Full wwPDB X-ray Structure Validation Report (i)

Jan 17, 2023 – 02:26 PM JST

PDB ID	:	7WMZ
Title	:	Crystal structure of methylenetetrahydrofolate reductase MSMEG_6649 from Mycobacterium smegmatis with NADH
Authors	:	Lin, W.; Wang, W.
Deposited on	:	2022-01-17
Resolution	:	1.92 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 1.92 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.
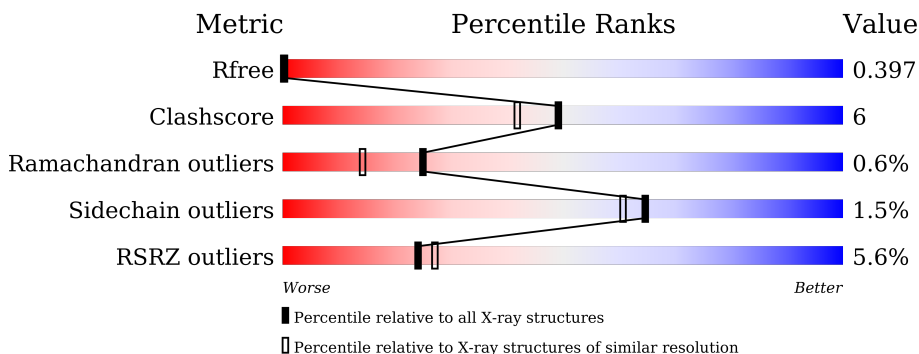
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	296	6% / 80% / 17% / ..
1	B	296	6% / 85% / 11% / ..
1	C	296	6% / 79% / 19% / ..
1	D	296	5% / 84% / 14% / .
1	E	296	4% / 90% / 8% / .
1	F	296	7% / 85% / 14% / .

2 Entity composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 14441 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 Methylenetetrahydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	290	Total	C	N	O	S	0	0	0
			2263	1446	390	416	11			
1	A	290	Total	C	N	O	S	0	0	0
			2259	1443	389	416	11			
1	B	288	Total	C	N	O	S	0	0	0
			2239	1432	382	414	11			
1	C	292	Total	C	N	O	S	0	0	0
			2260	1445	385	420	10			
1	D	290	Total	C	N	O	S	0	0	0
			2258	1443	392	412	11			
1	F	292	Total	C	N	O	S	0	0	0
			2267	1447	389	420	11			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).
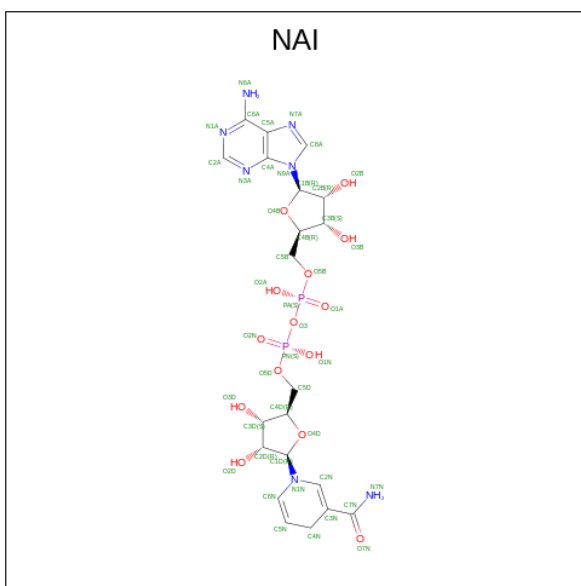
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

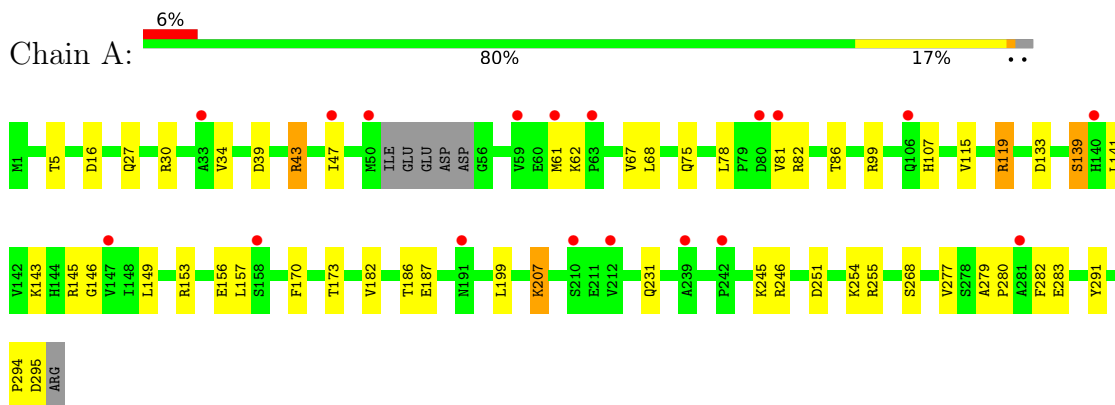| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	115	Total	O	0	0
			115	115		
3	A	98	Total	O	0	0
			98	98		
3	B	114	Total	O	0	0
			114	114		
3	C	108	Total	O	0	0
			108	108		
3	D	96	Total	O	0	0
			96	96		
3	F	100	Total	O	0	0
			100	100		

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.
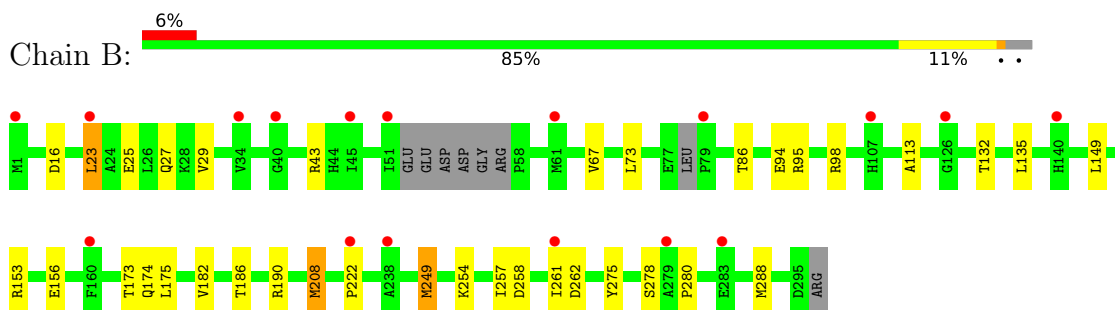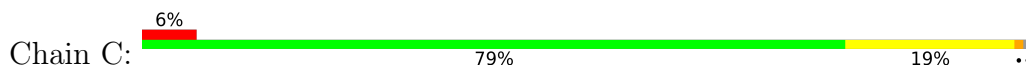
- Molecule 1: Methylenetetrahydrofolate reductase
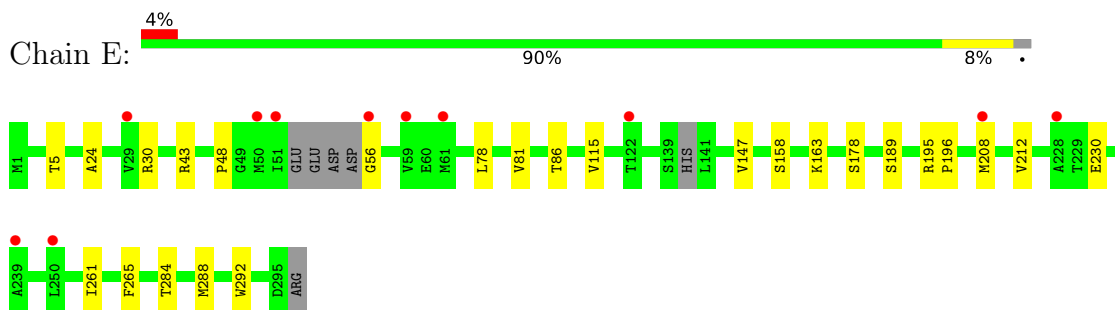
- Molecule 1: Methylenetetrahydrofolate reductase
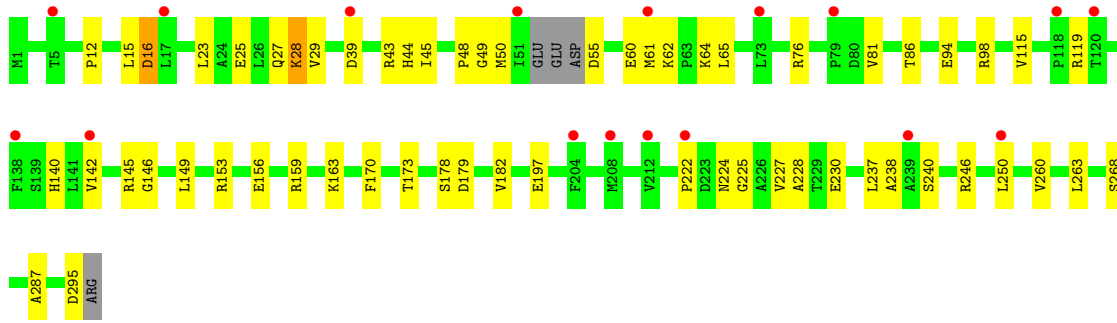

