



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:03 AM UTC

PDB ID : 4I4Z / pdb_00004i4z
Title : Synechocystis sp. PCC 6803 1,4-dihydroxy-2-naphthoyl-coenzyme A synthase (MenB) in complex with salicylyl-CoA
Authors : Song, H.G.; Sun, Y.R.; Li, J.; Li, Y.; Jiang, M.; Zhou, J.H.; Guo, Z.H.
Deposited on : 2012-11-28
Resolution : 2.00 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

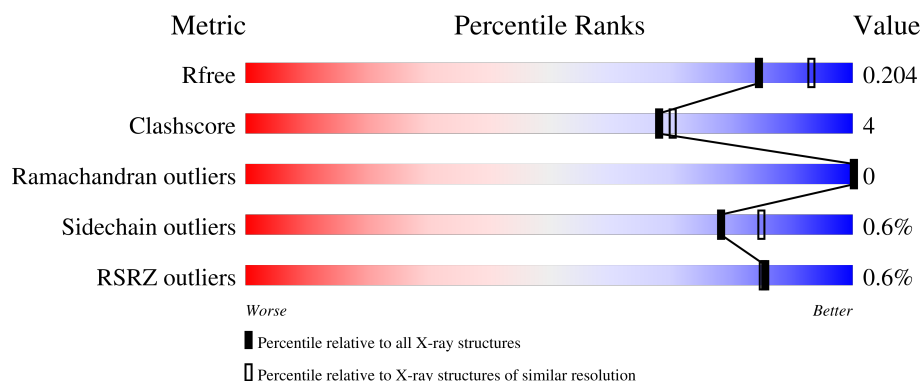
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

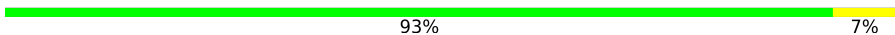
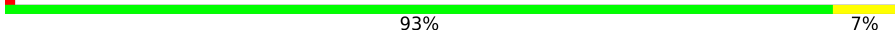
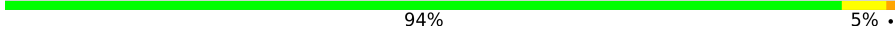
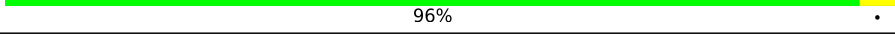
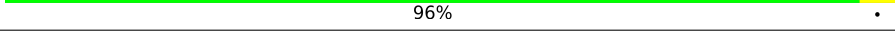
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	275	 93% 7%
1	B	275	 93% 7%
1	C	275	 94% 5%
1	D	275	 96%
1	E	275	 96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	275	% 95% 5%
1	G	275	92% 8%
1	H	275	2% 92% 8%
1	I	275	% 92% 8%

2 Entry composition

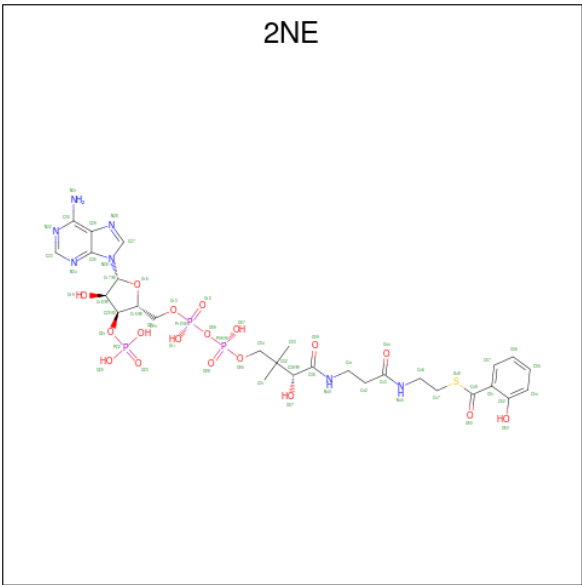
There are 5 unique types of molecules in this entry. The entry contains 20593 atoms, of which 4 are hydrogens and 0 are deuteriums.

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 Naphthoate synthase.

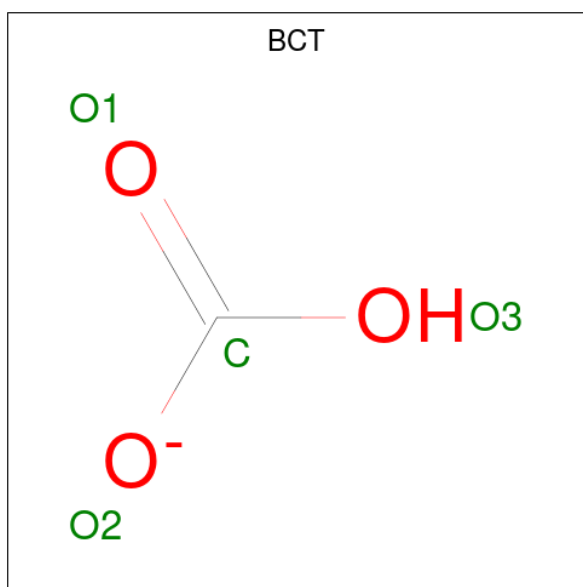
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2135	1354	375	395	11			
1	B	274	Total	C	N	O	S	0	0	0
			2120	1346	374	390	10			
1	C	275	Total	C	N	O	S	0	1	0
			2142	1359	378	394	11			
1	D	275	Total	C	N	O	S	0	2	0
			2144	1361	377	395	11			
1	E	275	Total	C	N	O	S	0	0	0
			2125	1350	370	394	11			
1	F	275	Total	C	N	O	S	0	0	0
			2120	1348	370	391	11			
1	G	275	Total	C	N	O	S	0	0	0
			2121	1347	372	391	11			
1	H	275	Total	C	N	O	S	0	0	0
			2109	1341	364	393	11			
1	I	275	Total	C	N	O	S	0	0	0
			2127	1349	374	393	11			

- Molecule 2 is Salicylyl CoA (CCD ID: 2NE) (formula: $C_{28}H_{40}N_7O_{18}P_3S$).



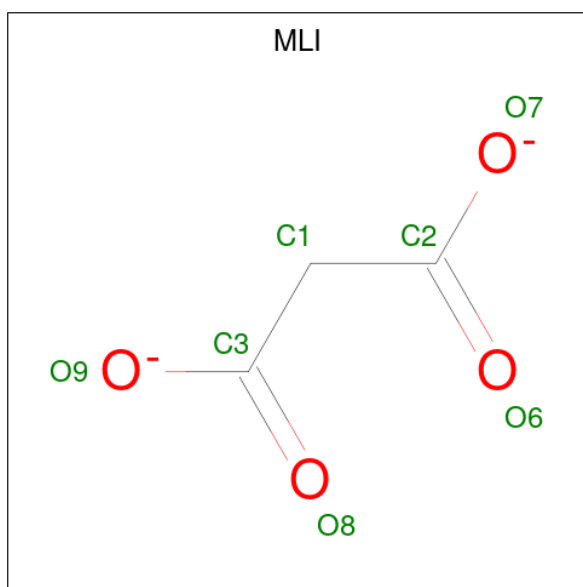
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			57	28	7	18	3	1		

- Molecule 3 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		
3	C	1	Total	C	O	0	0
			4	1	3		
3	D	1	Total	C	O	0	0
			4	1	3		
3	E	1	Total	C	O	0	0
			4	1	3		
3	F	1	Total	C	O	0	0
			4	1	3		
3	G	1	Total	C	O	0	0
			4	1	3		
3	H	1	Total	C	O	0	0
			4	1	3		
3	I	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			9	3	2	4		
4	I	1	Total	C	H	O	0	0
			9	3	2	4		

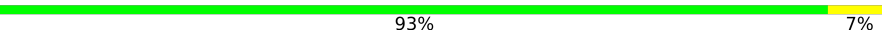
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	114	Total	O	0	0
			114	114		
5	B	89	Total	O	0	0
			89	89		
5	C	132	Total	O	0	0
			132	132		
5	D	103	Total	O	0	0
			103	103		
5	E	120	Total	O	0	0
			120	120		
5	F	104	Total	O	0	0
			104	104		
5	G	62	Total	O	0	0
			62	62		
5	H	60	Total	O	0	0
			60	60		
5	I	99	Total	O	0	0
			99	99		

3 Residue-property plots

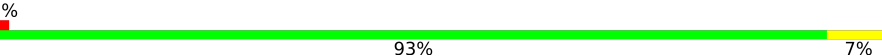
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Naphthoate synthase

Chain A:  93% 7%



- Molecule 1: Naphthoate synthase

Chain B:  93% 7%

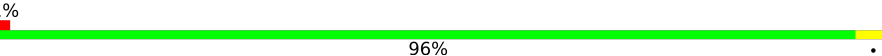


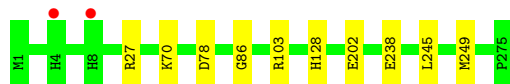
- Molecule 1: Naphthoate synthase

Chain C:  94% 5%

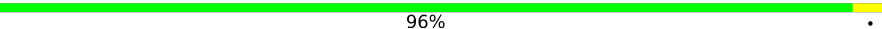


- Molecule 1: Naphthoate synthase

Chain D:  96%



- Molecule 1: Naphthoate synthase

Chain E:  96%



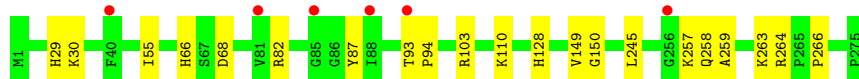
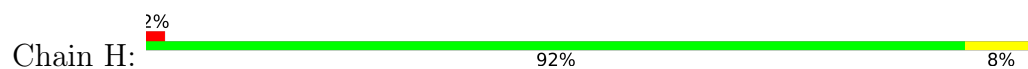
- Molecule 1: Naphthoate synthase



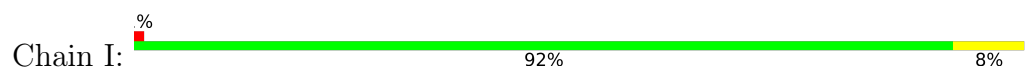
- Molecule 1: Naphthoate synthase



- Molecule 1: Naphthoate synthase



- Molecule 1: Naphthoate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.21Å 139.21Å 220.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.67 – 2.00 44.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.67-2.00) 99.7 (44.67-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.198 , 0.221 0.170 , 0.204	Depositor DCC
R_{free} test set	8411 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20593	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.70% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2NE, MLI, BCT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/2183	0.72	0/2951
1	B	0.42	0/2168	0.75	0/2932
1	C	0.45	0/2191	0.72	0/2962
1	D	0.44	0/2194	0.73	0/2968
1	E	0.45	0/2173	0.74	0/2939
1	F	0.46	0/2168	0.73	0/2932
1	G	0.40	0/2169	0.75	0/2934
1	H	0.39	0/2157	0.75	2/2921 (0.1%)
1	I	0.42	0/2173	0.75	0/2937
All	All	0.43	0/19576	0.74	2/26476 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	264	ARG	CA-C-N	-5.19	115.03	120.38
1	H	264	ARG	C-N-CA	-5.19	115.03	120.38

