



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:09 PM UTC

PDB ID : 1NFQ / pdb_00001nfq
Title : Rv2002 gene product from Mycobacterium tuberculosis
Authors : Yang, J.K.; Park, M.S.; Waldo, G.S.; Suh, S.W.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2002-12-15
Resolution : 2.40 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

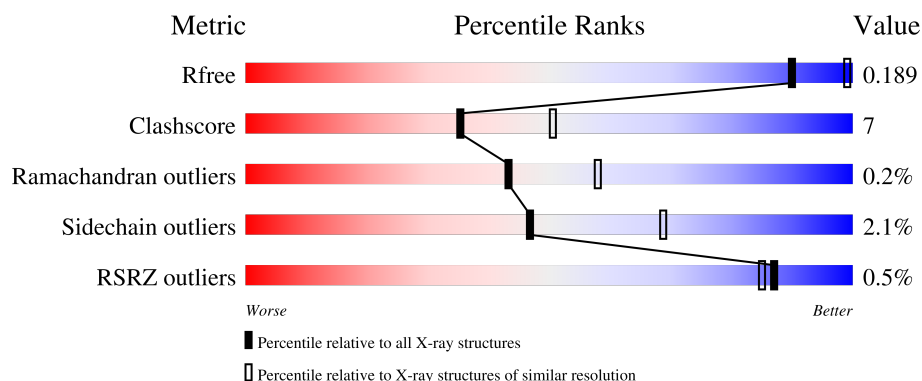
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	260	
1	B	260	
1	C	260	
1	D	260	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AOI	A	401	X	-	-	-
3	AOI	B	1401	X	-	-	-
3	AOI	C	2401	X	-	-	-
3	AOI	D	3401	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7618 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.

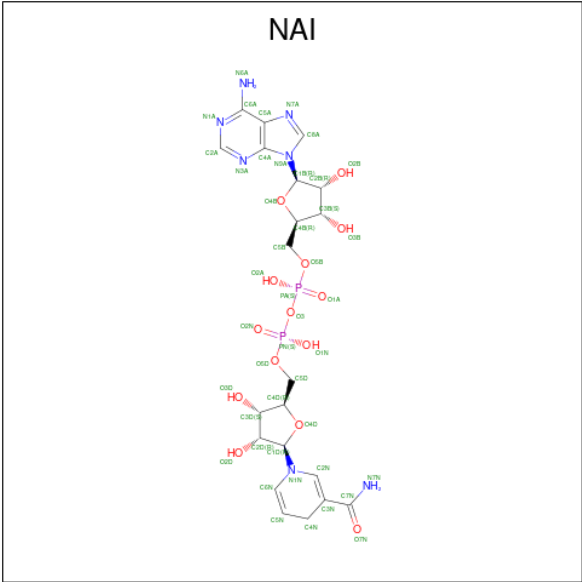
- Molecule 1 is a protein called Putative oxidoreductase Rv2002.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1780	1122	310	342	6			
1	B	244	Total	C	N	O	S	0	0	0
			1780	1122	310	342	6			
1	C	244	Total	C	N	O	S	0	0	0
			1780	1122	310	342	6			
1	D	244	Total	C	N	O	S	0	0	0
			1780	1122	310	342	6			

There are 12 discrepancies between the modelled and reference sequences:

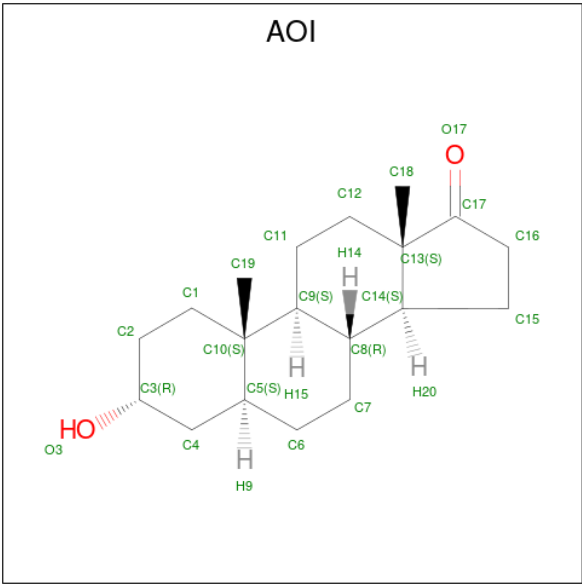
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	THR	ILE	engineered mutation	UNP P69167
A	47	MET	VAL	engineered mutation	UNP P69167
A	69	LYS	THR	engineered mutation	UNP P69167
B	6	THR	ILE	engineered mutation	UNP P69167
B	47	MET	VAL	engineered mutation	UNP P69167
B	69	LYS	THR	engineered mutation	UNP P69167
C	6	THR	ILE	engineered mutation	UNP P69167
C	47	MET	VAL	engineered mutation	UNP P69167
C	69	LYS	THR	engineered mutation	UNP P69167
D	6	THR	ILE	engineered mutation	UNP P69167
D	47	MET	VAL	engineered mutation	UNP P69167
D	69	LYS	THR	engineered mutation	UNP P69167

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is Androsterone (CCD ID: AOI) (formula: C₁₉H₃₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	19	2		
3	B	1	Total	C	O	0	0
			21	19	2		
3	C	1	Total	C	O	0	0
			21	19	2		
3	D	1	Total	C	O	0	0
			21	19	2		

- Molecule 4 is water.

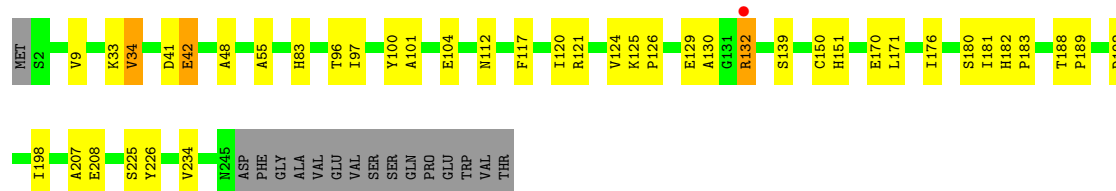
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	70	Total	O	0	0
			70	70		
4	C	61	Total	O	0	0
			61	61		
4	D	48	Total	O	0	0
			48	48		

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.