- Molecule 1: Methylenetetrahydrofolate reductase

- Molecule 1: Methylenetetrahydrofolate reductase
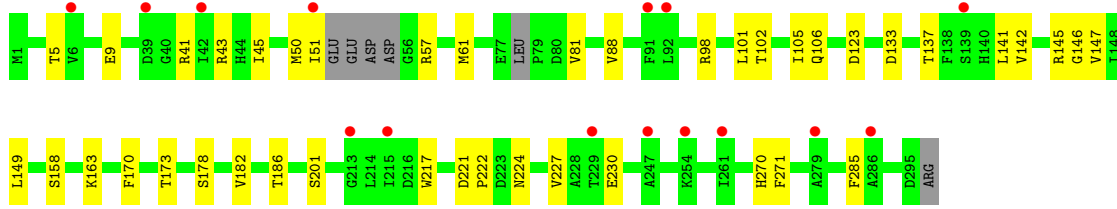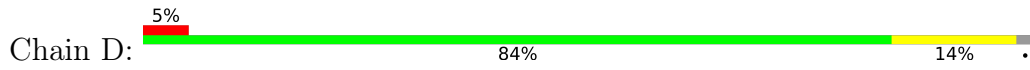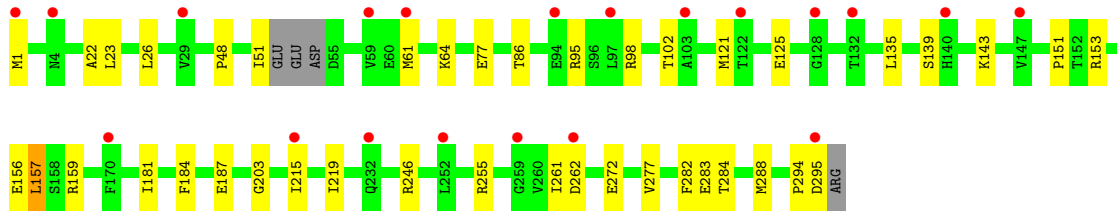
• Molecule 1: Methylenetetrahydrofolate reductase
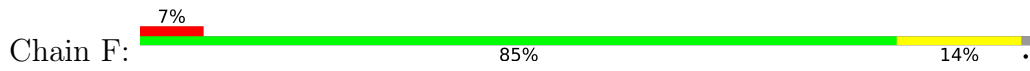
Chain D:

• Molecule 1: Methylenetetrahydrofolate reductase

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	70.93Å　　104.29Å　　318.53Å 90.00°　　94.08°　　90.00°	Depositor
Resolution (Å)	19.52 – 1.92 19.52 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.52-1.92) 98.3 (19.52-1.92)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.355　,　0.403 0.355　,　0.397	Depositor DCC
R_{free} test set	8736 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	1.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.8	EDS
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14441	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.1105e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.49	0/2307	0.55	0/3128
1	B	0.45	0/2285	0.56	0/3096
1	C	0.38	0/2308	0.53	0/3133
1	D	0.41	0/2305	0.57	0/3122
1	E	0.35	0/2309	0.51	0/3128
1	F	0.43	0/2314	0.55	0/3138
All	All	0.42	0/13828	0.54	0/18745

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2259	0	2262	35	0
1	B	2239	0	2242	27	0
1	C	2260	0	2248	34	0
1	D	2258	0	2267	26	0
1	E	2263	0	2276	15	0
1	F	2267	0	2263	25	0
2	A	44	0	27	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	27	0	0
2	C	44	0	27	0	0
2	D	44	0	27	1	0
2	E	44	0	27	0	0
2	F	44	0	27	0	0
3	A	98	0	0	5	0
3	B	114	0	0	3	0
3	C	108	0	0	4	0
3	D	96	0	0	0	0
3	E	115	0	0	3	0
3	F	100	0	0	3	0
All	All	14441	0	13720	162	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 6.

All (162) 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:B:249:MET:CE	1:B:288:MET:HE1	1.77	1.12
1:B:249:MET:HE2	1:B:288:MET:CE	1.84	1.07
1:B:249:MET:CE	1:B:288:MET:CE	2.37	1.01
1:E:147:VAL:HG21	1:E:163:LYS:HD3	1.44	0.97
1:C:45:ILE:HG12	1:C:81:VAL:HG11	1.46	0.96
1:B:249:MET:HE2	1:B:288:MET:HE1	0.98	0.96
1:D:45:ILE:HG12	1:D:81:VAL:HG11	1.61	0.83
1:F:261:ILE:HD12	1:F:262:ASP:N	1.97	0.80
1:B:23:LEU:HD11	1:B:73:LEU:HD22	1.67	0.76
1:E:178:SER:HB3	1:E:230:GLU:HG2	1.68	0.74
1:C:55:ASP:N	3:C:402:HOH:O	2.20	0.74
1:D:221:ASP:HB3	1:D:227:VAL:HG21	1.70	0.73
1:D:178:SER:HB3	1:D:230:GLU:HG2	1.72	0.72
1:A:141:LEU:HA	1:C:140:HIS:HB2	1.73	0.71
1:E:147:VAL:CG2	1:E:163:LYS:HD3	2.21	0.71
1:C:178:SER:HB3	1:C:230:GLU:HG2	1.74	0.69
1:B:249:MET:CE	1:B:288:MET:HE3	2.21	0.69
1:D:147:VAL:HG11	1:D:163:LYS:HD3	1.74	0.69
1:D:224:ASN:HB3	1:D:227:VAL:HG22	1.75	0.68
1:A:27:GLN:NE2	3:A:403:HOH:O	2.29	0.66
1:B:190:ARG:NH1	3:B:401:HOH:O	2.28	0.64
1:C:179:ASP:O	1:C:182:VAL:HG12	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:GLY:N	3:E:403:HOH:O	2.31	0.63
1:C:142:VAL:O	1:C:145:ARG:NH1	2.29	0.63
1:C:15:LEU:HD23	1:C:65:LEU:HD12	1.81	0.61
1:D:182:VAL:O	1:D:186:THR:HG23	2.01	0.61
1:E:147:VAL:HG22	3:E:446:HOH:O	2.02	0.60
1:C:246:ARG:O	1:C:250:LEU:HD12	2.00	0.60
1:A:279:ALA:O	1:A:283:GLU:HG2	2.01	0.60
1:D:102:THR:HG22	1:D:141:LEU:HD11	1.83	0.60
1:B:249:MET:HE3	1:B:288:MET:HE3	1.83	0.60
1:A:294:PRO:O	1:A:295:ASP:HB2	2.00	0.59
1:B:94:GLU:OE1	1:B:98:ARG:NH2	2.35	0.59
1:B:261:ILE:HD12	1:B:262:ASP:N	2.18	0.58
1:D:45:ILE:CG1	1:D:81:VAL:HG11	2.33	0.57
1:B:86:THR:HG22	1:B:113:ALA:HB3	1.86	0.56
1:B:182:VAL:O	1:B:186:THR:HG23	2.06	0.55
1:A:207:LYS:HD3	1:A:245:LYS:HZ1	1.72	0.55
1:C:260:VAL:HA	1:C:263:LEU:HD12	1.88	0.55
1:A:149:LEU:O	1:A:173:THR:HA	2.07	0.54
1:A:251:ASP:OD2	1:A:255:ARG:NH2	2.28	0.54
1:C:94:GLU:OE1	1:C:98:ARG:NH2	2.41	0.53
1:A:139:SER:HA	1:A:145:ARG:HD3	1.90	0.53
1:A:30:ARG:O	1:A:34:VAL:HG23	2.10	0.52
1:D:45:ILE:HG12	1:D:81:VAL:CG1	2.38	0.52
1:C:16:ASP:OD2	1:C:62:LYS:NZ	2.39	0.51
1:F:261:ILE:HD12	1:F:261:ILE:C	2.30	0.51
1:F:48:PRO:HA	1:F:86:THR:HB	1.92	0.51
1:D:142:VAL:HB	1:D:145:ARG:HG2	1.93	0.51
1:A:99:ARG:NH2	3:A:411:HOH:O	2.39	0.51
1:C:25:GLU:O	1:C:29:VAL:HG23	2.10	0.50
1:C:48:PRO:HA	1:C:86:THR:HB	1.92	0.50
1:F:22:ALA:O	1:F:26:LEU:HD13	2.12	0.50
1:F:157:LEU:HG	1:F:184:PHE:CE2	2.46	0.50
1:D:146:GLY:HA3	1:D:170:PHE:CZ	2.47	0.50
1:A:199:LEU:HD12	1:A:268:SER:HB2	1.93	0.50
1:A:254:LYS:HG2	1:A:291:TYR:CZ	2.47	0.50
1:A:5:THR:OG1	1:A:43:ARG:HB3	2.12	0.50
1:A:75:GLN:NE2	3:A:416:HOH:O	2.44	0.50
1:A:277:VAL:HG13	1:A:282:PHE:CZ	2.47	0.50
1:D:133:ASP:O	1:D:137:THR:HG23	2.12	0.49
1:F:51:ILE:N	3:F:407:HOH:O	2.46	0.49
1:C:250:LEU:HD21	1:C:287:ALA:HB1	1.94	0.49