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	2135	0	2101	21	0
1	B	2120	0	2083	13	0
1	C	2142	0	2105	25	0
1	D	2144	0	2093	8	0
1	E	2125	0	2081	10	1
1	F	2120	0	2080	17	0
1	G	2121	0	2082	20	0
1	H	2109	0	2049	12	2
1	I	2127	0	2086	19	1
2	A	57	0	37	2	0
2	B	57	0	35	2	0
2	C	57	0	35	1	0
2	D	57	0	35	3	0
2	E	57	0	35	2	0
2	F	57	0	35	2	0
2	G	57	0	35	5	0
2	H	57	0	35	4	1
2	I	57	0	35	4	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	1	0	0
3	D	4	0	0	0	0
3	E	4	0	1	0	0
3	F	4	0	1	0	0
3	G	4	0	1	1	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
4	C	7	2	2	0	0
4	I	7	2	2	0	0
5	A	114	0	0	2	0
5	B	89	0	0	0	0
5	C	132	0	0	2	0
5	D	103	0	0	3	0
5	E	120	0	0	1	0
5	F	104	0	0	2	0
5	G	62	0	0	2	0
5	H	60	0	0	0	0
5	I	99	0	0	3	0
All	All	20589	4	19085	138	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ARG:HG2	1:E:257:LYS:HD3	1.29	1.11
2:I:301:2NE:O50	2:I:301:2NE:H33	1.78	0.83
1:I:53:ASN:O	1:I:54:ARG:N	2.14	0.80
1:I:149:VAL:HG21	2:I:301:2NE:H35	1.64	0.78
1:H:257:LYS:HE3	1:H:258:GLN:OE1	1.83	0.77
1:C:82:ARG:HD2	5:C:414:HOH:O	1.84	0.76
1:G:89:ASP:OD2	1:G:93:THR:HG23	1.84	0.76
1:A:103:ARG:NH2	1:F:238:GLU:OE2	2.18	0.75
1:C:5:ILE:HD12	1:C:15:TYR:CD2	2.23	0.72
1:C:82:ARG:HG2	1:E:257:LYS:CD	2.14	0.72
1:C:238:GLU:OE2	1:E:103:ARG:NH2	2.21	0.71
2:G:301:2NE:O53	3:G:302:BCT:O1	2.09	0.71
2:H:301:2NE:H33	2:H:301:2NE:O50	1.91	0.69
1:I:53:ASN:CA	1:I:54:ARG:N	2.55	0.69
1:G:203:GLU:OE2	5:G:454:HOH:O	2.11	0.68
1:G:89:ASP:CG	1:G:93:THR:HG23	2.19	0.68
1:F:103:ARG:NH2	5:F:437:HOH:O	2.27	0.66
1:G:41:GLU:OE2	5:G:428:HOH:O	2.12	0.66
1:B:103:ARG:NH2	1:D:238:GLU:OE2	2.29	0.64
1:A:103:ARG:NH1	1:F:103:ARG:NH1	2.45	0.64
1:C:103:ARG:NH2	1:E:238:GLU:OE2	2.31	0.63
1:I:2:ASP:OD2	1:I:4:HIS:NE2	2.32	0.62
1:B:16:LYS:NZ	1:B:52:ASP:OD2	2.30	0.62
1:D:245:LEU:HD23	1:D:245:LEU:C	2.24	0.61
1:G:210:GLU:O	1:G:214:LYS:NZ	2.29	0.60
1:F:103:ARG:HD2	5:F:437:HOH:O	2.02	0.59
1:I:53:ASN:O	1:I:53:ASN:CA	2.51	0.59
2:D:301:2NE:C54	5:D:440:HOH:O	2.49	0.59
1:H:149:VAL:HG21	2:H:301:2NE:H34	1.85	0.59
1:A:149:VAL:HG21	2:A:301:2NE:H32	1.84	0.58
1:C:5:ILE:CD1	1:C:5:ILE:N	2.66	0.58
1:G:16:LYS:NZ	1:G:52:ASP:OD2	2.23	0.57
1:C:5:ILE:HD11	1:C:15:TYR:HE2	1.70	0.56
1:I:245:LEU:C	1:I:245:LEU:HD23	2.31	0.55
2:D:301:2NE:H37	5:D:440:HOH:O	2.07	0.55
1:C:5:ILE:CD1	1:C:15:TYR:CE2	2.90	0.54
1:A:103:ARG:HH11	1:F:103:ARG:NH1	2.06	0.54
1:B:149:VAL:HG21	2:B:301:2NE:H32	1.90	0.54
1:C:5:ILE:HD12	1:C:15:TYR:HD2	1.72	0.54
1:G:31:ARG:NH2	2:G:301:2NE:O09	2.41	0.53
1:E:55:ILE:O	1:E:110:LYS:HD2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLN:HG3	5:C:428:HOH:O	2.08	0.52
1:B:79:GLN:NE2	2:B:301:2NE:H35	2.25	0.51
2:H:301:2NE:H3	2:H:301:2NE:O39	2.10	0.51
1:B:199:ARG:O	1:B:199:ARG:HG3	2.11	0.50
1:B:184:GLU:HG2	1:B:187:ARG:HH22	1.76	0.50
1:A:245:LEU:C	1:A:245:LEU:HD23	2.36	0.50
1:H:66:HIS:HB3	1:H:68:ASP:OD1	2.12	0.49
1:I:31:ARG:NH1	1:I:70:LYS:HG3	2.27	0.49
1:H:245:LEU:C	1:H:245:LEU:HD23	2.38	0.49
1:I:251:GLU:HG3	1:I:252:GLU:N	2.27	0.49
2:F:301:2NE:O50	2:F:301:2NE:H33	2.11	0.49
1:B:103:ARG:HH11	1:D:103:ARG:HH21	1.60	0.48
1:A:7:LYS:HG3	1:A:8:HIS:N	2.28	0.48
2:E:301:2NE:H15	2:E:301:2NE:O13	2.13	0.48
1:C:5:ILE:HD11	1:C:15:TYR:CE2	2.47	0.48
1:E:199:ARG:O	1:E:199:ARG:HG3	2.14	0.48
1:A:103:ARG:HH21	1:F:238:GLU:HG3	1.78	0.48
1:E:245:LEU:C	1:E:245:LEU:HD23	2.38	0.47
1:G:31:ARG:HH21	2:G:301:2NE:P06	2.36	0.47
1:G:79:GLN:NE2	2:G:301:2NE:H35	2.28	0.47
1:B:137:ALA:HA	1:B:195:VAL:O	2.14	0.47
1:G:245:LEU:HD21	1:G:249:MET:HE3	1.97	0.47
1:F:90:ASP:HB3	1:H:29:HIS:HD2	1.79	0.47
1:A:187:ARG:NH1	5:A:497:HOH:O	1.84	0.47
1:C:137:ALA:HA	1:C:195:VAL:O	2.14	0.47
1:I:251:GLU:CG	5:I:449:HOH:O	2.63	0.47
1:G:199:ARG:O	1:G:199:ARG:HG3	2.15	0.46
1:C:5:ILE:HD12	1:C:5:ILE:N	2.31	0.46
1:I:147:PRO:HD2	1:I:177:CYS:SG	2.55	0.46
1:A:103:ARG:NH2	1:F:238:GLU:HG3	2.31	0.46
1:C:55:ILE:O	1:C:110:LYS:HD2	2.16	0.46
1:I:77:GLY:HA3	2:I:301:2NE:H40	1.98	0.46
1:A:199:ARG:HG3	1:A:199:ARG:O	2.16	0.46
1:H:82:ARG:NH1	1:H:150:GLY:O	2.49	0.46
1:F:137:ALA:HB1	1:F:197:VAL:HA	1.98	0.45
1:C:5:ILE:HD12	1:C:15:TYR:CE2	2.49	0.45
1:F:245:LEU:C	1:F:245:LEU:HD23	2.42	0.45
1:G:245:LEU:CD2	1:G:249:MET:HE3	2.47	0.45
1:A:103:ARG:NH1	1:F:103:ARG:HH11	2.14	0.45
1:G:137:ALA:HB1	1:G:197:VAL:HG22	1.99	0.45
1:A:103:ARG:NH2	1:F:238:GLU:CG	2.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:LEU:HD21	1:D:249:MET:HE3	2.00	0.44
1:G:245:LEU:C	1:G:245:LEU:HD23	2.43	0.44
1:H:87:TYR:OH	2:H:301:2NE:S48	2.75	0.44
1:I:89:ASP:OD1	1:I:89:ASP:C	2.61	0.44
1:A:86:GLY:HA2	1:F:248:TYR:HD2	1.81	0.44
1:G:89:ASP:OD2	1:G:93:THR:CG2	2.60	0.44
1:H:55:ILE:O	1:H:110:LYS:HD2	2.18	0.44
1:C:245:LEU:C	1:C:245:LEU:HD23	2.43	0.44
2:D:301:2NE:O13	2:D:301:2NE:H15	2.17	0.44
1:H:29:HIS:CD2	1:H:30:LYS:HG2	2.52	0.44
1:B:55:ILE:O	1:B:110:LYS:HD2	2.18	0.43
1:C:7:LYS:HD3	1:C:9:TYR:OH	2.18	0.43
1:F:55:ILE:O	1:F:110:LYS:HD2	2.18	0.43
1:F:149:VAL:HG21	2:F:301:2NE:H35	2.01	0.43
1:A:66:HIS:CG	1:A:67:SER:H	2.37	0.43
1:D:70:LYS:HA	1:D:70:LYS:HD2	1.80	0.43
1:B:248:TYR:HD2	1:D:86:GLY:HA2	1.84	0.43
1:E:137:ALA:HA	1:E:195:VAL:O	2.18	0.43
1:I:251:GLU:HG2	5:I:449:HOH:O	2.18	0.43
1:I:11:ASP:HB2	1:I:41:GLU:OE1	2.18	0.42
1:A:210:GLU:O	1:A:214:LYS:NZ	2.50	0.42
2:C:301:2NE:H15	2:C:301:2NE:O13	2.19	0.42
1:C:103:ARG:NH2	1:E:238:GLU:HG3	2.35	0.42
1:A:274:LEU:HB3	1:A:275:PRO:HD2	2.02	0.42
1:G:93:THR:HA	1:G:94:PRO:HD3	1.86	0.42
1:A:103:ARG:HH21	1:F:238:GLU:CG	2.32	0.42
1:B:245:LEU:CD2	1:B:249:MET:HE3	2.50	0.41
1:C:103:ARG:HH21	1:E:238:GLU:HG3	1.84	0.41
1:D:202:GLU:OE1	5:D:435:HOH:O	2.21	0.41
1:I:251:GLU:HG3	5:I:449:HOH:O	2.20	0.41
1:B:245:LEU:C	1:B:245:LEU:HD23	2.45	0.41
1:G:35:ARG:HG2	1:G:38:THR:OG1	2.20	0.41
1:I:19:GLY:HA2	1:I:54:ARG:O	2.20	0.41
1:A:59:LEU:HD13	1:A:115:LEU:HD11	2.02	0.41
1:G:89:ASP:OD1	1:G:89:ASP:C	2.64	0.41
1:H:259:ALA:CB	1:H:266:PRO:HA	2.49	0.41
1:I:27:ARG:NH2	1:I:78:ASP:OD2	2.37	0.41
1:D:27:ARG:NH2	1:D:78:ASP:OD2	2.40	0.41
1:G:149:VAL:HG21	2:G:301:2NE:H32	2.02	0.41
1:H:93:THR:HA	1:H:94:PRO:HD3	1.98	0.41
1:A:9:TYR:HB3	1:A:41:GLU:CD	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:THR:HA	1:C:94:PRO:HD3	1.91	0.41
1:F:93:THR:HA	1:F:94:PRO:HD3	1.92	0.41
1:H:257:LYS:HE2	1:H:257:LYS:HB3	1.69	0.41
2:E:301:2NE:C54	5:E:414:HOH:O	2.68	0.41
1:I:149:VAL:CG2	2:I:301:2NE:H35	2.43	0.41
1:A:148:LYS:NZ	5:A:467:HOH:O	2.54	0.40
1:B:82:ARG:NH1	1:B:150:GLY:O	2.54	0.40
1:C:199:ARG:O	1:C:199:ARG:HG3	2.20	0.40
1:A:66:HIS:CG	1:A:67:SER:N	2.89	0.40
2:A:301:2NE:H15	2:A:301:2NE:O13	2.21	0.40
1:G:125:HIS:CD2	1:G:142:PHE:HB3	2.56	0.40
1:I:268:PHE:HA	1:I:271:TYR:HD2	1.86	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:263:LYS:NZ	2:H:301:2NE:O25[6_554]	1.59	0.61
1:H:103:ARG:NH2	1:H:103:ARG:NH2[6_554]	2.05	0.15
1:E:26:ASN:ND2	1:I:91:GLN:OE1[1_655]	2.16	0.04