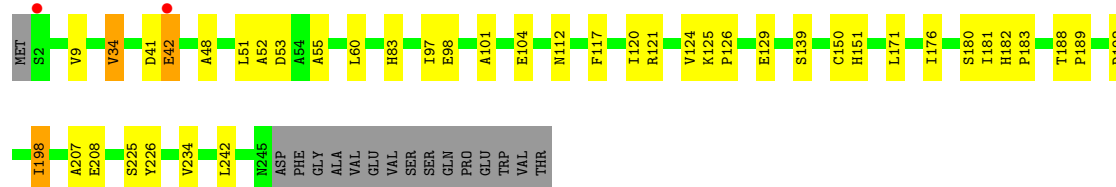
- Molecule 1: Putative oxidoreductase Rv2002

Chain A: 



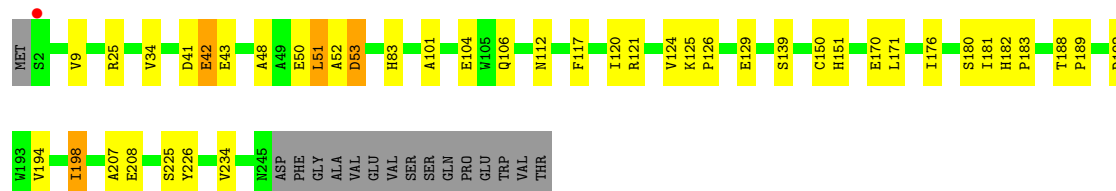
- Molecule 1: Putative oxidoreductase Rv2002

Chain B: 



- Molecule 1: Putative oxidoreductase Rv2002

Chain C: 



- Molecule 1: Putative oxidoreductase Rv2002

Chain D: 



H182	P183		T188	P189		D192	W193	V194		T198		A207	E208		S225	Y226		E231		R245	ASP	PHE	GLY	ALA	VAL	GLU	VAL	SER	SER	GLN	PRO	GLU	TRP	VAL	THR
------	------	--	------	------	--	------	------	------	--	------	--	------	------	--	------	------	--	------	--	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	122.16Å 122.16Å 141.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.40 19.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (19.91-2.40) 96.1 (19.91-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.162 , 0.189 0.162 , 0.189	Depositor DCC
R_{free} test set	4036 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for -h,k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7618	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: AOI, 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	0.44	0/1809	0.96	8/2460 (0.3%)
1	B	0.43	0/1809	0.95	10/2460 (0.4%)
1	C	0.51	3/1809 (0.2%)	0.99	11/2460 (0.4%)
1	D	0.39	0/1809	0.94	7/2460 (0.3%)
All	All	0.45	3/7236 (0.0%)	0.96	36/9840 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	ASP	CA-CB	5.91	1.64	1.53
1	C	53	ASP	CB-CG	5.28	1.65	1.52
1	C	53	ASP	CA-C	-5.08	1.45	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	52	ALA	CB-CA-C	-8.27	107.03	116.54
1	D	34	VAL	N-CA-C	6.65	117.42	108.11
1	A	208	GLU	N-CA-C	-6.65	101.70	110.07
1	A	34	VAL	N-CA-C	6.63	117.40	108.11
1	C	34	VAL	N-CA-C	6.63	117.39	108.11
1	C	208	GLU	N-CA-C	-6.53	101.85	110.07
1	B	208	GLU	N-CA-C	-6.52	101.85	110.07
1	B	34	VAL	N-CA-C	6.48	117.19	108.11
1	D	208	GLU	N-CA-C	-6.34	102.08	110.07
1	C	151	HIS	N-CA-C	6.31	117.82	111.07
1	A	151	HIS	N-CA-C	6.23	118.07	111.28
1	B	151	HIS	N-CA-C	6.20	117.70	111.07
1	D	151	HIS	N-CA-C	6.02	117.84	111.28
1	C	139	SER	N-CA-C	-5.85	103.98	108.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ASP	N-CA-C	5.73	117.53	111.28
1	A	41	ASP	N-CA-C	5.72	117.52	111.28
1	C	52	ALA	N-CA-C	5.69	116.95	108.31
1	D	41	ASP	N-CA-C	5.58	117.36	111.28
1	D	139	SER	N-CA-C	-5.57	104.21	108.78
1	B	139	SER	N-CA-C	-5.55	104.23	108.78
1	C	48	ALA	N-CA-C	-5.54	105.78	112.54
1	C	41	ASP	N-CA-C	5.54	117.31	111.28
1	D	112	ASN	N-CA-C	5.53	118.23	111.82
1	A	48	ALA	N-CA-C	-5.46	105.88	112.54
1	C	225	SER	N-CA-C	5.46	118.74	111.75
1	B	48	ALA	N-CA-C	-5.42	105.54	111.82
1	A	112	ASN	N-CA-C	5.40	118.08	111.82
1	B	112	ASN	N-CA-C	5.39	118.07	111.82
1	B	98	GLU	N-CA-C	5.37	116.94	111.14
1	C	112	ASN	N-CA-C	5.36	118.04	111.82
1	A	139	SER	N-CA-C	-5.31	104.42	108.78
1	C	51	LEU	N-CA-C	-5.28	106.79	113.18
1	B	225	SER	N-CA-C	5.24	118.46	111.75
1	D	225	SER	N-CA-C	5.15	118.34	111.75
1	A	225	SER	N-CA-C	5.11	118.29	111.75
1	B	53	ASP	N-CA-C	5.08	118.74	112.54

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	1780	0	1791	32	0
1	B	1780	0	1791	26	0
1	C	1780	0	1791	29	0
1	D	1780	0	1791	34	0
2	A	44	0	27	1	0
2	B	44	0	27	2	0
2	C	44	0	27	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	44	0	27	2	0
3	A	21	0	28	0	0
3	B	21	0	28	1	0
3	C	21	0	28	3	0
3	D	21	0	28	4	0
4	A	59	0	0	0	0
4	B	70	0	0	1	0
4	C	61	0	0	1	0
4	D	48	0	0	1	0
All	All	7618	0	7384	109	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 7.