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:ARG:O	1:F:102:THR:HG23	2.12	0.49
1:D:51:ILE:HG13	1:D:88:VAL:HG21	1.95	0.49
1:C:153:ARG:O	3:C:401:HOH:O	2.20	0.49
1:B:132:THR:HA	1:B:135:LEU:HD12	1.95	0.48
1:E:86:THR:HG23	1:E:115:VAL:HG21	1.94	0.48
1:C:39:ASP:OD1	1:C:39:ASP:N	2.42	0.48
1:F:157:LEU:HD22	1:F:187:GLU:HG2	1.95	0.48
1:A:30:ARG:NH1	1:A:39:ASP:OD1	2.41	0.47
1:C:238:ALA:C	1:C:240:SER:H	2.18	0.47
1:B:257:ILE:O	1:B:261:ILE:HG13	2.14	0.47
1:A:231:GLN:NE2	3:A:421:HOH:O	2.47	0.47
1:F:153:ARG:NE	1:F:156:GLU:OE1	2.45	0.47
1:C:86:THR:HG23	1:C:115:VAL:HG21	1.96	0.47
1:F:135:LEU:O	1:F:139:SER:HB3	2.15	0.47
1:C:12:PRO:O	1:C:64:LYS:HD3	2.14	0.47
1:D:178:SER:HB3	1:D:230:GLU:CG	2.43	0.47
1:D:147:VAL:CG1	1:D:163:LYS:HD3	2.44	0.47
1:F:294:PRO:O	1:F:295:ASP:HB2	2.14	0.47
1:F:277:VAL:HG13	1:F:282:PHE:CZ	2.50	0.46
1:B:249:MET:HE3	1:B:288:MET:CE	2.32	0.46
1:B:254:LYS:HD2	3:B:425:HOH:O	2.15	0.46
1:C:28:LYS:HG2	3:C:457:HOH:O	2.15	0.46
1:A:47:ILE:HG22	1:A:67:VAL:HG22	1.98	0.46
1:C:76:ARG:HA	1:C:76:ARG:HD2	1.70	0.46
1:C:153:ARG:O	1:C:156:GLU:HB2	2.16	0.45
1:C:197:GLU:OE2	1:C:268:SER:OG	2.30	0.45
1:A:153:ARG:NE	1:A:156:GLU:OE1	2.46	0.45
1:C:225:GLY:HA2	1:C:228:ALA:HB3	1.99	0.45
1:A:43:ARG:HA	1:A:82:ARG:HH21	1.82	0.44
1:B:25:GLU:O	1:B:29:VAL:HG23	2.17	0.44
1:B:254:LYS:NZ	1:B:258:ASP:OD2	2.33	0.44
1:D:101:LEU:O	1:D:105:ILE:HG12	2.18	0.44
1:B:261:ILE:HD12	1:B:262:ASP:H	1.80	0.44
1:E:5:THR:OG1	1:E:43:ARG:HB3	2.17	0.44
1:E:78:LEU:O	1:E:81:VAL:HG22	2.17	0.44
1:D:98:ARG:O	1:D:102:THR:HG23	2.18	0.44
1:E:189:SER:O	1:E:195:ARG:NH2	2.51	0.44
1:B:174:GLN:HG3	1:B:175:LEU:N	2.31	0.44
1:C:159:ARG:HG2	1:C:163:LYS:HE3	2.00	0.44
1:A:207:LYS:H	1:A:207:LYS:CE	2.31	0.44
1:F:246:ARG:NH2	1:F:283:GLU:HG3	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:O	1:A:81:VAL:HG22	2.18	0.43
1:A:246:ARG:NH2	1:A:283:GLU:HG3	2.33	0.43
1:C:43:ARG:NH1	1:C:44:HIS:HE1	2.16	0.43
2:D:301:NAI:H2N	2:D:301:NAI:H2D	1.82	0.43
1:B:23:LEU:O	1:B:27:GLN:HG3	2.19	0.43
1:F:156:GLU:OE1	1:F:159:ARG:HD2	2.18	0.43
1:E:261:ILE:HD12	1:E:292:TRP:NE1	2.34	0.43
1:A:157:LEU:HD11	1:A:187:GLU:HG2	2.01	0.43
1:B:23:LEU:HG	1:B:73:LEU:HB3	2.01	0.43
1:B:67:VAL:HG23	3:B:483:HOH:O	2.18	0.43
1:C:142:VAL:HB	1:C:145:ARG:HG2	2.01	0.43
1:F:153:ARG:HH21	1:F:156:GLU:CD	2.18	0.43
1:E:208:MET:HG2	1:E:212:VAL:HG23	2.00	0.43
1:F:23:LEU:HD22	1:F:77:GLU:OE1	2.19	0.42
1:B:153:ARG:O	1:B:156:GLU:HB2	2.18	0.42
1:F:203:GLY:HA2	1:F:272:GLU:O	2.19	0.42
1:C:119:ARG:NH1	3:C:419:HOH:O	2.51	0.42
1:C:146:GLY:HA2	1:C:170:PHE:O	2.19	0.42
1:C:224:ASN:HB3	1:C:227:VAL:HB	2.02	0.42
1:D:5:THR:OG1	1:D:43:ARG:HB2	2.19	0.42
1:D:57:ARG:HG3	1:D:217:TRP:CZ3	2.54	0.42
1:F:215:ILE:O	1:F:219:ILE:HG12	2.19	0.42
1:F:255:ARG:HG3	3:F:451:HOH:O	2.19	0.42
1:D:149:LEU:O	1:D:173:THR:HA	2.19	0.42
1:A:182:VAL:O	1:A:186:THR:HG23	2.20	0.42
1:F:261:ILE:C	1:F:261:ILE:CD1	2.88	0.42
1:F:284:THR:HG22	1:F:288:MET:CE	2.49	0.42
1:E:48:PRO:HA	1:E:86:THR:HB	2.02	0.41
1:D:41:ARG:HH11	1:D:41:ARG:HG3	1.85	0.41
1:A:68:LEU:HD22	1:A:107:HIS:CG	2.55	0.41
1:A:133:ASP:OD2	3:A:401:HOH:O	2.22	0.41
1:B:149:LEU:O	1:B:173:THR:HA	2.20	0.41
1:C:149:LEU:O	1:C:173:THR:HA	2.20	0.41
1:F:121:MET:HB3	1:F:125:GLU:HB3	2.02	0.41
1:B:208:MET:HG2	1:B:275:TYR:CE1	2.55	0.41
1:B:278:SER:OG	1:B:280:PRO:HD2	2.21	0.41
1:F:64:LYS:NZ	3:F:416:HOH:O	2.52	0.41
1:D:102:THR:O	1:D:106:GLN:HG3	2.20	0.41
1:C:49:GLY:H	1:C:86:THR:HB	1.86	0.41
1:E:284:THR:O	1:E:288:MET:HG3	2.20	0.41
1:D:201:SER:HA	1:D:270:HIS:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LYS:HG2	1:A:291:TYR:CE2	2.56	0.41
1:E:24:ALA:HB3	3:E:409:HOH:O	2.21	0.41
1:A:86:THR:HG23	1:A:115:VAL:HG21	2.03	0.41
1:D:41:ARG:HG3	1:D:41:ARG:NH1	2.36	0.41
1:E:196:PRO:HD2	1:E:265:PHE:CE2	2.56	0.40
1:A:279:ALA:HB3	1:A:280:PRO:HD3	2.03	0.40
1:C:23:LEU:O	1:C:27:GLN:HG3	2.20	0.40
1:D:9:GLU:HB2	1:D:270:HIS:HE2	1.86	0.40
1:A:146:GLY:HA2	1:A:170:PHE:O	2.21	0.40
1:A:119:ARG:HH11	1:A:119:ARG:HD3	1.75	0.40
1:C:237:LEU:HD23	1:C:237:LEU:HA	1.83	0.40
1:F:95:ARG:HD3	1:F:98:ARG:HE	1.86	0.40
1:A:207:LYS:HB2	1:A:207:LYS:HE2	1.85	0.40
1:F:151:PRO:HG3	1:F:181:ILE:HD13	2.02	0.40
1:A:16:ASP:OD2	1:A:62:LYS:NZ	2.48	0.40
1:A:207:LYS:H	1:A:207:LYS:HE2	1.86	0.40
1:D:271:PHE:HB3	1:D:285:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/296 (97%)	281 (98%)	4 (1%)	1 (0%)	41	31
1	B	282/296 (95%)	270 (96%)	10 (4%)	2 (1%)	22	11
1	C	288/296 (97%)	275 (96%)	9 (3%)	4 (1%)	11	3
1	D	284/296 (96%)	277 (98%)	5 (2%)	2 (1%)	22	11
1	E	284/296 (96%)	271 (95%)	13 (5%)	0	100	100
1	F	288/296 (97%)	284 (99%)	3 (1%)	1 (0%)	41	31
All	All	1712/1776 (96%)	1658 (97%)	44 (3%)	10 (1%)	25	14