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	273/275 (99%)	266 (97%)	7 (3%)	0	100	100
1	B	272/275 (99%)	266 (98%)	6 (2%)	0	100	100
1	C	274/275 (100%)	268 (98%)	6 (2%)	0	100	100
1	D	275/275 (100%)	269 (98%)	6 (2%)	0	100	100
1	E	273/275 (99%)	267 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	273/275 (99%)	267 (98%)	6 (2%)	0	100	100
1	G	273/275 (99%)	267 (98%)	6 (2%)	0	100	100
1	H	273/275 (99%)	266 (97%)	7 (3%)	0	100	100
1	I	271/275 (98%)	265 (98%)	6 (2%)	0	100	100
All	All	2457/2475 (99%)	2401 (98%)	56 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/218 (100%)	217 (100%)	1 (0%)	81	87
1	B	215/218 (99%)	214 (100%)	1 (0%)	81	87
1	C	218/218 (100%)	215 (99%)	3 (1%)	59	66
1	D	217/218 (100%)	216 (100%)	1 (0%)	81	87
1	E	215/218 (99%)	214 (100%)	1 (0%)	81	87
1	F	214/218 (98%)	213 (100%)	1 (0%)	81	87
1	G	215/218 (99%)	213 (99%)	2 (1%)	70	78
1	H	212/218 (97%)	211 (100%)	1 (0%)	81	87
1	I	216/218 (99%)	215 (100%)	1 (0%)	81	87
All	All	1940/1962 (99%)	1928 (99%)	12 (1%)	78	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	B	128	HIS
1	C	5	ILE
1	C	82	ARG
1	C	128	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	128	HIS
1	E	128	HIS
1	F	128	HIS
1	G	93	THR
1	G	128	HIS
1	H	128	HIS
1	I	128	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	B	8	HIS
1	B	144	GLN
1	B	233	GLN
1	C	233	GLN
1	D	233	GLN
1	E	8	HIS
1	F	233	GLN
1	H	4	HIS
1	H	29	HIS
1	I	8	HIS
1	I	37	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	2NE	D	301	-	58,60,60	2.28	22 (37%)	83,89,89	2.05	14 (16%)
3	BCT	D	302	-	3,3,3	2.30	1 (33%)	2,3,3	0.14	0
3	BCT	H	302	-	3,3,3	2.31	1 (33%)	2,3,3	0.20	0
2	2NE	G	301	-	58,60,60	2.00	18 (31%)	83,89,89	2.06	23 (27%)
2	2NE	E	301	-	58,60,60	2.17	21 (36%)	83,89,89	1.90	17 (20%)
3	BCT	E	302	-	3,3,3	0.95	0	2,3,3	0.26	0
4	MLI	C	303	-	6,6,6	1.40	0	7,7,7	0.89	0
2	2NE	A	301	-	58,60,60	1.88	10 (17%)	83,89,89	1.87	19 (22%)
2	2NE	B	301	-	58,60,60	2.03	16 (27%)	83,89,89	2.01	20 (24%)
3	BCT	G	302	-	3,3,3	0.94	0	2,3,3	0.15	0
2	2NE	H	301	-	58,60,60	1.87	14 (24%)	83,89,89	2.12	20 (24%)
2	2NE	F	301	-	58,60,60	2.15	20 (34%)	83,89,89	2.05	20 (24%)
2	2NE	C	301	-	58,60,60	2.19	24 (41%)	83,89,89	2.01	18 (21%)
3	BCT	C	302	-	3,3,3	0.93	0	2,3,3	0.28	0
3	BCT	I	302	-	3,3,3	2.36	1 (33%)	2,3,3	0.21	0
3	BCT	A	302	-	3,3,3	2.27	1 (33%)	2,3,3	0.37	0
4	MLI	I	303	-	6,6,6	1.19	0	7,7,7	1.43	0
3	BCT	F	302	-	3,3,3	1.00	0	2,3,3	0.62	0
3	BCT	B	302	-	3,3,3	2.28	1 (33%)	2,3,3	0.25	0
2	2NE	I	301	-	58,60,60	2.25	23 (39%)	83,89,89	2.23	19 (22%)

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	2NE	G	301	-	-	7/55/71/71	0/4/4/4
2	2NE	E	301	-	-	3/55/71/71	0/4/4/4
2	2NE	H	301	-	-	11/55/71/71	0/4/4/4
2	2NE	D	301	-	-	3/55/71/71	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2NE	F	301	-	-	7/55/71/71	0/4/4/4
2	2NE	C	301	-	-	4/55/71/71	0/4/4/4
4	MLI	C	303	-	-	0/4/4/4	-
2	2NE	A	301	-	-	4/55/71/71	0/4/4/4
2	2NE	I	301	-	-	5/55/71/71	0/4/4/4
4	MLI	I	303	-	-	0/4/4/4	-
2	2NE	B	301	-	-	8/55/71/71	0/4/4/4

All (173) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	2NE	C38-N40	6.05	1.47	1.33
2	A	301	2NE	C43-N45	5.71	1.46	1.33
2	F	301	2NE	O37-C36	-5.57	1.32	1.42
2	B	301	2NE	C18-C20	-5.56	1.40	1.53
2	C	301	2NE	C18-C20	-5.42	1.41	1.53
2	G	301	2NE	C18-C20	-5.30	1.41	1.53
2	I	301	2NE	C18-C20	-5.30	1.41	1.53
2	H	301	2NE	C38-N40	5.21	1.45	1.33
2	A	301	2NE	C18-C20	-5.21	1.41	1.53
2	H	301	2NE	C18-C20	-5.11	1.41	1.53
2	D	301	2NE	O37-C36	-4.84	1.33	1.42
2	D	301	2NE	C18-C20	-4.82	1.42	1.53
2	E	301	2NE	C18-C20	-4.81	1.42	1.53
2	E	301	2NE	O37-C36	-4.76	1.33	1.42
2	F	301	2NE	C18-C20	-4.76	1.42	1.53
2	I	301	2NE	O37-C36	-4.73	1.34	1.42
2	F	301	2NE	C38-N40	4.73	1.44	1.33
2	D	301	2NE	P06-O09	-4.64	1.54	1.59
2	I	301	2NE	P06-O09	-4.64	1.54	1.59
2	A	301	2NE	C30-N31	4.60	1.46	1.34
2	B	301	2NE	O37-C36	-4.59	1.34	1.42
2	H	301	2NE	C43-N45	4.48	1.44	1.33
2	B	301	2NE	C38-N40	4.43	1.44	1.33
2	D	301	2NE	C38-N40	4.37	1.43	1.33
2	C	301	2NE	C38-N40	4.34	1.43	1.33
2	G	301	2NE	O37-C36	-4.32	1.34	1.42
2	E	301	2NE	C43-N45	4.26	1.43	1.33
2	A	301	2NE	O16-C17	4.25	1.51	1.42
2	F	301	2NE	C43-N45	4.25	1.43	1.33
2	C	301	2NE	O37-C36	-4.21	1.34	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	2NE	C43-N45	4.17	1.43	1.33
2	I	301	2NE	C29-N28	-4.15	1.31	1.39
2	I	301	2NE	C38-N40	4.14	1.43	1.33
2	G	301	2NE	C38-N40	4.12	1.43	1.33
2	D	301	2NE	C20-C15	-4.08	1.42	1.52
2	H	301	2NE	O37-C36	-4.04	1.35	1.42
2	E	301	2NE	C38-N40	3.92	1.42	1.33
2	C	301	2NE	C43-N45	3.91	1.42	1.33
2	G	301	2NE	C18-C17	-3.91	1.41	1.53
2	D	301	2NE	P10-O09	-3.89	1.55	1.59
2	E	301	2NE	C18-C17	-3.86	1.41	1.53
2	D	301	2NE	C18-C17	-3.86	1.41	1.53
2	E	301	2NE	C20-C15	-3.74	1.43	1.52
3	I	302	BCT	O1-C	3.69	1.38	1.25
2	G	301	2NE	C20-C15	-3.68	1.43	1.52
2	B	301	2NE	C29-N28	-3.64	1.32	1.39
2	I	301	2NE	C43-N45	3.64	1.42	1.33
2	C	301	2NE	C29-N28	-3.62	1.32	1.39
3	H	302	BCT	O1-C	3.60	1.38	1.25
2	D	301	2NE	P22-O21	-3.59	1.53	1.59
3	D	302	BCT	O1-C	3.57	1.38	1.25
2	F	301	2NE	C20-C15	-3.57	1.43	1.52
2	C	301	2NE	C20-C15	-3.55	1.43	1.52
3	A	302	BCT	O1-C	3.53	1.37	1.25
3	B	302	BCT	O1-C	3.51	1.37	1.25
2	B	301	2NE	C20-C15	-3.50	1.43	1.52
2	I	301	2NE	C20-C15	-3.49	1.43	1.52
2	H	301	2NE	C20-C15	-3.47	1.43	1.52
2	E	301	2NE	P06-O09	-3.45	1.55	1.59
2	D	301	2NE	C43-N45	3.43	1.41	1.33
2	G	301	2NE	C29-N28	-3.42	1.32	1.39
2	F	301	2NE	C18-C17	-3.42	1.42	1.53
2	I	301	2NE	C18-C17	-3.38	1.42	1.53
2	D	301	2NE	C29-N28	-3.37	1.32	1.39
2	G	301	2NE	C30-N31	3.34	1.42	1.34
2	C	301	2NE	P06-O09	-3.33	1.55	1.59
2	D	301	2NE	C49-S48	3.31	1.83	1.76
2	F	301	2NE	C29-N28	-3.30	1.33	1.39
2	H	301	2NE	O16-C17	3.27	1.49	1.42
2	G	301	2NE	C43-N45	3.26	1.41	1.33
2	E	301	2NE	C29-N28	-3.25	1.33	1.39
2	E	301	2NE	C30-N31	3.22	1.42	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	2NE	C18-C17	-3.17	1.43	1.53
2	C	301	2NE	P06-O07	-3.16	1.40	1.55
2	C	301	2NE	C18-C17	-3.16	1.43	1.53
2	E	301	2NE	C27-N26	-3.15	1.32	1.37
2	H	301	2NE	C30-N31	3.12	1.42	1.34
2	D	301	2NE	P06-O07	-3.09	1.41	1.55
2	I	301	2NE	P06-O07	-3.09	1.41	1.55
2	G	301	2NE	O16-C17	3.06	1.49	1.42
2	D	301	2NE	P10-O11	-3.04	1.41	1.55
2	C	301	2NE	C30-N31	3.02	1.41	1.34
2	F	301	2NE	C49-S48	3.02	1.83	1.76
2	I	301	2NE	P22-O25	-3.01	1.43	1.54
2	F	301	2NE	P06-O09	-3.01	1.56	1.59
2	E	301	2NE	P22-O25	-3.00	1.43	1.54
2	I	301	2NE	C49-S48	3.00	1.83	1.76
2	C	301	2NE	C27-N26	-2.97	1.32	1.37
2	B	301	2NE	C30-N31	2.90	1.41	1.34
2	A	301	2NE	C18-C17	-2.87	1.44	1.53
2	B	301	2NE	C51-C49	2.86	1.54	1.49
2	I	301	2NE	C30-N31	2.84	1.41	1.34
2	I	301	2NE	P22-O24	-2.84	1.44	1.54
2	C	301	2NE	P22-O25	-2.82	1.44	1.54
2	I	301	2NE	C35-N26	-2.81	1.31	1.37
2	E	301	2NE	P22-O21	-2.80	1.54	1.59
2	D	301	2NE	C27-N26	-2.79	1.32	1.37
2	F	301	2NE	P10-O11	-2.79	1.42	1.55
2	I	301	2NE	C27-N26	-2.78	1.32	1.37
2	B	301	2NE	C17-N26	-2.76	1.38	1.46
2	E	301	2NE	P06-O07	-2.76	1.42	1.55
2	I	301	2NE	P10-O11	-2.75	1.42	1.55
2	H	301	2NE	P22-O21	-2.73	1.54	1.59
2	C	301	2NE	P10-O11	-2.72	1.42	1.55
2	E	301	2NE	P10-O11	-2.72	1.42	1.55
2	I	301	2NE	C51-C49	2.71	1.53	1.49
2	C	301	2NE	P22-O24	-2.71	1.44	1.54
2	F	301	2NE	C30-N31	2.71	1.41	1.34
2	F	301	2NE	C27-N26	-2.70	1.32	1.37
2	A	301	2NE	C20-C15	-2.70	1.45	1.52
2	H	301	2NE	P06-O09	-2.69	1.56	1.59
2	D	301	2NE	C30-N31	2.68	1.41	1.34
2	G	301	2NE	P22-O21	-2.67	1.54	1.59
2	D	301	2NE	C17-N26	-2.66	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	2NE	P22-O23	-2.65	1.42	1.50
2	F	301	2NE	C17-N26	-2.64	1.39	1.46
2	B	301	2NE	P22-O25	-2.64	1.45	1.54
2	A	301	2NE	O37-C36	-2.64	1.37	1.42
2	H	301	2NE	C18-C17	-2.64	1.45	1.53
2	B	301	2NE	O16-C17	2.63	1.48	1.42
2	C	301	2NE	P22-O21	-2.61	1.54	1.59
2	F	301	2NE	P22-O21	-2.60	1.55	1.59
2	B	301	2NE	C27-N26	-2.60	1.33	1.37
2	C	301	2NE	C49-S48	2.57	1.82	1.76
2	C	301	2NE	O39-C38	-2.55	1.18	1.23
2	F	301	2NE	P06-O07	-2.54	1.43	1.55
2	F	301	2NE	P22-O23	-2.54	1.42	1.50
2	D	301	2NE	C35-N26	-2.54	1.32	1.37
2	A	301	2NE	C17-N26	-2.53	1.39	1.46
2	D	301	2NE	O39-C38	-2.52	1.18	1.23
2	E	301	2NE	O39-C38	-2.49	1.18	1.23
2	C	301	2NE	C17-N26	-2.47	1.39	1.46
2	A	301	2NE	O16-C15	2.46	1.50	1.45
2	D	301	2NE	P22-O25	-2.46	1.45	1.54
2	E	301	2NE	P22-O24	-2.44	1.45	1.54
2	B	301	2NE	P06-O07	-2.43	1.44	1.55
2	I	301	2NE	C17-N26	-2.41	1.39	1.46
2	H	301	2NE	C29-N28	-2.39	1.34	1.39
2	E	301	2NE	C35-N26	-2.36	1.32	1.37
2	B	301	2NE	C35-N26	-2.36	1.32	1.37
2	F	301	2NE	O53-C52	2.35	1.41	1.36
2	F	301	2NE	P22-O24	-2.34	1.46	1.54
2	C	301	2NE	O50-C49	-2.33	1.17	1.21
2	D	301	2NE	O16-C17	2.31	1.47	1.42
2	G	301	2NE	C42-C43	-2.30	1.46	1.51
2	F	301	2NE	O16-C17	2.29	1.47	1.42
2	C	301	2NE	C35-N26	-2.29	1.32	1.37
2	G	301	2NE	P06-O09	-2.29	1.57	1.59
2	F	301	2NE	P22-O25	-2.29	1.46	1.54
2	C	301	2NE	P10-O09	-2.27	1.57	1.59
2	H	301	2NE	O16-C15	2.27	1.50	1.45
2	G	301	2NE	P06-O07	-2.26	1.44	1.55
2	G	301	2NE	P10-O11	-2.26	1.44	1.55
2	E	301	2NE	O16-C17	2.25	1.47	1.42
2	G	301	2NE	C17-N26	-2.25	1.40	1.46
2	E	301	2NE	C17-N26	-2.25	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	2NE	P22-O25	-2.24	1.46	1.54
2	I	301	2NE	O16-C17	2.24	1.47	1.42
2	C	301	2NE	P22-O23	-2.22	1.43	1.50
2	I	301	2NE	O39-C38	-2.22	1.19	1.23
2	I	301	2NE	P22-O21	-2.20	1.55	1.59
2	E	301	2NE	P10-O12	-2.19	1.43	1.50
2	C	301	2NE	P06-O08	-2.15	1.43	1.50
2	B	301	2NE	P10-O11	-2.12	1.45	1.55
2	I	301	2NE	P10-O09	-2.11	1.57	1.59
2	G	301	2NE	C46-N45	-2.11	1.41	1.46
2	H	301	2NE	C17-N26	-2.10	1.40	1.46
2	G	301	2NE	P22-O24	-2.09	1.47	1.54
2	C	301	2NE	O16-C17	2.09	1.46	1.42
2	H	301	2NE	C51-C49	2.07	1.52	1.49
2	E	301	2NE	P10-O09	-2.06	1.57	1.59
2	D	301	2NE	P22-O24	-2.06	1.47	1.54
2	I	301	2NE	P22-O23	-2.03	1.44	1.50

