



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:54 AM EDT

PDB ID : 1YL7 / pdb_00001yl7
Title : the crystal structure of Mycobacterium tuberculosis dihydrodipicolinate reductase (Rv2773c) in complex with NADH (crystal form C)
Authors : Janowski, R.; Kefala, G.; Weiss, M.S.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2005-01-19
Resolution : 2.34 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

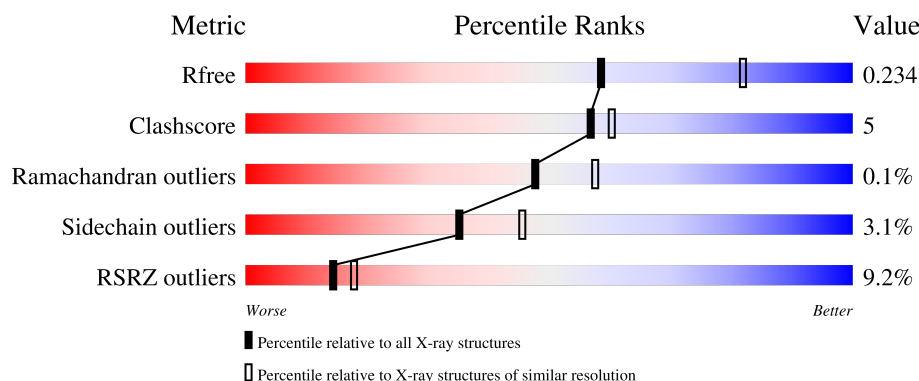
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	245	2% 87% 13%
1	B	245	87% 11%
1	C	245	38% 81% 17%
1	D	245	90% 10%

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Mol	Chain	Length	Quality of chain
1	E	245	91% 9%
1	F	245	3% 82% 16%
1	G	245	90% 9%
1	H	245	30% 90% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15209 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 Dihydrodipicolinate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1806	1140	320	343	3			
1	B	245	Total	C	N	O	S	0	3	1
			1820	1150	323	343	4			
1	C	245	Total	C	N	O	S	0	1	0
			1811	1144	320	343	4			
1	D	245	Total	C	N	O	S	0	1	0
			1811	1144	320	343	4			
1	E	245	Total	C	N	O	S	0	4	1
			1823	1151	323	346	3			
1	F	245	Total	C	N	O	S	0	2	1
			1809	1143	320	342	4			
1	G	245	Total	C	N	O	S	0	1	1
			1809	1142	323	341	3			
1	H	245	Total	C	N	O	S	0	0	0
			1806	1140	320	343	3			

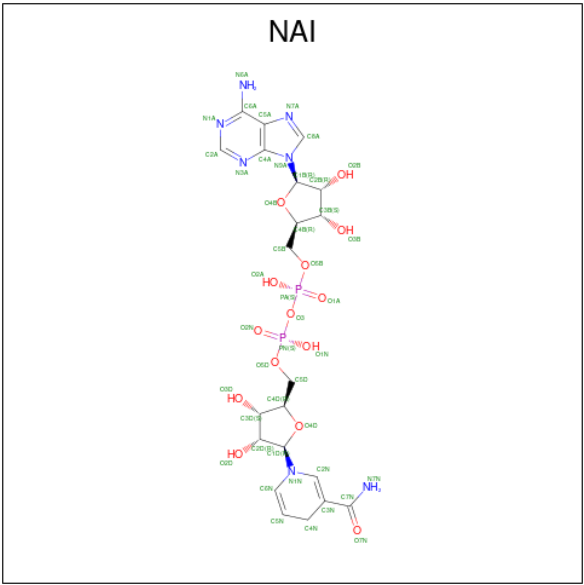
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	cloning artifact	UNP P72024
B	1	ALA	-	cloning artifact	UNP P72024
C	1	ALA	-	cloning artifact	UNP P72024
D	1	ALA	-	cloning artifact	UNP P72024
E	1	ALA	-	cloning artifact	UNP P72024
F	1	ALA	-	cloning artifact	UNP P72024
G	1	ALA	-	cloning artifact	UNP P72024
H	1	ALA	-	cloning artifact	UNP P72024

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

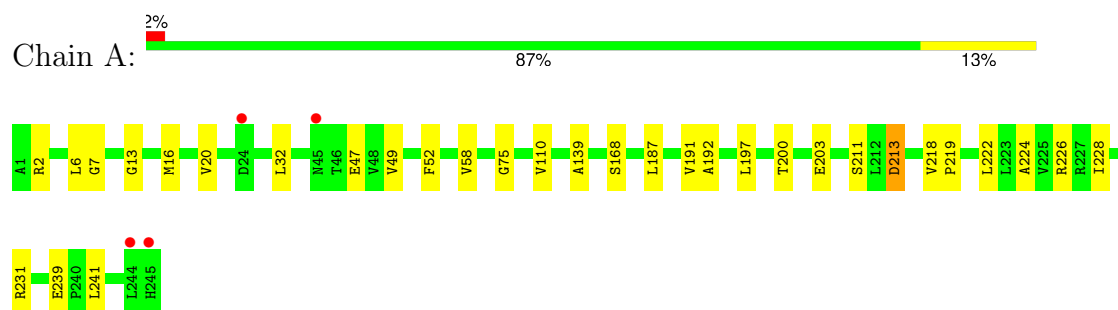
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O	0	0
			49	49		
4	B	61	Total	O	0	0
			61	61		
4	C	27	Total	O	0	0
			27	27		
4	D	84	Total	O	0	0
			84	84		
4	E	32	Total	O	0	0
			32	32		
4	F	20	Total	O	0	0
			20	20		
4	G	59	Total	O	0	0
			59	59		
4	H	24	Total	O	0	0
			24	24		

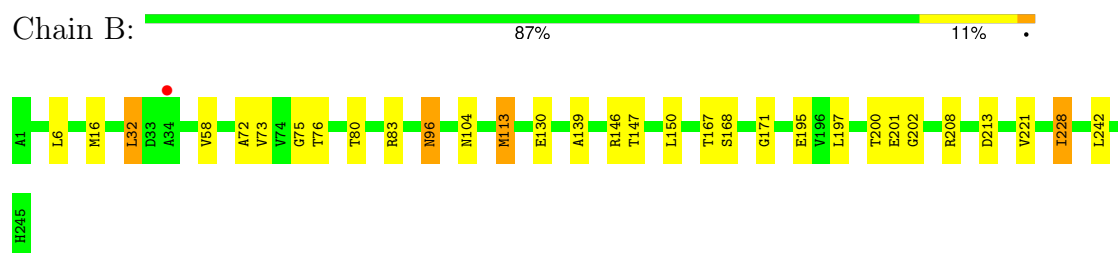
3 Residue-property plots [i](#)

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

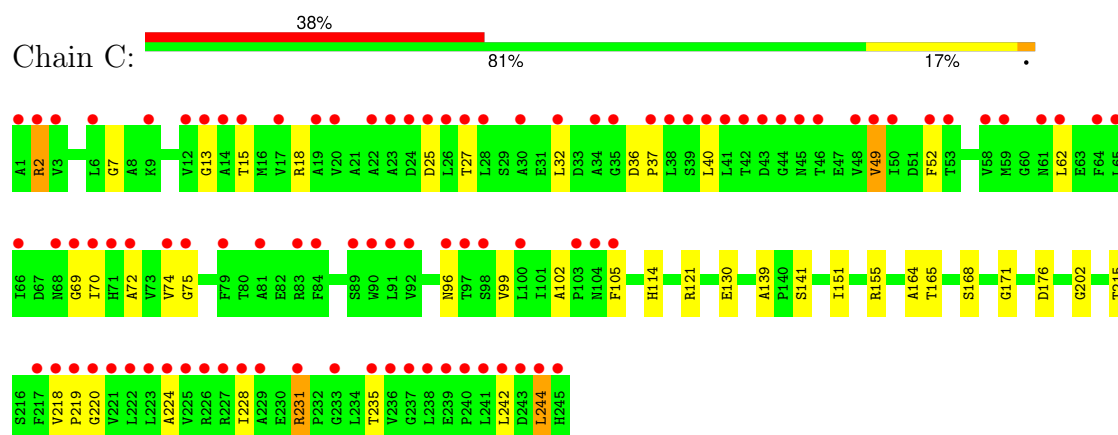
- Molecule 1: Dihydrodipicolinate reductase



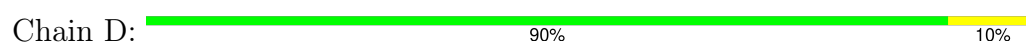
- Molecule 1: Dihydrodipicolinate reductase



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- Molecule 1: Dihydrodipicolinate reductase

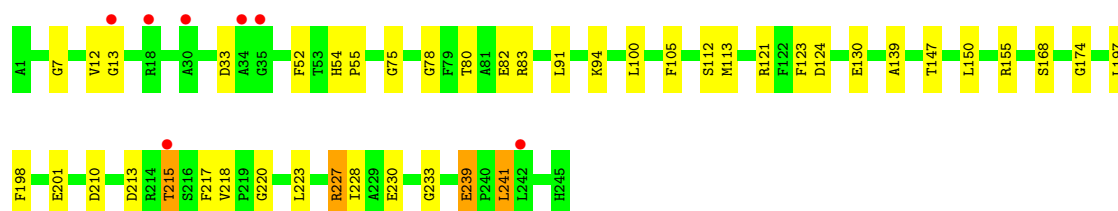
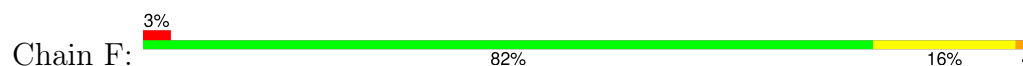




- Molecule 1: Dihydrodipicolinate reductase



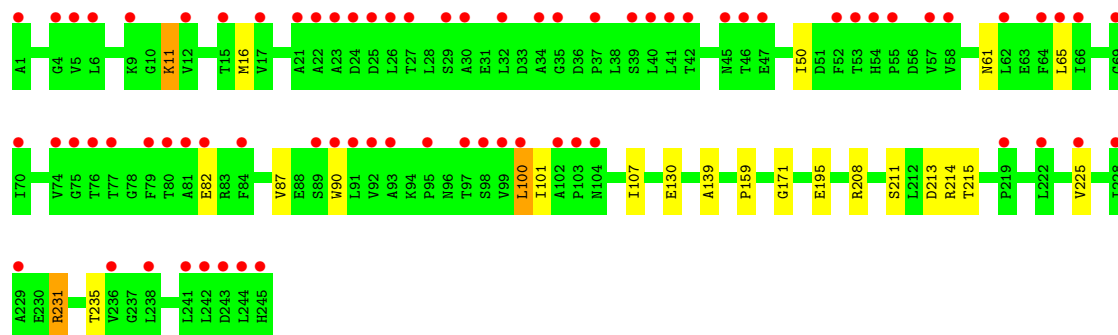
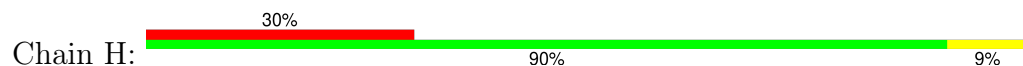
- Molecule 1: Dihydrodipicolinate reductase



- Molecule 1: Dihydrodipicolinate reductase



- Molecule 1: Dihydrodipicolinate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	238.60Å 67.52Å 154.49Å 90.00° 117.08° 90.00°	Depositor
Resolution (Å)	30.00 – 2.34 30.00 – 2.34	Depositor EDS
% Data completeness (in resolution range)	86.6 (30.00-2.34) 86.5 (30.00-2.34)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.181 , 0.238 0.179 , 0.234	Depositor DCC
R_{free} test set	2428 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15209	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% 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: NAI, MG