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	222	PRO
1	C	60	GLU
1	F	61	MET
1	B	208	MET
1	C	61	MET
1	D	61	MET
1	D	222	PRO
1	A	61	MET
1	C	16	ASP
1	C	222	PRO

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	241/248 (97%)	236 (98%)	5 (2%)	53	46
1	B	239/248 (96%)	234 (98%)	5 (2%)	53	46
1	C	240/248 (97%)	237 (99%)	3 (1%)	69	66
1	D	240/248 (97%)	237 (99%)	3 (1%)	69	66
1	E	242/248 (98%)	240 (99%)	2 (1%)	81	81
1	F	241/248 (97%)	238 (99%)	3 (1%)	71	69
All	All	1443/1488 (97%)	1422 (98%)	21 (2%)	65	61

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	30	ARG
1	E	158	SER
1	A	43	ARG
1	A	119	ARG
1	A	139	SER
1	A	143	LYS
1	A	207	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	16	ASP
1	B	23	LEU
1	B	43	ARG
1	B	95	ARG
1	B	249	MET
1	C	28	LYS
1	C	50	MET
1	C	295	ASP
1	D	50	MET
1	D	123	ASP
1	D	158	SER
1	F	1	MET
1	F	143	LYS
1	F	157	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	183	ASN
1	A	75	GLN
1	A	231	GLN
1	A	248	GLN
1	C	140	HIS
1	C	231	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	NAI	B	301	-	42,48,48	1.30	4 (9%)	47,73,73	0.83	2 (4%)
2	NAI	D	301	-	42,48,48	1.34	3 (7%)	47,73,73	0.98	3 (6%)
2	NAI	C	301	-	42,48,48	1.35	4 (9%)	47,73,73	0.77	1 (2%)
2	NAI	F	301	-	42,48,48	1.37	4 (9%)	47,73,73	0.76	2 (4%)
2	NAI	E	301	-	42,48,48	1.36	4 (9%)	47,73,73	0.76	3 (6%)
2	NAI	A	301	-	42,48,48	1.35	4 (9%)	47,73,73	0.76	2 (4%)

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	NAI	B	301	-	-	4/25/72/72	0/5/5/5
2	NAI	D	301	-	-	7/25/72/72	0/5/5/5
2	NAI	C	301	-	-	6/25/72/72	0/5/5/5
2	NAI	F	301	-	-	8/25/72/72	0/5/5/5
2	NAI	E	301	-	-	5/25/72/72	0/5/5/5
2	NAI	A	301	-	-	7/25/72/72	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NAI	C4N-C3N	-5.82	1.38	1.49
2	D	301	NAI	C4N-C3N	-5.74	1.38	1.49
2	E	301	NAI	C4N-C3N	-5.64	1.38	1.49
2	A	301	NAI	C4N-C3N	-5.57	1.39	1.49
2	C	301	NAI	C4N-C3N	-5.54	1.39	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAI	C4N-C3N	-5.30	1.39	1.49
2	E	301	NAI	C4N-C5N	-4.51	1.37	1.48
2	F	301	NAI	C4N-C5N	-4.44	1.37	1.48
2	A	301	NAI	C4N-C5N	-4.42	1.37	1.48
2	D	301	NAI	C4N-C5N	-4.30	1.37	1.48
2	C	301	NAI	C4N-C5N	-4.21	1.37	1.48
2	B	301	NAI	C4N-C5N	-4.13	1.38	1.48
2	C	301	NAI	C6N-C5N	2.62	1.38	1.33
2	E	301	NAI	C6N-C5N	2.53	1.37	1.33
2	D	301	NAI	C6N-C5N	2.45	1.37	1.33
2	B	301	NAI	C6N-C5N	2.45	1.37	1.33
2	A	301	NAI	C6N-C5N	2.43	1.37	1.33
2	F	301	NAI	C6N-C5N	2.38	1.37	1.33
2	A	301	NAI	C8A-N7A	-2.17	1.30	1.34
2	C	301	NAI	C8A-N7A	-2.10	1.31	1.34
2	F	301	NAI	C8A-N7A	-2.08	1.31	1.34
2	E	301	NAI	C8A-N7A	-2.07	1.31	1.34
2	B	301	NAI	C8A-N7A	-2.07	1.31	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	NAI	C3N-C2N-N1N	-4.25	117.03	123.10
2	B	301	NAI	C3D-C2D-C1D	2.61	106.38	101.43
2	B	301	NAI	C3N-C2N-N1N	-2.59	119.40	123.10
2	A	301	NAI	C3N-C2N-N1N	-2.59	119.40	123.10
2	D	301	NAI	C3D-C2D-C1D	2.51	106.19	101.43
2	C	301	NAI	C3D-C2D-C1D	2.44	106.06	101.43
2	E	301	NAI	C3N-C2N-N1N	-2.44	119.62	123.10
2	E	301	NAI	C3D-C2D-C1D	2.34	105.87	101.43
2	D	301	NAI	C5A-C6A-N6A	2.31	123.87	120.35
2	A	301	NAI	C3D-C2D-C1D	2.31	105.81	101.43
2	F	301	NAI	C3D-C2D-C1D	2.24	105.68	101.43
2	E	301	NAI	C5A-C6A-N6A	2.12	123.58	120.35
2	F	301	NAI	C5A-C6A-N6A	2.01	123.41	120.35

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	NAI	C5B-O5B-PA-O1A
2	F	301	NAI	C5B-O5B-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	301	NAI	C3B-C4B-C5B-O5B
2	D	301	NAI	C3B-C4B-C5B-O5B
2	A	301	NAI	O4B-C4B-C5B-O5B
2	A	301	NAI	C2D-C1D-N1N-C6N
2	D	301	NAI	C2D-C1D-N1N-C6N
2	C	301	NAI	C5B-O5B-PA-O3
2	F	301	NAI	C5B-O5B-PA-O3
2	D	301	NAI	O4B-C4B-C5B-O5B
2	F	301	NAI	PA-O3-PN-O1N
2	C	301	NAI	C5B-O5B-PA-O2A
2	E	301	NAI	O4D-C1D-N1N-C6N
2	A	301	NAI	O4D-C1D-N1N-C6N
2	A	301	NAI	C2D-C1D-N1N-C2N
2	D	301	NAI	C2D-C1D-N1N-C2N
2	F	301	NAI	C2D-C1D-N1N-C6N
2	D	301	NAI	O4D-C1D-N1N-C6N
2	F	301	NAI	O4D-C1D-N1N-C6N
2	B	301	NAI	O4D-C1D-N1N-C6N
2	E	301	NAI	PA-O3-PN-O1N
2	A	301	NAI	PA-O3-PN-O1N
2	C	301	NAI	PA-O3-PN-O1N
2	D	301	NAI	PA-O3-PN-O1N
2	B	301	NAI	C2D-C1D-N1N-C6N
2	C	301	NAI	C2D-C1D-N1N-C6N
2	C	301	NAI	O4D-C1D-N1N-C6N
2	D	301	NAI	O4D-C1D-N1N-C2N
2	F	301	NAI	C2D-C1D-N1N-C2N
2	A	301	NAI	O4D-C1D-N1N-C2N
2	F	301	NAI	O4D-C1D-N1N-C2N
2	E	301	NAI	C3B-C4B-C5B-O5B
2	E	301	NAI	PA-O3-PN-O2N
2	B	301	NAI	PA-O3-PN-O1N
2	B	301	NAI	PA-O3-PN-O2N
2	F	301	NAI	PA-O3-PN-O2N
2	E	301	NAI	C2N-C3N-C7N-N7N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAI B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI F 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI E 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI A 301