All (109) 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:9:VAL:H	1:C:83:HIS:HD2	1.14	0.89
1:D:9:VAL:H	1:D:83:HIS:HD2	1.14	0.89
1:A:9:VAL:H	1:A:83:HIS:HD2	1.18	0.87
1:B:9:VAL:H	1:B:83:HIS:HD2	1.18	0.86
1:B:42:GLU:H	1:B:42:GLU:CD	1.88	0.81
1:C:42:GLU:H	1:C:42:GLU:CD	1.89	0.81
1:A:42:GLU:H	1:A:42:GLU:CD	1.90	0.79
1:D:42:GLU:H	1:D:42:GLU:CD	1.88	0.78
1:D:9:VAL:H	1:D:83:HIS:CD2	2.05	0.69
1:D:9:VAL:N	1:D:83:HIS:HD2	1.91	0.67
1:C:9:VAL:N	1:C:83:HIS:HD2	1.91	0.67
1:C:9:VAL:H	1:C:83:HIS:CD2	2.05	0.67
1:A:132:ARG:HH11	1:A:132:ARG:HG3	1.61	0.66
1:C:181:ILE:HG22	1:C:183:PRO:HD3	1.77	0.66
1:D:181:ILE:HG22	1:D:183:PRO:HD3	1.78	0.65
1:A:181:ILE:HG22	1:A:183:PRO:HD3	1.78	0.65
1:A:9:VAL:H	1:A:83:HIS:CD2	2.09	0.65
1:B:9:VAL:H	1:B:83:HIS:CD2	2.09	0.64
1:B:181:ILE:HG22	1:B:183:PRO:HD3	1.77	0.64
1:B:9:VAL:N	1:B:83:HIS:HD2	1.95	0.62
1:D:132:ARG:HB3	1:D:132:ARG:HH11	1.64	0.62
1:D:132:ARG:HB3	1:D:132:ARG:NH1	2.17	0.59
1:B:117:PHE:CE2	1:B:121:ARG:HD2	2.39	0.58
1:D:188:THR:HB	1:D:189:PRO:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:N	1:A:83:HIS:HD2	1.95	0.57
1:A:132:ARG:HG3	1:A:132:ARG:NH1	2.20	0.57
1:C:188:THR:HB	1:C:189:PRO:HD2	1.86	0.57
1:C:117:PHE:CE2	1:C:121:ARG:HD2	2.40	0.56
1:C:120:ILE:O	1:C:124:VAL:HG13	2.05	0.56
1:A:188:THR:HB	1:A:189:PRO:HD2	1.86	0.56
1:B:188:THR:HB	1:B:189:PRO:HD2	1.86	0.56
1:D:120:ILE:O	1:D:124:VAL:HG13	2.05	0.56
1:A:120:ILE:O	1:A:124:VAL:HG13	2.06	0.56
1:D:117:PHE:CE2	1:D:121:ARG:HD2	2.41	0.56
1:A:117:PHE:CE2	1:A:121:ARG:HD2	2.41	0.55
1:B:120:ILE:O	1:B:124:VAL:HG13	2.06	0.55
1:C:226:TYR:CE2	1:D:207:ALA:HB2	2.43	0.54
1:A:226:TYR:CE2	1:B:207:ALA:HB2	2.43	0.53
1:A:207:ALA:HB2	1:B:226:TYR:CE2	2.43	0.53
1:D:183:PRO:HG2	2:D:3300:NAI:C5N	2.39	0.52
1:C:207:ALA:HB2	1:D:226:TYR:CE2	2.45	0.51
1:D:4:ARG:HG3	1:D:30:GLU:OE1	2.10	0.51
1:A:183:PRO:HG2	2:A:300:NAI:C5N	2.41	0.51
1:C:43:GLU:HG2	4:C:662:HOH:O	2.11	0.50
1:A:207:ALA:HB2	1:B:226:TYR:CD2	2.48	0.48
1:C:226:TYR:CD2	1:D:207:ALA:HB2	2.48	0.48
1:A:226:TYR:CD2	1:B:207:ALA:HB2	2.49	0.48
1:B:125:LYS:HB3	1:B:126:PRO:CD	2.44	0.48
1:A:34:VAL:O	1:A:55:ALA:HA	2.14	0.48
1:A:170:GLU:OE2	1:D:97:ILE:HG13	2.14	0.48
1:B:183:PRO:HG2	2:B:1300:NAI:C5N	2.44	0.48
1:D:101:ALA:HB3	1:D:104:GLU:HG3	1.96	0.48
1:C:42:GLU:CD	1:C:42:GLU:N	2.67	0.47
1:D:198:ILE:HG12	3:D:3401:AOI:H17	1.96	0.47
1:C:207:ALA:HB2	1:D:226:TYR:CD2	2.49	0.47
1:A:97:ILE:HG13	1:D:170:GLU:OE2	2.13	0.47
1:A:101:ALA:HB3	1:A:104:GLU:HG3	1.96	0.47
1:C:198:ILE:HG12	3:C:2401:AOI:H17	1.96	0.47
1:C:101:ALA:HB3	1:C:104:GLU:HG3	1.97	0.47
1:C:180:SER:OG	1:C:182:HIS:HE1	1.96	0.47
1:B:101:ALA:HB3	1:B:104:GLU:HG3	1.97	0.47
1:C:25:ARG:NH2	1:C:50:GLU:OE2	2.47	0.47