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	0.69	0/1840	0.89	3/2509 (0.1%)
1	B	0.71	0/1863	0.95	3/2541 (0.1%)
1	C	0.76	1/1848 (0.1%)	0.92	4/2519 (0.2%)
1	D	0.78	0/1848	0.89	0/2519
1	E	0.69	0/1869	0.88	0/2550
1	F	0.66	1/1849 (0.1%)	0.88	1/2522 (0.0%)
1	G	0.72	0/1846	0.90	2/2519 (0.1%)
1	H	0.63	1/1840 (0.1%)	0.86	0/2509
All	All	0.71	3/14803 (0.0%)	0.90	13/20188 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2	ARG	NE-CZ	10.60	1.44	1.33
1	F	218	VAL	CA-CB	7.09	1.57	1.54
1	H	159	PRO	CA-C	5.49	1.54	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	VAL	N-CA-C	6.43	117.18	110.62
1	C	102	ALA	CA-C-N	6.39	126.01	119.56
1	C	102	ALA	C-N-CA	6.39	126.01	119.56
1	B	58	VAL	N-CA-C	6.35	117.10	110.62
1	G	203	GLU	N-CA-C	5.76	117.86	108.76
1	A	203	GLU	N-CA-C	5.75	117.85	108.76
1	A	228	ILE	N-CA-C	5.60	116.33	110.62
1	C	2	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	B	228	ILE	N-CA-C	5.38	116.75	110.62
1	C	49	VAL	N-CA-C	5.31	115.60	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	120	ALA	N-CA-C	5.20	117.62	111.33
1	B	242	LEU	N-CA-C	-5.07	106.68	112.92
1	F	228	ILE	N-CA-C	5.03	116.36	110.62

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	1806	0	1822	16	0
1	B	1820	0	1848	21	0
1	C	1811	0	1831	32	0
1	D	1811	0	1831	17	0
1	E	1823	0	1848	14	0
1	F	1809	0	1834	23	0
1	G	1809	0	1833	16	0
1	H	1806	0	1822	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
3	A	44	0	27	0	0
3	B	44	0	27	0	0
3	C	44	0	27	0	0
3	D	44	0	27	1	0
3	E	44	0	27	1	0
3	F	44	0	27	0	0
3	G	44	0	27	1	0
3	H	44	0	27	0	0
4	A	49	0	0	0	0
4	B	61	0	0	0	0
4	C	27	0	0	2	0
4	D	84	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	32	0	0	0	0
4	F	20	0	0	1	0
4	G	59	0	0	1	0
4	H	24	0	0	1	0
All	All	15209	0	14885	137	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 5.

All (137) 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:32:LEU:HD22	1:C:40:LEU:HD12	1.36	1.04
1:C:32:LEU:CD2	1:C:40:LEU:HD12	1.98	0.93
1:C:32:LEU:HD21	1:C:40:LEU:HB2	1.53	0.90
1:B:113[B]:MET:HE3	1:B:147:THR:HG23	1.62	0.79
1:C:231:ARG:HH11	1:C:231:ARG:HG3	1.46	0.79
1:H:16:MET:HE3	1:H:16:MET:HA	1.67	0.76
1:C:32:LEU:CD2	1:C:40:LEU:CD1	2.67	0.72
1:E:75:GLY:O	3:E:505:NAI:H2N	1.91	0.71
1:E:195:GLU:HG3	1:E:208:ARG:HD3	1.74	0.70
1:G:195:GLU:HG2	1:G:197:LEU:HD11	1.75	0.69
1:H:231:ARG:HH11	1:H:231:ARG:HG3	1.58	0.68
1:D:113[B]:MET:HE1	1:D:147:THR:HG23	1.77	0.67
1:G:195:GLU:HG2	1:G:197:LEU:CD1	2.25	0.66
1:A:2:ARG:HB2	1:A:47:GLU:HG3	1.79	0.65
1:C:32:LEU:HD22	1:C:40:LEU:CD1	2.20	0.64
1:G:216:SER:HA	4:H:522:HOH:O	1.98	0.63
1:G:222:LEU:O	1:G:226:ARG:HG3	1.98	0.62
1:C:121:ARG:HB2	4:C:527:HOH:O	1.97	0.62
1:A:139:ALA:O	1:D:168:SER:HA	2.01	0.60
1:E:110:VAL:HG13	1:E:239[A]:GLU:HG3	1.83	0.60
1:F:168:SER:HA	1:G:139:ALA:O	2.00	0.60
1:A:213:ASP:HB2	1:B:202:GLY:HA2	1.82	0.60
1:D:75:GLY:O	3:D:504:NAI:H2N	2.02	0.60
1:E:168:SER:HA	1:H:139:ALA:O	2.02	0.60
1:B:168:SER:HA	1:C:139:ALA:O	2.03	0.58
1:H:213:ASP:HB3	1:H:215:THR:H	1.69	0.58
1:B:113[B]:MET:SD	1:B:150:LEU:HD12	2.43	0.57
1:F:121:ARG:HG2	4:F:520:HOH:O	2.06	0.55
1:F:78:GLY:O	1:F:83:ARG:HD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:GLY:O	1:C:13:GLY:HA3	2.08	0.54
1:E:239[A]:GLU:H	1:E:239[A]:GLU:CD	2.16	0.54
1:G:71:HIS:HB3	1:G:228:ILE:HG12	1.89	0.54
1:D:113[B]:MET:CE	1:D:147:THR:HG23	2.38	0.53
1:B:73:VAL:HG22	1:B:228:ILE:HD12	1.91	0.53
1:E:189:GLY:O	1:G:212:LEU:HD13	2.09	0.52
1:F:124:ASP:O	1:F:155:ARG:NH2	2.42	0.52
1:F:139:ALA:O	1:G:168:SER:HA	2.09	0.52
1:B:113[B]:MET:SD	1:B:150:LEU:CD1	2.98	0.52
1:B:171:GLY:HA2	1:C:171:GLY:HA2	1.91	0.52
1:B:72:ALA:O	1:B:228:ILE:HD11	2.11	0.51
1:E:110:VAL:CG1	1:E:239[A]:GLU:HG3	2.41	0.51
1:H:61:ASN:O	1:H:65:LEU:HB2	2.11	0.51
1:B:104:ASN:HD22	1:B:146[A]:ARG:HH21	1.59	0.50
1:C:242:LEU:HB2	1:C:244:LEU:HD22	1.93	0.50
1:E:197:LEU:HD23	1:E:206:THR:HG23	1.92	0.50
1:F:239:GLU:H	1:F:239:GLU:CD	2.19	0.50
1:F:215:THR:CG2	1:F:215:THR:O	2.60	0.49
1:C:15:THR:HG23	1:C:18:ARG:HH21	1.78	0.49
1:C:32:LEU:HD21	1:C:40:LEU:CB	2.33	0.49
1:D:202:GLY:O	1:D:203:GLU:HB3	2.12	0.49
1:F:227:ARG:HB3	1:F:241:LEU:HD13	1.95	0.49
1:F:227:ARG:HG3	1:F:230:GLU:OE2	2.12	0.48
1:G:122:PHE:HB3	1:H:107:ILE:HG21	1.96	0.48
1:D:113[B]:MET:SD	1:D:147:THR:HA	2.53	0.48
1:F:7:GLY:O	1:F:13:GLY:HA3	2.13	0.48
1:D:52:PHE:CE2	1:D:75:GLY:HA3	2.50	0.47
1:G:231[A]:ARG:HD2	4:G:544:HOH:O	2.14	0.47
1:B:16:MET:HE2	1:B:221:VAL:HG11	1.96	0.47
1:C:49:VAL:HG23	1:C:70:ILE:HG21	1.95	0.47
1:G:52:PHE:CE2	1:G:75:GLY:HA3	2.50	0.47
1:C:164:ALA:O	1:C:165:THR:C	2.58	0.47
1:B:104:ASN:HD22	1:B:146[A]:ARG:NH2	2.13	0.46
1:F:80:THR:OG1	1:F:83:ARG:HG3	2.15	0.46
1:B:80:THR:H	1:B:83:ARG:HB2	1.80	0.46
1:F:52:PHE:CE1	1:F:75:GLY:HA3	2.49	0.46
1:H:11:LYS:HB3	1:H:214:ARG:HE	1.79	0.46
1:C:105:PHE:O	1:C:220:GLY:HA3	2.16	0.46
1:C:215:THR:HA	1:C:218:VAL:HG23	1.98	0.46
1:G:124:ASP:O	1:G:155:ARG:NH2	2.49	0.46
1:H:16:MET:HA	1:H:16:MET:CE	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:HIS:CD2	1:C:244:LEU:HG	2.51	0.46
1:G:6:LEU:HD12	1:G:49:VAL:HG11	1.98	0.46
1:H:195:GLU:HG2	1:H:208:ARG:HD2	1.96	0.46
1:A:7:GLY:O	1:A:13:GLY:HA3	2.16	0.46
1:A:231:ARG:HH21	1:A:241:LEU:HD23	1.80	0.46
1:H:50:ILE:HD11	1:H:225:VAL:HG21	1.98	0.45
1:C:72:ALA:HB3	1:C:99:VAL:HG22	1.98	0.45
1:F:241:LEU:N	1:F:241:LEU:HD23	2.31	0.45
1:C:176:ASP:OD2	1:C:176:ASP:C	2.60	0.45
1:A:52:PHE:CE2	1:A:75:GLY:HA3	2.52	0.45
1:E:133:HIS:HB3	1:E:190:LEU:O	2.17	0.45
1:F:12:VAL:HG13	1:F:217:PHE:CE1	2.52	0.45
1:D:12:VAL:O	1:D:15:THR:HB	2.17	0.45
1:E:74:VAL:HB	1:E:101:ILE:HG12	1.99	0.45
1:F:113[B]:MET:HE1	1:F:147:THR:HA	1.99	0.45
1:B:139:ALA:O	1:C:168:SER:HA	2.16	0.44
1:C:224:ALA:O	1:C:228:ILE:HB	2.17	0.44
1:F:123:PHE:CG	1:F:198:PHE:HB3	2.52	0.44
1:C:231:ARG:HG3	1:C:231:ARG:NH1	2.23	0.44
1:B:6:LEU:HD23	1:B:32:LEU:HB2	1.99	0.44
1:C:62:LEU:HD21	1:C:74:VAL:HG21	2.00	0.44
1:F:91:LEU:HD13	1:F:233:GLY:HA2	1.99	0.44
1:A:224:ALA:HA	1:A:241:LEU:CD1	2.48	0.44
1:F:174:GLY:HA2	1:G:171:GLY:O	2.18	0.43
1:C:202:GLY:HA2	1:D:213:ASP:HB3	2.00	0.43
1:C:218:VAL:HB	1:C:219:PRO:HD3	2.00	0.43
1:H:87:VAL:HA	1:H:90:TRP:CE3	2.53	0.43
1:B:197:LEU:N	1:B:197:LEU:HD12	2.34	0.43
1:C:32:LEU:HD21	1:C:40:LEU:HD12	1.91	0.43
1:F:105:PHE:O	1:F:220:GLY:HA3	2.18	0.43
1:C:32:LEU:HD21	1:C:40:LEU:CD1	2.45	0.43
1:D:66:ILE:O	1:D:94:LYS:HG3	2.19	0.43
1:F:197:LEU:N	1:F:197:LEU:HD12	2.34	0.43
1:E:6:LEU:HD23	1:E:32:LEU:HB2	2.00	0.43
1:F:54:HIS:HA	1:F:55:PRO:HD2	1.85	0.43
1:D:7:GLY:O	1:D:13:GLY:HA3	2.19	0.42
1:G:75:GLY:O	3:G:507:NAI:H2N	2.19	0.42
1:B:195:GLU:HG3	1:B:208:ARG:HB2	2.02	0.42
1:E:204:THR:OG1	1:F:210:ASP:HB2	2.20	0.42
1:D:138:ASP:OD1	1:D:138:ASP:N	2.50	0.42
1:A:110:VAL:HG13	1:A:239:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:PHE:CE2	1:C:75:GLY:HA3	2.55	0.42
1:G:41:LEU:HD22	1:G:49:VAL:CG2	2.50	0.42
1:A:168:SER:HA	1:D:139:ALA:O	2.20	0.42
1:A:239:GLU:CD	1:A:239:GLU:H	2.28	0.41
1:C:141:SER:HB2	4:C:517:HOH:O	2.20	0.41
1:B:75:GLY:O	1:B:76:THR:C	2.63	0.41
1:B:200:THR:O	1:B:201:GLU:C	2.64	0.41
1:D:239:GLU:HB2	1:D:240:PRO:HD3	2.03	0.41
1:A:218:VAL:HB	1:A:219:PRO:HD3	2.01	0.41
1:B:16:MET:HE2	1:B:221:VAL:CG1	2.51	0.41
1:B:96:ASN:ND2	1:B:96:ASN:H	2.15	0.41
1:E:171:GLY:HA2	1:H:171:GLY:HA2	2.03	0.41
1:F:113[B]:MET:SD	1:F:150:LEU:HD12	2.61	0.41
1:H:100:LEU:HD12	1:H:101:ILE:N	2.35	0.41
1:D:71:HIS:HB3	1:D:228:ILE:HG12	2.03	0.41
1:A:16:MET:O	1:A:20:VAL:HG23	2.21	0.41
1:A:197:LEU:HD12	1:A:197:LEU:N	2.35	0.41
1:C:36:ASP:HA	1:C:37:PRO:HD3	1.97	0.41
1:E:176:ASP:OD2	1:E:176:ASP:C	2.64	0.41
1:D:200:THR:O	1:D:201:GLU:C	2.64	0.40
1:C:151:ILE:HG22	1:C:155:ARG:HD3	2.04	0.40
1:A:6:LEU:HD12	1:A:49:VAL:HG11	2.04	0.40
1:A:192:ALA:HB3	1:A:211:SER:HB3	2.03	0.40
1:D:130:GLU:C	1:D:131:LEU:HD12	2.47	0.40
1:A:222:LEU:O	1:A:226:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	243/245 (99%)	233 (96%)	9 (4%)	1 (0%)	30 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	246/245 (100%)	235 (96%)	11 (4%)	0	100	100
1	C	244/245 (100%)	230 (94%)	13 (5%)	1 (0%)	30	32
1	D	244/245 (100%)	238 (98%)	6 (2%)	0	100	100
1	E	247/245 (101%)	241 (98%)	6 (2%)	0	100	100
1	F	245/245 (100%)	234 (96%)	11 (4%)	0	100	100
1	G	244/245 (100%)	235 (96%)	9 (4%)	0	100	100
1	H	243/245 (99%)	237 (98%)	6 (2%)	0	100	100
All	All	1956/1960 (100%)	1883 (96%)	71 (4%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	69	GLY
1	A	191	VAL