Bond lengths

Bond angles

Torsions

Rings
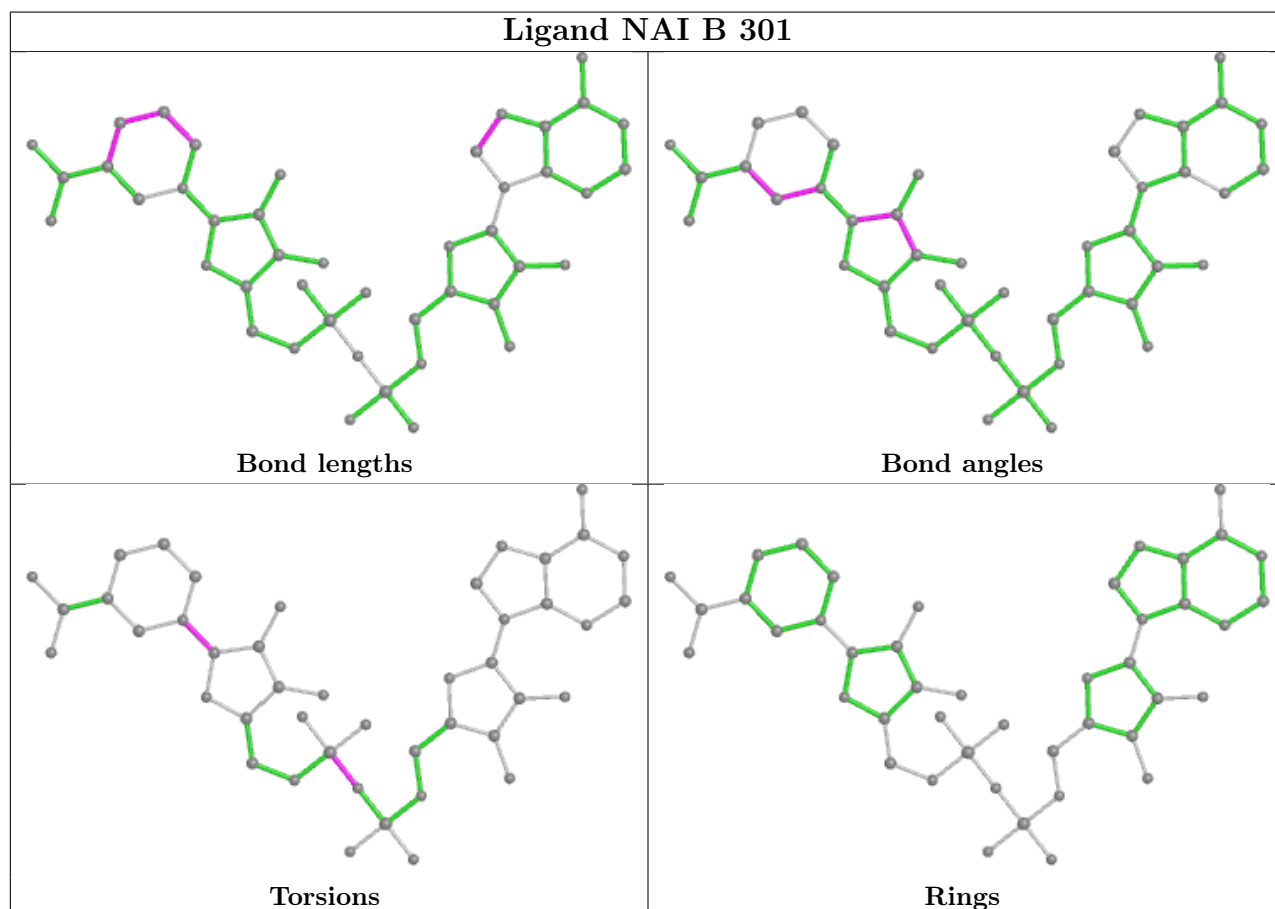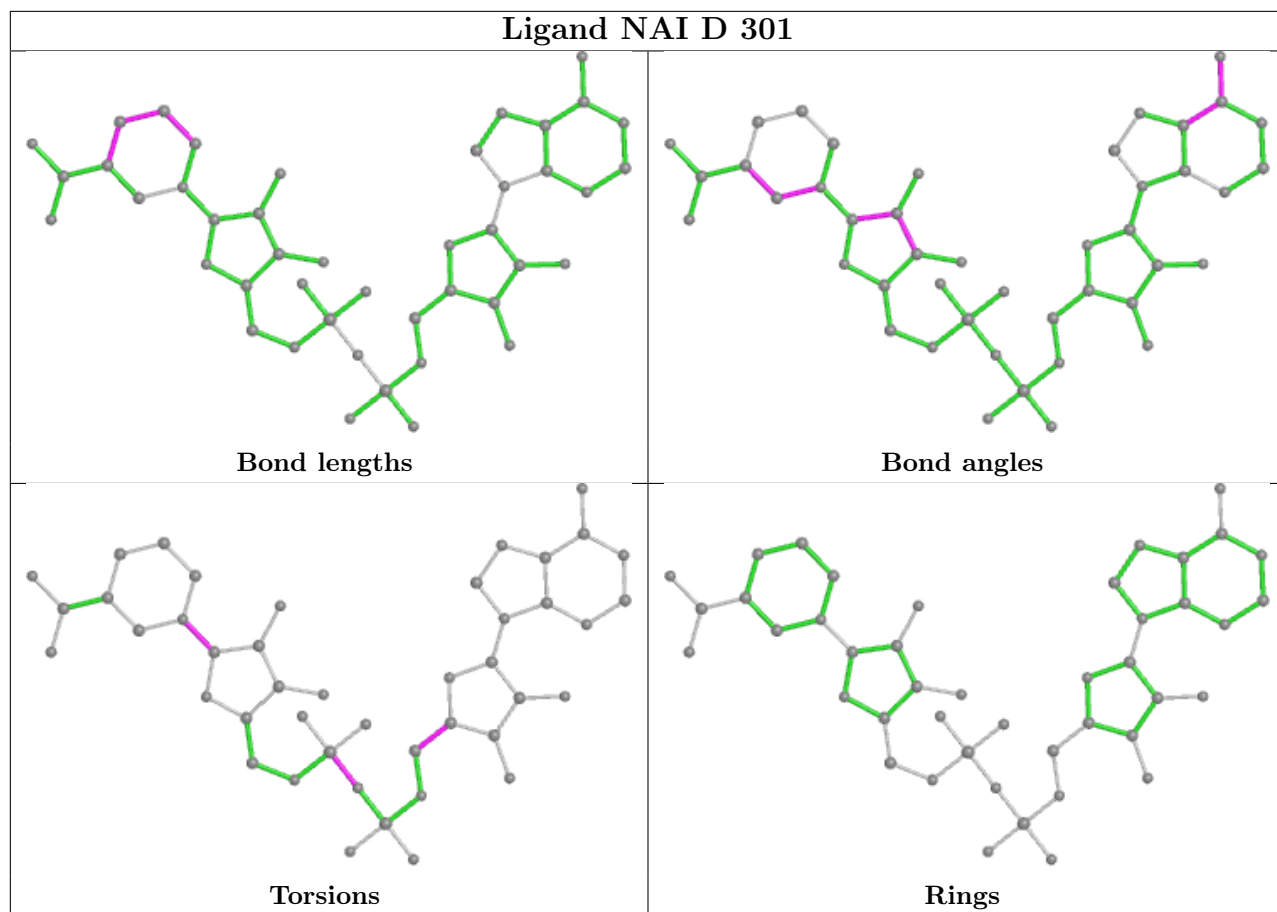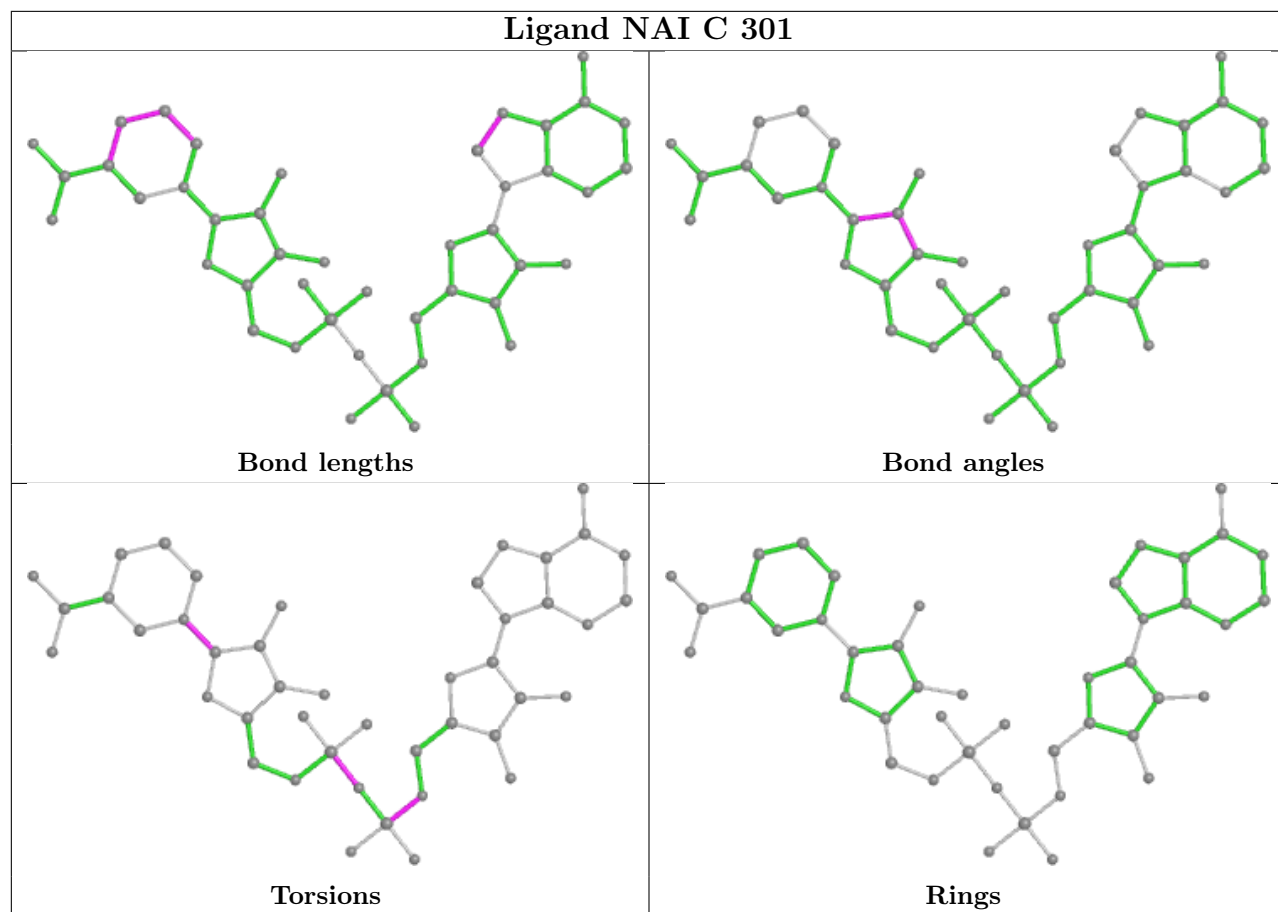