:202:MET:CG	3:D:302:L8U:BR1	3.18	0.47
1:D:199:VAL:HG23	1:D:236:GLY:O	2.15	0.47
1:D:43:VAL:O	1:D:68:ALA:HA	2.14	0.47
1:D:109:HIS:O	1:D:110:LEU:C	2.58	0.47
1:B:85:PHE:HB3	1:B:139:HIS:CD2	2.49	0.47
1:A:202:MET:HE1	2:A:301:NAP:H2D	1.97	0.47
1:B:47:TYR:CZ	1:B:72:LYS:HB2	2.50	0.47
1:A:107:PHE:HZ	1:A:206:VAL:HG12	1.81	0.46
1:A:11:PRO:HG3	1:C:11:PRO:O	2.15	0.46
1:C:75:VAL:HG23	1:C:124:LEU:CD1	2.45	0.46
1:B:165:TYR:O	1:B:168:SER:OG	2.29	0.46
1:A:43:VAL:O	1:A:68:ALA:HA	2.16	0.46
1:C:182:ASP:HB3	1:D:109:HIS:CE1	2.50	0.46
1:C:115:GLU:HG2	1:D:78:VAL:HG21	1.97	0.45
1:D:176:VAL:HG11	1:D:192:ALA:HB2	1.98	0.45
1:D:45:VAL:O	1:D:70:ALA:HA	2.16	0.45
1:D:73:ALA:HA	1:D:80:GLU:OE1	2.16	0.45
1:D:46:ASN:ND2	1:D:73:ALA:HB3	2.31	0.45
1:D:45:VAL:HG21	1:D:57:VAL:HG12	1.97	0.45
1:B:28:ILE:HG12	1:B:198:THR:HG21	1.98	0.45
1:A:268:ALA:HB1	3:A:302:L8U:BR2	2.72	0.45
1:C:10:ILE:HG22	1:C:11:PRO:HD2	1.99	0.45
1:A:211:ILE:HD13	1:A:211:ILE:HA	1.85	0.45
1:B:252:GLU:HG3	1:D:243:ARG:HD3	1.99	0.45
1:C:134:ARG:HA	1:D:110:LEU:HG	1.98	0.45
1:A:118:PHE:CE1	1:B:127:ARG:HG3	2.52	0.44
1:C:104:VAL:HG13	1:C:124:LEU:CD2	2.46	0.44
1:B:21:VAL:HG12	1:B:24:SER:HB3	2.00	0.44
1:B:220:GLU:HA	1:B:223:GLN:HB3	2.00	0.44
1:A:111:LYS:HD3	1:B:137:TYR:CE2	2.51	0.44
1:A:268:ALA:HA	3:A:302:L8U:BR2	2.73	0.44
1:B:83:ARG:HG2	1:B:87:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:THR:HG21	1:C:241:ILE:HD13	1.99	0.44
1:B:152:ASN:HD22	1:B:152:ASN:H	1.64	0.44
1:A:125:ASN:O	1:A:172:ILE:HD11	2.18	0.43
1:A:118:PHE:C	1:A:118:PHE:CD1	2.96	0.43
1:D:111:LYS:HG3	1:D:112:ASP:CG	2.43	0.43
1:B:248:LEU:HD11	1:B:261:LEU:HD22	1.99	0.43
1:C:206:VAL:HG11	3:C:302:L8U:C08	2.48	0.43
1:C:248:LEU:HD21	1:C:261:LEU:HD22	2.00	0.43
1:D:23:GLY:O	1:D:29:GLY:HA3	2.19	0.43
1:A:140:LEU:HD12	1:A:140:LEU:HA	1.91	0.43
1:B:230:SER:C	1:B:232:LEU:N	2.74	0.43
1:B:264:ASP:CG	1:D:259:LYS:HZ1	2.27	0.43
1:C:176:VAL:HG11	1:C:192:ALA:HB2	2.01	0.43
1:D:146:ILE:HB	1:D:190:VAL:HG22	2.00	0.43
1:B:103:GLY:HA2	1:B:125:ASN:OD1	2.18	0.43
1:C:152:ASN:O	1:C:156:ASP:HB2	2.18	0.42
1:C:155:ARG:O	1:C:156:ASP:C	2.62	0.42
1:C:13:ARG:NH1	1:C:38:LEU:O	2.53	0.42
1:C:148:MET:O	1:C:192:ALA:HA	2.20	0.42
1:A:162:PHE:HZ	3:A:302:L8U:C08	2.32	0.42
1:A:175:PHE:CE1	1:B:167:GLY:HA3	2.55	0.42
1:B:117:GLU:O	1:B:118:PHE:C	2.63	0.42
1:A:194:ALA:N	1:A:261:LEU:O	2.48	0.42
1:B:207:SER:C	1:B:209:HIS:N	2.78	0.42
1:B:69:ILE:HD12	1:B:71:ILE:HD11	2.02	0.42
1:B:262:THR:HB	1:D:259:LYS:HE2	2.00	0.42
1:A:94:GLN:HA	4:A:401:HOH:O	2.19	0.41
1:B:198:THR:HG23	1:B:241:ILE:HD13	2.02	0.41
1:A:263:VAL:CG1	1:C:255:TRP:HB3	2.49	0.41
1:A:232:LEU:O	1:A:233:HIS:C	2.62	0.41
1:B:17:LYS:HA	1:B:96:ASP:OD2	2.20	0.41
1:A:45:VAL:O	1:A:70:ALA:HA	2.19	0.41
1:A:83:ARG:HG2	1:A:87:GLU:OE1	2.19	0.41
1:A:97:ILE:HG12	1:A:249:VAL:HB	2.02	0.41
1:B:148:MET:O	1:B:192:ALA:HA	2.21	0.41
1:D:24:SER:HA	1:D:29:GLY:C	2.45	0.41
1:A:117:GLU:HA	1:A:117:GLU:OE1	2.21	0.41
1:C:89:VAL:O	1:C:93:GLY:N	2.53	0.41
1:A:28:ILE:HD11	1:A:198:THR:HG21	2.03	0.41
1:B:50:SER:OG	2:B:301:NAP:O1X	2.32	0.41
2:C:301:NAP:O1N	2:C:301:NAP:N7N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:TYR:CZ	1:D:72:LYS:HB2	2.56	0.41
1:A:178:ILE:HD12	1:B:159:VAL:O	2.20	0.41
1:C:136:ALA:O	1:C:140:LEU:HB2	2.20	0.41
1:A:22:THR:O	1:A:101:ASN:HB3	2.20	0.41
1:A:22:THR:HA	1:A:46:ASN:HB3	2.03	0.41
1:B:244:VAL:HG21	1:B:263:VAL:HG11	2.03	0.41
1:C:75:VAL:HG22	2:C:301:NAP:N1A	2.36	0.41
1:C:26:ARG:HG3	2:C:301:NAP:H3B	2.03	0.41
1:A:145:ARG:HD3	1:A:189:THR:OG1	2.21	0.40
1:B:109:HIS:O	1:B:110:LEU:C	2.64	0.40
1:B:119:ASP:O	1:B:120:ARG:C	2.64	0.40
1:C:152:ASN:ND2	3:C:302:L8U:O10	2.52	0.40
1:C:137:TYR:CE1	1:C:186:LYS:HD3	2.56	0.40
1:C:149:THR:HG21	2:C:301:NAP:H4D	2.04	0.40
1:B:43:VAL:O	1:B:68:ALA:HA	2.20	0.40
1:A:69:ILE:HG21	1:A:91:HIS:NE2	2.36	0.40
1:C:27:GLY:O	1:C:28:ILE:C	2.64	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	255/279 (91%)	235 (92%)	19 (8%)	1 (0%)	30	59
1	B	249/279 (89%)	228 (92%)	19 (8%)	2 (1%)	16	44
1	C	247/279 (88%)	224 (91%)	23 (9%)	0	100	100
1	D	252/279 (90%)	233 (92%)	18 (7%)	1 (0%)	30	59
All	All	1003/1116 (90%)	920 (92%)	79 (8%)	4 (0%)	30	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	D	212	PRO
1	B	156	ASP
1	B	228	HIS

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	204/225 (91%)	185 (91%)	19 (9%)	8	27
1	B	196/225 (87%)	183 (93%)	13 (7%)	15	43
1	C	197/225 (88%)	182 (92%)	15 (8%)	12	36
1	D	198/225 (88%)	186 (94%)	12 (6%)	17	46
All	All	795/900 (88%)	736 (93%)	59 (7%)	13	38

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	64	LEU
1	A	69	ILE
1	A	89	VAL
1	A	110	LEU
1	A	152	ASN
1	A	154	SER
1	A	158	SER
1	A	162	PHE
1	A	172	ILE
1	A	176	VAL
1	A	198	THR
1	A	199	VAL
1	A	206	VAL
1	A	211	ILE
1	A	212	PRO
1	A	221	GLU
1	A	225	MET