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	188/189 (100%)	184 (98%)	4 (2%)	47	60
1	B	191/189 (101%)	184 (96%)	7 (4%)	30	39
1	C	189/189 (100%)	181 (96%)	8 (4%)	26	34
1	D	189/189 (100%)	188 (100%)	1 (0%)	81	88
1	E	192/189 (102%)	187 (97%)	5 (3%)	40	53
1	F	190/189 (100%)	177 (93%)	13 (7%)	14	16
1	G	189/189 (100%)	186 (98%)	3 (2%)	55	67
1	H	188/189 (100%)	181 (96%)	7 (4%)	30	39
All	All	1516/1512 (100%)	1468 (97%)	48 (3%)	35	44

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	187	LEU
1	A	200	THR
1	A	213	ASP
1	B	32	LEU
1	B	96	ASN
1	B	113[A]	MET
1	B	113[B]	MET
1	B	130	GLU
1	B	167	THR
1	B	213	ASP
1	C	2	ARG
1	C	25	ASP
1	C	27	THR
1	C	96	ASN
1	C	130	GLU
1	C	231	ARG
1	C	235	THR
1	C	244	LEU
1	D	187	LEU
1	E	32	LEU
1	E	112	SER
1	E	187	LEU
1	E	200	THR
1	E	231	ARG
1	F	33	ASP
1	F	82	GLU
1	F	94	LYS
1	F	100	LEU
1	F	112	SER
1	F	130	GLU
1	F	201	GLU
1	F	213	ASP
1	F	215	THR
1	F	223	LEU
1	F	227	ARG
1	F	239	GLU
1	F	241	LEU
1	G	24	ASP
1	G	187	LEU
1	G	212	LEU
1	H	11	LYS
1	H	82	GLU

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Mol	Chain	Res	Type
1	H	100	LEU
1	H	130	GLU
1	H	211	SER
1	H	231	ARG
1	H	235	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	114	HIS
1	B	104	ASN
1	B	114	HIS
1	C	86	GLN
1	C	114	HIS
1	C	118	GLN
1	C	135	HIS
1	D	96	ASN
1	D	114	HIS
1	E	45	ASN
1	E	86	GLN
1	E	114	HIS
1	E	118	GLN
1	F	61	ASN
1	F	68	ASN
1	F	118	GLN
1	G	114	HIS
1	H	114	HIS
1	H	194	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAI	E	505	-	47,48,48	1.78	10 (21%)	64,73,73	1.67	11 (17%)
3	NAI	D	504	-	47,48,48	1.68	8 (17%)	64,73,73	1.65	12 (18%)
3	NAI	A	501	-	47,48,48	1.67	7 (14%)	64,73,73	1.71	11 (17%)
3	NAI	H	508	-	47,48,48	1.82	10 (21%)	64,73,73	1.65	9 (14%)
3	NAI	B	502	-	47,48,48	1.75	8 (17%)	64,73,73	1.65	11 (17%)
3	NAI	G	507	-	47,48,48	1.92	12 (25%)	64,73,73	1.67	12 (18%)
3	NAI	C	503	-	47,48,48	1.82	11 (23%)	64,73,73	1.70	12 (18%)
3	NAI	F	506	-	47,48,48	1.88	10 (21%)	64,73,73	1.58	9 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAI	E	505	-	-	6/29/72/72	0/5/5/5
3	NAI	D	504	-	-	6/29/72/72	0/5/5/5
3	NAI	A	501	-	-	9/29/72/72	0/5/5/5
3	NAI	H	508	-	-	7/29/72/72	0/5/5/5
3	NAI	B	502	-	-	8/29/72/72	0/5/5/5
3	NAI	G	507	-	-	5/29/72/72	0/5/5/5
3	NAI	C	503	-	-	9/29/72/72	0/5/5/5
3	NAI	F	506	-	-	8/29/72/72	0/5/5/5

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	506	NAI	O7N-C7N	7.24	1.41	1.24
3	H	508	NAI	O7N-C7N	7.12	1.41	1.24
3	G	507	NAI	O7N-C7N	6.95	1.40	1.24
3	E	505	NAI	O7N-C7N	6.52	1.39	1.24
3	B	502	NAI	O7N-C7N	6.29	1.39	1.24
3	C	503	NAI	O7N-C7N	6.24	1.39	1.24
3	A	501	NAI	O7N-C7N	6.19	1.38	1.24
3	D	504	NAI	O7N-C7N	6.04	1.38	1.24
3	C	503	NAI	C4N-C3N	-5.31	1.40	1.50
3	F	506	NAI	C4N-C3N	-5.22	1.40	1.50
3	H	508	NAI	C4N-C3N	-5.17	1.40	1.50
3	B	502	NAI	C4N-C3N	-5.09	1.40	1.50
3	D	504	NAI	C4N-C3N	-4.77	1.41	1.50
3	G	507	NAI	C4N-C3N	-4.74	1.41	1.50
3	E	505	NAI	C4N-C3N	-4.69	1.41	1.50
3	A	501	NAI	C4N-C3N	-4.04	1.42	1.50
3	B	502	NAI	C4N-C5N	-3.69	1.39	1.49
3	F	506	NAI	C4N-C5N	-3.60	1.39	1.49
3	C	503	NAI	C4N-C5N	-3.44	1.40	1.49
3	H	508	NAI	C4N-C5N	-3.39	1.40	1.49
3	A	501	NAI	C4N-C5N	-3.38	1.40	1.49
3	G	507	NAI	C4N-C5N	-3.36	1.40	1.49
3	D	504	NAI	PA-O3	3.31	1.63	1.59
3	E	505	NAI	C4N-C5N	-3.28	1.40	1.49
3	B	502	NAI	C2A-N3A	3.27	1.39	1.33
3	G	507	NAI	C2A-N1A	3.25	1.39	1.33
3	G	507	NAI	PA-O3	3.20	1.63	1.59
3	A	501	NAI	C1D-N1N	3.12	1.54	1.46
3	D	504	NAI	C4N-C5N	-3.10	1.41	1.49
3	B	502	NAI	C2A-N1A	3.07	1.39	1.33
3	A	501	NAI	C2A-N3A	3.02	1.39	1.33
3	F	506	NAI	C2A-N3A	2.99	1.39	1.33
3	E	505	NAI	C7N-C3N	-2.94	1.42	1.48
3	C	503	NAI	PA-O3	2.94	1.62	1.59
3	F	506	NAI	C2A-N1A	2.93	1.39	1.33
3	E	505	NAI	PA-O3	2.93	1.62	1.59
3	E	505	NAI	C2A-N3A	2.92	1.39	1.33
3	A	501	NAI	C6N-C5N	2.87	1.41	1.33
3	H	508	NAI	C2A-N3A	2.77	1.38	1.33
3	G	507	NAI	C6N-C5N	2.76	1.41	1.33
3	G	507	NAI	C2A-N3A	2.74	1.38	1.33
3	H	508	NAI	C2A-N1A	2.73	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	504	NAI	C8A-N7A	2.73	1.36	1.31
3	C	503	NAI	C2A-N1A	2.71	1.38	1.33
3	F	506	NAI	PN-O3	2.69	1.62	1.59
3	A	501	NAI	C2A-N1A	2.69	1.38	1.33
3	E	505	NAI	C2A-N1A	2.65	1.38	1.33
3	C	503	NAI	C2A-N3A	2.64	1.38	1.33
3	C	503	NAI	PN-O3	2.55	1.62	1.59
3	G	507	NAI	C7N-C3N	-2.53	1.43	1.48
3	F	506	NAI	PA-O3	2.51	1.62	1.59
3	G	507	NAI	C7N-N7N	-2.45	1.26	1.33
3	E	505	NAI	C6N-C5N	2.45	1.40	1.33
3	F	506	NAI	C6A-N6A	-2.44	1.28	1.34
3	B	502	NAI	C6N-C5N	2.44	1.40	1.33
3	H	508	NAI	PN-O3	2.43	1.62	1.59
3	B	502	NAI	C7N-C3N	-2.43	1.43	1.48
3	D	504	NAI	C2A-N3A	2.39	1.38	1.33
3	G	507	NAI	C5A-N7A	-2.39	1.34	1.39
3	C	503	NAI	C6A-N6A	2.37	1.40	1.34
3	H	508	NAI	C6A-N6A	-2.33	1.28	1.34
3	H	508	NAI	PA-O3	2.31	1.62	1.59
3	G	507	NAI	PN-O3	2.31	1.62	1.59
3	D	504	NAI	C2A-N1A	2.30	1.38	1.33
3	F	506	NAI	C6N-C5N	2.28	1.40	1.33
3	B	502	NAI	C8A-N7A	2.27	1.36	1.31
3	C	503	NAI	C6N-C5N	2.26	1.40	1.33
3	H	508	NAI	C6N-C5N	2.20	1.39	1.33
3	C	503	NAI	C8A-N7A	2.17	1.35	1.31
3	H	508	NAI	C8A-N7A	2.15	1.35	1.31
3	E	505	NAI	C8A-N7A	2.14	1.35	1.31
3	E	505	NAI	C7N-N7N	-2.10	1.27	1.33
3	D	504	NAI	C6N-C5N	2.09	1.39	1.33
3	C	503	NAI	C1D-N1N	2.03	1.51	1.46
3	F	506	NAI	C8A-N7A	2.02	1.35	1.31
3	G	507	NAI	O4B-C4B	-2.01	1.40	1.45