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301	2NE	C47-S48-C49	11.23	113.08	99.85
2	H	301	2NE	C47-S48-C49	11.01	112.83	99.85
2	D	301	2NE	O50-C49-C51	-10.78	106.67	123.18
2	B	301	2NE	C47-S48-C49	7.88	109.13	99.85
2	C	301	2NE	C51-C49-S48	7.60	128.36	114.94
2	D	301	2NE	C51-C49-S48	7.50	128.19	114.94
2	A	301	2NE	C47-S48-C49	7.30	108.46	99.85
2	F	301	2NE	C47-S48-C49	7.24	108.39	99.85
2	C	301	2NE	O50-C49-C51	-6.73	112.88	123.18
2	G	301	2NE	C51-C49-S48	6.72	126.80	114.94
2	F	301	2NE	O50-C49-C51	-6.71	112.90	123.18
2	E	301	2NE	C51-C49-S48	6.23	125.94	114.94
2	F	301	2NE	C29-C35-N34	-6.20	118.18	126.72
2	C	301	2NE	C29-C35-N34	-6.15	118.25	126.72
2	G	301	2NE	C29-C35-N34	-6.10	118.31	126.72
2	E	301	2NE	O50-C49-C51	-6.03	113.95	123.18
2	G	301	2NE	O50-C49-C51	-6.02	113.96	123.18
2	E	301	2NE	C29-C35-N34	-6.01	118.44	126.72
2	I	301	2NE	C29-C35-N34	-5.97	118.50	126.72
2	B	301	2NE	C51-C49-S48	5.84	125.26	114.94
2	I	301	2NE	C51-C49-S48	5.65	124.92	114.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	2NE	C29-C35-N34	-5.63	118.97	126.72
2	D	301	2NE	C29-C35-N34	-5.58	119.03	126.72
2	A	301	2NE	C29-C35-N34	-5.52	119.11	126.72
2	I	301	2NE	O50-C49-C51	-5.41	114.90	123.18
2	H	301	2NE	C29-C35-N34	-5.25	119.48	126.72
2	G	301	2NE	C47-S48-C49	5.22	106.00	99.85
2	E	301	2NE	C47-S48-C49	5.15	105.92	99.85
2	B	301	2NE	O50-C49-C51	-4.90	115.67	123.18
2	C	301	2NE	C35-C29-N28	-4.88	105.00	110.58
2	E	301	2NE	C35-C29-N28	-4.78	105.12	110.58
2	F	301	2NE	C46-N45-C43	4.59	131.37	122.82
2	H	301	2NE	C51-C49-S48	4.58	123.02	114.94
2	A	301	2NE	N34-C33-N32	-4.57	121.66	128.58
2	H	301	2NE	N34-C33-N32	-4.45	121.85	128.58
2	G	301	2NE	C41-C42-C43	-4.42	105.04	112.39
2	C	301	2NE	C47-S48-C49	4.29	104.90	99.85
2	F	301	2NE	C35-C29-N28	-4.23	105.75	110.58
2	A	301	2NE	C41-N40-C38	-3.89	115.56	122.55
2	B	301	2NE	N34-C35-N26	3.87	133.74	127.17
2	C	301	2NE	C29-N28-C27	3.82	109.46	103.45
2	I	301	2NE	C35-C29-N28	-3.81	106.22	110.58
2	A	301	2NE	C41-C42-C43	-3.77	106.11	112.39
2	D	301	2NE	N34-C35-N26	3.74	133.53	127.17
2	G	301	2NE	N34-C35-N26	3.73	133.50	127.17
2	A	301	2NE	C33-N34-C35	3.72	120.92	111.83
2	G	301	2NE	N34-C33-N32	-3.70	122.98	128.58
2	F	301	2NE	C51-C49-S48	3.67	121.41	114.94
2	B	301	2NE	N34-C33-N32	-3.65	123.05	128.58
2	I	301	2NE	C46-N45-C43	3.63	129.58	122.82
2	F	301	2NE	N34-C35-N26	3.62	133.33	127.17
2	F	301	2NE	C29-N28-C27	3.60	109.10	103.45
2	D	301	2NE	N34-C33-N32	-3.55	123.21	128.58
2	H	301	2NE	P22-O21-C20	-3.50	114.08	123.43
2	E	301	2NE	C29-N28-C27	3.47	108.90	103.45
2	B	301	2NE	C15-O16-C17	-3.46	101.82	109.47
2	H	301	2NE	C41-N40-C38	-3.45	116.36	122.55
2	B	301	2NE	C35-C29-N28	-3.40	106.69	110.58
2	C	301	2NE	N34-C33-N32	-3.38	123.46	128.58
2	B	301	2NE	C29-N28-C27	3.38	108.77	103.45
2	I	301	2NE	N34-C35-N26	3.34	132.85	127.17
2	A	301	2NE	N34-C35-N26	3.34	132.84	127.17
2	I	301	2NE	C15-O16-C17	-3.34	102.10	109.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	2NE	C35-C29-N28	-3.33	106.78	110.58
2	G	301	2NE	C35-C29-N28	-3.31	106.79	110.58
2	F	301	2NE	O07-P06-O09	3.31	116.22	107.27
2	H	301	2NE	C33-N34-C35	3.31	119.91	111.83
2	B	301	2NE	C33-N34-C35	3.30	119.90	111.83
2	G	301	2NE	C33-N34-C35	3.30	119.88	111.83
2	I	301	2NE	C33-N34-C35	3.29	119.86	111.83
2	D	301	2NE	C15-O16-C17	-3.28	102.23	109.47
2	A	301	2NE	C15-O16-C17	-3.27	102.24	109.47
2	F	301	2NE	C47-C46-N45	3.21	119.12	112.41
2	G	301	2NE	C15-O16-C17	-3.21	102.39	109.47
2	C	301	2NE	C15-O16-C17	-3.18	102.44	109.47
2	C	301	2NE	C33-N34-C35	3.18	119.61	111.83
2	E	301	2NE	C33-N34-C35	3.18	119.60	111.83
2	C	301	2NE	C29-C35-N26	3.17	109.27	105.81
2	H	301	2NE	O50-C49-C51	-3.17	118.33	123.18
2	A	301	2NE	C35-C29-N28	-3.15	106.98	110.58
2	B	301	2NE	N26-C27-N28	-3.14	109.48	113.94
2	F	301	2NE	C33-N34-C35	3.12	119.46	111.83
2	C	301	2NE	N34-C35-N26	3.12	132.48	127.17
2	I	301	2NE	N34-C33-N32	-3.11	123.87	128.58
2	E	301	2NE	C29-C35-N26	3.11	109.20	105.81
2	A	301	2NE	N26-C27-N28	-3.10	109.54	113.94
2	I	301	2NE	C20-C18-C17	3.10	106.70	99.89
2	D	301	2NE	C29-N28-C27	3.07	108.27	103.45
2	G	301	2NE	C29-N28-C27	3.06	108.26	103.45
2	H	301	2NE	N34-C35-N26	3.06	132.37	127.17
2	A	301	2NE	C46-N45-C43	-3.05	117.14	122.82
2	E	301	2NE	N34-C35-N26	3.05	132.36	127.17
2	E	301	2NE	O09-P06-O08	-3.05	101.52	110.70
2	B	301	2NE	C46-N45-C43	-3.05	117.14	122.82
2	D	301	2NE	C33-N34-C35	3.05	119.27	111.83
2	F	301	2NE	N34-C33-N32	-3.04	123.98	128.58
2	I	301	2NE	C29-N28-C27	3.01	108.18	103.45
2	C	301	2NE	N26-C27-N28	-3.01	109.67	113.94
2	F	301	2NE	N26-C27-N28	-3.00	109.68	113.94
2	G	301	2NE	O11-P10-O12	-2.98	98.58	112.44
2	A	301	2NE	C29-N28-C27	2.98	108.13	103.45
2	F	301	2NE	C20-C18-C17	2.95	106.38	99.89
2	E	301	2NE	C15-O16-C17	-2.95	102.95	109.47
2	H	301	2NE	C35-C29-N28	-2.95	107.21	110.58
2	H	301	2NE	N26-C27-N28	-2.93	109.78	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	2NE	N34-C33-N32	-2.90	124.20	128.58
2	H	301	2NE	O09-P06-O08	-2.88	102.05	110.70
2	G	301	2NE	O11-P10-O09	2.81	114.88	107.27
2	A	301	2NE	O39-C38-N40	-2.79	117.07	122.98
2	H	301	2NE	C15-O16-C17	-2.76	103.37	109.47
2	G	301	2NE	O50-C49-S48	-2.74	116.55	122.37
2	C	301	2NE	C20-C18-C17	2.71	105.84	99.89
2	G	301	2NE	C46-N45-C43	-2.70	117.80	122.82
2	H	301	2NE	C29-N28-C27	2.66	107.62	103.45
2	E	301	2NE	N26-C27-N28	-2.65	110.17	113.94
2	D	301	2NE	N26-C27-N28	-2.64	110.19	113.94
2	G	301	2NE	O09-P10-O12	2.62	118.58	110.70
2	F	301	2NE	O25-P22-O21	2.61	116.00	105.85
2	I	301	2NE	C29-C35-N26	2.60	108.65	105.81
2	B	301	2NE	C03-C02-C36	2.58	113.16	108.77
2	H	301	2NE	C20-C18-C17	2.56	105.52	99.89
2	B	301	2NE	C20-C18-C17	2.56	105.51	99.89
2	E	301	2NE	O07-P06-O09	2.55	114.18	107.27
2	A	301	2NE	C42-C43-N45	2.53	120.95	116.34
2	C	301	2NE	C30-C29-C35	2.52	120.62	117.18
2	A	301	2NE	C51-C49-S48	2.52	119.38	114.94
2	G	301	2NE	C30-C29-C35	2.51	120.61	117.18
2	E	301	2NE	C20-C18-C17	2.49	105.38	99.89
2	B	301	2NE	C47-C46-N45	2.47	117.56	112.41
2	F	301	2NE	O11-P10-O09	2.46	113.91	107.27
2	F	301	2NE	C29-C35-N26	2.46	108.49	105.81
2	F	301	2NE	C15-O16-C17	-2.43	104.10	109.47
2	E	301	2NE	C30-C29-C35	2.41	120.47	117.18
2	G	301	2NE	N26-C27-N28	-2.39	110.54	113.94
2	I	301	2NE	N26-C27-N28	-2.39	110.54	113.94
2	B	301	2NE	O39-C38-N40	-2.37	117.97	122.98
2	H	301	2NE	C01-C02-C04	2.36	112.12	108.22
2	I	301	2NE	O09-P06-O08	-2.35	103.64	110.70
2	B	301	2NE	O09-P06-O08	-2.33	103.69	110.70
2	C	301	2NE	O09-P06-O08	-2.32	103.72	110.70
2	D	301	2NE	C20-C18-C17	2.31	104.96	99.89
2	G	301	2NE	C41-N40-C38	-2.28	118.44	122.55
2	F	301	2NE	C30-C29-C35	2.28	120.30	117.18
2	I	301	2NE	O25-P22-O21	2.27	114.71	105.85
2	E	301	2NE	C47-C46-N45	2.24	117.09	112.41
2	I	301	2NE	C30-C29-C35	2.24	120.23	117.18
2	G	301	2NE	C42-C41-N40	-2.23	107.25	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	2NE	C03-C02-C36	2.18	112.49	108.77
2	D	301	2NE	O25-P22-O23	-2.17	102.37	110.83
2	G	301	2NE	C29-C35-N26	2.17	108.17	105.81
2	B	301	2NE	O07-P06-O09	2.15	113.07	107.27
2	H	301	2NE	C29-C35-N26	2.14	108.14	105.81
2	H	301	2NE	O50-C49-S48	-2.14	117.82	122.37
2	C	301	2NE	O16-C17-N26	2.13	112.18	108.09
2	C	301	2NE	C03-C02-C36	2.12	112.38	108.77
2	F	301	2NE	O09-P06-O08	-2.12	104.33	110.70
2	A	301	2NE	O09-P06-O08	-2.11	104.35	110.70
2	A	301	2NE	C03-C02-C36	2.10	112.34	108.77
2	B	301	2NE	C41-C42-C43	-2.10	108.90	112.39
2	D	301	2NE	C47-S48-C49	2.09	102.31	99.85
2	I	301	2NE	O07-P06-O09	2.08	112.90	107.27
2	B	301	2NE	C30-C29-C35	2.08	120.02	117.18
2	G	301	2NE	P22-O21-C20	-2.06	117.93	123.43
2	H	301	2NE	P10-O13-C14	-2.06	109.57	121.35
2	A	301	2NE	C29-C35-N26	2.05	108.04	105.81
2	I	301	2NE	O39-C38-N40	-2.04	118.66	122.98
2	A	301	2NE	O16-C17-N26	2.03	112.00	108.09
2	D	301	2NE	C30-C29-C35	2.03	119.95	117.18
2	C	301	2NE	C56-C55-C54	-2.03	117.74	120.24
2	H	301	2NE	O25-P22-O24	2.02	115.39	107.80