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Mol	Chain	Res	Type
1	A	241	ILE
1	B	26	ARG
1	B	52	THR
1	B	94	GLN
1	B	107	PHE
1	B	140	LEU
1	B	150	SER
1	B	152	ASN
1	B	193	VAL
1	B	198	THR
1	B	206	VAL
1	B	217	TYR
1	B	218	THR
1	B	263	VAL
1	C	10	ILE
1	C	26	ARG
1	C	94	GLN
1	C	142	ASN
1	C	150	SER
1	C	152	ASN
1	C	159	VAL
1	C	160	PRO
1	C	161	LYS
1	C	162	PHE
1	C	209	HIS
1	C	218	THR
1	C	225	MET
1	C	235	ASN
1	C	263	VAL
1	D	24	SER
1	D	69	ILE
1	D	111	LYS
1	D	140	LEU
1	D	152	ASN
1	D	163	SER
1	D	205	ASP
1	D	211	ILE
1	D	212	PRO
1	D	216	THR
1	D	218	THR
1	D	241	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	94	GLN
1	A	101	ASN
1	A	152	ASN
1	A	191	ASN
1	A	208	GLN
1	A	209	HIS
1	B	46	ASN
1	B	94	GLN
1	B	152	ASN
1	B	208	GLN
1	B	233	HIS
1	C	49	ASN
1	C	91	HIS
1	C	141	ASN
1	C	152	ASN
1	C	223	GLN
1	D	35	HIS
1	D	49	ASN
1	D	101	ASN
1	D	152	ASN
1	D	233	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](#)

8 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	NAP	A	301	-	50,52,52	2.41	28 (56%)	71,80,80	1.74	17 (23%)
3	L8U	D	302	-	12,12,12	1.34	2 (16%)	16,16,16	1.49	1 (6%)
2	NAP	D	301	-	50,52,52	2.27	23 (46%)	71,80,80	2.06	19 (26%)
3	L8U	A	302	-	12,12,12	1.48	2 (16%)	16,16,16	2.37	6 (37%)
3	L8U	B	302	-	12,12,12	1.42	3 (25%)	16,16,16	1.10	1 (6%)
2	NAP	B	301	-	50,52,52	2.32	26 (52%)	71,80,80	1.78	13 (18%)
3	L8U	C	302	-	12,12,12	1.32	1 (8%)	16,16,16	1.54	3 (18%)
2	NAP	C	301	-	50,52,52	2.25	20 (40%)	71,80,80	1.75	13 (18%)

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	NAP	A	301	-	-	5/35/67/67	0/5/5/5
3	L8U	D	302	-	-	0/6/6/6	0/1/1/1
2	NAP	D	301	-	-	11/35/67/67	0/5/5/5
3	L8U	A	302	-	-	4/6/6/6	0/1/1/1
3	L8U	B	302	-	-	0/6/6/6	0/1/1/1
2	NAP	B	301	-	-	0/35/67/67	0/5/5/5
3	L8U	C	302	-	-	2/6/6/6	0/1/1/1
2	NAP	C	301	-	-	5/35/67/67	0/5/5/5

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C2N-N1N	-5.35	1.29	1.35
2	C	301	NAP	C2N-N1N	-4.94	1.29	1.35
2	A	301	NAP	C4A-N9A	-4.77	1.27	1.37
2	B	301	NAP	C8A-N9A	-4.65	1.29	1.37
2	A	301	NAP	C2N-N1N	-4.50	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAP	C5A-N7A	-4.37	1.31	1.39
2	B	301	NAP	C5A-N7A	-4.34	1.31	1.39
2	C	301	NAP	C8A-N9A	-4.25	1.30	1.37
2	D	301	NAP	C5A-N7A	-4.19	1.31	1.39
2	B	301	NAP	C4A-N9A	-4.02	1.29	1.37
2	A	301	NAP	C8A-N9A	-4.02	1.30	1.37
2	D	301	NAP	C2N-N1N	-3.91	1.30	1.35
2	A	301	NAP	PA-O3	-3.82	1.55	1.59
2	D	301	NAP	C8A-N9A	-3.79	1.31	1.37
2	D	301	NAP	PN-O3	-3.77	1.55	1.59
2	A	301	NAP	O7N-C7N	-3.77	1.17	1.24
2	A	301	NAP	C5A-N7A	-3.77	1.32	1.39
2	B	301	NAP	O7N-C7N	-3.69	1.17	1.24
2	A	301	NAP	PN-O3	-3.63	1.55	1.59
2	D	301	NAP	P2B-O2B	-3.61	1.53	1.59
2	D	301	NAP	C4A-N9A	-3.60	1.30	1.37
2	D	301	NAP	P2B-O2X	-3.56	1.41	1.54
2	C	301	NAP	O7N-C7N	-3.47	1.17	1.24
2	A	301	NAP	C3N-C7N	-3.46	1.45	1.50
2	A	301	NAP	P2B-O2B	-3.45	1.53	1.59
2	D	301	NAP	O7N-C7N	-3.42	1.17	1.24
2	C	301	NAP	C4A-N9A	-3.38	1.30	1.37
2	B	301	NAP	C3N-C7N	-3.23	1.45	1.50
2	A	301	NAP	P2B-O3X	-3.23	1.42	1.54
2	A	301	NAP	PN-O2N	-3.15	1.40	1.55
2	C	301	NAP	P2B-O3X	-3.14	1.43	1.54
2	C	301	NAP	PA-O3	-3.14	1.56	1.59
2	B	301	NAP	P2B-O3X	-3.09	1.43	1.54
2	D	301	NAP	PN-O1N	-3.07	1.40	1.50
2	D	301	NAP	P2B-O3X	-3.04	1.43	1.54
2	A	301	NAP	PA-O2A	-3.04	1.41	1.55
2	B	301	NAP	C6N-N1N	-3.03	1.28	1.35
2	D	301	NAP	PN-O2N	-2.98	1.41	1.55
2	C	301	NAP	PA-O2A	-2.96	1.41	1.55
2	A	301	NAP	P2B-O2X	-2.93	1.43	1.54
2	B	301	NAP	PN-O2N	-2.93	1.41	1.55
2	D	301	NAP	O4B-C4B	-2.92	1.38	1.45
2	C	301	NAP	P2B-O2X	-2.86	1.44	1.54
2	D	301	NAP	C6N-N1N	-2.85	1.28	1.35
2	C	301	NAP	O4D-C4D	-2.85	1.38	1.45
2	A	301	NAP	O4D-C4D	-2.83	1.38	1.45
2	C	301	NAP	PN-O3	-2.83	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	L8U	O09-C07	-2.82	1.17	1.22
2	A	301	NAP	C7N-N7N	-2.78	1.27	1.33
2	B	301	NAP	P2B-O2B	-2.75	1.54	1.59
2	D	301	NAP	P2B-O1X	-2.75	1.41	1.50
2	B	301	NAP	O4D-C4D	-2.74	1.38	1.45
2	C	301	NAP	C2A-N3A	-2.74	1.29	1.33
2	B	301	NAP	O4B-C4B	-2.73	1.38	1.45
2	C	301	NAP	C3N-C7N	-2.71	1.46	1.50
3	B	302	L8U	BR2-C02	2.64	1.95	1.90
2	B	301	NAP	C5N-C4N	-2.63	1.34	1.38
2	C	301	NAP	O4B-C4B	-2.62	1.39	1.45
2	D	301	NAP	C4N-C3N	-2.62	1.35	1.39
2	B	301	NAP	P2B-O2X	-2.62	1.45	1.54
2	B	301	NAP	C4N-C3N	-2.62	1.35	1.39
3	A	302	L8U	C05-C04	-2.61	1.36	1.40
2	C	301	NAP	PA-O1A	-2.60	1.41	1.50
2	A	301	NAP	C5A-C4A	2.57	1.43	1.39
2	C	301	NAP	PN-O2N	-2.56	1.43	1.55
2	B	301	NAP	P2B-O1X	-2.54	1.42	1.50
2	D	301	NAP	PA-O2A	-2.54	1.43	1.55
2	B	301	NAP	PN-O1N	-2.49	1.42	1.50
2	A	301	NAP	PA-O5B	-2.45	1.49	1.59
2	B	301	NAP	PA-O2A	-2.42	1.44	1.55
3	C	302	L8U	O09-C07	-2.41	1.18	1.22
2	D	301	NAP	PA-O1A	-2.40	1.42	1.50
2	C	301	NAP	C5N-C4N	-2.38	1.34	1.38
2	A	301	NAP	O4B-C4B	-2.34	1.39	1.45
2	D	301	NAP	C2A-N3A	-2.33	1.29	1.33
2	A	301	NAP	C2A-N3A	-2.33	1.29	1.33
3	B	302	L8U	C05-C07	2.33	1.53	1.48
2	B	301	NAP	C7N-N7N	-2.32	1.28	1.33
2	A	301	NAP	P2B-O1X	-2.29	1.43	1.50
2	D	301	NAP	O4D-C4D	-2.29	1.39	1.45
2	B	301	NAP	C2N-C3N	-2.28	1.35	1.39
2	D	301	NAP	C2B-C1B	-2.28	1.47	1.53
2	C	301	NAP	PN-O1N	-2.27	1.43	1.50
2	C	301	NAP	C2A-N1A	-2.27	1.29	1.33
2	A	301	NAP	C6N-N1N	-2.25	1.30	1.35
2	C	301	NAP	P2B-O2B	-2.25	1.55	1.59
2	B	301	NAP	PN-O5D	-2.24	1.50	1.59
2	A	301	NAP	PN-O1N	-2.19	1.43	1.50
2	A	301	NAP	C3D-C4D	-2.19	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C5A-C4A	2.18	1.43	1.39
2	A	301	NAP	C4N-C3N	-2.16	1.36	1.39
2	B	301	NAP	PA-O1A	-2.15	1.43	1.50
2	A	301	NAP	C2N-C3N	-2.15	1.35	1.39
3	B	302	L8U	O09-C07	-2.15	1.18	1.22
2	D	301	NAP	PN-O5D	-2.13	1.51	1.59
2	A	301	NAP	PA-O1A	-2.13	1.43	1.50
3	D	302	L8U	BR2-C02	2.13	1.94	1.90
2	D	301	NAP	C3B-C2B	-2.12	1.48	1.53
3	D	302	L8U	O10-C04	2.11	1.40	1.36
2	A	301	NAP	C5N-C4N	-2.10	1.35	1.38
2	B	301	NAP	C3B-C4B	-2.09	1.47	1.53
2	A	301	NAP	C6A-N1A	-2.08	1.30	1.35
2	D	301	NAP	C5A-C6A	2.05	1.46	1.41
2	B	301	NAP	C6N-C5N	-2.05	1.34	1.38
2	B	301	NAP	C6A-N1A	-2.01	1.30	1.35