1:C:125:LYS:HB3	1:C:126:PRO:CD	2.45	0.47
1:A:130:ALA:CB	1:A:132:ARG:HH22	2.28	0.47
1:A:132:ARG:O	1:A:132:ARG:CZ	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLU:CD	1:B:42:GLU:N	2.66	0.46
1:A:125:LYS:O	1:A:129:GLU:HG3	2.15	0.46
1:A:125:LYS:HB3	1:A:126:PRO:CD	2.45	0.46
1:A:180:SER:OG	1:A:182:HIS:HE1	1.98	0.46
1:D:180:SER:OG	1:D:182:HIS:HE1	1.99	0.46
1:D:189:PRO:HA	1:D:192:ASP:OD2	2.15	0.46
1:A:189:PRO:HA	1:A:192:ASP:OD2	2.16	0.46
1:D:125:LYS:HB3	1:D:126:PRO:CD	2.45	0.46
1:B:180:SER:OG	1:B:182:HIS:HE1	1.99	0.45
1:D:125:LYS:O	1:D:129:GLU:HG3	2.17	0.45
1:C:125:LYS:O	1:C:129:GLU:HG3	2.16	0.44
1:B:125:LYS:O	1:B:129:GLU:HG3	2.17	0.44
1:D:60:LEU:O	2:D:3300:NAI:H2A	2.18	0.44
1:C:189:PRO:HA	1:C:192:ASP:OD2	2.17	0.44
1:B:60:LEU:O	2:B:1300:NAI:H2A	2.18	0.44
1:B:189:PRO:HA	1:B:192:ASP:OD2	2.16	0.44
1:A:96:THR:O	1:A:100:TYR:HB2	2.18	0.43
1:C:183:PRO:HG2	2:C:2300:NAI:C5N	2.48	0.43
1:C:51:LEU:HD23	1:C:51:LEU:HA	1.84	0.43
4:B:551:HOH:O	1:C:106:GLN:NE2	2.45	0.43
1:D:194:VAL:HG21	3:D:3401:AOI:C19	2.49	0.43
1:D:96:THR:O	1:D:100:TYR:HB2	2.19	0.43
1:A:130:ALA:HB1	1:A:132:ARG:HH12	1.83	0.42
1:B:242:LEU:CD2	1:D:145:ALA:HB3	2.49	0.42
1:A:171:LEU:HB3	1:A:176:ILE:HB	2.00	0.42
1:C:234:VAL:O	1:C:234:VAL:HG13	2.20	0.42
1:D:171:LEU:HB3	1:D:176:ILE:HB	2.00	0.42
1:D:33:LYS:HA	1:D:33:LYS:HD3	1.83	0.42
1:B:198:ILE:HG12	3:B:1401:AOI:H17	2.02	0.41
1:B:234:VAL:O	1:B:234:VAL:HG13	2.19	0.41
1:D:231:GLU:HG3	4:D:526:HOH:O	2.19	0.41
1:B:97:ILE:HG13	1:C:170:GLU:OE2	2.20	0.41
1:D:132:ARG:HH11	1:D:132:ARG:CB	2.29	0.41
1:C:194:VAL:HG21	3:C:2401:AOI:C19	2.49	0.41
1:A:234:VAL:HG13	1:A:234:VAL:O	2.21	0.41
1:C:194:VAL:HG11	3:C:2401:AOI:H30	2.02	0.41
1:B:171:LEU:HB3	1:B:176:ILE:HB	2.02	0.41
1:D:92:LEU:HD21	3:D:3401:AOI:H11	2.02	0.41
1:C:171:LEU:HB3	1:C:176:ILE:HB	2.01	0.41
1:A:33:LYS:HA	1:A:33:LYS:HD3	1.83	0.41
1:A:132:ARG:O	1:A:132:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:VAL:HG11	3:D:3401:AOI:H30	2.02	0.41
1:B:34:VAL:O	1:B:55:ALA:HA	2.21	0.40
1:A:130:ALA:HB1	1:A:132:ARG:HH22	1.87	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	242/260 (93%)	232 (96%)	10 (4%)	0	100	100
1	B	242/260 (93%)	232 (96%)	9 (4%)	1 (0%)	30	43
1	C	242/260 (93%)	232 (96%)	10 (4%)	0	100	100
1	D	242/260 (93%)	229 (95%)	12 (5%)	1 (0%)	30	43
All	All	968/1040 (93%)	925 (96%)	41 (4%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	ALA
1	D	52	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/196 (93%)	178 (98%)	4 (2%)	45	67
1	B	182/196 (93%)	178 (98%)	4 (2%)	45	67
1	C	182/196 (93%)	178 (98%)	4 (2%)	45	67
1	D	182/196 (93%)	179 (98%)	3 (2%)	55	76
All	All	728/784 (93%)	713 (98%)	15 (2%)	47	69