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	NAI	N3A-C2A-N1A	-5.92	119.63	128.58
3	D	504	NAI	N3A-C2A-N1A	-5.80	119.80	128.58
3	A	501	NAI	N3A-C2A-N1A	-5.67	120.00	128.58
3	H	508	NAI	N3A-C2A-N1A	-5.67	120.00	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	507	NAI	N3A-C2A-N1A	-5.57	120.15	128.58
3	F	506	NAI	N3A-C2A-N1A	-5.57	120.16	128.58
3	B	502	NAI	N3A-C2A-N1A	-5.44	120.35	128.58
3	E	505	NAI	N3A-C2A-N1A	-5.34	120.50	128.58
3	F	506	NAI	C5A-C4A-N3A	-4.94	119.91	126.72
3	E	505	NAI	C5A-C4A-N3A	-4.77	120.16	126.72
3	D	504	NAI	C5A-C4A-N3A	-4.74	120.19	126.72
3	H	508	NAI	C5A-C4A-N3A	-4.64	120.33	126.72
3	C	503	NAI	C5A-C4A-N3A	-4.58	120.41	126.72
3	G	507	NAI	N9A-C8A-N7A	-4.49	107.56	113.94
3	A	501	NAI	N9A-C8A-N7A	-4.49	107.57	113.94
3	A	501	NAI	C5A-C4A-N3A	-4.45	120.59	126.72
3	E	505	NAI	N9A-C8A-N7A	-4.43	107.65	113.94
3	B	502	NAI	N9A-C8A-N7A	-4.35	107.77	113.94
3	E	505	NAI	C5A-N7A-C8A	4.18	110.03	103.45
3	B	502	NAI	C5A-C4A-N3A	-4.04	121.16	126.72
3	A	501	NAI	C5A-N7A-C8A	3.96	109.67	103.45
3	H	508	NAI	O4B-C1B-N9A	3.95	115.68	108.09
3	C	503	NAI	N9A-C8A-N7A	-3.92	108.38	113.94
3	H	508	NAI	N9A-C8A-N7A	-3.87	108.44	113.94
3	B	502	NAI	C5A-N7A-C8A	3.86	109.51	103.45
3	D	504	NAI	C2A-N3A-C4A	3.81	121.14	111.83
3	G	507	NAI	C5A-N7A-C8A	3.77	109.38	103.45
3	A	501	NAI	C1D-N1N-C2N	-3.71	115.03	121.14
3	D	504	NAI	N9A-C8A-N7A	-3.70	108.69	113.94
3	G	507	NAI	C1D-N1N-C2N	-3.65	115.12	121.14
3	H	508	NAI	C5A-N7A-C8A	3.65	109.19	103.45
3	G	507	NAI	C5A-C4A-N3A	-3.63	121.72	126.72
3	F	506	NAI	C2A-N3A-C4A	3.57	120.55	111.83
3	C	503	NAI	C5A-N7A-C8A	3.54	109.02	103.45
3	C	503	NAI	C2A-N3A-C4A	3.53	120.45	111.83
3	E	505	NAI	C2A-N3A-C4A	3.50	120.37	111.83
3	A	501	NAI	C2A-N3A-C4A	3.48	120.34	111.83
3	H	508	NAI	C2A-N3A-C4A	3.46	120.29	111.83
3	C	503	NAI	N6A-C6A-N1A	-3.40	110.80	118.38
3	D	504	NAI	C5A-N7A-C8A	3.34	108.70	103.45
3	B	502	NAI	C2A-N3A-C4A	3.33	119.96	111.83
3	F	506	NAI	N9A-C8A-N7A	-3.31	109.24	113.94
3	F	506	NAI	C5A-N7A-C8A	3.30	108.64	103.45
3	F	506	NAI	O4B-C1B-N9A	3.23	114.30	108.09
3	F	506	NAI	N3A-C4A-N9A	3.20	132.61	127.17
3	D	504	NAI	C1D-N1N-C2N	-3.15	115.95	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	NAI	N3A-C4A-N9A	3.13	132.50	127.17
3	E	505	NAI	N3A-C4A-N9A	3.12	132.47	127.17
3	B	502	NAI	C4A-C5A-N7A	-3.08	107.06	110.58
3	G	507	NAI	C2A-N3A-C4A	3.04	119.27	111.83
3	E	505	NAI	C4A-C5A-N7A	-3.02	107.13	110.58
3	H	508	NAI	N3A-C4A-N9A	2.93	132.15	127.17
3	A	501	NAI	N3A-C4A-N9A	2.91	132.12	127.17
3	A	501	NAI	C4A-C5A-N7A	-2.86	107.31	110.58
3	A	501	NAI	O4B-C1B-N9A	2.86	113.58	108.09
3	D	504	NAI	N3A-C4A-N9A	2.86	132.02	127.17
3	E	505	NAI	C1D-N1N-C2N	-2.85	116.44	121.14
3	G	507	NAI	C4A-N9A-C8A	2.84	108.72	105.74
3	C	503	NAI	O7N-C7N-N7N	-2.78	116.66	122.89
3	H	508	NAI	C4A-C5A-N7A	-2.76	107.43	110.58
3	B	502	NAI	C1D-N1N-C2N	-2.70	116.69	121.14
3	G	507	NAI	N3A-C4A-N9A	2.68	131.72	127.17
3	G	507	NAI	O4B-C1B-N9A	2.66	113.20	108.09
3	C	503	NAI	C5A-C6A-N6A	2.64	129.81	123.29
3	C	503	NAI	O4B-C1B-N9A	2.59	113.06	108.09
3	D	504	NAI	C3N-C2N-N1N	-2.57	119.44	123.20
3	A	501	NAI	O1N-PN-O2N	2.53	124.21	112.44
3	D	504	NAI	C6N-N1N-C2N	2.50	121.99	119.32
3	E	505	NAI	C2D-C1D-N1N	2.48	119.39	113.31
3	F	506	NAI	C4A-C5A-N7A	-2.47	107.76	110.58
3	B	502	NAI	C3N-C2N-N1N	-2.45	119.60	123.20
3	G	507	NAI	C4A-C5A-N7A	-2.45	107.78	110.58
3	D	504	NAI	C4A-C5A-N7A	-2.42	107.81	110.58
3	C	503	NAI	C4A-C5A-N7A	-2.40	107.84	110.58
3	B	502	NAI	O7N-C7N-C3N	-2.40	116.38	120.90
3	A	501	NAI	C4A-N9A-C8A	2.31	108.17	105.74
3	B	502	NAI	N3A-C4A-N9A	2.28	131.05	127.17
3	C	503	NAI	C1D-N1N-C2N	-2.22	117.48	121.14
3	D	504	NAI	O1N-PN-O2N	2.08	122.13	112.44
3	H	508	NAI	C6A-C5A-C4A	2.07	120.00	117.18
3	F	506	NAI	C6A-C5A-C4A	2.06	120.00	117.18
3	G	507	NAI	C2D-C1D-N1N	2.06	118.37	113.31
3	D	504	NAI	O4B-C1B-N9A	2.05	112.02	108.09
3	E	505	NAI	O4B-C1B-N9A	2.04	112.00	108.09
3	B	502	NAI	C4A-N9A-C8A	2.03	107.87	105.74
3	G	507	NAI	O1N-PN-O2N	2.02	121.85	112.44
3	E	505	NAI	C6A-C5A-C4A	2.00	119.91	117.18

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NAI	C5D-O5D-PN-O2N
3	C	503	NAI	C5D-O5D-PN-O3
3	C	503	NAI	C5D-O5D-PN-O1N
3	C	503	NAI	C5D-O5D-PN-O2N
3	H	508	NAI	C5D-O5D-PN-O2N
3	F	506	NAI	O4B-C4B-C5B-O5B
3	F	506	NAI	C3B-C4B-C5B-O5B
3	E	505	NAI	O4B-C4B-C5B-O5B
3	C	503	NAI	C2D-C1D-N1N-C2N
3	H	508	NAI	C2D-C1D-N1N-C2N
3	B	502	NAI	C2B-C1B-N9A-C8A
3	F	506	NAI	C2B-C1B-N9A-C8A
3	A	501	NAI	C2D-C1D-N1N-C2N
3	B	502	NAI	C2D-C1D-N1N-C2N
3	C	503	NAI	O4B-C4B-C5B-O5B
3	A	501	NAI	C5D-O5D-PN-O3
3	F	506	NAI	C5D-O5D-PN-O2N
3	D	504	NAI	C2D-C1D-N1N-C2N
3	A	501	NAI	O4D-C1D-N1N-C2N
3	B	502	NAI	O4D-C1D-N1N-C2N
3	H	508	NAI	O4D-C1D-N1N-C2N
3	C	503	NAI	O4D-C1D-N1N-C2N
3	E	505	NAI	C3B-C4B-C5B-O5B
3	A	501	NAI	C2B-C1B-N9A-C8A
3	D	504	NAI	C2B-C1B-N9A-C8A
3	D	504	NAI	O4D-C1D-N1N-C2N
3	F	506	NAI	O4D-C1D-N1N-C2N
3	G	507	NAI	O4D-C1D-N1N-C2N
3	C	503	NAI	C2D-C1D-N1N-C6N
3	A	501	NAI	C2N-C3N-C7N-N7N
3	B	502	NAI	O4B-C4B-C5B-O5B
3	B	502	NAI	O4D-C1D-N1N-C6N
3	B	502	NAI	C2N-C3N-C7N-N7N
3	D	504	NAI	O4D-C1D-N1N-C6N
3	D	504	NAI	C2N-C3N-C7N-N7N
3	E	505	NAI	O4D-C1D-N1N-C2N
3	E	505	NAI	C2N-C3N-C7N-N7N
3	G	507	NAI	C2N-C3N-C7N-N7N
3	H	508	NAI	C2N-C3N-C7N-N7N
3	F	506	NAI	C2D-C1D-N1N-C2N
3	G	507	NAI	C2D-C1D-N1N-C2N
3	A	501	NAI	O4D-C1D-N1N-C6N

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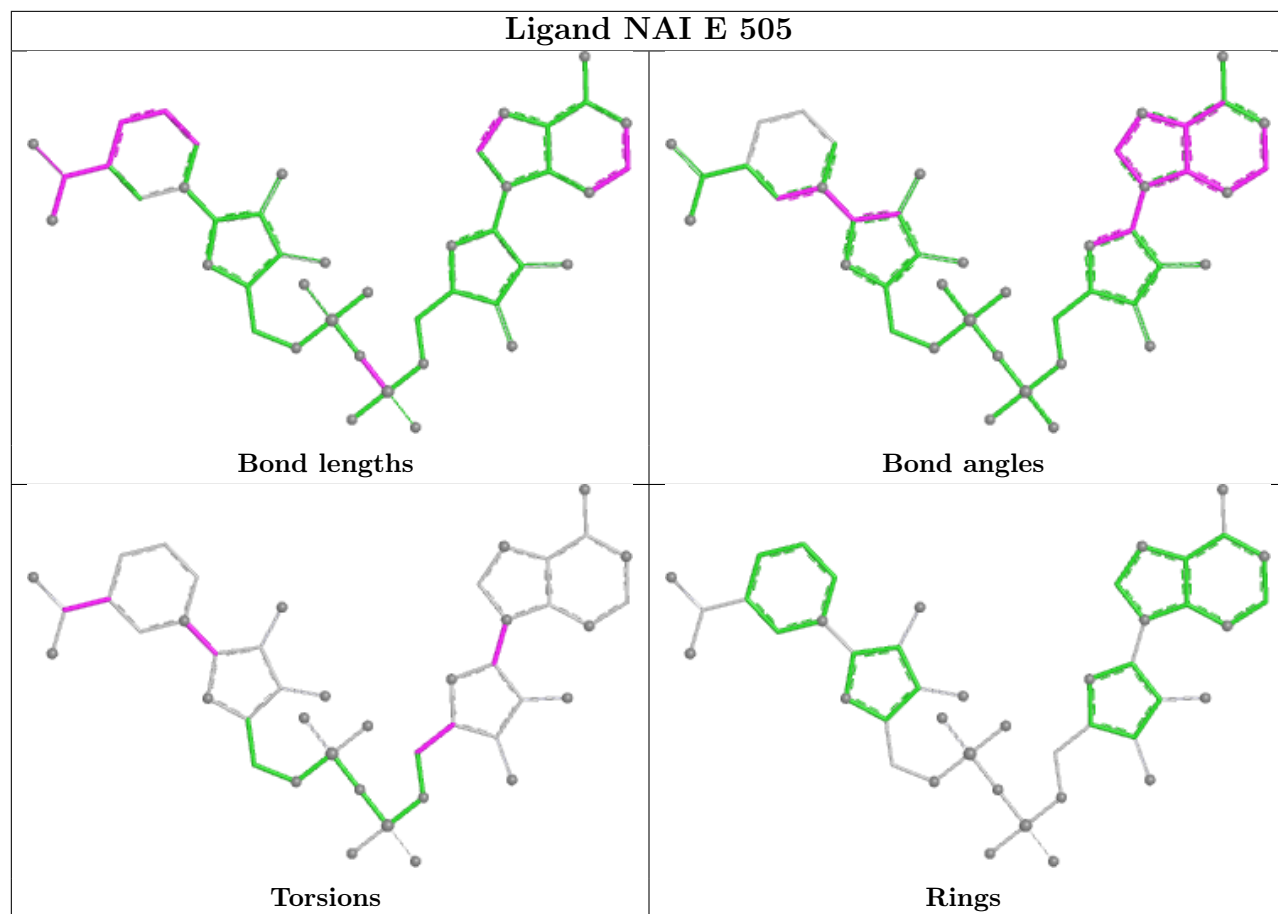
Mol	Chain	Res	Type	Atoms
3	C	503	NAI	O4D-C1D-N1N-C6N
3	H	508	NAI	O4D-C1D-N1N-C6N
3	B	502	NAI	C2D-C1D-N1N-C6N
3	D	504	NAI	C2D-C1D-N1N-C6N
3	H	508	NAI	C2D-C1D-N1N-C6N
3	B	502	NAI	O4B-C1B-N9A-C8A
3	F	506	NAI	O4B-C1B-N9A-C8A
3	E	505	NAI	C2D-C1D-N1N-C2N
3	C	503	NAI	C3B-C4B-C5B-O5B
3	E	505	NAI	C2B-C1B-N9A-C8A
3	G	507	NAI	C2B-C1B-N9A-C8A
3	A	501	NAI	O4B-C1B-N9A-C8A
3	F	506	NAI	O4D-C1D-N1N-C6N
3	A	501	NAI	C2D-C1D-N1N-C6N
3	H	508	NAI	O4B-C4B-C5B-O5B
3	G	507	NAI	O4D-C1D-N1N-C6N

There are no ring outliers.