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAP	C5A-C4A-N3A	-6.64	117.58	126.72
2	D	301	NAP	C2B-C1B-N9A	-5.88	104.08	113.75
2	C	301	NAP	C5A-C4A-N3A	-5.53	119.10	126.72
2	D	301	NAP	C5A-C4A-N3A	-5.53	119.11	126.72
3	A	302	L8U	BR1-C08-C07	-5.14	98.60	112.14
2	D	301	NAP	C3N-C7N-N7N	5.03	123.94	117.74
3	A	302	L8U	C04-C05-C07	-4.93	116.36	120.09
2	B	301	NAP	C4A-C5A-N7A	-4.41	105.55	110.58
2	C	301	NAP	N3A-C2A-N1A	-4.30	122.08	128.58
2	B	301	NAP	N3A-C4A-N9A	4.29	134.46	127.17
2	B	301	NAP	C2A-N3A-C4A	4.27	122.25	111.83
2	C	301	NAP	C4A-C5A-N7A	-4.25	105.73	110.58
2	D	301	NAP	O4B-C1B-N9A	4.24	116.23	108.09
3	D	302	L8U	C06-C05-C04	4.23	123.46	118.15
2	C	301	NAP	C2A-N3A-C4A	4.18	122.03	111.83
2	A	301	NAP	C4D-O4D-C1D	4.12	113.70	109.92
2	D	301	NAP	C4A-C5A-N7A	-4.09	105.91	110.58
2	A	301	NAP	C5A-C4A-N3A	-3.97	121.24	126.72
2	D	301	NAP	C2A-N3A-C4A	3.97	121.52	111.83
2	D	301	NAP	N3A-C4A-N9A	3.97	133.91	127.17
2	B	301	NAP	N3A-C2A-N1A	-3.76	122.90	128.58
2	C	301	NAP	N3A-C4A-N9A	3.73	133.51	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAP	O4B-C1B-C2B	-3.72	100.18	106.59
2	D	301	NAP	N3A-C2A-N1A	-3.70	122.98	128.58
2	A	301	NAP	O3D-C3D-C4D	-3.56	100.85	111.08
2	A	301	NAP	O4B-C1B-N9A	3.39	114.60	108.09
2	B	301	NAP	C5N-C4N-C3N	-3.34	117.08	120.36
2	A	301	NAP	C4A-C5A-N7A	-3.27	106.84	110.58
2	C	301	NAP	C6A-C5A-N7A	3.25	138.35	132.09
3	A	302	L8U	C06-C05-C04	3.15	122.11	118.15
2	B	301	NAP	O4B-C1B-C2B	-3.15	101.17	106.59
2	A	301	NAP	C2B-C1B-N9A	-3.06	108.72	113.75
3	C	302	L8U	BR1-C08-C07	-3.05	104.12	112.14
2	C	301	NAP	O2N-PN-O3	3.04	115.50	107.27
2	C	301	NAP	C2A-N1A-C6A	2.98	123.63	118.73
3	C	302	L8U	C04-C05-C07	-2.95	117.86	120.09
3	A	302	L8U	BR2-C02-C03	-2.95	115.06	119.23
2	D	301	NAP	C5A-N7A-C8A	2.88	107.97	103.45
2	A	301	NAP	C2A-N1A-C6A	2.88	123.45	118.73
2	B	301	NAP	O3X-P2B-O2X	2.82	118.36	107.80
2	C	301	NAP	C5A-N7A-C8A	2.80	107.84	103.45
2	A	301	NAP	N3A-C2A-N1A	-2.78	124.37	128.58
2	D	301	NAP	C6A-C5A-N7A	2.76	137.42	132.09
2	C	301	NAP	O4B-C1B-N9A	2.69	113.25	108.09
3	A	302	L8U	BR2-C02-C01	2.67	122.93	119.30
2	A	301	NAP	C2A-N3A-C4A	2.66	118.33	111.83
2	B	301	NAP	C6A-C5A-N7A	2.65	137.21	132.09
2	C	301	NAP	O4B-C1B-C2B	-2.63	102.06	106.59
2	A	301	NAP	N3A-C4A-N9A	2.60	131.58	127.17
2	A	301	NAP	O3X-P2B-O2X	2.56	117.41	107.80
2	A	301	NAP	C3N-C7N-N7N	2.55	120.88	117.74
2	B	301	NAP	O2A-PA-O3	2.49	114.00	107.27
2	A	301	NAP	C3B-C2B-C1B	-2.45	98.12	102.81
2	A	301	NAP	O3-PA-O1A	2.44	118.05	110.70
2	A	301	NAP	C6A-C5A-N7A	2.44	136.79	132.09
2	D	301	NAP	O7N-C7N-N7N	-2.43	119.10	122.62
2	D	301	NAP	O3X-P2B-O2X	2.37	116.70	107.80
2	D	301	NAP	C5N-C4N-C3N	-2.37	118.03	120.36
2	D	301	NAP	O5D-C5D-C4D	2.37	117.05	108.99
3	C	302	L8U	C06-C05-C04	2.36	121.11	118.15
2	D	301	NAP	C2A-N1A-C6A	2.33	122.56	118.73
2	C	301	NAP	C5N-C4N-C3N	-2.30	118.10	120.36
3	A	302	L8U	C08-C07-C05	2.27	121.09	117.14
2	D	301	NAP	O2B-P2B-O1X	-2.27	101.24	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	L8U	C04-C03-C02	2.26	120.18	118.87
2	B	301	NAP	C5A-N7A-C8A	2.18	106.88	103.45
2	D	301	NAP	O7N-C7N-C3N	-2.17	116.95	119.60
2	C	301	NAP	C6N-N1N-C2N	-2.15	120.05	121.88
2	B	301	NAP	O2N-PN-O3	2.15	113.08	107.27
2	A	301	NAP	C4A-N9A-C8A	2.13	107.98	105.74
2	B	301	NAP	O5B-PA-O1A	-2.09	100.65	108.94
2	D	301	NAP	C4A-N9A-C8A	2.09	107.93	105.74
2	A	301	NAP	C4A-N9A-C1B	-2.07	121.79	126.63

There are no chirality outliers.