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	2NE	N45-C46-C47-S48
2	A	301	2NE	O50-C49-S48-C47
2	A	301	2NE	C51-C49-S48-C47
2	B	301	2NE	N45-C46-C47-S48
2	B	301	2NE	O50-C49-S48-C47
2	B	301	2NE	C51-C49-S48-C47
2	B	301	2NE	S48-C49-C51-C52
2	D	301	2NE	C51-C49-S48-C47
2	G	301	2NE	C46-C47-S48-C49
2	G	301	2NE	O50-C49-S48-C47
2	H	301	2NE	C01-C02-C04-O05
2	H	301	2NE	C04-O05-P06-O08
2	H	301	2NE	N45-C46-C47-S48
2	H	301	2NE	C46-C47-S48-C49

Continued on next page...

Continued from previous page...

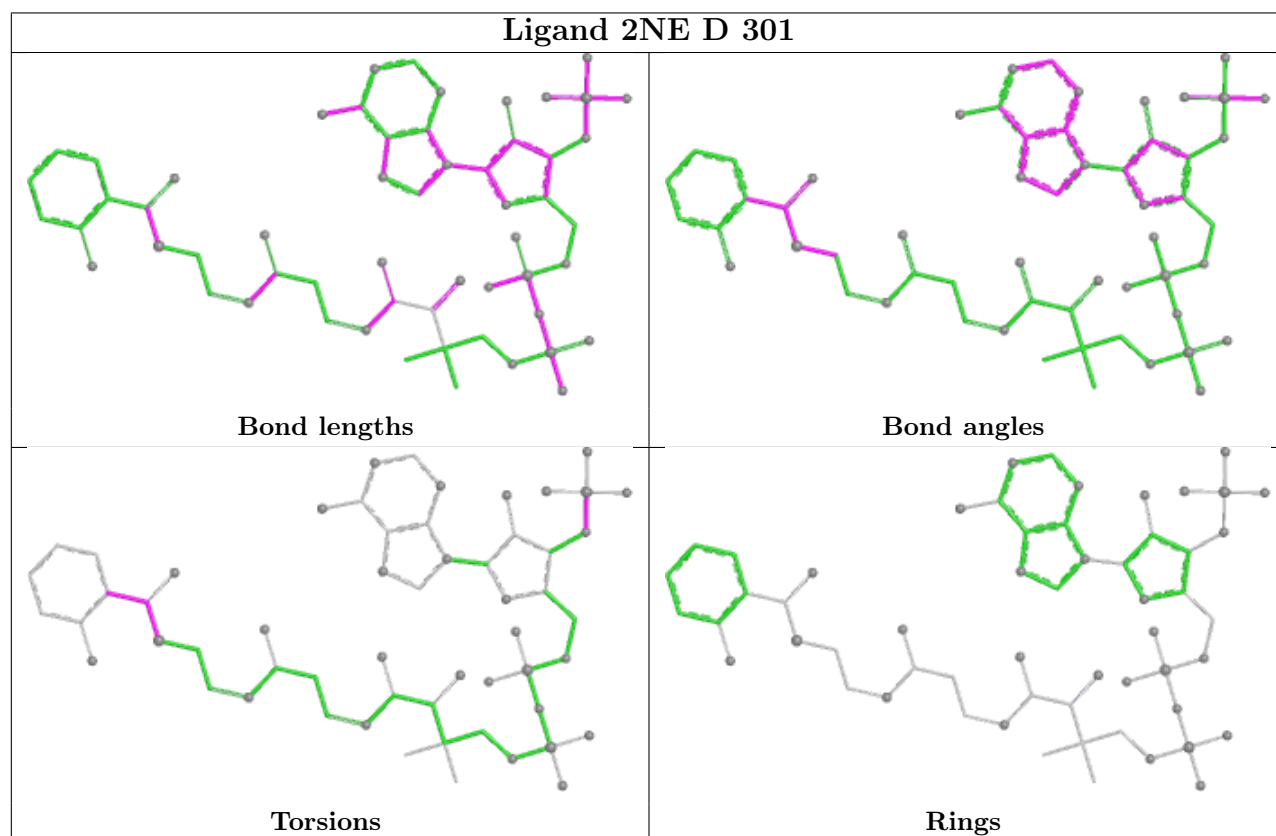
Mol	Chain	Res	Type	Atoms
2	H	301	2NE	O50-C49-S48-C47
2	H	301	2NE	C51-C49-S48-C47
2	I	301	2NE	C46-C47-S48-C49
2	A	301	2NE	O50-C49-C51-C57
2	B	301	2NE	O50-C49-C51-C57
2	C	301	2NE	O50-C49-C51-C57
2	D	301	2NE	O50-C49-C51-C57
2	E	301	2NE	O50-C49-C51-C57
2	H	301	2NE	O50-C49-C51-C57
2	I	301	2NE	O50-C49-C51-C57
2	G	301	2NE	O50-C49-C51-C57
2	C	301	2NE	O50-C49-S48-C47
2	C	301	2NE	C51-C49-S48-C47
2	E	301	2NE	O50-C49-S48-C47
2	E	301	2NE	C51-C49-S48-C47
2	G	301	2NE	C51-C49-S48-C47
2	I	301	2NE	O50-C49-S48-C47
2	B	301	2NE	O50-C49-C51-C52
2	F	301	2NE	O50-C49-C51-C52
2	F	301	2NE	O50-C49-C51-C57
2	H	301	2NE	C03-C02-C04-O05
2	B	301	2NE	C46-C47-S48-C49
2	F	301	2NE	C46-C47-S48-C49
2	F	301	2NE	S48-C49-C51-C52
2	H	301	2NE	C36-C02-C04-O05
2	H	301	2NE	C04-O05-P06-O09
2	C	301	2NE	C20-O21-P22-O25
2	D	301	2NE	C20-O21-P22-O24
2	G	301	2NE	C20-O21-P22-O25
2	G	301	2NE	N45-C46-C47-S48
2	I	301	2NE	N45-C46-C47-S48
2	F	301	2NE	C20-O21-P22-O23
2	F	301	2NE	C51-C49-S48-C47
2	G	301	2NE	C20-O21-P22-O23
2	H	301	2NE	S48-C49-C51-C52
2	I	301	2NE	S48-C49-C51-C52
2	B	301	2NE	S48-C49-C51-C57
2	F	301	2NE	S48-C49-C51-C57

There are no ring outliers.

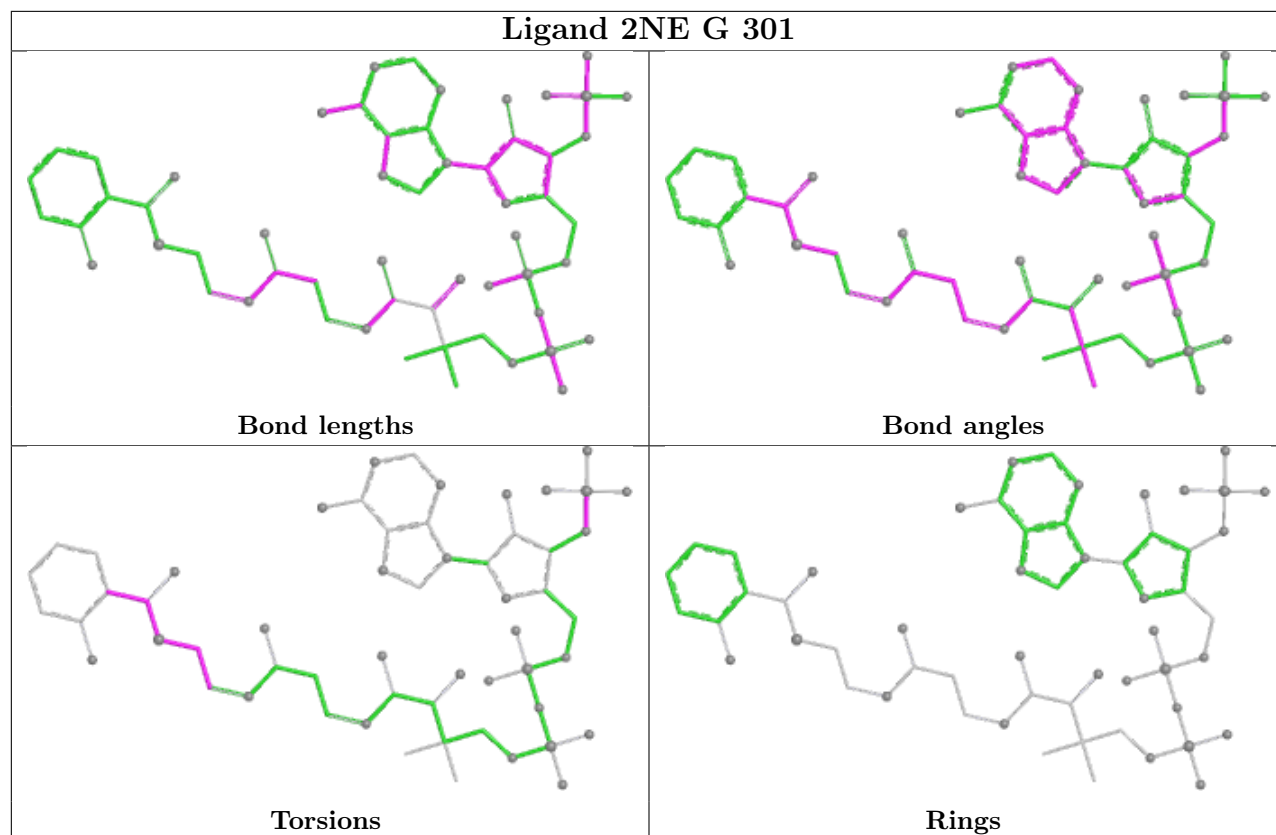
10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	2NE	3	0
2	G	301	2NE	5	0
2	E	301	2NE	2	0
2	A	301	2NE	2	0
2	B	301	2NE	2	0
3	G	302	BCT	1	0
2	H	301	2NE	4	1
2	F	301	2NE	2	0
2	C	301	2NE	1	0
2	I	301	2NE	4	0