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	132	ARG
1	A	150	CYS
1	A	198	ILE
1	B	42	GLU
1	B	51	LEU
1	B	150	CYS
1	B	198	ILE
1	C	42	GLU
1	C	53	ASP
1	C	150	CYS
1	C	198	ILE
1	D	42	GLU
1	D	150	CYS
1	D	198	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	87	ASN
1	A	182	HIS
1	A	200	GLN
1	A	244	HIS
1	B	64	GLN
1	B	83	HIS
1	B	87	ASN
1	B	88	ASN
1	B	182	HIS
1	B	244	HIS
1	C	59	HIS

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Mol	Chain	Res	Type
1	C	83	HIS
1	C	87	ASN
1	C	106	GLN
1	C	182	HIS
1	C	200	GLN
1	C	244	HIS
1	D	83	HIS
1	D	87	ASN
1	D	88	ASN
1	D	182	HIS
1	D	200	GLN
1	D	244	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AOI	D	3401	-	24,24,24	7.13	21 (87%)	39,39,39	5.12	26 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAI	C	2300	-	47,48,48	1.20	5 (10%)	64,73,73	1.12	5 (7%)
3	AOI	A	401	-	24,24,24	7.15	21 (87%)	39,39,39	5.14	26 (66%)
3	AOI	B	1401	-	24,24,24	7.14	21 (87%)	39,39,39	5.15	26 (66%)
2	NAI	B	1300	-	47,48,48	1.27	5 (10%)	64,73,73	1.20	5 (7%)
2	NAI	A	300	-	47,48,48	1.26	4 (8%)	64,73,73	1.08	4 (6%)
2	NAI	D	3300	-	47,48,48	1.16	3 (6%)	64,73,73	1.06	4 (6%)
3	AOI	C	2401	-	24,24,24	7.13	21 (87%)	39,39,39	5.16	26 (66%)

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	AOI	D	3401	-	2/2/8/8	-	0/4/4/4
2	NAI	C	2300	-	-	2/29/72/72	0/5/5/5
3	AOI	B	1401	-	2/2/8/8	-	0/4/4/4
3	AOI	A	401	-	2/2/8/8	-	0/4/4/4
2	NAI	B	1300	-	-	5/29/72/72	0/5/5/5
2	NAI	A	300	-	-	3/29/72/72	0/5/5/5
2	NAI	D	3300	-	-	3/29/72/72	0/5/5/5
3	AOI	C	2401	-	2/2/8/8	-	0/4/4/4