All (27) torsion outliers are listed below:

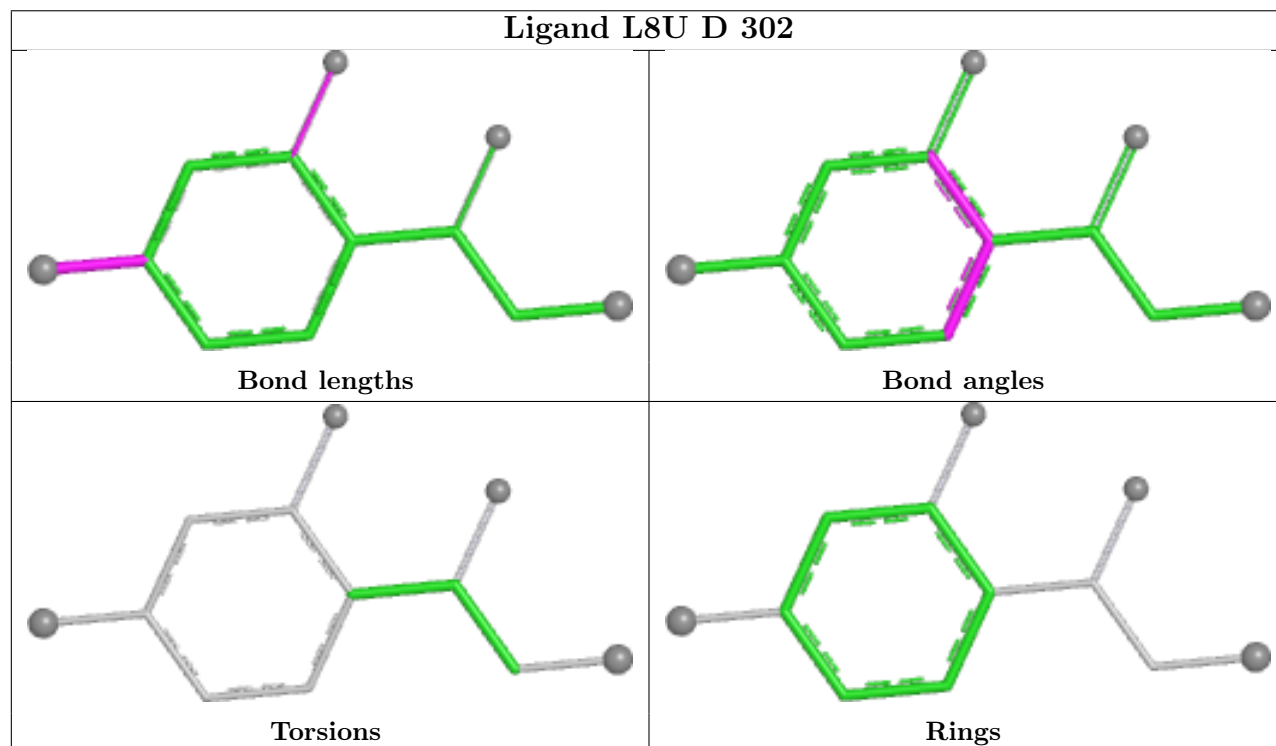
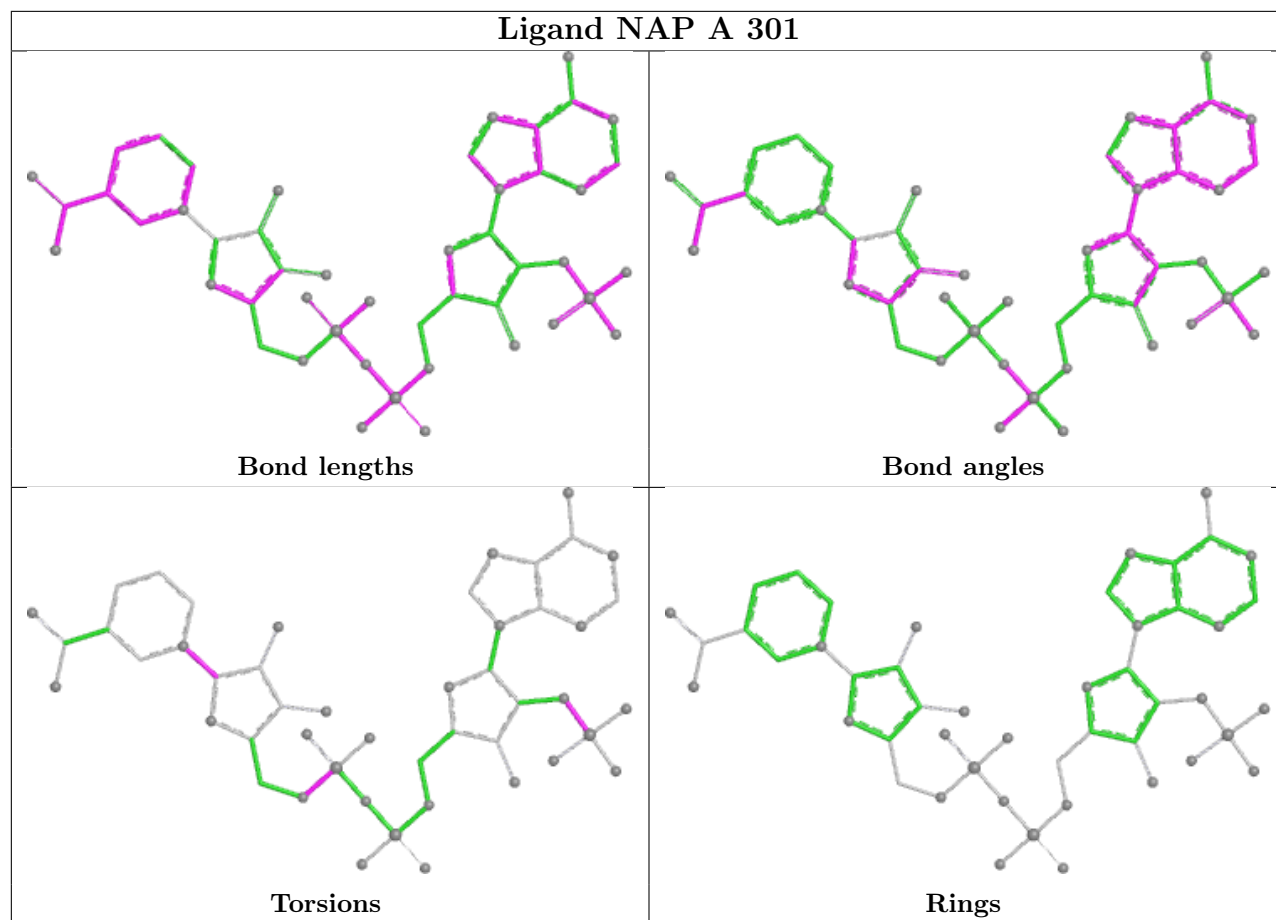
Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C5D-O5D-PN-O3
2	A	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	C5D-O5D-PN-O2N
2	C	301	NAP	C5D-O5D-PN-O3
2	C	301	NAP	C5D-O5D-PN-O1N
2	C	301	NAP	C5D-O5D-PN-O2N
2	D	301	NAP	C5B-O5B-PA-O1A
2	D	301	NAP	C5B-O5B-PA-O3
2	D	301	NAP	PN-O3-PA-O5B
2	D	301	NAP	C5D-O5D-PN-O3
3	A	302	L8U	C05-C07-C08-BR1
3	A	302	L8U	O09-C07-C08-BR1
2	D	301	NAP	C3B-C4B-C5B-O5B
2	D	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	C2B-O2B-P2B-O1X
3	A	302	L8U	C04-C05-C07-O09
3	A	302	L8U	C04-C05-C07-C08
2	D	301	NAP	PA-O3-PN-O1N
3	C	302	L8U	C04-C05-C07-O09
3	C	302	L8U	C04-C05-C07-C08
2	D	301	NAP	C5B-O5B-PA-O2A
2	D	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	O4D-C1D-N1N-C6N
2	D	301	NAP	PA-O3-PN-O2N
2	C	301	NAP	O4B-C4B-C5B-O5B
2	C	301	NAP	C3B-C4B-C5B-O5B
2	A	301	NAP	C2B-O2B-P2B-O1X