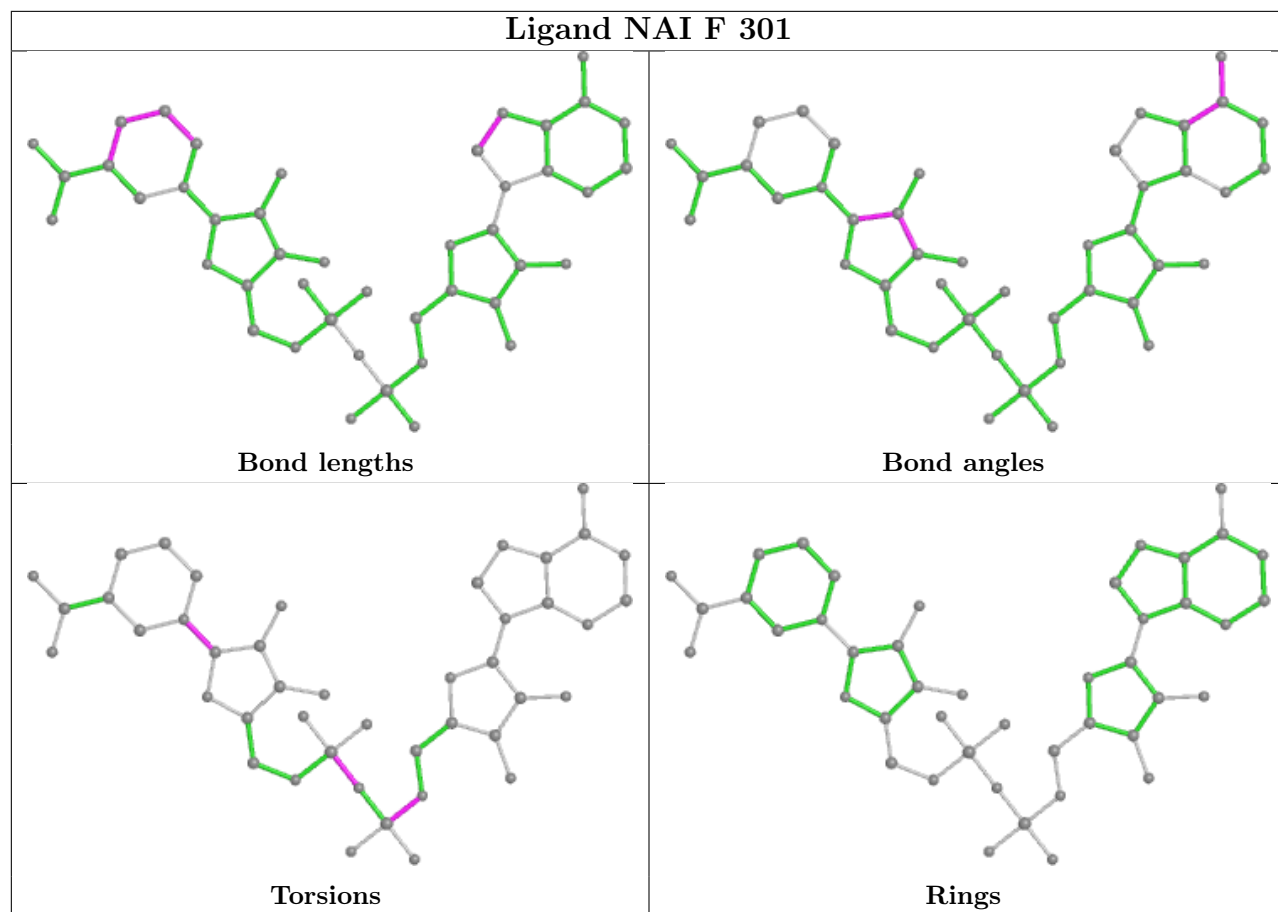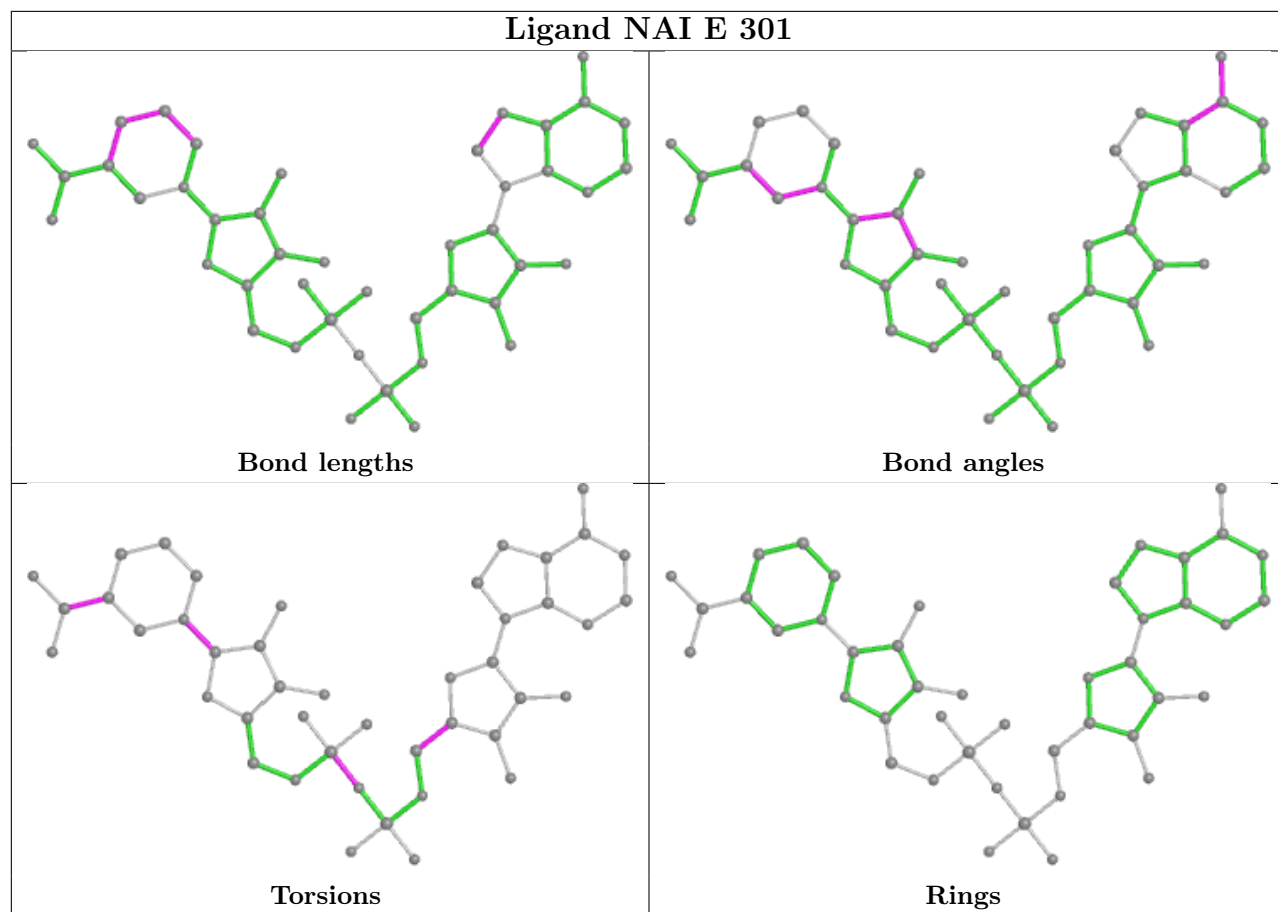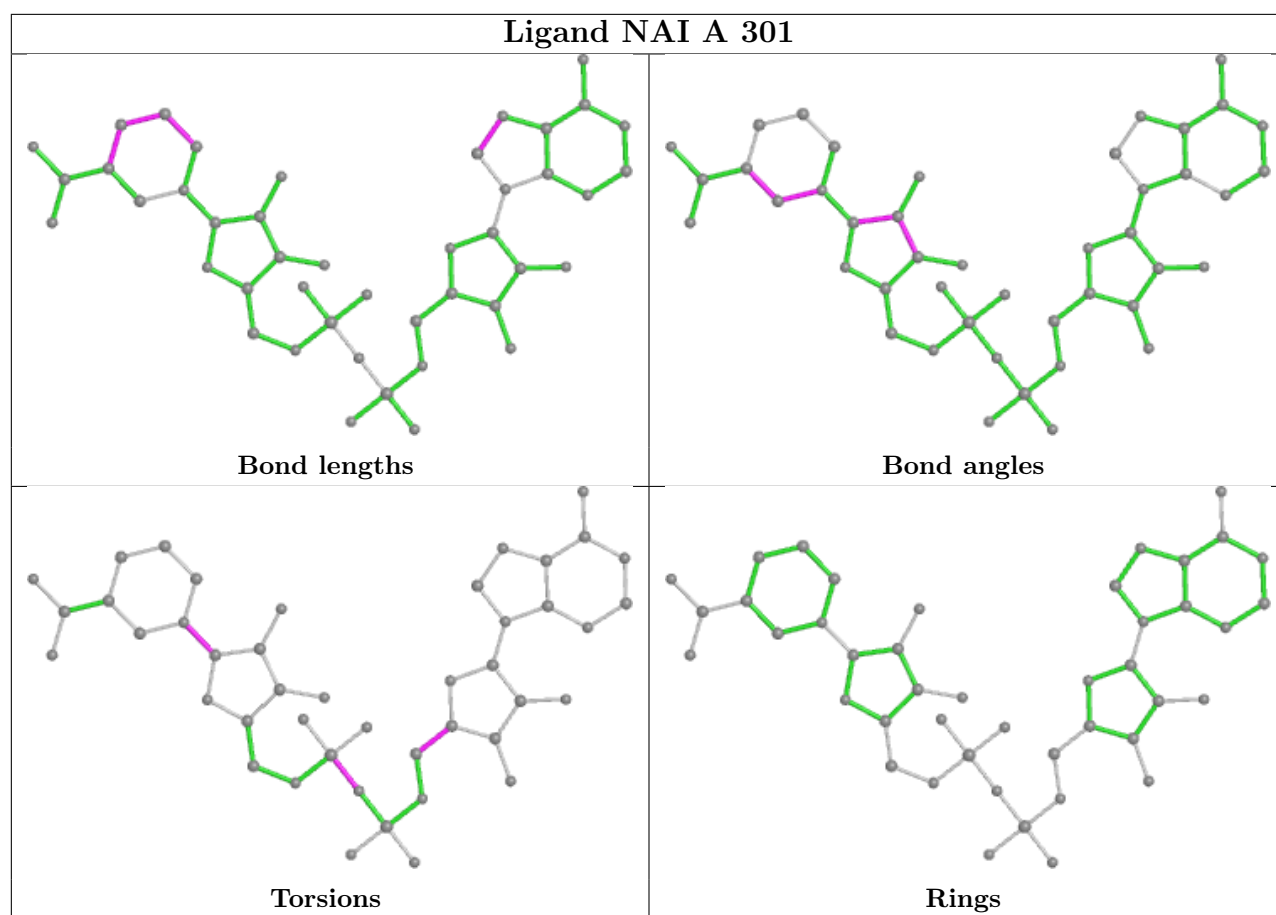
5.7 Other polymers ⓘ