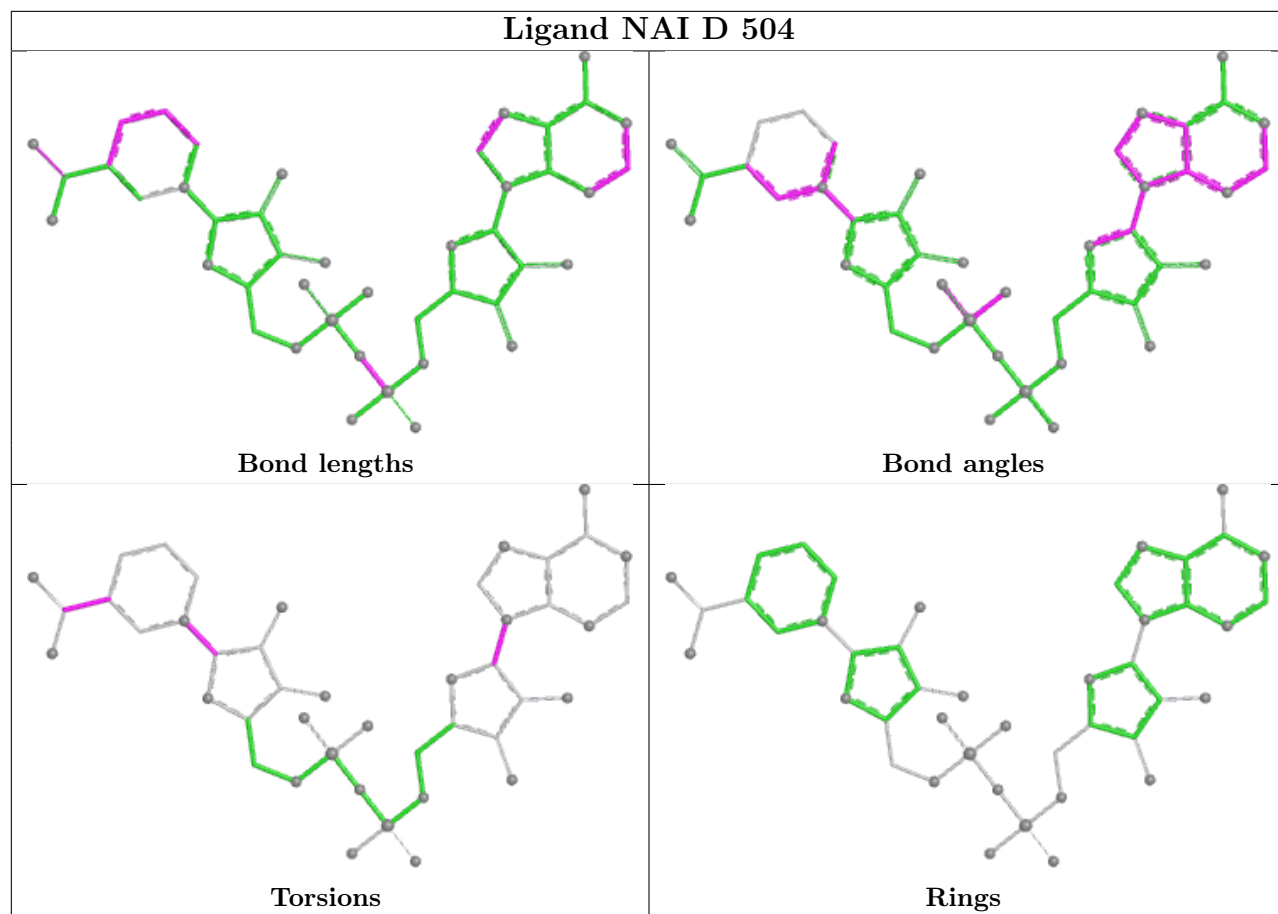
3 monomers are involved in 3 short contacts:

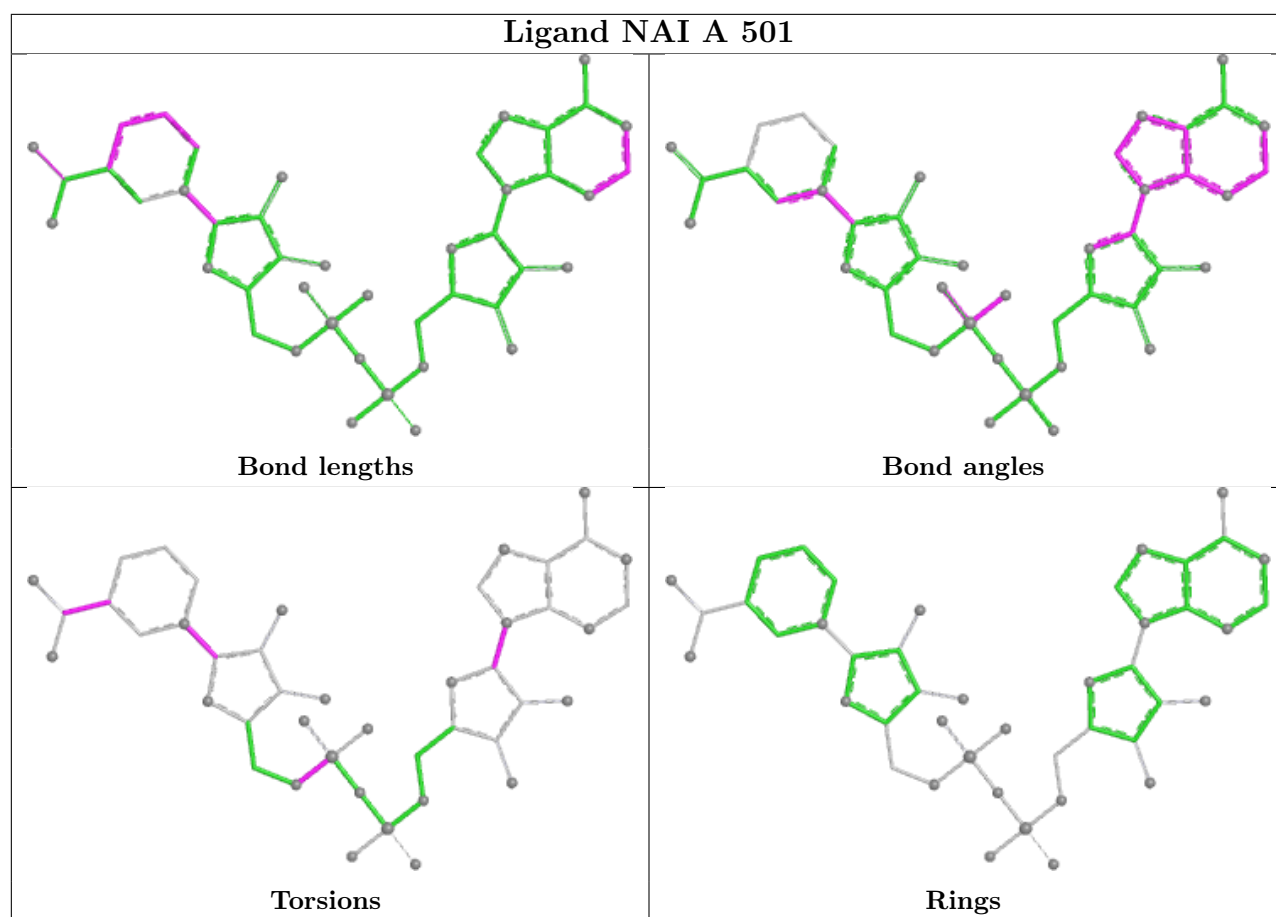
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	505	NAI	1	0
3	D	504	NAI	1	0
3	G	507	NAI	1	0

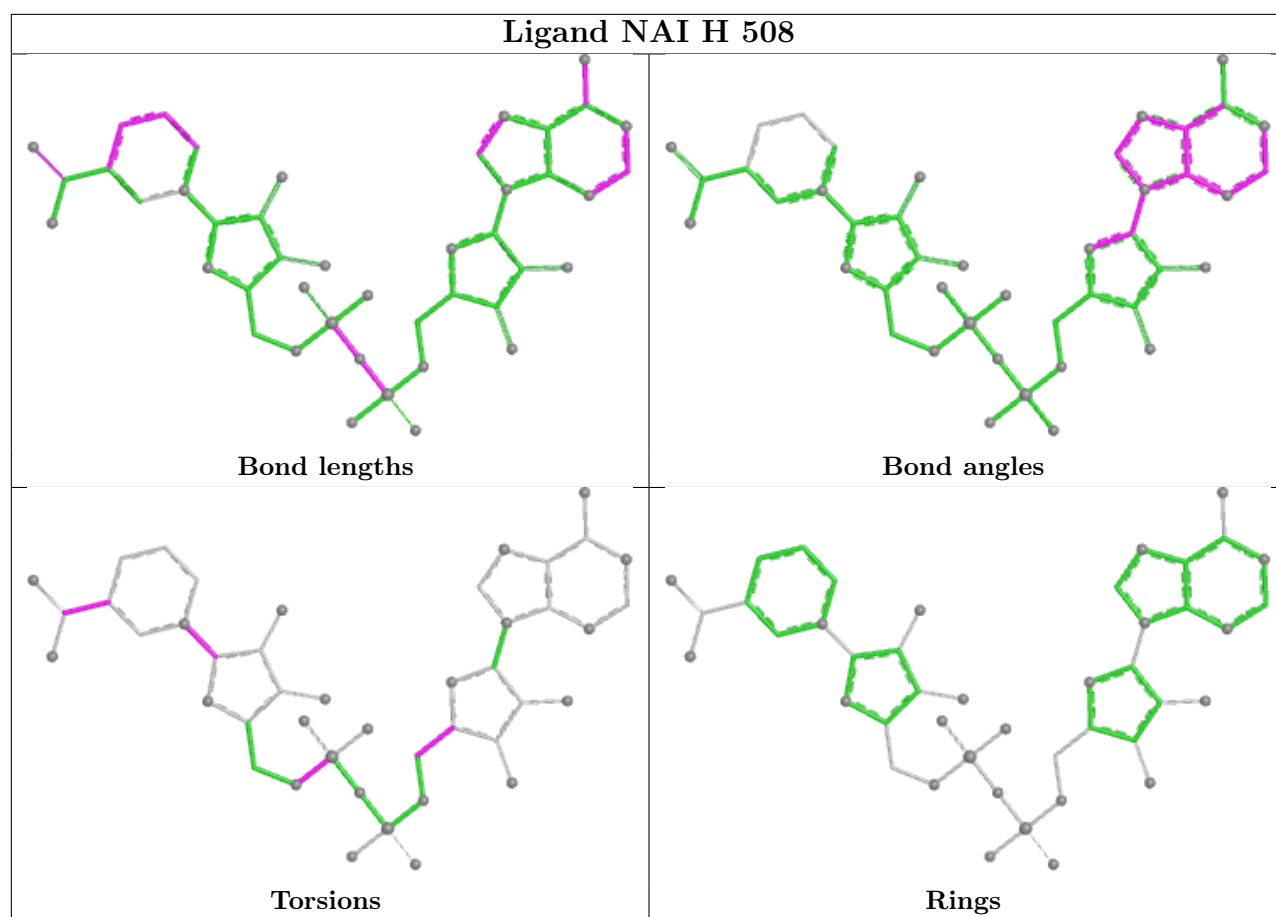
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