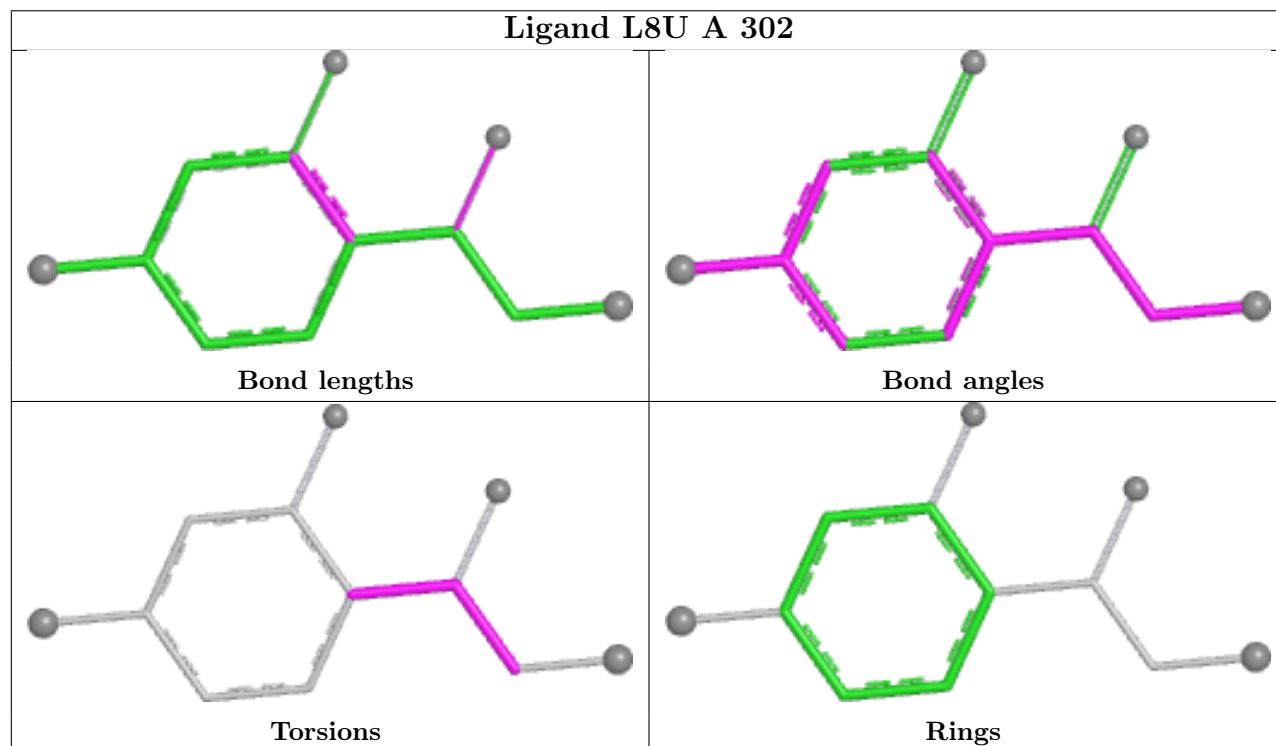
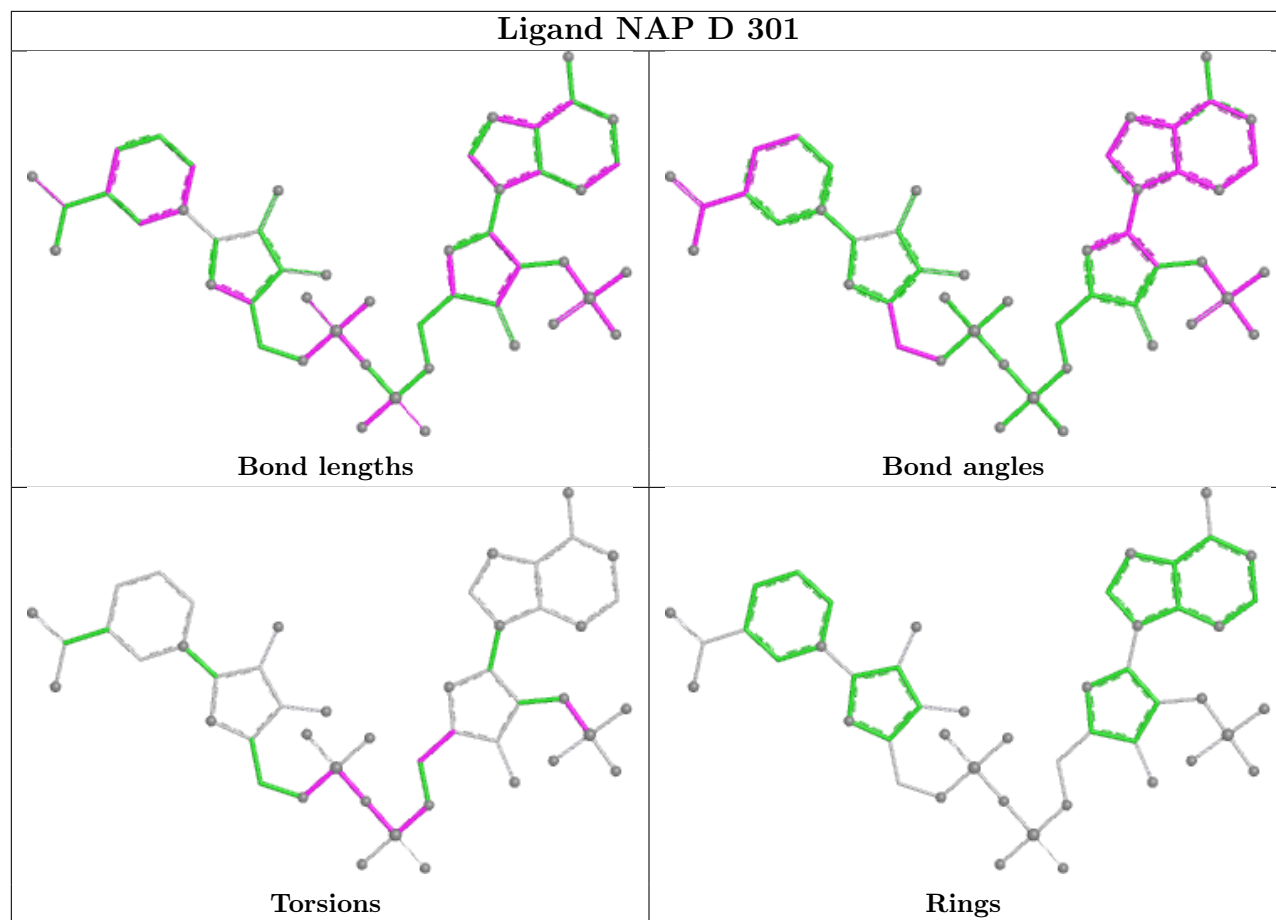
There are no ring outliers.

7 monomers are involved in 21 short contacts:

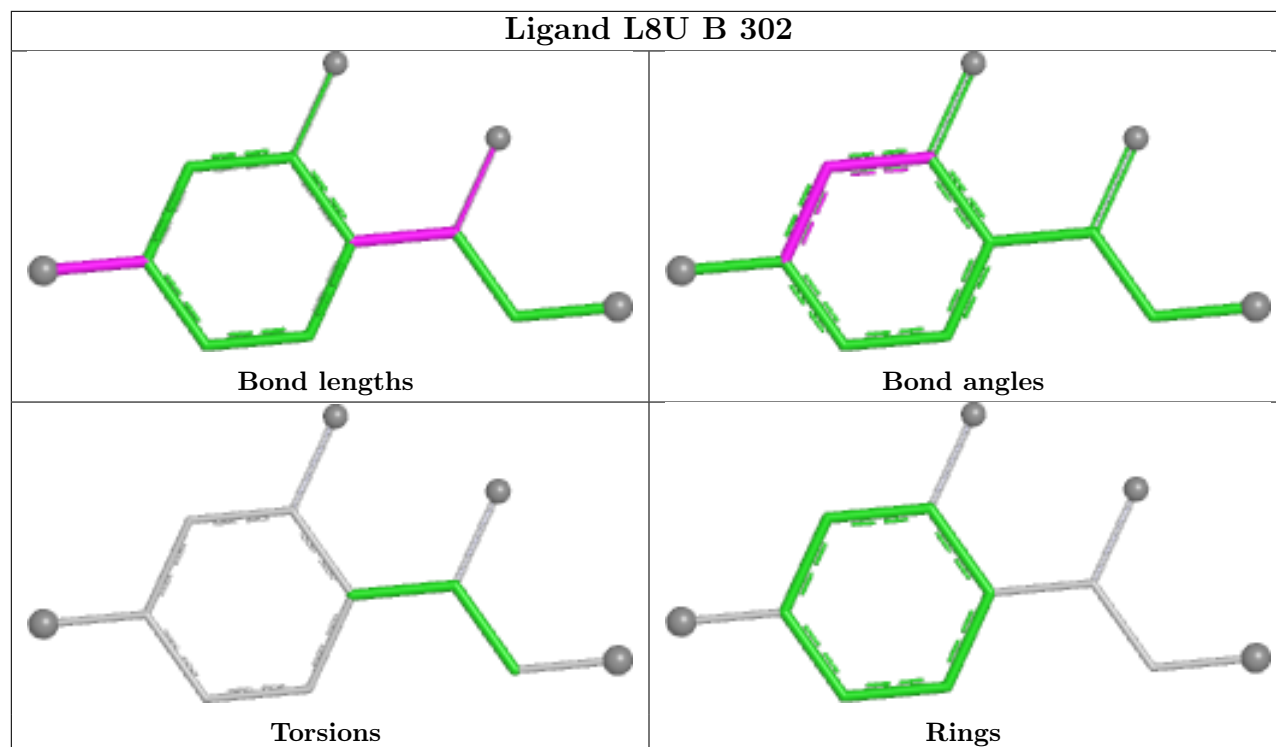
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAP	3	0
3	D	302	L8U	4	0
2	D	301	NAP	1	0
3	A	302	L8U	5	0
2	B	301	NAP	2	0
3	C	302	L8U	2	0
2	C	301	NAP	4	0