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1401	AOI	O17-C17	14.27	1.43	1.21
3	D	3401	AOI	O17-C17	14.22	1.43	1.21
3	C	2401	AOI	O17-C17	14.15	1.43	1.21
3	A	401	AOI	O17-C17	14.13	1.43	1.21
3	A	401	AOI	C11-C9	13.06	1.75	1.53
3	B	1401	AOI	C11-C9	12.94	1.75	1.53
3	C	2401	AOI	C11-C9	12.87	1.75	1.53
3	D	3401	AOI	C11-C9	12.86	1.74	1.53
3	C	2401	AOI	C8-C9	11.07	1.74	1.53
3	D	3401	AOI	C8-C9	11.01	1.74	1.53
3	B	1401	AOI	C8-C9	11.01	1.74	1.53
3	A	401	AOI	C8-C9	10.97	1.74	1.53
3	D	3401	AOI	C16-C17	9.27	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	AOI	C16-C17	9.27	1.66	1.51
3	C	2401	AOI	C16-C17	9.23	1.66	1.51
3	B	1401	AOI	C16-C17	9.22	1.66	1.51
3	A	401	AOI	C10-C9	8.98	1.71	1.56
3	B	1401	AOI	C1-C2	8.94	1.71	1.53
3	C	2401	AOI	C10-C9	8.92	1.71	1.56
3	A	401	AOI	C1-C2	8.90	1.71	1.53
3	B	1401	AOI	C10-C9	8.86	1.71	1.56
3	D	3401	AOI	C10-C9	8.86	1.71	1.56
3	C	2401	AOI	C1-C2	8.85	1.71	1.53
3	D	3401	AOI	C1-C2	8.84	1.71	1.53
3	C	2401	AOI	C15-C14	8.55	1.71	1.54
3	D	3401	AOI	C15-C14	8.54	1.71	1.54
3	A	401	AOI	C15-C14	8.51	1.71	1.54
3	B	1401	AOI	C15-C14	8.43	1.71	1.54
3	D	3401	AOI	C12-C13	7.91	1.68	1.54
3	C	2401	AOI	C18-C13	7.90	1.67	1.54
3	B	1401	AOI	C12-C13	7.90	1.68	1.54
3	D	3401	AOI	C18-C13	7.88	1.67	1.54
3	B	1401	AOI	C18-C13	7.87	1.67	1.54
3	A	401	AOI	C18-C13	7.84	1.67	1.54
3	A	401	AOI	C12-C13	7.83	1.68	1.54
3	C	2401	AOI	C12-C13	7.74	1.68	1.54
3	D	3401	AOI	C12-C11	6.88	1.67	1.53
3	C	2401	AOI	C12-C11	6.80	1.67	1.53
3	B	1401	AOI	C12-C11	6.76	1.66	1.53
3	A	401	AOI	C12-C11	6.75	1.66	1.53
3	D	3401	AOI	C15-C16	6.15	1.67	1.53
3	A	401	AOI	C15-C16	6.14	1.67	1.53
3	B	1401	AOI	C15-C16	6.14	1.67	1.53
3	C	2401	AOI	C15-C16	6.13	1.67	1.53
3	A	401	AOI	C19-C10	5.84	1.64	1.54
3	C	2401	AOI	C19-C10	5.77	1.63	1.54
3	D	3401	AOI	C8-C14	5.71	1.64	1.53
3	B	1401	AOI	C19-C10	5.69	1.63	1.54
3	C	2401	AOI	C7-C6	5.69	1.66	1.52
3	C	2401	AOI	C8-C14	5.68	1.64	1.53
3	B	1401	AOI	C8-C14	5.64	1.64	1.53
3	A	401	AOI	C8-C14	5.63	1.64	1.53
3	A	401	AOI	C7-C6	5.63	1.66	1.52
3	D	3401	AOI	C19-C10	5.61	1.63	1.54
3	D	3401	AOI	C7-C6	5.59	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	AOI	C2-C3	5.58	1.64	1.51
3	B	1401	AOI	C7-C6	5.56	1.66	1.52
3	B	1401	AOI	C2-C3	5.51	1.64	1.51
3	D	3401	AOI	C2-C3	5.46	1.64	1.51
3	C	2401	AOI	C2-C3	5.43	1.64	1.51
3	A	401	AOI	C1-C10	5.41	1.63	1.54
3	C	2401	AOI	C1-C10	5.29	1.63	1.54
3	B	1401	AOI	C1-C10	5.25	1.63	1.54
3	D	3401	AOI	C1-C10	5.24	1.63	1.54
2	A	300	NAI	C2N-C3N	5.02	1.49	1.35
2	C	2300	NAI	C2N-C3N	4.95	1.48	1.35
2	B	1300	NAI	C2N-C3N	4.93	1.48	1.35
2	D	3300	NAI	C2N-C3N	4.88	1.48	1.35
3	C	2401	AOI	C4-C3	-4.09	1.44	1.52
3	A	401	AOI	C4-C3	-4.04	1.44	1.52
3	B	1401	AOI	C4-C3	-4.04	1.44	1.52
3	D	3401	AOI	C4-C3	-4.02	1.44	1.52
3	D	3401	AOI	C13-C17	3.90	1.57	1.52
3	B	1401	AOI	C13-C17	3.89	1.57	1.52
3	C	2401	AOI	C13-C17	3.83	1.57	1.52
3	A	401	AOI	C13-C17	3.80	1.57	1.52
3	D	3401	AOI	C10-C5	3.62	1.61	1.55
3	C	2401	AOI	C10-C5	3.61	1.61	1.55
3	A	401	AOI	C10-C5	3.61	1.61	1.55
3	B	1401	AOI	C10-C5	3.51	1.60	1.55
2	A	300	NAI	PN-O3	3.35	1.63	1.59
2	B	1300	NAI	PN-O3	2.99	1.62	1.59
2	D	3300	NAI	C6N-N1N	2.68	1.43	1.37
2	B	1300	NAI	C6N-N1N	2.67	1.43	1.37
2	C	2300	NAI	C6N-N1N	2.64	1.43	1.37
2	A	300	NAI	C6N-N1N	2.64	1.43	1.37
2	C	2300	NAI	C2A-N1A	2.46	1.38	1.33
2	B	1300	NAI	C2A-N1A	2.44	1.38	1.33
3	B	1401	AOI	C4-C5	2.42	1.57	1.53
3	A	401	AOI	C4-C5	2.42	1.57	1.53
2	B	1300	NAI	PA-O3	2.39	1.62	1.59
2	D	3300	NAI	C2A-N1A	2.38	1.38	1.33
2	A	300	NAI	C2A-N1A	2.36	1.38	1.33
3	B	1401	AOI	C13-C14	-2.31	1.50	1.54
3	A	401	AOI	C13-C14	-2.31	1.50	1.54
3	D	3401	AOI	C4-C5	2.31	1.57	1.53
3	C	2401	AOI	C4-C5	2.22	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2401	AOI	C13-C14	-2.22	1.50	1.54
2	C	2300	NAI	O4B-C1B	-2.17	1.37	1.42
3	D	3401	AOI	C13-C14	-2.16	1.50	1.54
2	C	2300	NAI	PN-O3	2.12	1.61	1.59