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	290/296 (97%)	0.79	18 (6%)	20	23	27, 35, 41, 47	0
1	B	288/296 (97%)	0.83	17 (5%)	22	25	26, 34, 39, 44	0
1	C	292/296 (98%)	0.80	17 (5%)	23	26	27, 36, 41, 45	0
1	D	290/296 (97%)	0.81	15 (5%)	27	30	27, 35, 41, 47	0
1	E	290/296 (97%)	0.79	11 (3%)	40	43	26, 35, 40, 44	0
1	F	292/296 (98%)	0.79	20 (6%)	17	19	26, 35, 40, 45	0
All	All	1742/1776 (98%)	0.80	98 (5%)	24	27	26, 35, 41, 47	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	HIS	4.6
1	A	33	ALA	4.5
1	C	51	ILE	3.8
1	B	34	VAL	3.5
1	C	239	ALA	3.5
1	A	281	ALA	3.4
1	C	208	MET	3.3
1	D	261	ILE	3.2
1	F	29	VAL	3.2
1	F	262	ASP	3.2
1	F	1	MET	3.1
1	E	29	VAL	3.1
1	A	158	SER	3.0
1	C	61	MET	3.0
1	D	279	ALA	3.0
1	E	59	VAL	3.0
1	F	147	VAL	3.0
1	B	126	GLY	2.9
1	C	118	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	222	PRO	2.9
1	D	51	ILE	2.9
1	E	51	ILE	2.8
1	A	61	MET	2.7
1	E	50	MET	2.7
1	F	259	GLY	2.7
1	A	147	VAL	2.7
1	E	250	LEU	2.7
1	F	4	ASN	2.6
1	F	132	THR	2.5
1	D	254	LYS	2.5
1	C	138	PHE	2.5
1	F	94	GLU	2.5
1	C	142	VAL	2.5
1	D	247	ALA	2.5
1	A	81	VAL	2.5
1	A	63	PRO	2.4
1	D	139	SER	2.4
1	A	80	ASP	2.4
1	B	45	ILE	2.4
1	B	238	ALA	2.4
1	B	279	ALA	2.4
1	E	122	THR	2.4
1	D	39	ASP	2.4
1	A	191	ASN	2.4
1	E	228	ALA	2.4
1	C	39	ASP	2.4
1	C	120	THR	2.4
1	C	79	PRO	2.4
1	F	61	MET	2.3
1	F	295	ASP	2.3
1	D	91	PHE	2.3
1	D	42	ILE	2.3
1	F	59	VAL	2.3
1	B	61	MET	2.3
1	F	128	GLY	2.3
1	A	239	ALA	2.3
1	C	73	LEU	2.3
1	C	204	PHE	2.3
1	F	170	PHE	2.3
1	B	107	HIS	2.3
1	B	1	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	92	LEU	2.3
1	B	222	PRO	2.2
1	E	239	ALA	2.2
1	A	212	VAL	2.2
1	E	56	GLY	2.2
1	F	97	LEU	2.2
1	B	160	PHE	2.2
1	D	286	ALA	2.2
1	F	140	HIS	2.2
1	A	106	GLN	2.2
1	D	215	ILE	2.2
1	F	215	ILE	2.2
1	C	250	LEU	2.2
1	B	23	LEU	2.2
1	F	122	THR	2.2
1	D	6	VAL	2.2
1	A	47	ILE	2.1
1	E	208	MET	2.1
1	A	50	MET	2.1
1	B	40	GLY	2.1
1	B	283	GLU	2.1
1	B	261	ILE	2.1
1	D	213	GLY	2.1