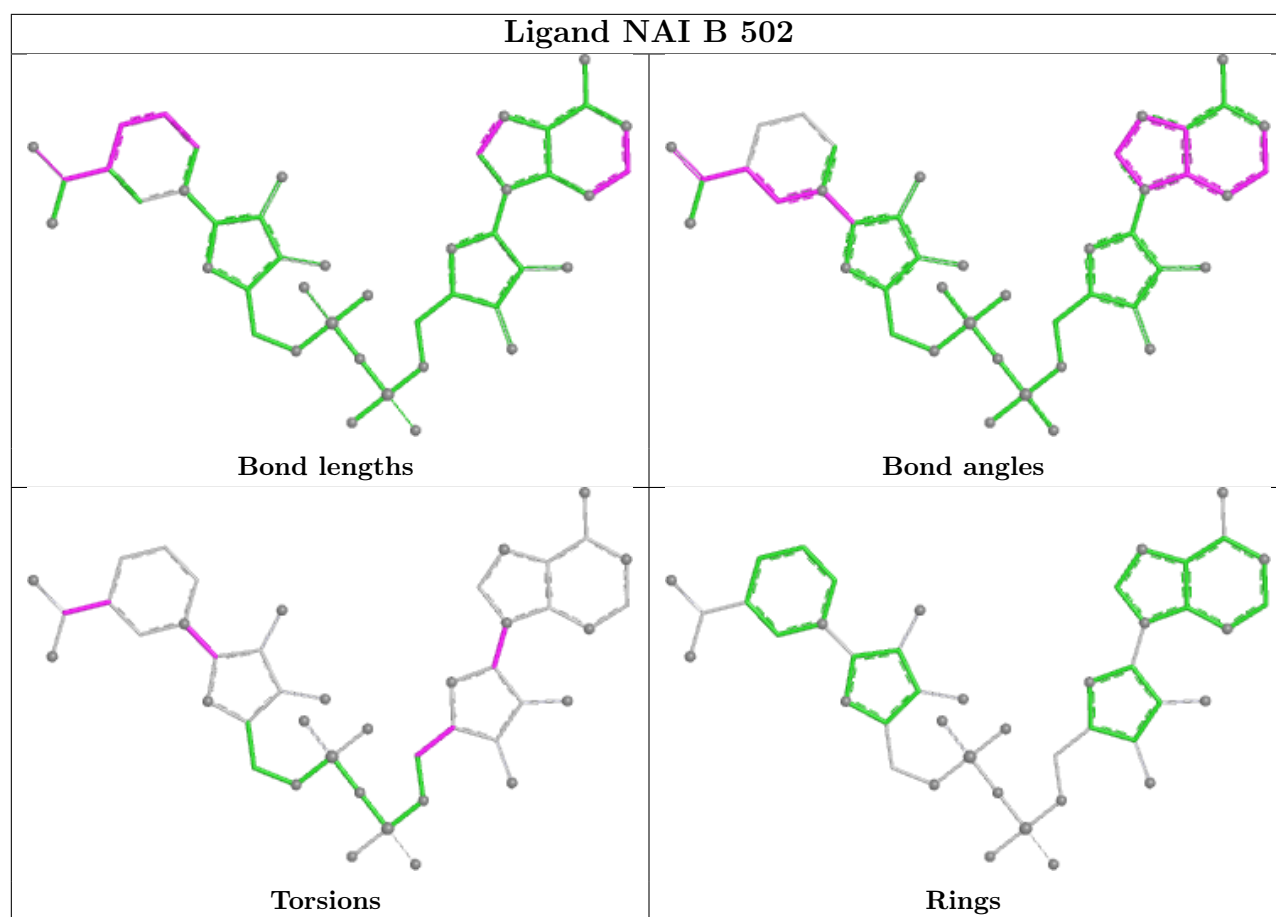


Ligand NAI D 504

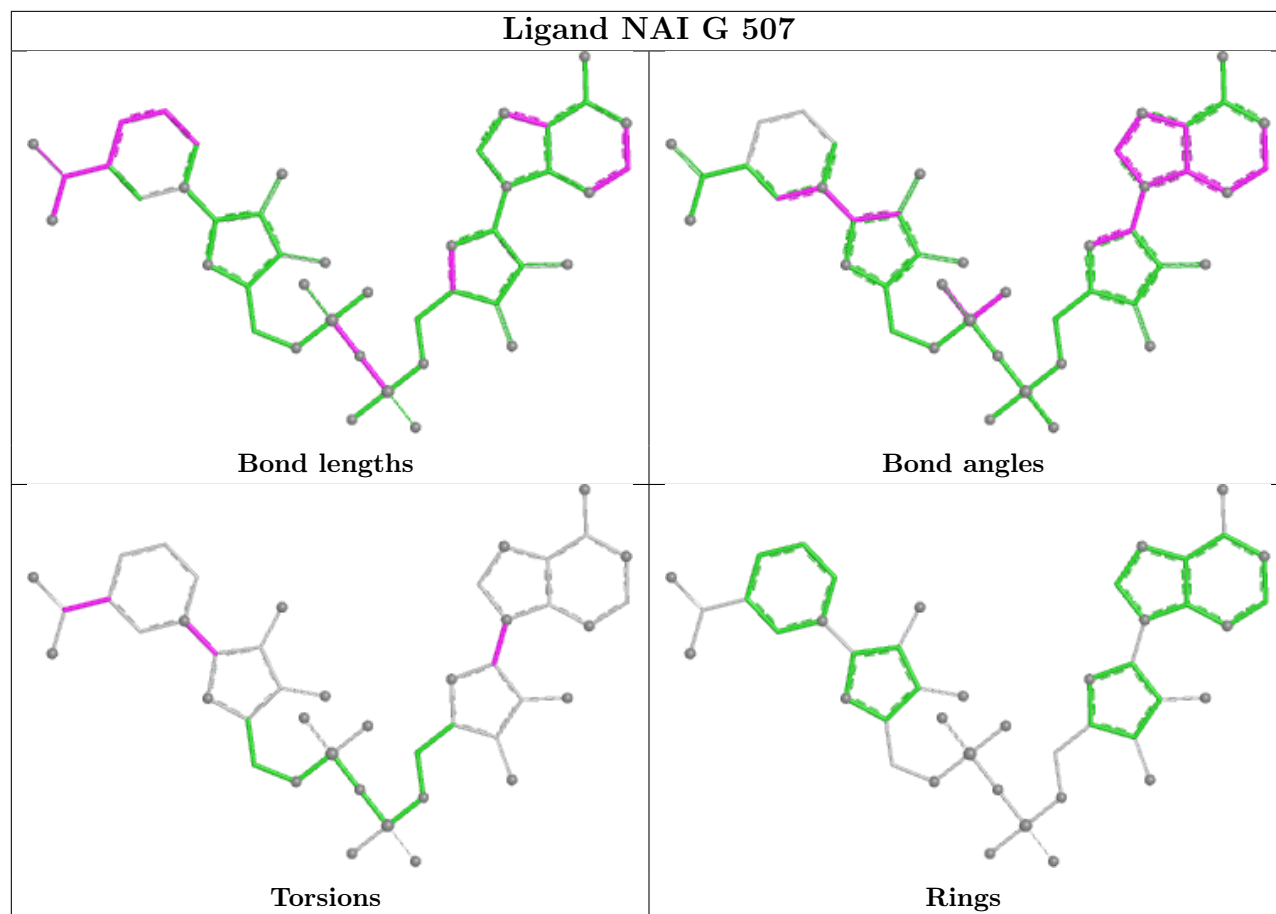




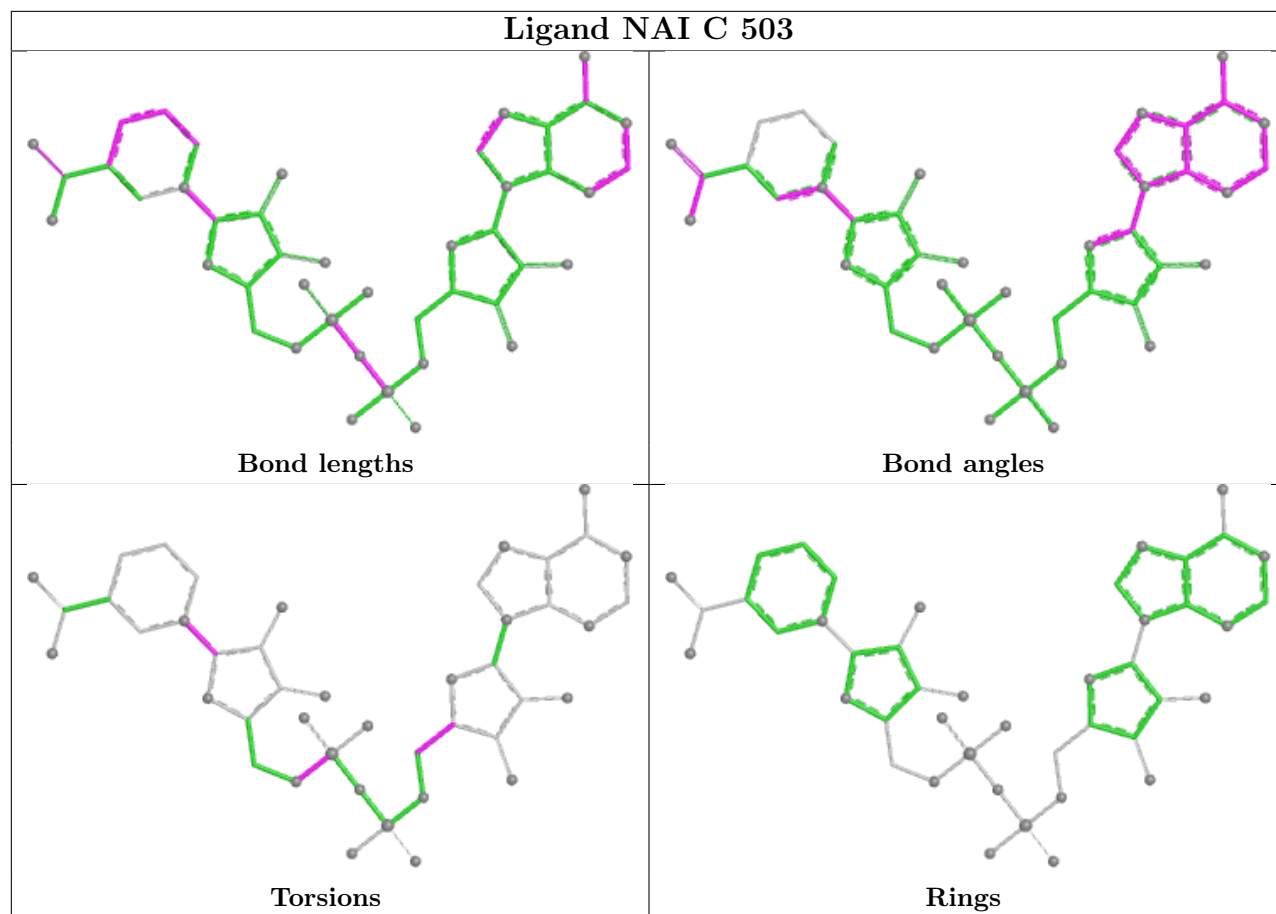


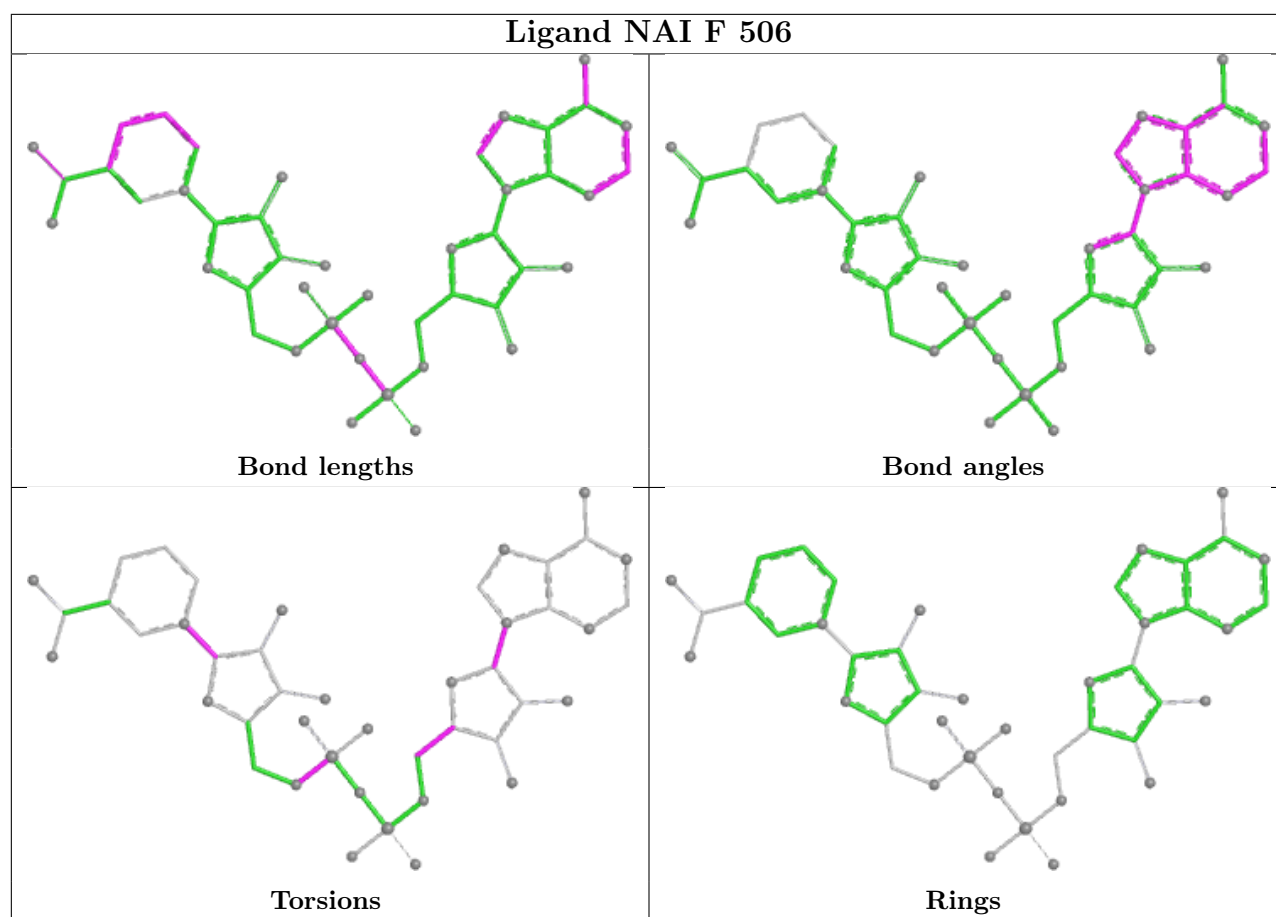


Ligand NAI G 507



Ligand NAI C 503





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	245/245 (100%)	-0.06	4 (1%) 70 75	21, 39, 47, 60	0
1	B	245/245 (100%)	-0.05	1 (0%) 88 90	19, 39, 54, 66	3 (1%)
1	C	245/245 (100%)	1.31	93 (37%) 1 0	20, 54, 75, 84	1 (0%)
1	D	245/245 (100%)	-0.46	1 (0%) 88 90	19, 29, 38, 57	1 (0%)
1	E	245/245 (100%)	-0.22	0 100 100	23, 38, 48, 56	4 (1%)
1	F	245/245 (100%)	0.34	7 (2%) 53 60	23, 46, 59, 66	2 (0%)
1	G	245/245 (100%)	-0.31	1 (0%) 88 90	25, 34, 41, 51	1 (0%)
1	H	245/245 (100%)	1.16	74 (30%) 1 1	32, 64, 84, 91	0
All	All	1960/1960 (100%)	0.21	181 (9%) 14 18	19, 37, 70, 91	12 (0%)

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	LEU	6.1
1	C	219	PRO	5.7
1	C	90	TRP	5.4
1	C	44	GLY	5.3
1	H	64	PHE	5.3
1	C	242	LEU	5.1
1	C	238	LEU	5.0
1	C	228	ILE	4.8
1	H	80	THR	4.6
1	C	1	ALA	4.6
1	C	240	PRO	4.6
1	C	66	ILE	4.3
1	H	24	ASP	4.3
1	H	93	ALA	4.2
1	C	32	LEU	4.2
1	C	24	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	52	PHE	4.1
1	C	81	ALA	4.0
1	H	90	TRP	3.9
1	C	220	GLY	3.9
1	C	245	HIS	3.8
1	C	58	VAL	3.8
1	C	221	VAL	3.8
1	D	245	HIS	3.8
1	C	229	ALA	3.8
1	H	26	LEU	3.7
1	C	225	VAL	3.7
1	C	45	ASN	3.7
1	C	2	ARG	3.7
1	C	34	ALA	3.7
1	C	22	ALA	3.7
1	C	105	PHE	3.6
1	C	41	LEU	3.6
1	C	25	ASP	3.6
1	C	26	LEU	3.6
1	H	245	HIS	3.6
1	H	27	THR	3.5
1	C	53	THR	3.5
1	C	97	THR	3.5
1	C	30	ALA	3.5
1	C	104	ASN	3.4
1	C	222	LEU	3.4
1	C	226	ARG	3.4
1	C	241	LEU	3.4
1	C	243	ASP	3.4
1	H	55	PRO	3.4
1	H	46	THR	3.4
1	C	23	ALA	3.4
1	H	219	PRO	3.3
1	A	245	HIS	3.3
1	H	58	VAL	3.3
1	C	69	GLY	3.3
1	C	75	GLY	3.3
1	H	41	LEU	3.2
1	C	48	VAL	3.2
1	H	21	ALA	3.2
1	H	30	ALA	3.2
1	H	75	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	98	SER	3.1
1	H	103	PRO	3.1
1	C	64	PHE	3.1
1	C	96	ASN	3.1
1	H	5	VAL	3.1
1	H	39	SER	3.1
1	C	20	VAL	3.1
1	C	218	VAL	3.1
1	C	3	VAL	3.1
1	H	242	LEU	3.0
1	C	50	ILE	3.0
1	H	79	PHE	3.0
1	H	34	ALA	3.0
1	H	77	THR	3.0
1	C	61	ASN	3.0
1	C	237	GLY	3.0
1	H	22	ALA	2.9
1	C	91	LEU	2.9
1	G	245	HIS	2.9
1	H	81	ALA	2.9
1	H	244	LEU	2.9
1	C	92	VAL	2.9
1	C	46	THR	2.9
1	C	239	GLU	2.9
1	C	37	PRO	2.9
1	C	223	LEU	2.9
1	H	229	ALA	2.9
1	B	34	ALA	2.8
1	C	217	PHE	2.8
1	H	92	VAL	2.8