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

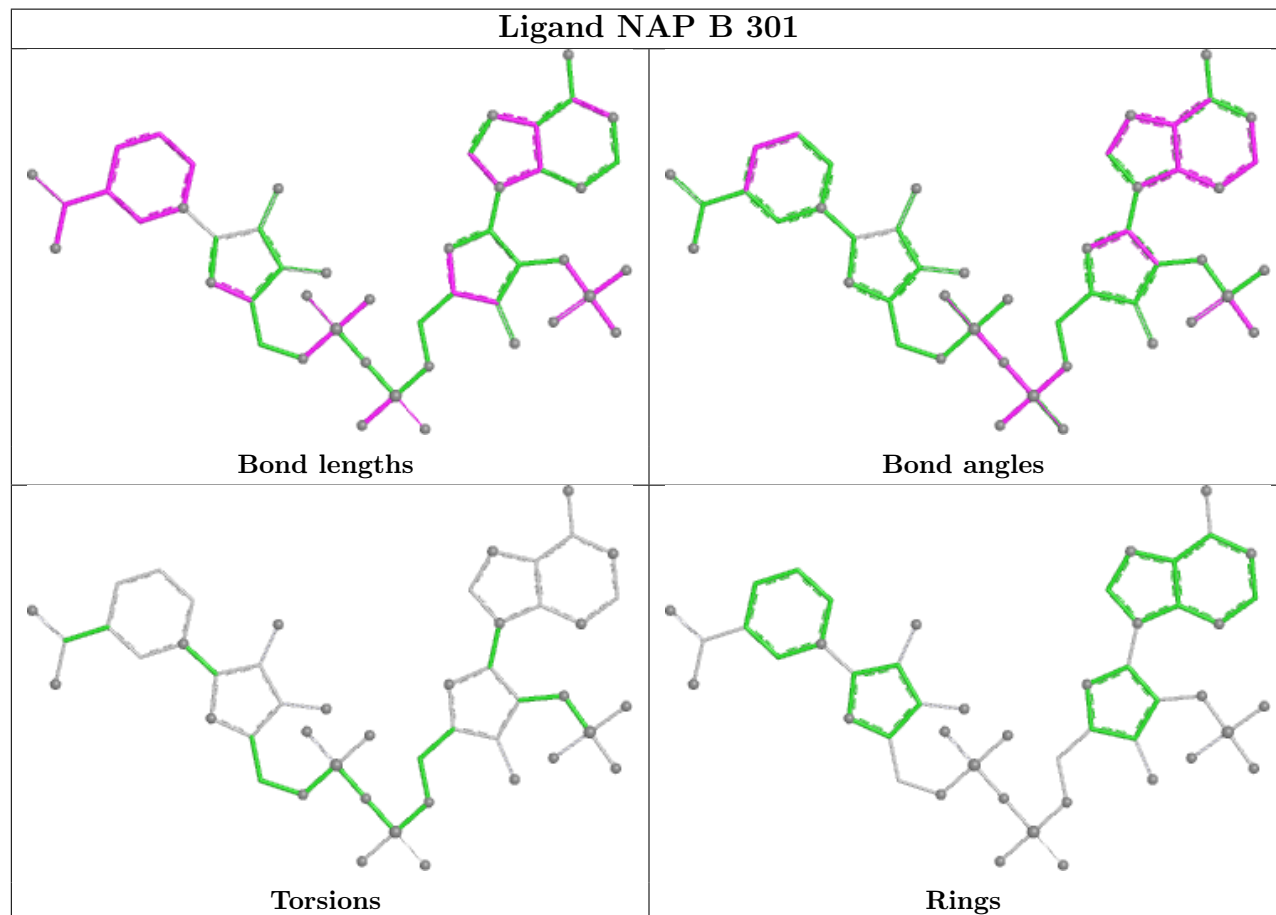




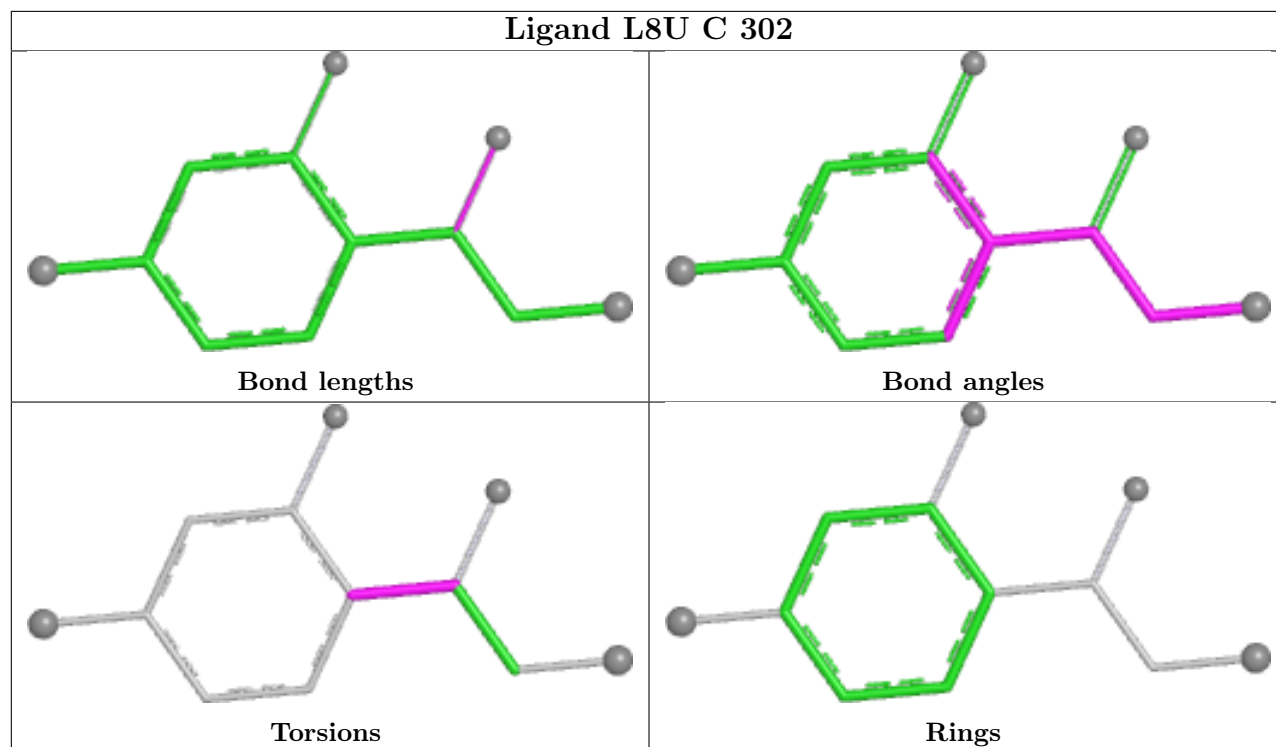
Ligand L8U B 302



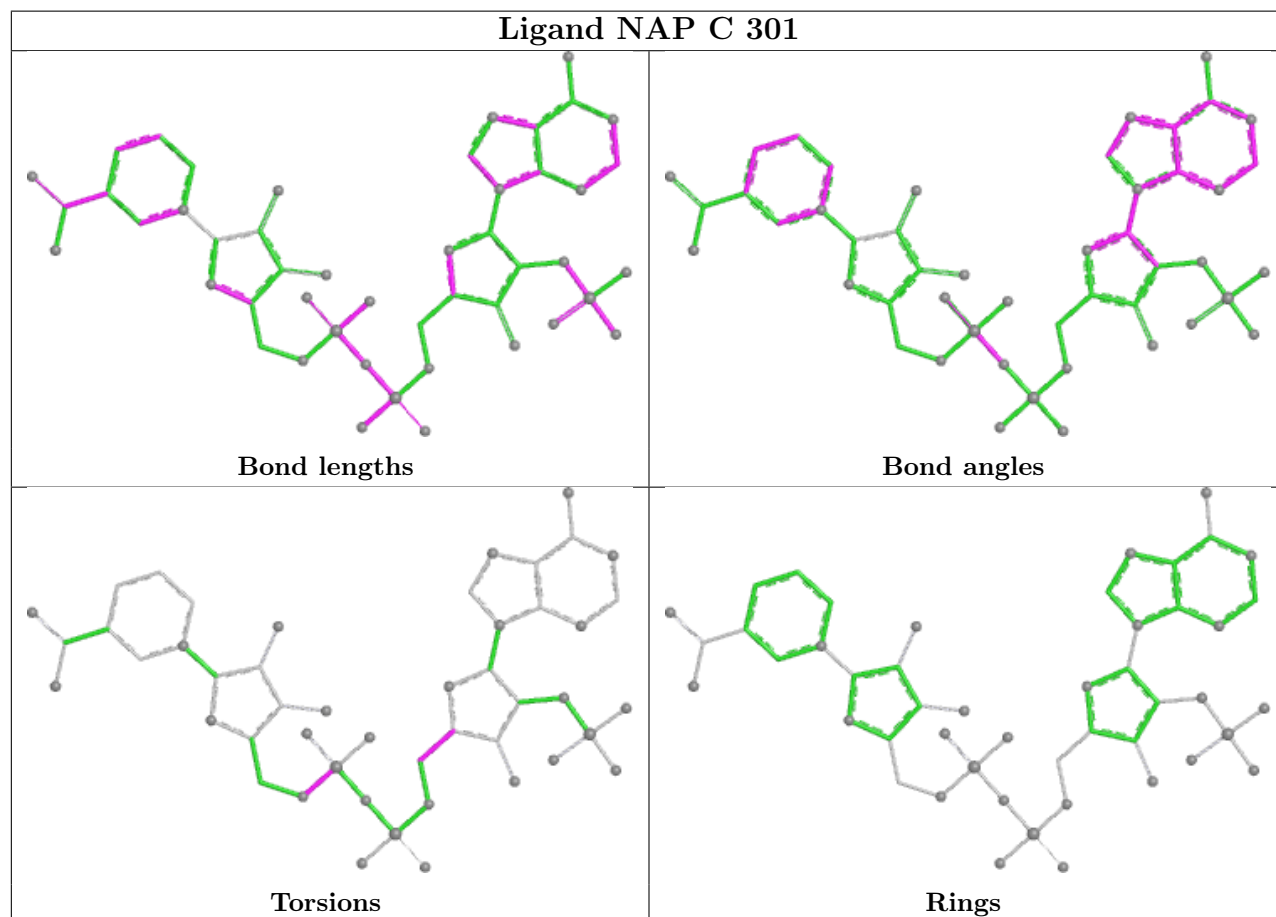
Ligand NAP B 301



Ligand L8U C 302



Ligand NAP C 301



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	259/279 (92%)	0.18	11 (4%) 40 32	16, 25, 45, 74	0
1	B	253/279 (90%)	0.27	18 (7%) 22 17	18, 30, 58, 77	0
1	C	251/279 (89%)	0.20	13 (5%) 33 26	16, 27, 56, 74	0
1	D	256/279 (91%)	0.16	13 (5%) 33 26	19, 29, 59, 86	0
All	All	1019/1116 (91%)	0.20	55 (5%) 31 24	16, 28, 56, 86	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	GLY	7.4
1	B	159	VAL	5.8
1	A	197	GLY	5.3
1	B	157	PHE	5.1
1	A	10	ILE	4.8
1	A	198	THR	4.0
1	B	228	HIS	3.9
1	A	9	HIS	3.9
1	B	156	ASP	3.9
1	B	160	PRO	3.8
1	C	10	ILE	3.6
1	D	153	THR	3.6
1	D	215	GLU	3.4
1	A	155	ARG	3.2
1	D	158	SER	3.2
1	B	218	THR	3.1
1	D	210	TYR	3.1
1	B	107	PHE	3.1
1	D	155	ARG	3.1
1	C	196	GLY	3.1
1	B	197	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	267	ALA	3.0
1	C	199	VAL	3.0
1	C	157	PHE	3.0
1	B	196	GLY	2.9
1	D	212	PRO	2.9
1	A	111	LYS	2.8
1	C	142	ASN	2.8
1	B	217	TYR	2.8
1	B	158	SER	2.7
1	C	156	ASP	2.6
1	C	264	ASP	2.6
1	D	214	GLY	2.6
1	A	109	HIS	2.5
1	B	219	PRO	2.5
1	C	154	SER	2.4
1	B	198	THR	2.4