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1401	AOI	C4-C5-C10	12.99	126.48	112.66
3	A	401	AOI	C4-C5-C10	12.98	126.47	112.66
3	C	2401	AOI	C4-C5-C10	12.86	126.34	112.66
3	D	3401	AOI	C4-C5-C10	12.80	126.28	112.66
3	C	2401	AOI	C4-C3-C2	11.72	124.92	110.62
3	B	1401	AOI	C4-C3-C2	11.66	124.84	110.62
3	D	3401	AOI	C4-C3-C2	11.63	124.80	110.62
3	C	2401	AOI	C18-C13-C12	-11.42	98.05	111.10
3	A	401	AOI	C4-C3-C2	11.40	124.52	110.62
3	A	401	AOI	C18-C13-C12	-11.29	98.20	111.10
3	D	3401	AOI	C18-C13-C12	-11.24	98.26	111.10
3	B	1401	AOI	C18-C13-C12	-11.22	98.28	111.10
3	A	401	AOI	O17-C17-C13	-9.61	113.38	125.98
3	C	2401	AOI	O17-C17-C13	-9.58	113.42	125.98
3	D	3401	AOI	O17-C17-C13	-9.48	113.55	125.98
3	B	1401	AOI	O17-C17-C13	-9.44	113.60	125.98
3	C	2401	AOI	O17-C17-C16	-8.96	114.84	125.75
3	B	1401	AOI	O17-C17-C16	-8.92	114.89	125.75
3	A	401	AOI	O17-C17-C16	-8.80	115.04	125.75
3	D	3401	AOI	O17-C17-C16	-8.74	115.11	125.75
3	A	401	AOI	C15-C16-C17	-7.28	98.67	105.70
3	B	1401	AOI	C15-C16-C17	-7.25	98.70	105.70
3	B	1401	AOI	C1-C10-C9	7.20	122.53	111.34
3	D	3401	AOI	C1-C10-C9	7.20	122.52	111.34
3	C	2401	AOI	C15-C16-C17	-7.20	98.75	105.70
3	C	2401	AOI	C1-C10-C9	7.19	122.50	111.34
3	A	401	AOI	C1-C10-C9	7.15	122.44	111.34
3	D	3401	AOI	C15-C16-C17	-7.15	98.80	105.70
3	D	3401	AOI	C19-C10-C1	-6.80	97.50	108.31
3	A	401	AOI	C19-C10-C1	-6.72	97.63	108.31
3	B	1401	AOI	C19-C10-C1	-6.70	97.65	108.31
3	C	2401	AOI	C19-C10-C1	-6.57	97.86	108.31
3	A	401	AOI	C2-C1-C10	6.41	123.55	112.74
3	C	2401	AOI	C2-C1-C10	6.40	123.54	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1401	AOI	C2-C1-C10	6.39	123.52	112.74
3	D	3401	AOI	C2-C1-C10	6.28	123.34	112.74
3	B	1401	AOI	C7-C6-C5	5.12	121.75	111.84
3	A	401	AOI	C7-C6-C5	5.02	121.56	111.84
3	A	401	AOI	C5-C4-C3	5.02	120.28	112.71
3	C	2401	AOI	C7-C6-C5	4.98	121.48	111.84
3	D	3401	AOI	C7-C6-C5	4.95	121.43	111.84
3	C	2401	AOI	C5-C4-C3	4.88	120.07	112.71
3	D	3401	AOI	C5-C4-C3	4.87	120.05	112.71
3	B	1401	AOI	C19-C10-C5	-4.85	102.33	110.44
3	C	2401	AOI	C19-C10-C5	-4.84	102.35	110.44
3	B	1401	AOI	C5-C4-C3	4.83	119.99	112.71
3	D	3401	AOI	C19-C10-C5	-4.74	102.52	110.44
3	A	401	AOI	C19-C10-C5	-4.65	102.66	110.44
3	A	401	AOI	O3-C3-C2	4.52	121.98	110.17
3	A	401	AOI	C12-C11-C9	-4.49	105.51	113.14
3	B	1401	AOI	C12-C11-C9	-4.48	105.52	113.14
3	C	2401	AOI	O3-C3-C2	4.47	121.85	110.17
3	B	1401	AOI	O3-C3-C2	4.45	121.79	110.17
3	D	3401	AOI	C12-C11-C9	-4.44	105.58	113.14
3	B	1401	AOI	C14-C8-C9	4.38	114.81	109.09
3	D	3401	AOI	O3-C3-C2	4.38	121.61	110.17
3	D	3401	AOI	C14-C8-C9	4.37	114.79	109.09
3	A	401	AOI	C14-C8-C9	4.33	114.75	109.09
3	C	2401	AOI	C12-C11-C9	-4.32	105.79	113.14
2	B	1300	NAI	O7N-C7N-C3N	-4.32	112.77	120.90
2	C	2300	NAI	O7N-C7N-C3N	-4.25	112.90	120.90
3	C	2401	AOI	C14-C8-C9	4.24	114.63	109.09
2	B	1300	NAI	C3N-C7N-N7N	4.22	125.17	117.67
2	D	3300	NAI	O7N-C7N-C3N	-4.11	113.16	120.90
2	C	2300	NAI	C3N-C7N-N7N	4.09	124.93	117.67
2	A	300	NAI	O7N-C7N-C3N	-3.96	113.43	120.90
2	A	300	NAI	C3N-C7N-N7N	3.88	124.55	117.67
3	D	3401	AOI	C6-C5-C10	3.81	118.70	112.31
2	D	3300	NAI	C3N-C7N-N7N	3.81	124.43	117.67
3	C	2401	AOI	C6-C5-C10	3.73	118.56	112.31
3	A	401	AOI	C6-C5-C10	3.70	118.52	112.31
3	B	1401	AOI	C6-C5-C10	3.69	118.50	112.31
3	B	1401	AOI	C12-C13-C14	3.28	113.97	108.88
3	A	401	AOI	C12-C13-C14	3.27	113.96	108.88
3	C	2401	AOI	C12-C13-C14	3.18	113.81	108.88
3	A	401	AOI	C10-C9-C8	-3.16	109.22	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3401	AOI	C12-C13-C14	3.15	113.78	108.88
3	D	3401	AOI	C15-C14-C8	3.15	124.13	119.10
3	A	401	AOI	C15-C14-C8	3.12	124.08	119.10
3	C	2401	AOI	C15-C14-C8	3.11	124.07	119.10
3	B	1401	AOI	C7-C8-C14	-3.10	106.94	112.08
3	D	3401	AOI	C15-C14-C13	-3.09	101.42	104.08
3	A	401	AOI	C7-C8-C14	-3.07	106.97	112.08
3	C	2401	AOI	C10-C9-C8	-3.07	109.31	112.43
3	B	1401	AOI	C15-C14-C8	3.07	123.99	119.10
3	C	2401	AOI	C15-C14-C13	-3.05	101.46	104.08
3	D	3401	AOI	C7-C8-C14	-3.02	107.06	112.08
3	D	3401	AOI	C10-C9-C8	-3.02	109.36	112.43
3	B	1401	AOI	C10-C9-C8	-2.97	109.42	112.43
3	C	2401	AOI	C11-C9-C8	-2.96	107.65	111.78
3	A	401	AOI	C15-C14-C13	-2.92	101.58	104.08
3	C	2401	AOI	C7-C8-C14	-2.90	107.25	112.08
3	B	1401	AOI	C15-C14-C13	-2.90	101.59	104.08
3	A	401	AOI	C11-C9-C8	-2.87	107.77	111.78
3	B	1401	AOI	C11-C9-C8	-2.86	107.79	111.78
2	B	1300	NAI	O1N-PN-O3	2.80	114.84	107.27
3	D	3401	AOI	C11-C9-C8	-2.78	107.90	111.78
3	C	2401	AOI	C18-C13-C17	2.75	110.26	105.18
2	A	300	NAI	O1N-PN-O3	2.75	114.71	107.27
3	B	1401	AOI	C18-C13-C17	2.71	110.18	105.18
3	C	2401	AOI	C9-C10-C5	2.71	112.27	108.51
2	B	1300	NAI	O5B-C5B-C4B	-2.69	99.82	108.99
3	A	401	AOI	C18-C13-C17	2.67	110.11	105.18
2	D	3300	NAI	O5B-C5B-C4B	-2.57	100.24	108.99
3	B	1401	AOI	C9-C10-C5	2.56	112.06	108.51
3	D	3401	AOI	C18-C13-C17	2.55	109.89	105.18
2	C	2300	NAI	O1N-PN-O3	2.51	114.06	107.27
3	A	401	AOI	C9-C10-C5	2.50	111.99	108.51
3	B	1401	AOI	C16-C17-C13	-2.50	106.07	108.56
2	B	1300	NAI	O2A-PA-O3	2.49	114.02	107.27
2	D	3300	NAI	O1N-PN-O3	2.48	113.98	107.27
3	D	3401	AOI	C16-C17-C13	-2.48	106.09	108.56
3	D	3401	AOI	C18-C13-C14	2.48	116.54	112.99
3	C	2401	AOI	C18-C13-C14	2.45	116.51	112.99
2	C	2300	NAI	O5B-C5B-C4B	-2.45	100.67	108.99
3	B	1401	AOI	C18-C13-C14	2.44	116.49	112.99
3	D	3401	AOI	C9-C10-C5	2.41	111.86	108.51
3	C	2401	AOI	C16-C17-C13	-2.40	106.17	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	AOI	C16-C17-C13	-2.39	106.18	108.56
3	A	401	AOI	C18-C13-C14	2.38	116.41	112.99
2	A	300	NAI	O5B-C5B-C4B	-2.37	100.94	108.99
2	C	2300	NAI	O4D-C1D-N1N	2.05	111.99	108.08