1	C	27	THR	2.8
1	H	99	VAL	2.8
1	H	53	THR	2.8
1	H	69	GLY	2.7
1	H	98	SER	2.7
1	C	89	SER	2.7
1	C	40	LEU	2.7
1	H	104	ASN	2.7
1	H	89	SER	2.7
1	H	238	LEU	2.7
1	C	42	THR	2.6
1	H	95	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	25	ASP	2.6
1	C	227	ARG	2.6
1	H	84	PHE	2.6
1	H	54	HIS	2.6
1	H	6	LEU	2.6
1	H	62	LEU	2.6
1	C	84	PHE	2.6
1	C	12	VAL	2.6
1	C	70	ILE	2.6
1	H	76	THR	2.5
1	C	236	VAL	2.5
1	H	225	VAL	2.5
1	C	100	LEU	2.5
1	C	68	ASN	2.5
1	H	1	ALA	2.5
1	H	91	LEU	2.5
1	C	52	PHE	2.5
1	H	32	LEU	2.5
1	H	228	ILE	2.4
1	C	231	ARG	2.4
1	H	4	GLY	2.4
1	C	38	LEU	2.4
1	C	13	GLY	2.4
1	F	215	THR	2.4
1	C	17	VAL	2.4
1	H	65	LEU	2.4
1	H	9	LYS	2.4
1	H	15	THR	2.4
1	H	12	VAL	2.4
1	C	71	HIS	2.4
1	C	19	ALA	2.3
1	C	224	ALA	2.3
1	H	23	ALA	2.3
1	H	70	ILE	2.3
1	H	236	VAL	2.3
1	H	100	LEU	2.3
1	A	45	ASN	2.3
1	F	34	ALA	2.3
1	H	17	VAL	2.3
1	H	74	VAL	2.3
1	A	24	ASP	2.3
1	C	103	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	42	THR	2.3
1	H	97	THR	2.3
1	C	49	VAL	2.3
1	C	74	VAL	2.3
1	C	6	LEU	2.3
1	H	243	ASP	2.3
1	C	59	MET	2.3
1	C	79	PHE	2.2
1	C	233	GLY	2.2
1	H	29	SER	2.2
1	F	35	GLY	2.2
1	C	15	THR	2.2
1	H	45	ASN	2.2
1	C	65	LEU	2.2
1	C	35	GLY	2.2
1	H	35	GLY	2.2
1	C	14	ALA	2.2
1	C	235	THR	2.2
1	F	18	ARG	2.1
1	H	222	LEU	2.1
1	H	241	LEU	2.1
1	H	82	GLU	2.1
1	H	57	VAL	2.1
1	C	72	ALA	2.1
1	C	28	LEU	2.1
1	H	40	LEU	2.1
1	C	83	ARG	2.1
1	C	39	SER	2.1
1	C	9	LYS	2.1
1	H	47	GLU	2.1
1	F	242	LEU	2.1
1	F	13	GLY	2.1
1	F	30	ALA	2.0
1	C	43	ASP	2.0
1	C	62	LEU	2.0
1	H	37	PRO	2.0
1	H	102	ALA	2.0
1	A	244	LEU	2.0
1	H	66	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

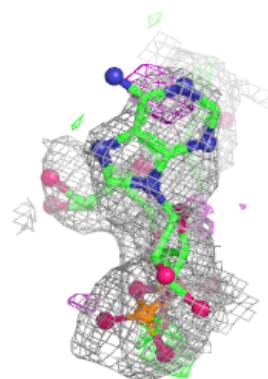
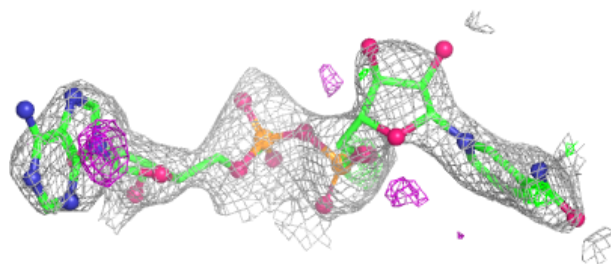
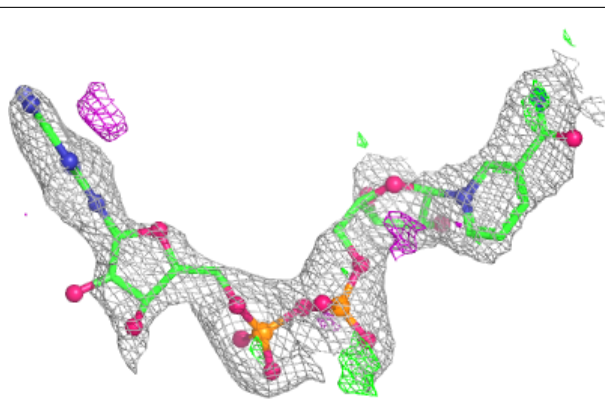
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAI	H	508	44/44	0.73	0.16	56,64,82,83	0
3	NAI	C	503	44/44	0.76	0.16	47,63,75,76	0
2	MG	E	403	1/1	0.80	0.22	35,35,35,35	0
3	NAI	F	506	44/44	0.81	0.13	60,69,72,76	0
2	MG	G	402	1/1	0.85	0.15	42,42,42,42	0
2	MG	F	406	1/1	0.87	0.08	80,80,80,80	0
3	NAI	B	502	44/44	0.90	0.11	26,49,53,56	0
3	NAI	A	501	44/44	0.91	0.10	23,39,44,45	0
2	MG	B	404	1/1	0.93	0.15	40,40,40,40	0
3	NAI	E	505	44/44	0.95	0.07	14,37,46,48	0
3	NAI	G	507	44/44	0.96	0.06	23,34,38,40	0
2	MG	A	405	1/1	0.96	0.15	52,52,52,52	0
3	NAI	D	504	44/44	0.97	0.06	12,28,33,34	0
2	MG	D	401	1/1	0.98	0.15	26,26,26,26	0