1	B	152	ASN	2.3
1	B	229	ALA	2.3
1	B	153	THR	2.3
1	D	216	THR	2.3
1	C	225	MET	2.3
1	D	228	HIS	2.3
1	A	210	TYR	2.2
1	D	232	LEU	2.2
1	A	156	ASP	2.2
1	C	153	THR	2.1
1	C	209	HIS	2.1
1	C	11	PRO	2.1
1	D	217	TYR	2.1
1	A	158	SER	2.0
1	B	225	MET	2.0
1	D	154	SER	2.0
1	D	229	ALA	2.0
1	B	206	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

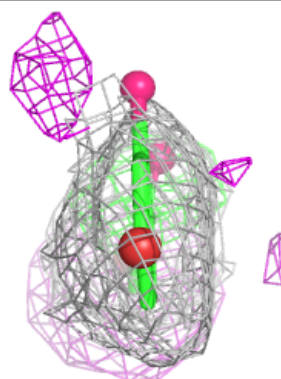
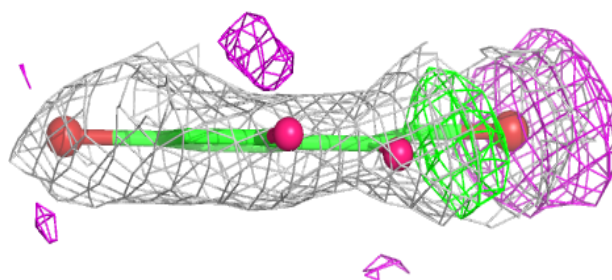
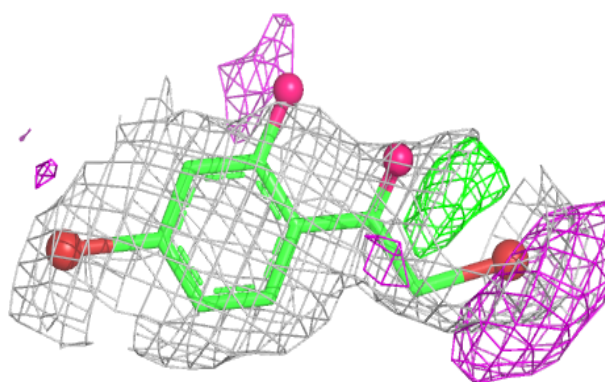
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	L8U	D	302	12/12	0.82	0.21	44,57,69,127	0
3	L8U	A	302	12/12	0.89	0.20	41,53,67,128	0
3	L8U	C	302	12/12	0.90	0.17	55,76,89,128	0
3	L8U	B	302	12/12	0.94	0.14	49,67,89,127	0
2	NAP	B	301	48/48	0.94	0.08	20,24,29,30	0
2	NAP	A	301	48/48	0.94	0.09	18,20,25,27	0
2	NAP	D	301	48/48	0.95	0.08	16,22,25,27	0
2	NAP	C	301	48/48	0.96	0.07	17,20,26,29	0

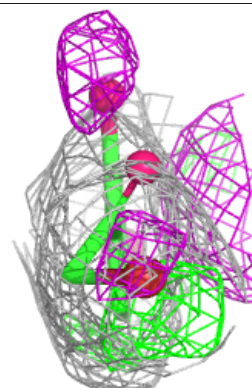
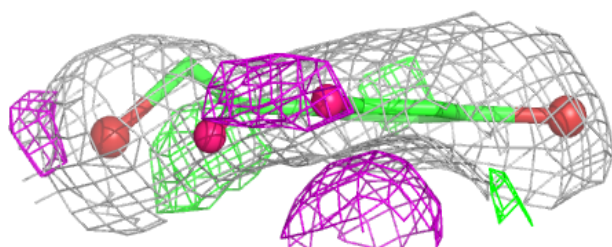
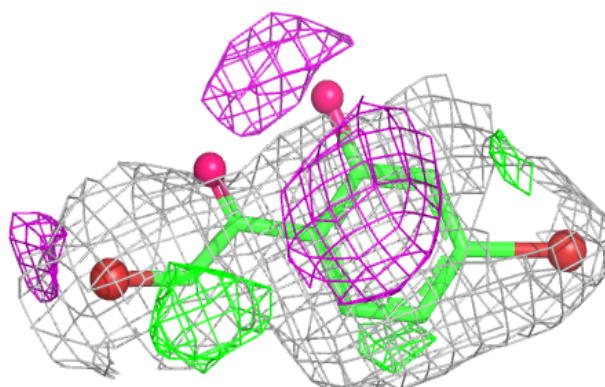
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around L8U D 302:

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

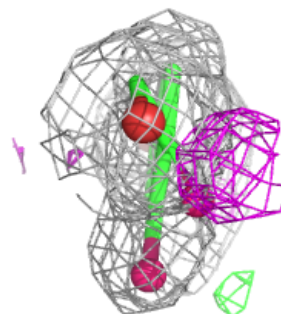
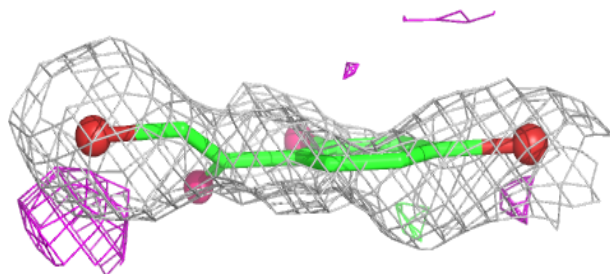
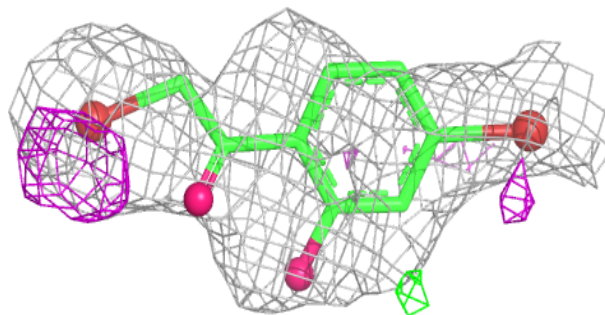
**Electron density around L8U A 302:**