1	D	229	THR	2.1
1	F	252	LEU	2.1
1	A	140	HIS	2.1
1	B	79	PRO	2.1
1	A	59	VAL	2.1
1	F	103	ALA	2.1
1	A	242	PRO	2.1
1	F	232	GLN	2.1
1	E	61	MET	2.0
1	A	210	SER	2.0
1	C	17	LEU	2.0
1	C	5	THR	2.0
1	C	212	VAL	2.0
1	B	51	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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
2	NAI	D	301	44/44	0.83	0.18	33,35,37,38	0
2	NAI	E	301	44/44	0.87	0.15	32,34,35,35	0
2	NAI	B	301	44/44	0.89	0.13	32,33,35,35	0
2	NAI	C	301	44/44	0.89	0.14	32,34,36,36	0
2	NAI	A	301	44/44	0.89	0.14	34,35,37,38	0
2	NAI	F	301	44/44	0.91	0.13	31,33,34,35	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.
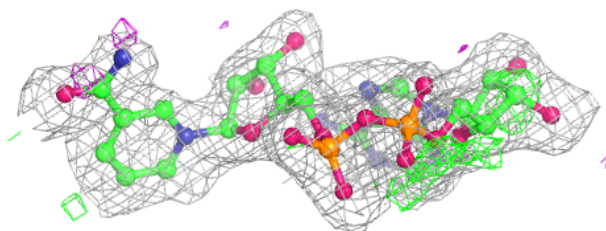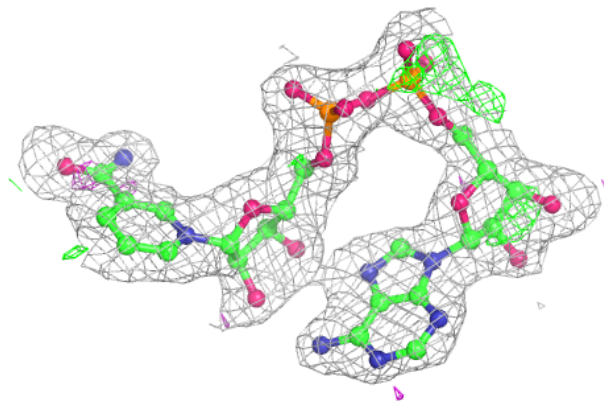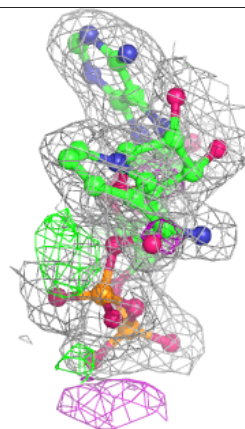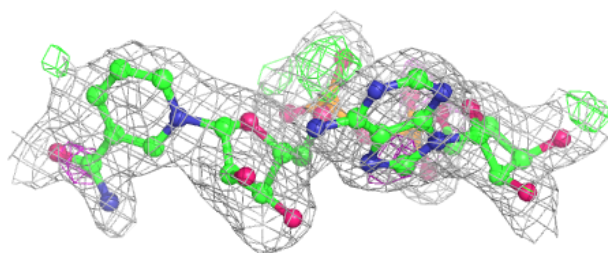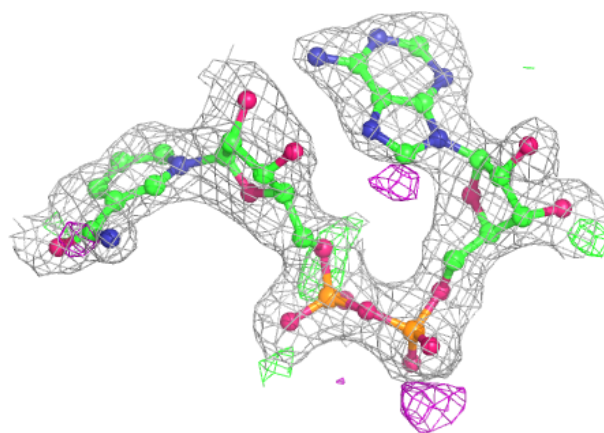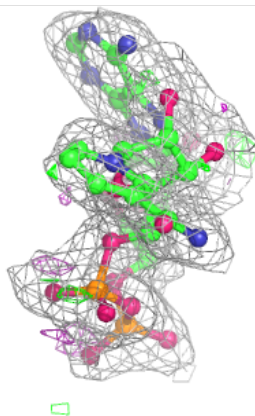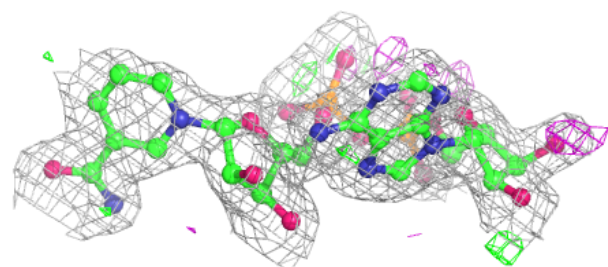
Electron density around NAI D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
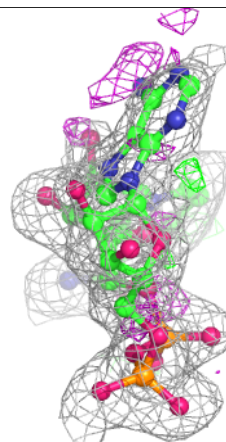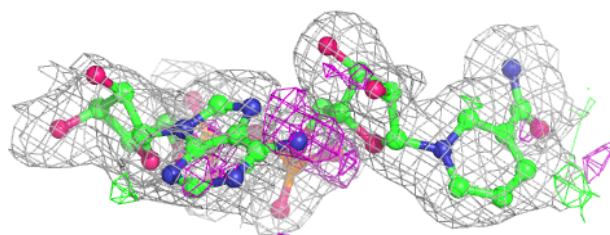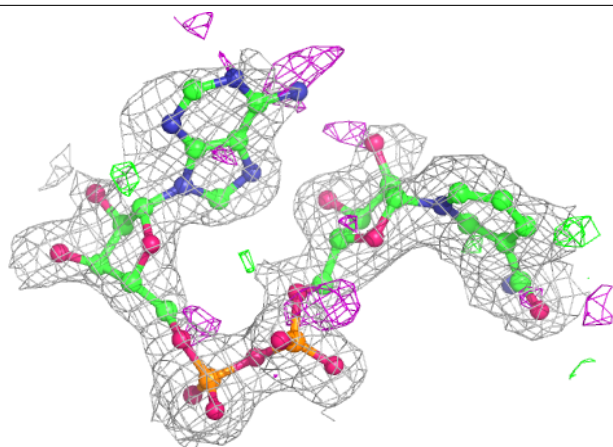
Electron density around NAI E 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
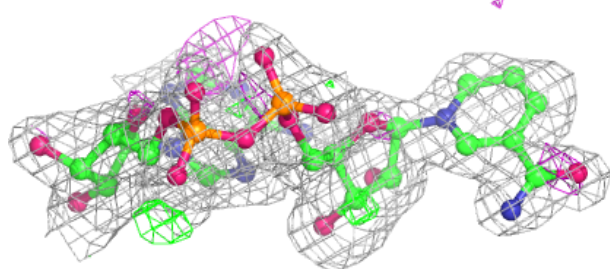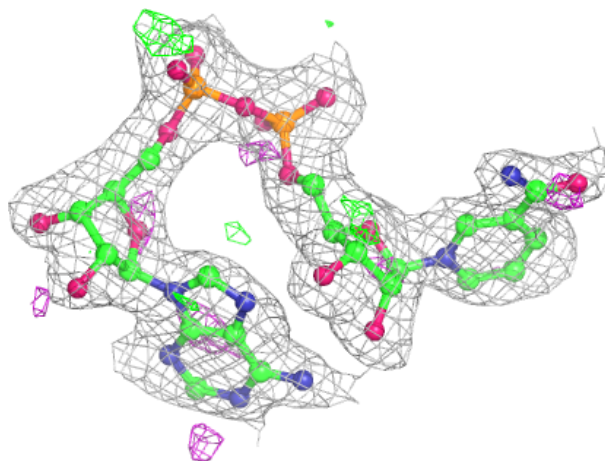
Electron density around NAI B 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
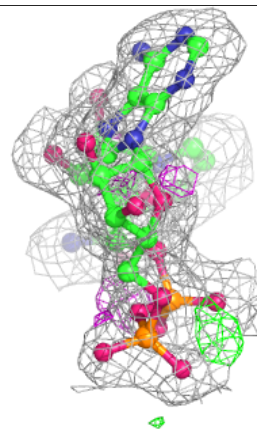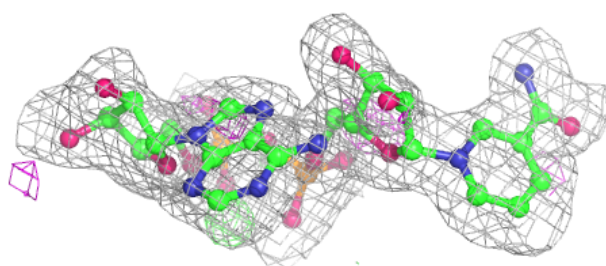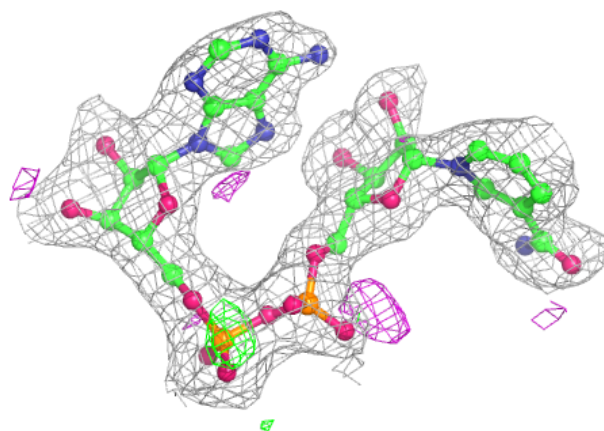
Electron density around NAI C 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
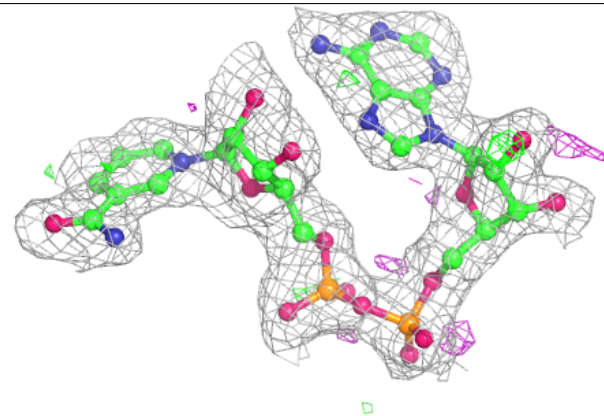$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
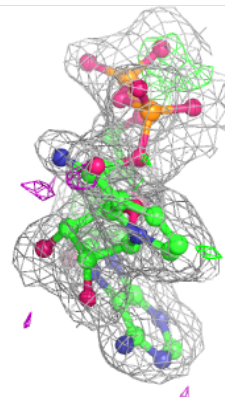
Electron density around NAI A 301:

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

Electron density around NAI 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.