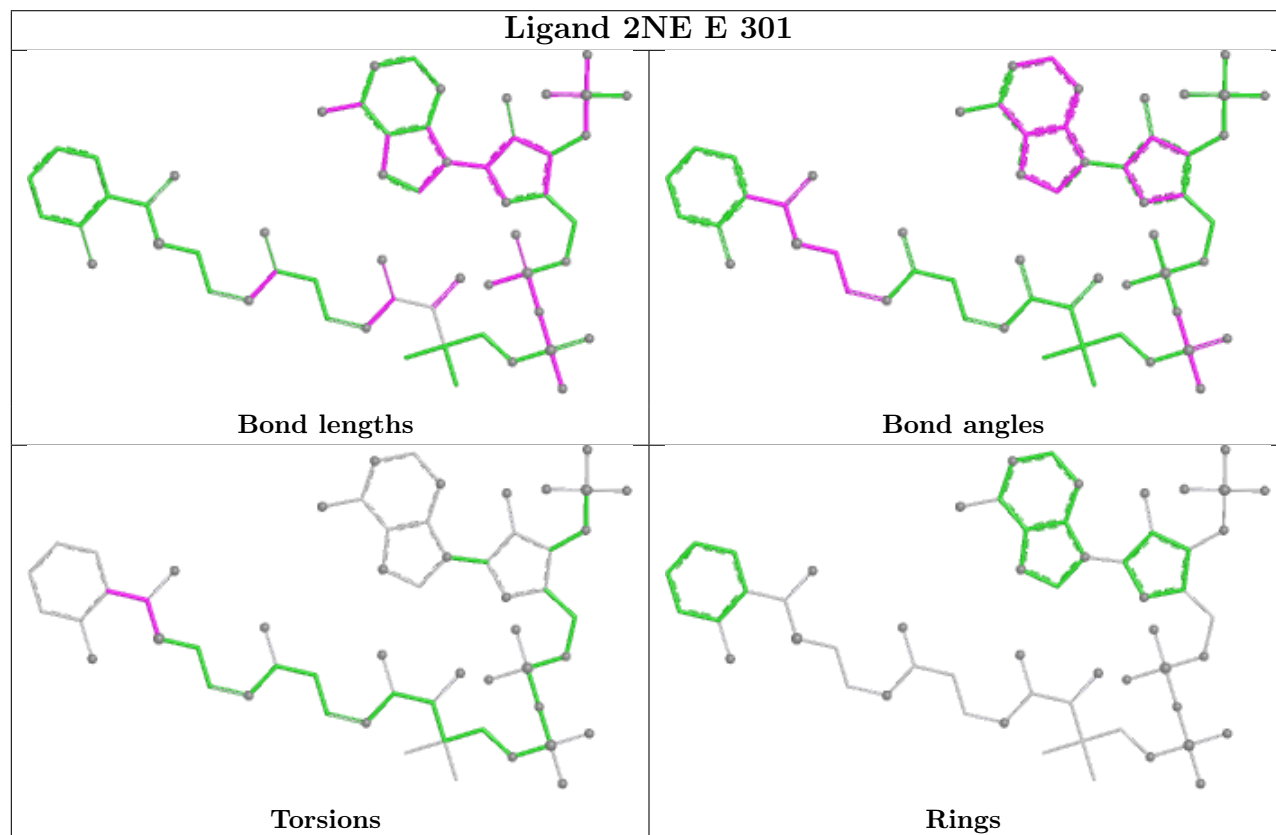
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