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

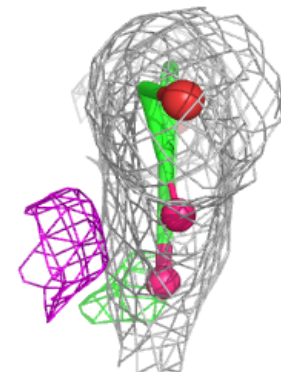
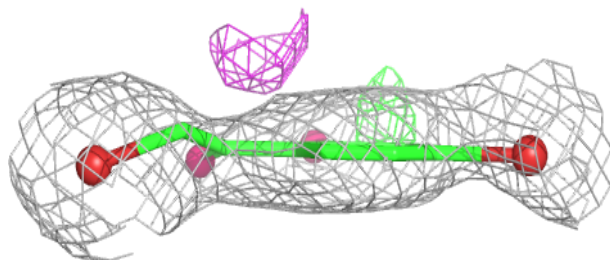
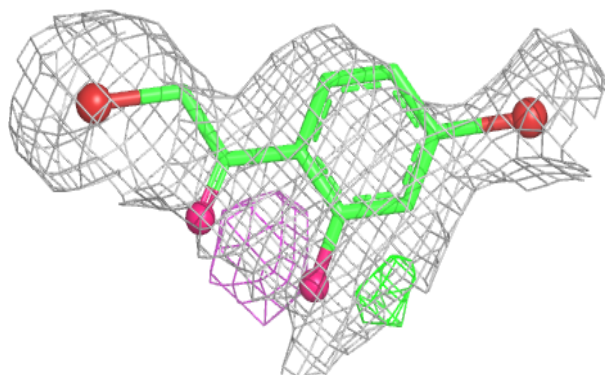


Electron density around L8U C 302:

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

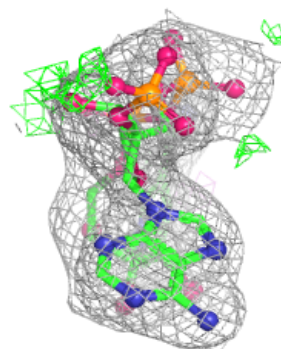
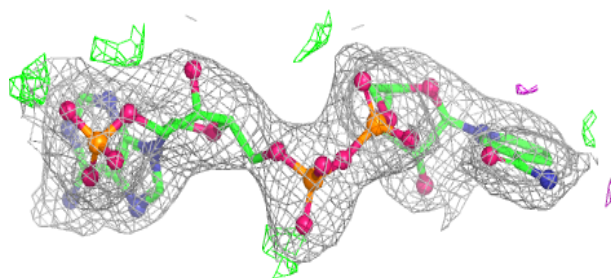
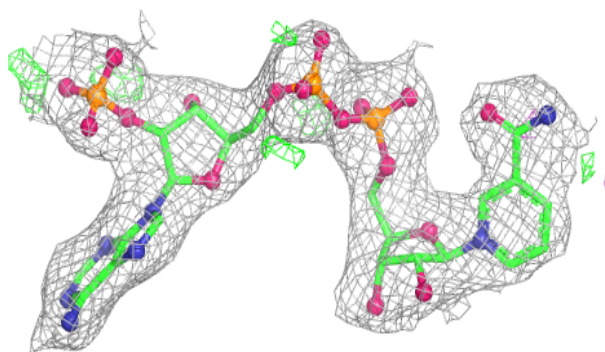
**Electron density around L8U B 302:**

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

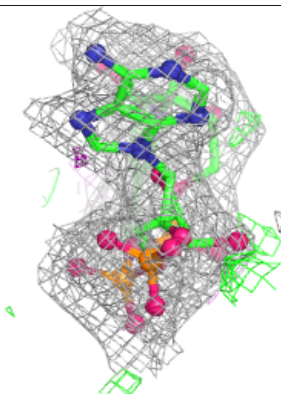
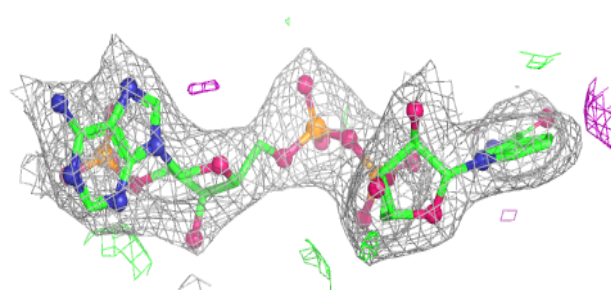
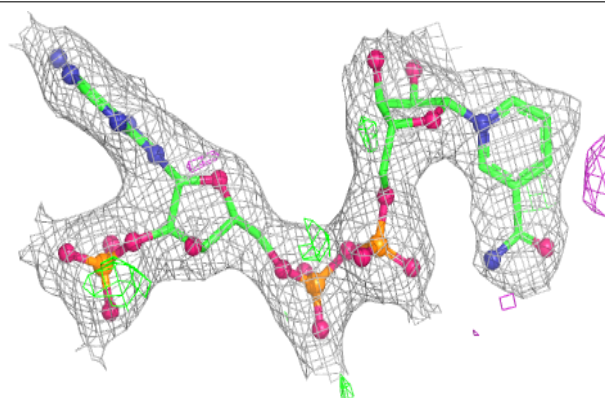


Electron density around NAP B 301:

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

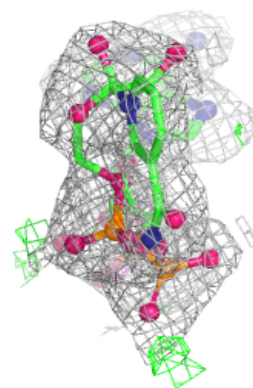
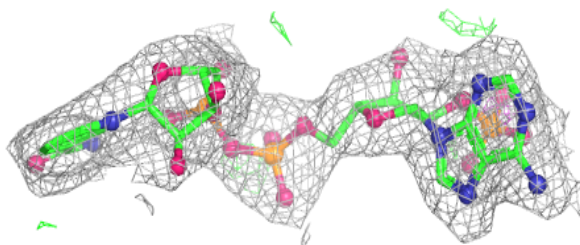
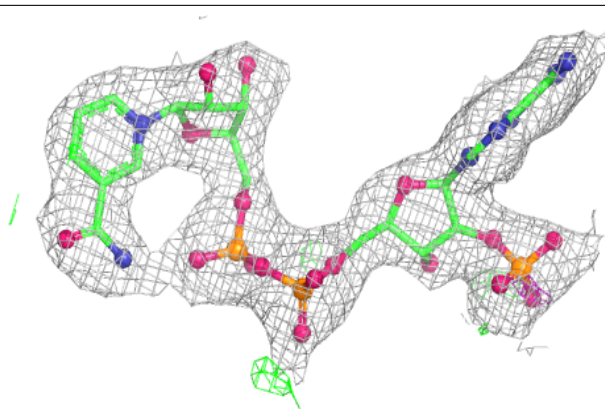
**Electron density around NAP A 301:**

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

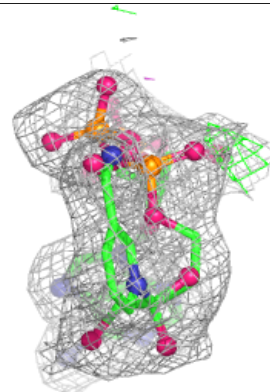
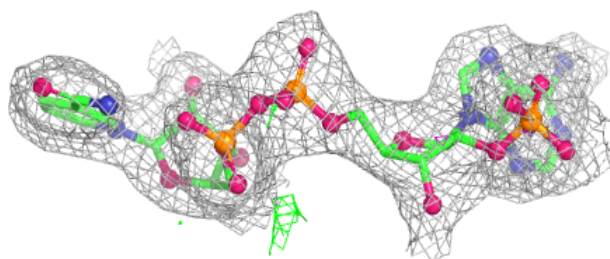
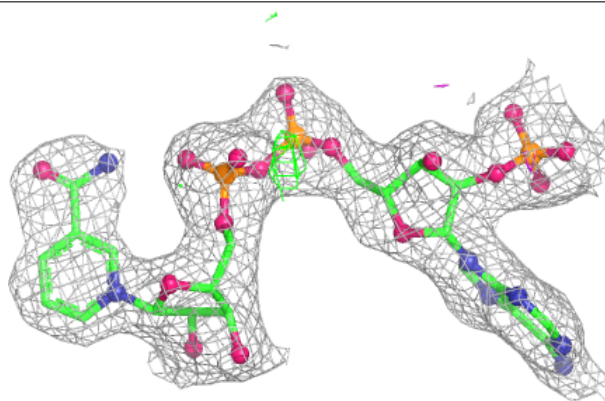


Electron density around NAP D 301:

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

**Electron density around NAP C 301:**

$2mF_o-DF_c$ (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.