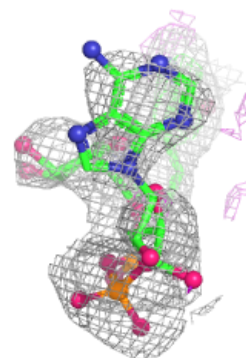
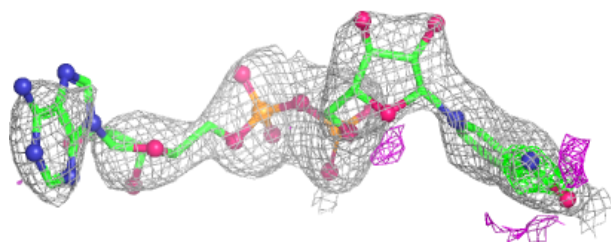
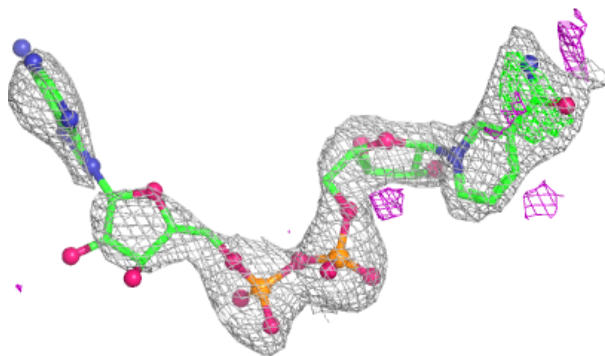
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI H 508:

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

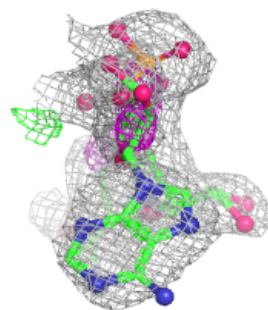
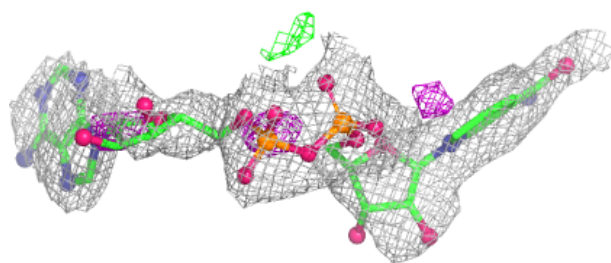
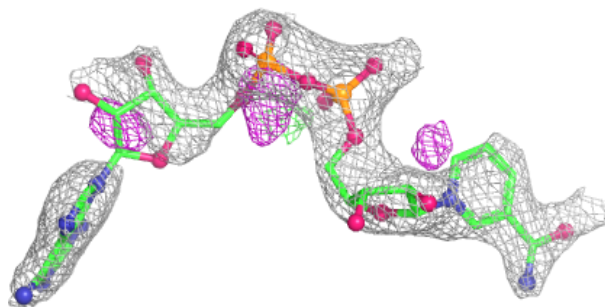
**Electron density around NAI C 503:**

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

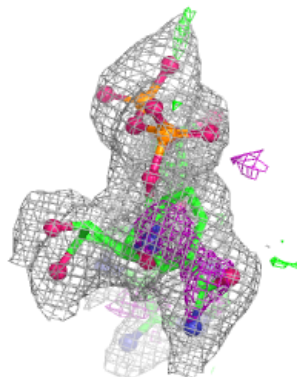
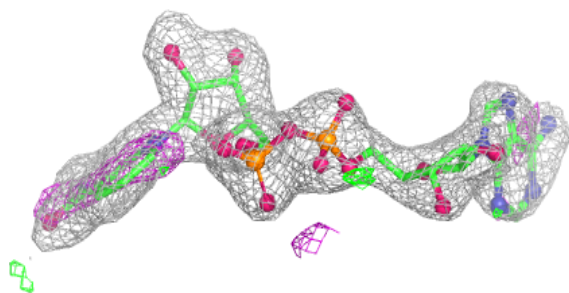
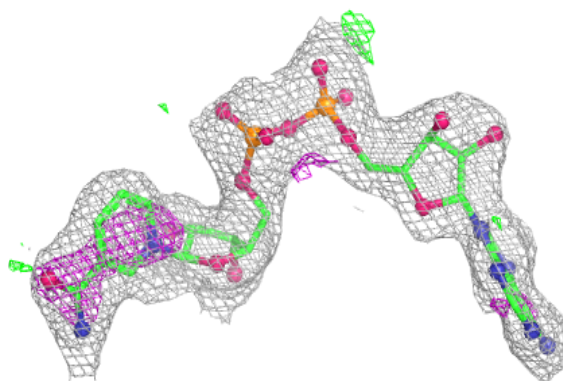


Electron density around NAI F 506:

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

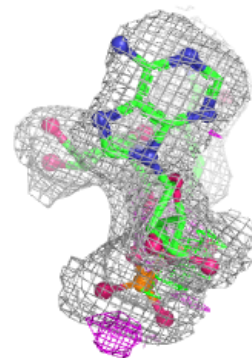
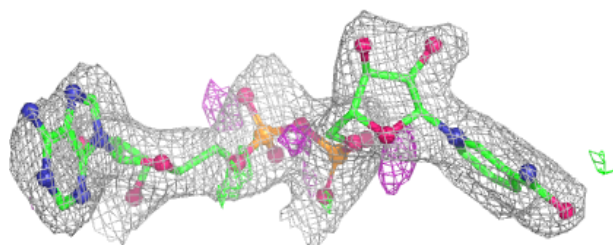
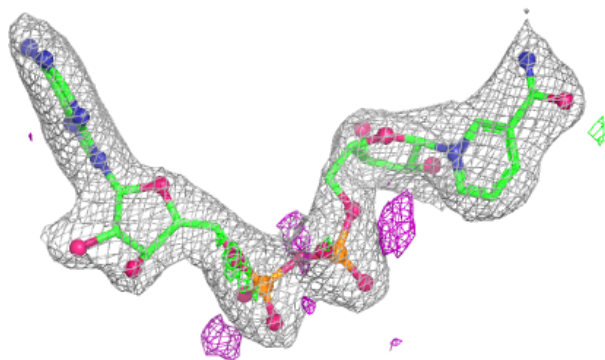
**Electron density around NAI B 502:**

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

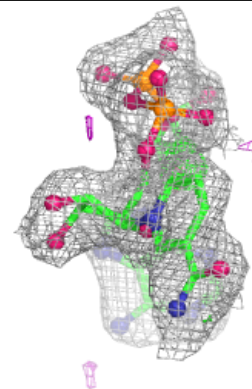
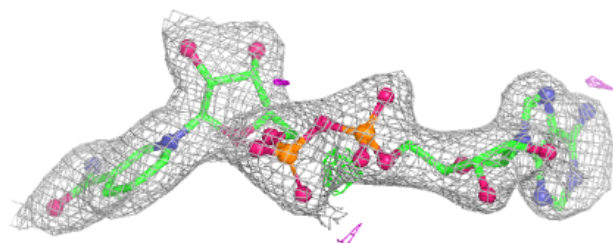
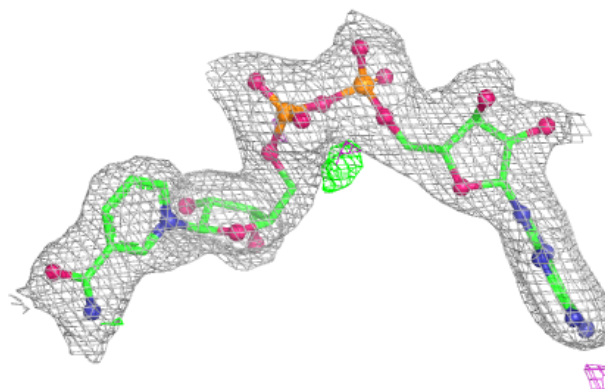


Electron density around NAI A 501:

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

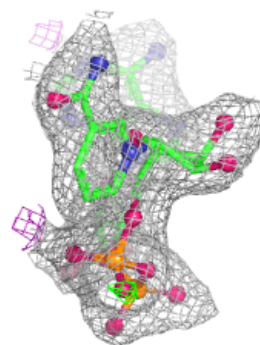
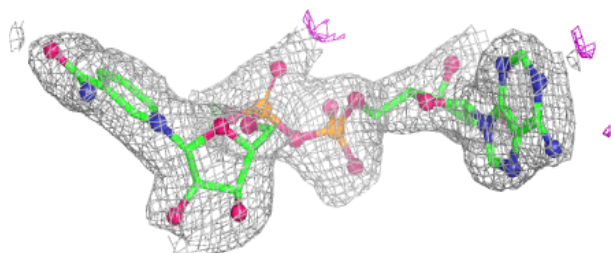
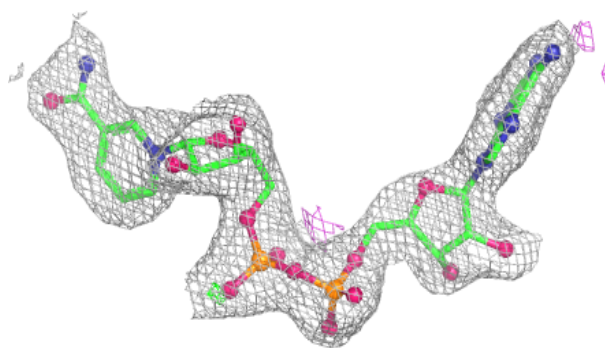
**Electron density around NAI E 505:**

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

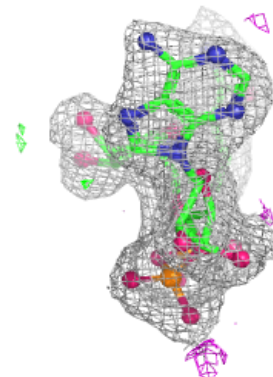
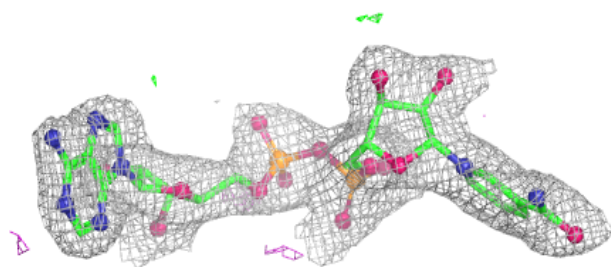
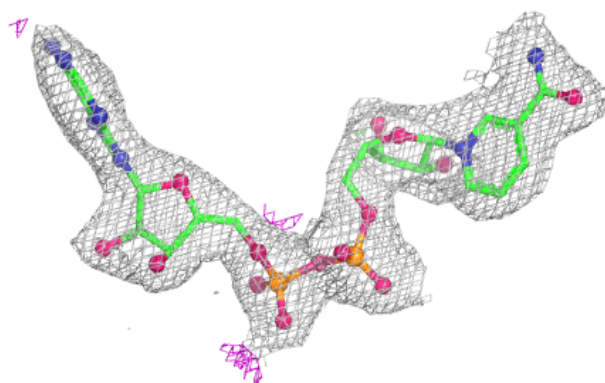


Electron density around NAI G 507:

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

**Electron density around NAI D 504:**

$2mF_o-DF_c$ (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.