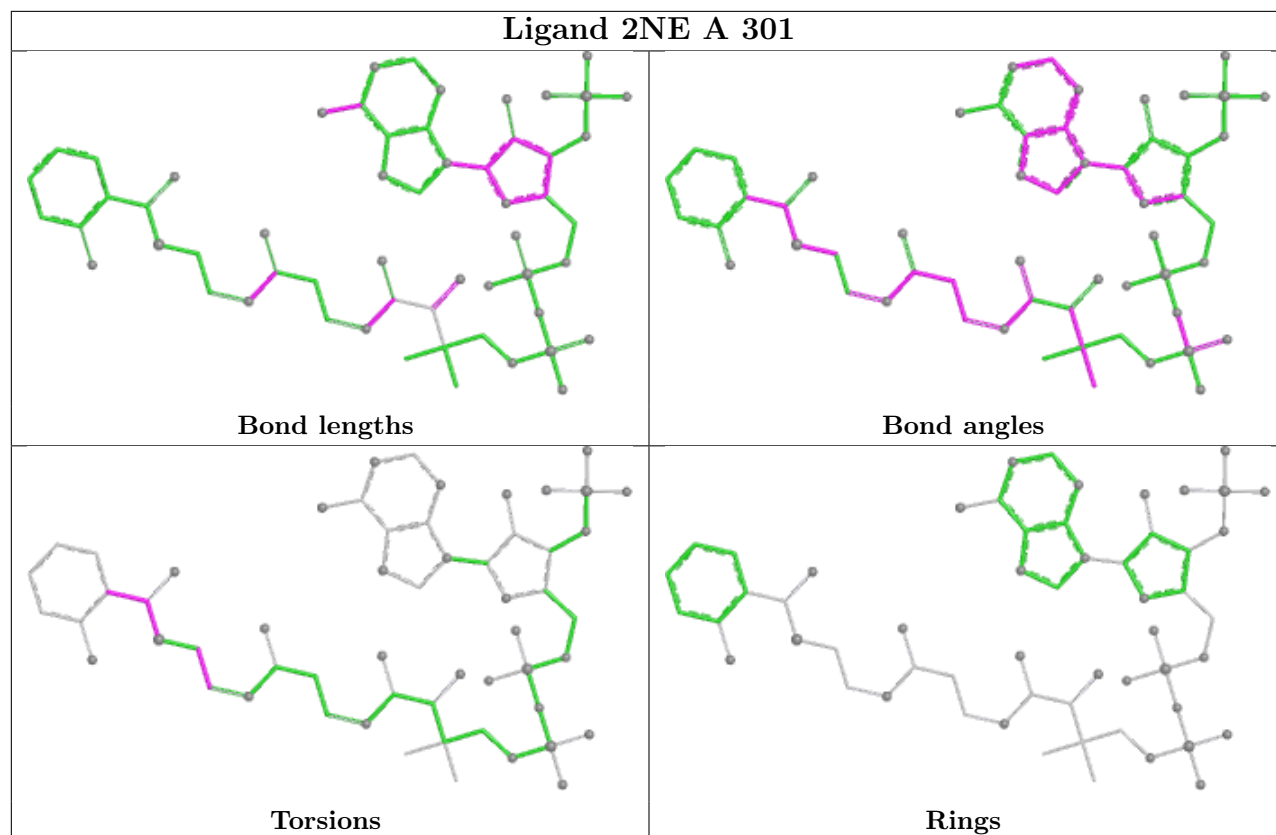
Ligand 2NE G 301



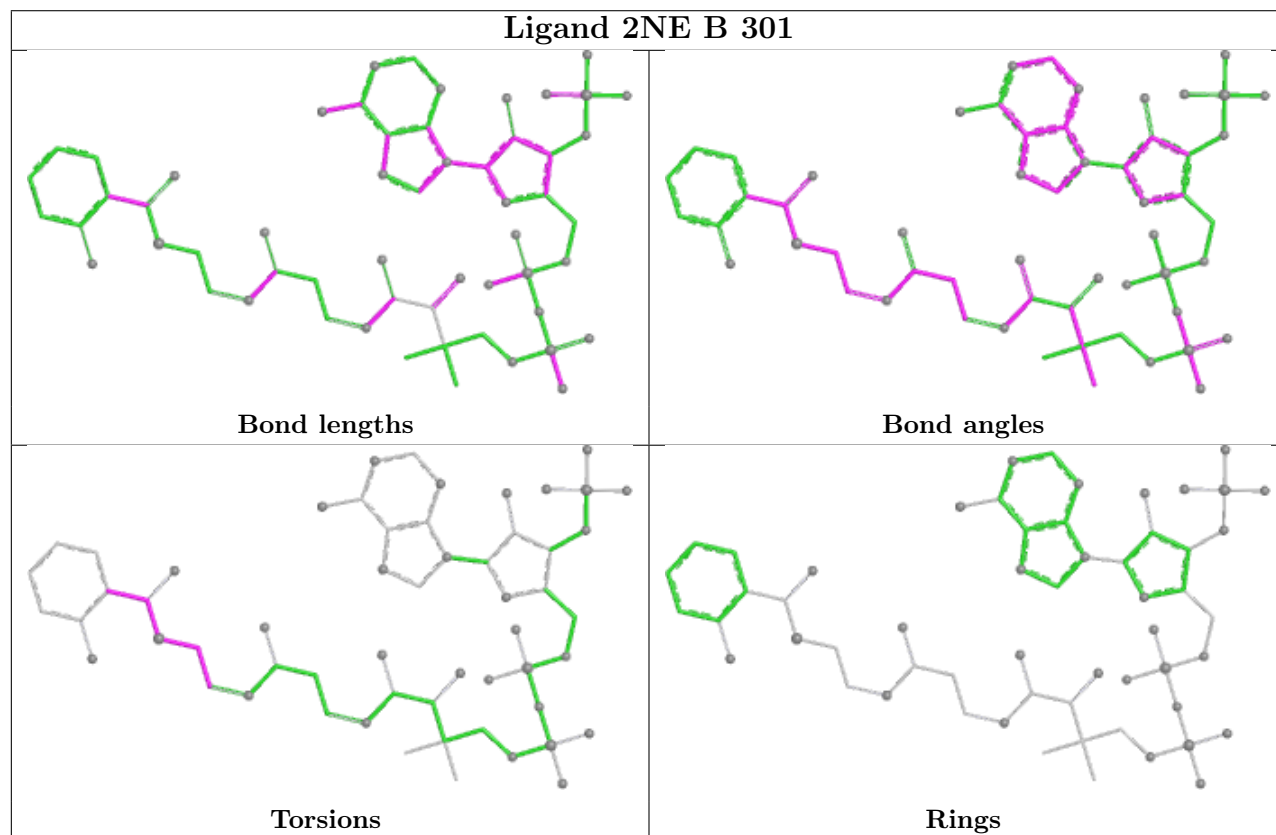
Ligand 2NE E 301



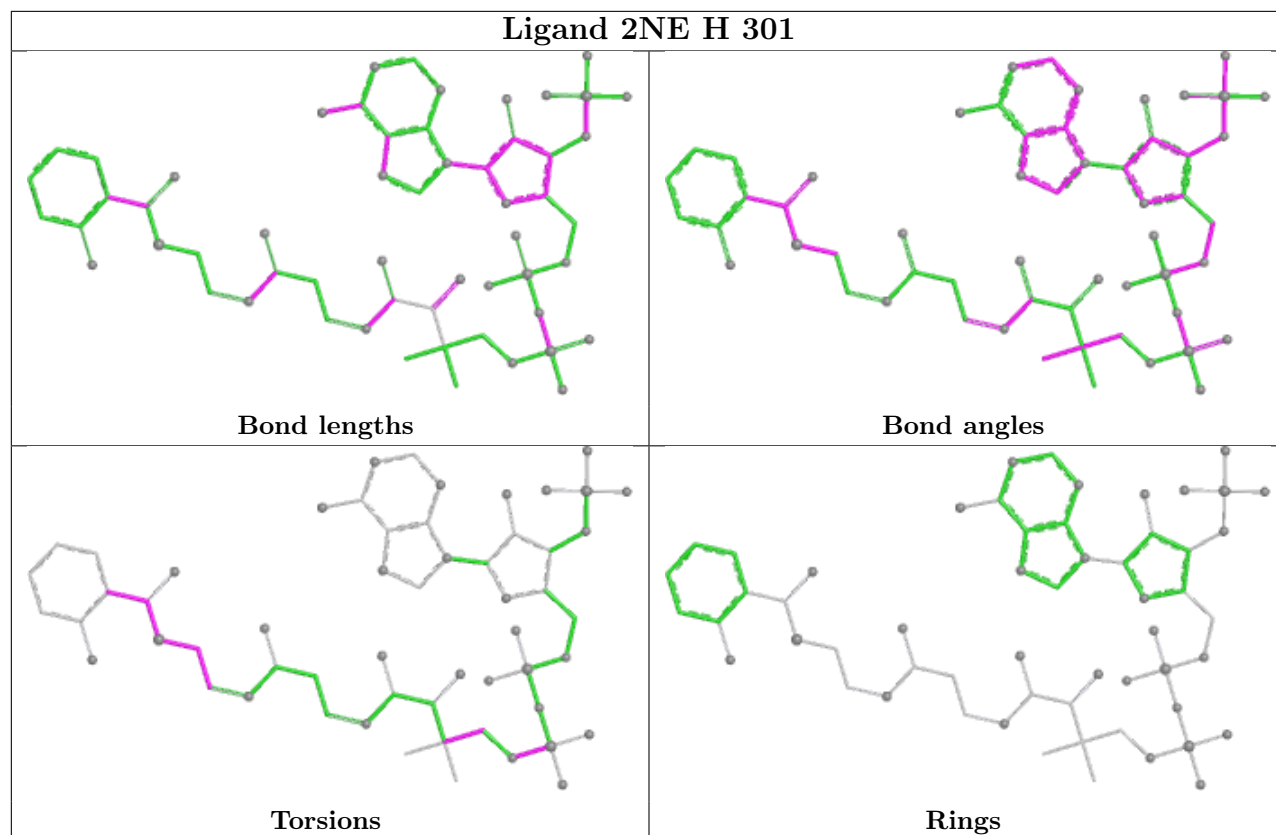
Ligand 2NE A 301



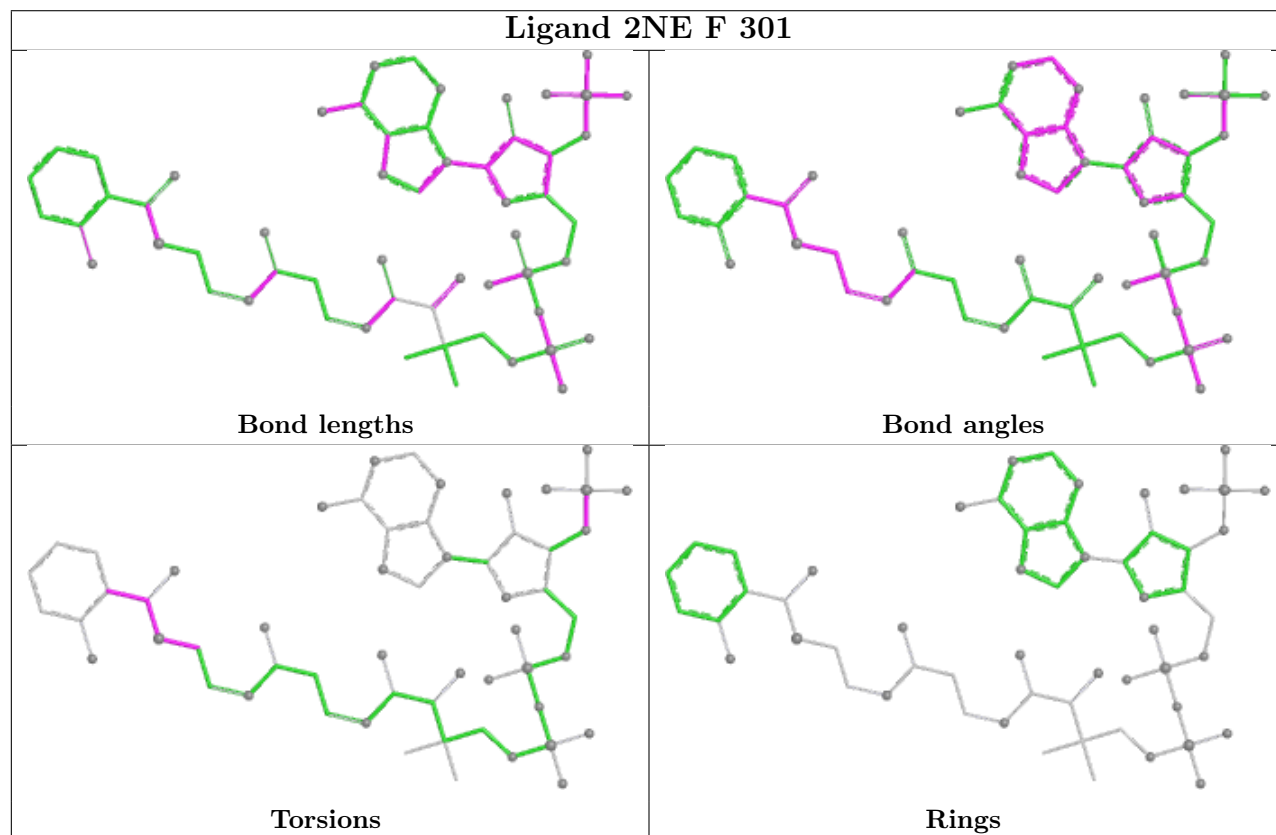
Ligand 2NE B 301



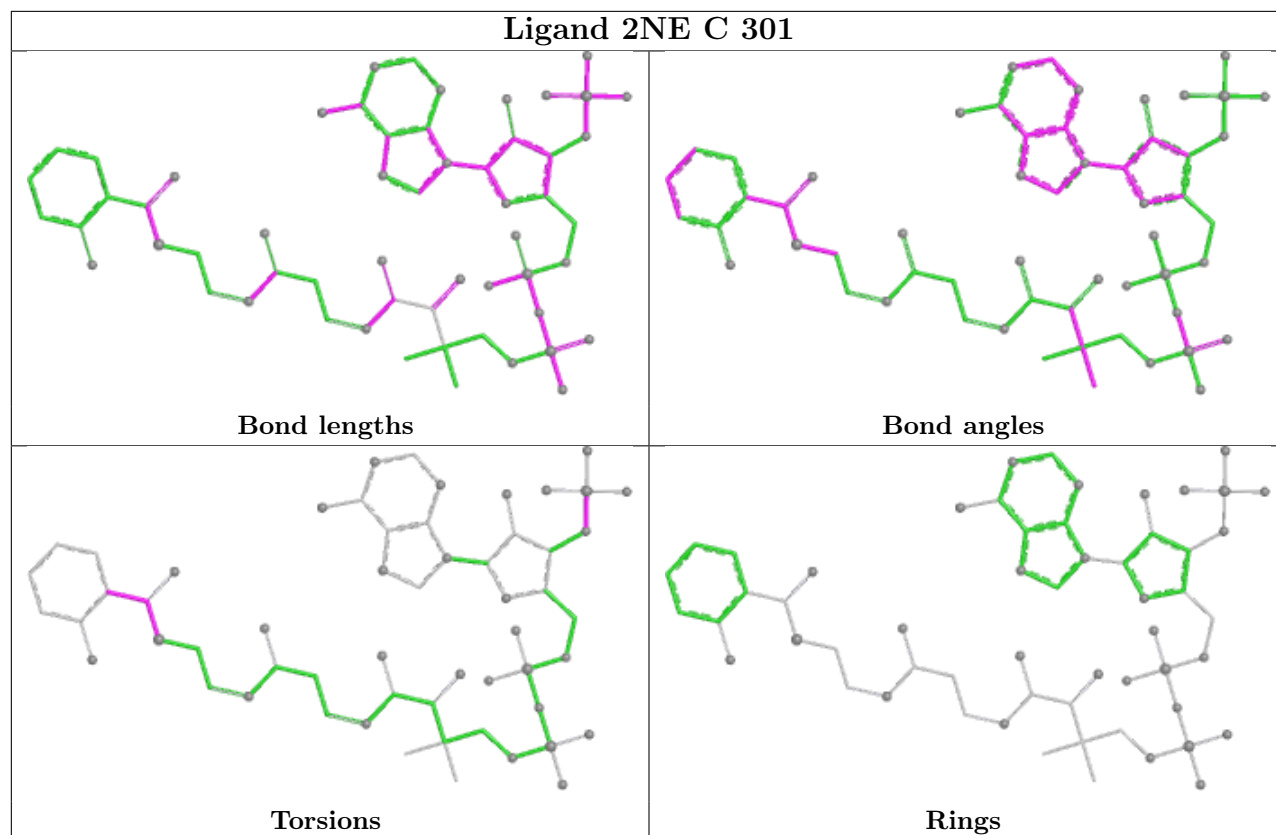
Ligand 2NE H 301



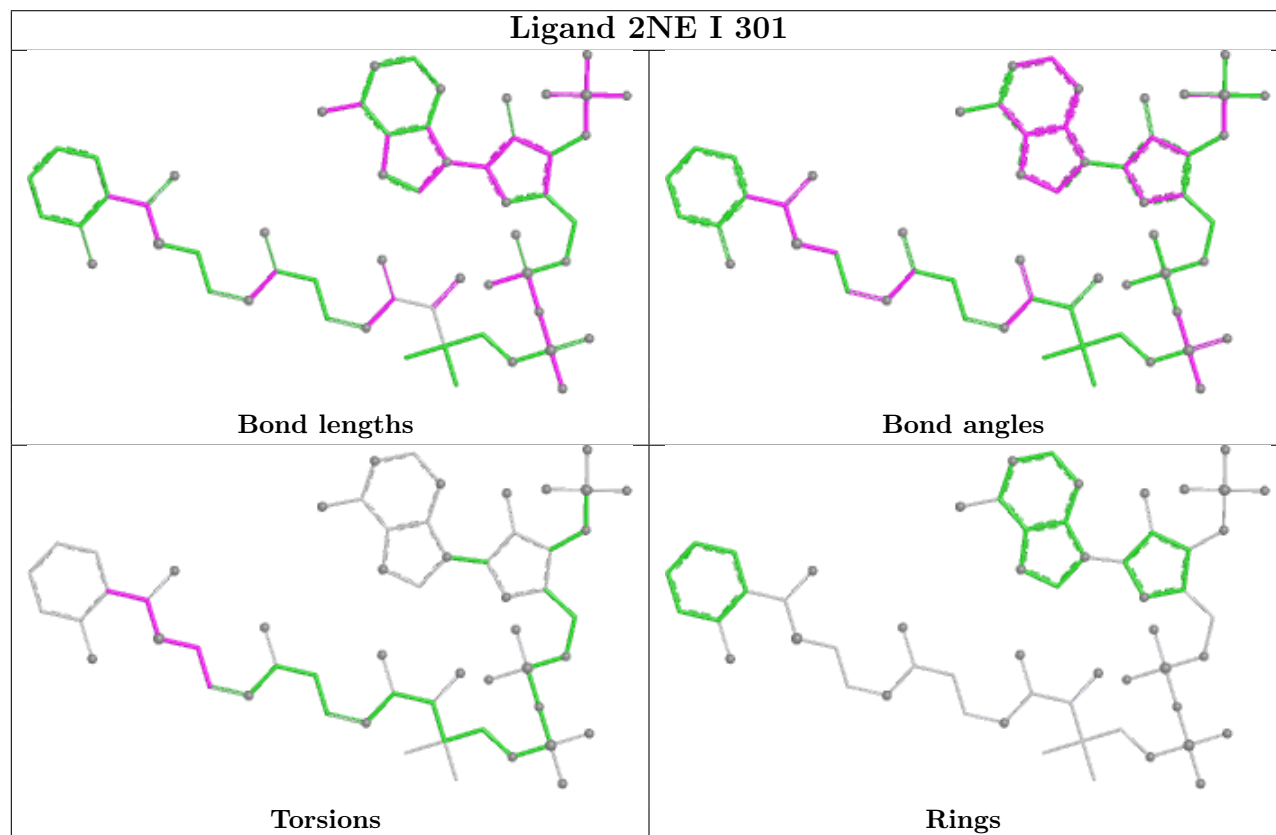
Ligand 2NE F 301



Ligand 2NE C 301



Ligand 2NE I 301



5.7 Other polymers

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 ⓘ

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	275/275 (100%)	-0.39	1 (0%) 88 88	21, 34, 53, 65	0
1	B	274/275 (99%)	-0.30	2 (0%) 84 84	21, 37, 58, 76	0
1	C	275/275 (100%)	-0.52	0 100 100	20, 29, 49, 68	1 (0%)
1	D	275/275 (100%)	-0.43	2 (0%) 84 84	20, 32, 53, 69	2 (0%)
1	E	275/275 (100%)	-0.48	0 100 100	22, 31, 51, 67	0
1	F	275/275 (100%)	-0.48	3 (1%) 78 77	20, 31, 52, 85	0
1	G	275/275 (100%)	-0.04	0 100 100	27, 45, 67, 88	0
1	H	275/275 (100%)	-0.04	6 (2%) 62 61	27, 40, 76, 101	0
1	I	275/275 (100%)	-0.36	2 (0%) 84 84	25, 34, 58, 76	0
All	All	2474/2475 (99%)	-0.34	16 (0%) 85 85	20, 34, 61, 101	3 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ASP	3.9
1	H	85	GLY	2.9
1	D	8[A]	HIS	2.8
1	F	8	HIS	2.8
1	H	88	ILE	2.7
1	H	93	THR	2.6
1	F	40	PHE	2.4
1	D	4[A]	HIS	2.2
1	I	91	GLN	2.2
1	H	81	VAL	2.2
1	H	256	GLY	2.2
1	I	40	PHE	2.2
1	F	91	GLN	2.1
1	H	40	PHE	2.1
1	A	138	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	40	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

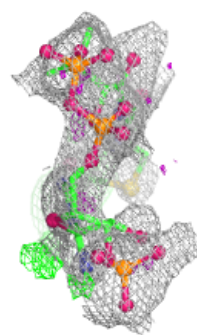
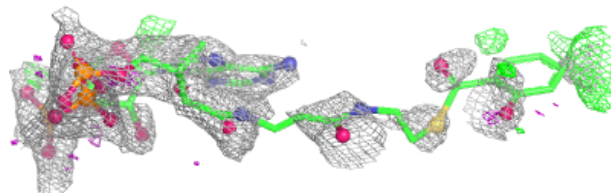
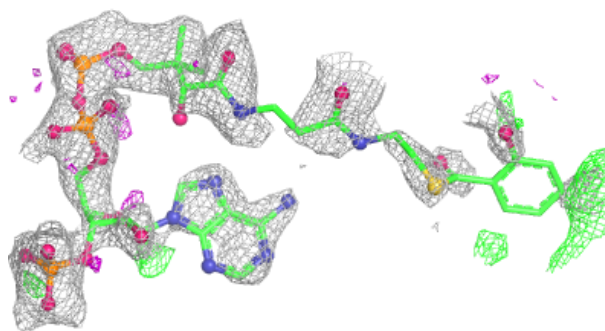
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MLI	C	303	7/7	0.74	0.17	40,56,69,69	0
2	2NE	H	301	57/57	0.75	0.18	40,89,101,133	57
3	BCT	G	302	4/4	0.80	0.14	51,63,66,69	0
2	2NE	G	301	57/57	0.83	0.13	36,62,99,100	0
3	BCT	H	302	4/4	0.85	0.12	52,63,63,70	0
2	2NE	B	301	57/57	0.85	0.12	35,49,84,92	0
2	2NE	A	301	57/57	0.87	0.12	30,47,76,97	0
4	MLI	I	303	7/7	0.87	0.15	45,52,60,67	0
3	BCT	A	302	4/4	0.88	0.12	36,53,56,61	0
3	BCT	C	302	4/4	0.89	0.18	31,38,44,51	0
3	BCT	E	302	4/4	0.89	0.17	36,45,50,56	0
2	2NE	E	301	57/57	0.89	0.11	27,44,77,84	0
3	BCT	I	302	4/4	0.90	0.13	35,47,52,55	0
2	2NE	C	301	57/57	0.91	0.10	22,37,68,97	0
3	BCT	F	302	4/4	0.92	0.12	32,37,46,49	0
2	2NE	I	301	57/57	0.92	0.10	26,38,70,136	0
2	2NE	F	301	57/57	0.92	0.10	24,35,79,102	0
3	BCT	D	302	4/4	0.93	0.11	30,42,48,56	0
3	BCT	B	302	4/4	0.93	0.13	35,50,56,61	0
2	2NE	D	301	57/57	0.94	0.09	26,37,84,125	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.

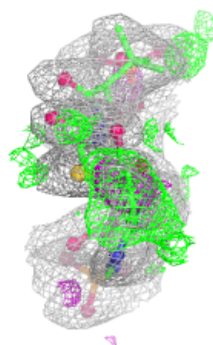
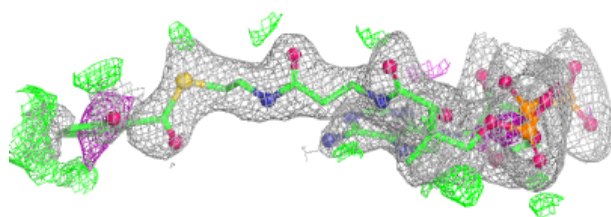
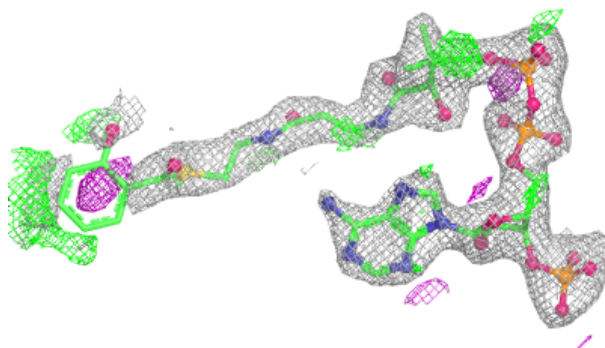
Electron density around 2NE H 301:

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

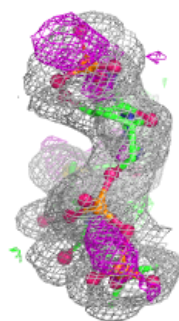
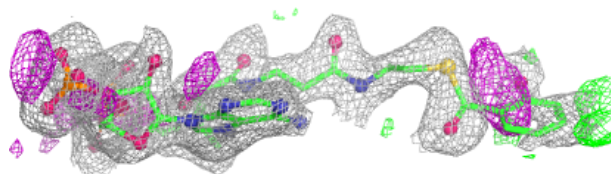
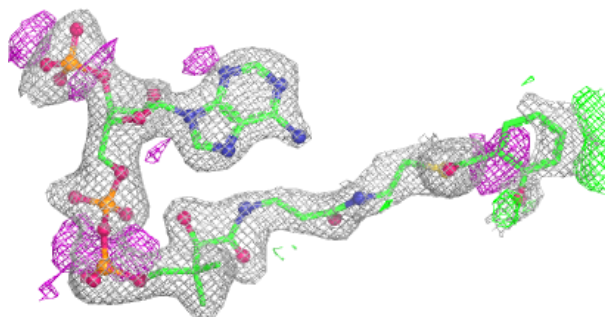


Electron density around 2NE G 301:

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

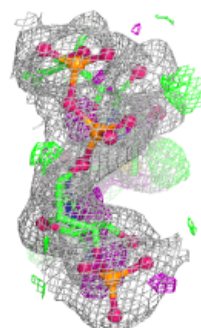
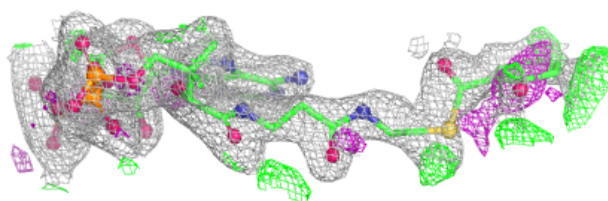
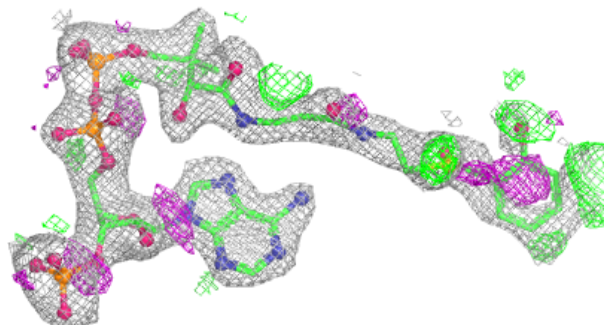
**Electron density around 2NE B 301:**

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

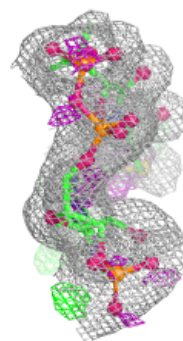
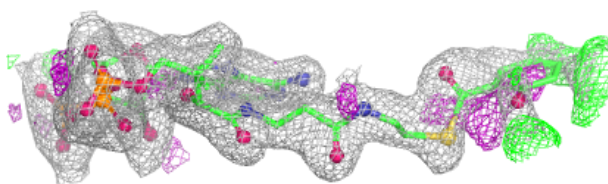
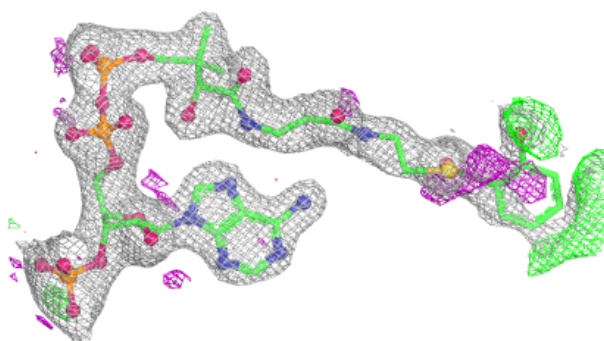


Electron density around 2NE A 301:

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

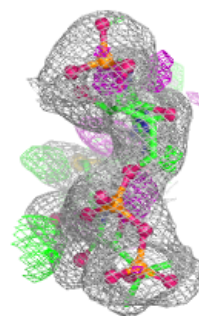
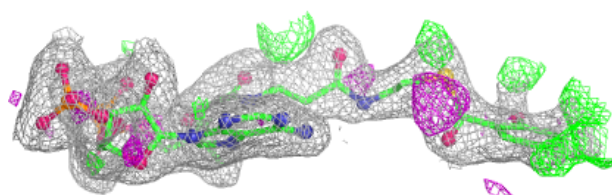
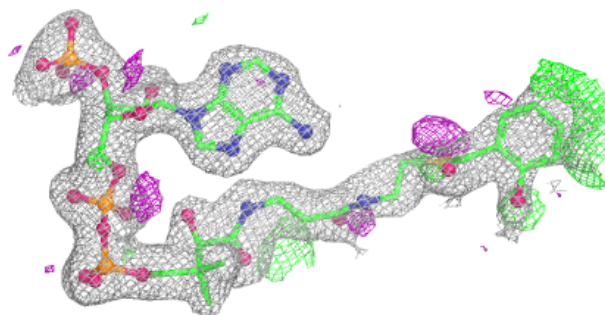
**Electron density around 2NE E 301:**

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

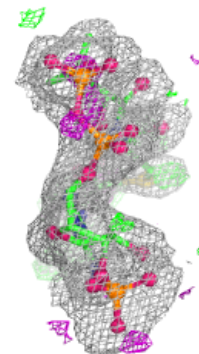
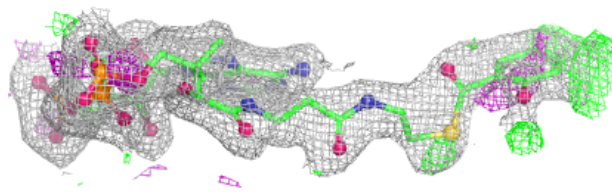
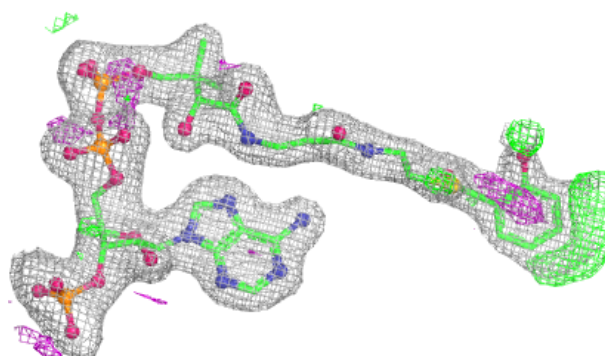


Electron density around 2NE C 301:

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

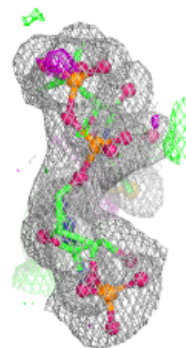
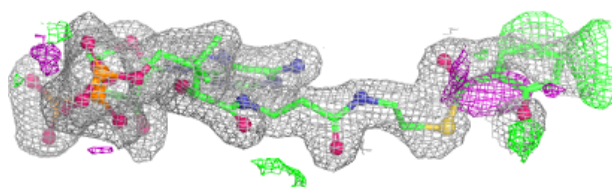
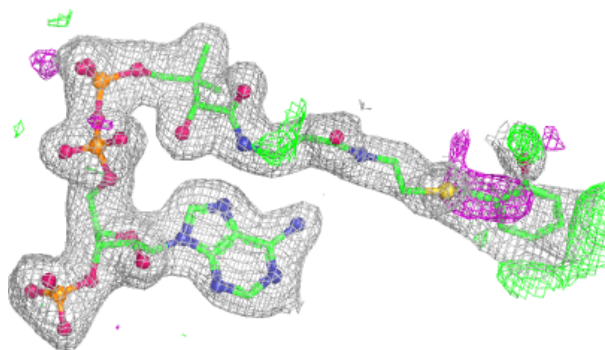
**Electron density around 2NE I 301:**

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

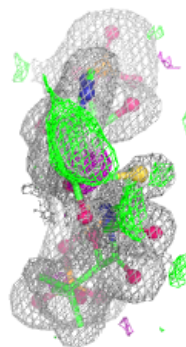
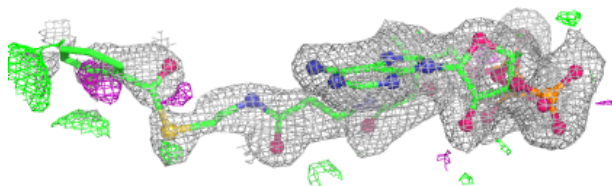
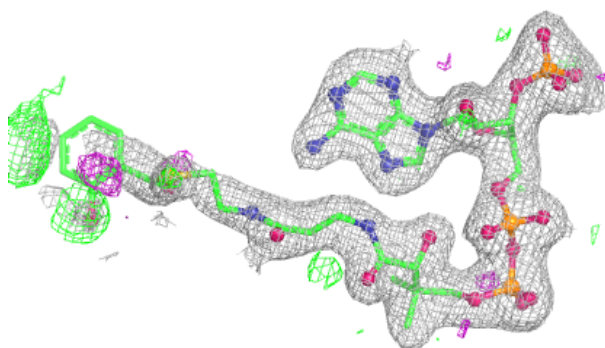


Electron density around 2NE F 301:

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

**Electron density around 2NE 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.