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	401	AOI	C5
3	A	401	AOI	C3
3	B	1401	AOI	C5
3	B	1401	AOI	C3
3	C	2401	AOI	C5
3	C	2401	AOI	C3
3	D	3401	AOI	C5
3	D	3401	AOI	C3

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1300	NAI	C5D-O5D-PN-O2N
2	A	300	NAI	O4D-C1D-N1N-C6N
2	D	3300	NAI	O4D-C1D-N1N-C6N
2	B	1300	NAI	C5D-O5D-PN-O3
2	B	1300	NAI	C5D-O5D-PN-O1N
2	C	2300	NAI	O4D-C1D-N1N-C6N
2	B	1300	NAI	O4D-C1D-N1N-C6N
2	A	300	NAI	C2N-C3N-C7N-N7N
2	B	1300	NAI	C2N-C3N-C7N-N7N
2	C	2300	NAI	C2N-C3N-C7N-N7N
2	D	3300	NAI	C2N-C3N-C7N-N7N
2	A	300	NAI	C2B-C1B-N9A-C8A
2	D	3300	NAI	C2B-C1B-N9A-C8A

There are no ring outliers.

7 monomers are involved in 14 short contacts:

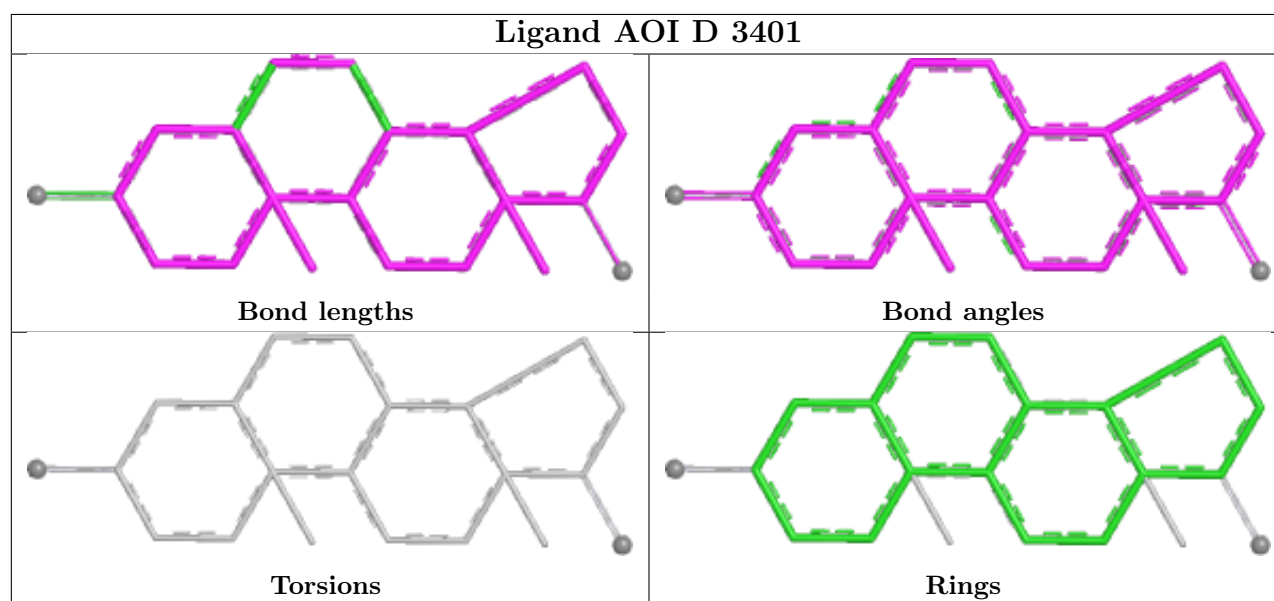
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3401	AOI	4	0
2	C	2300	NAI	1	0
3	B	1401	AOI	1	0

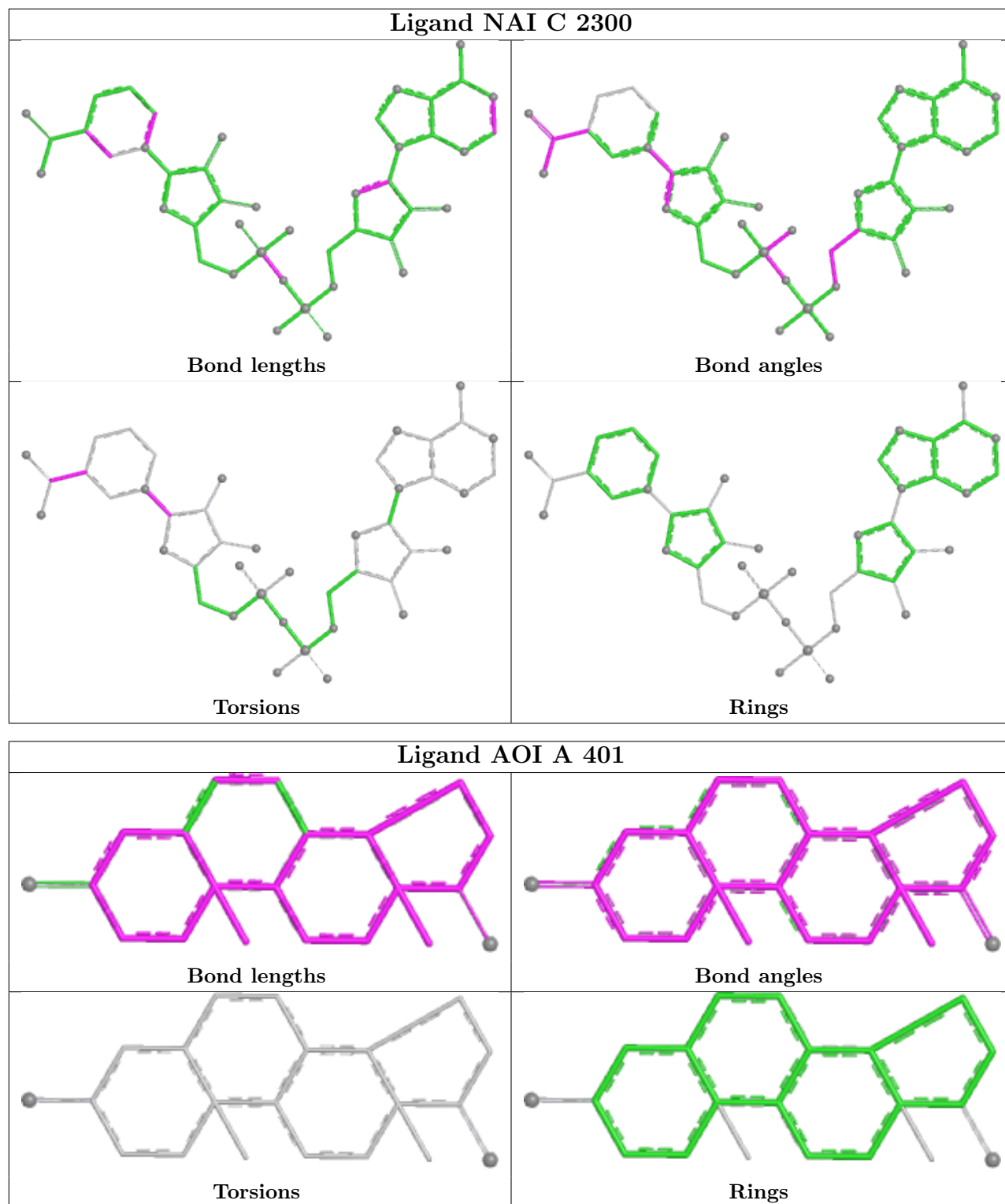
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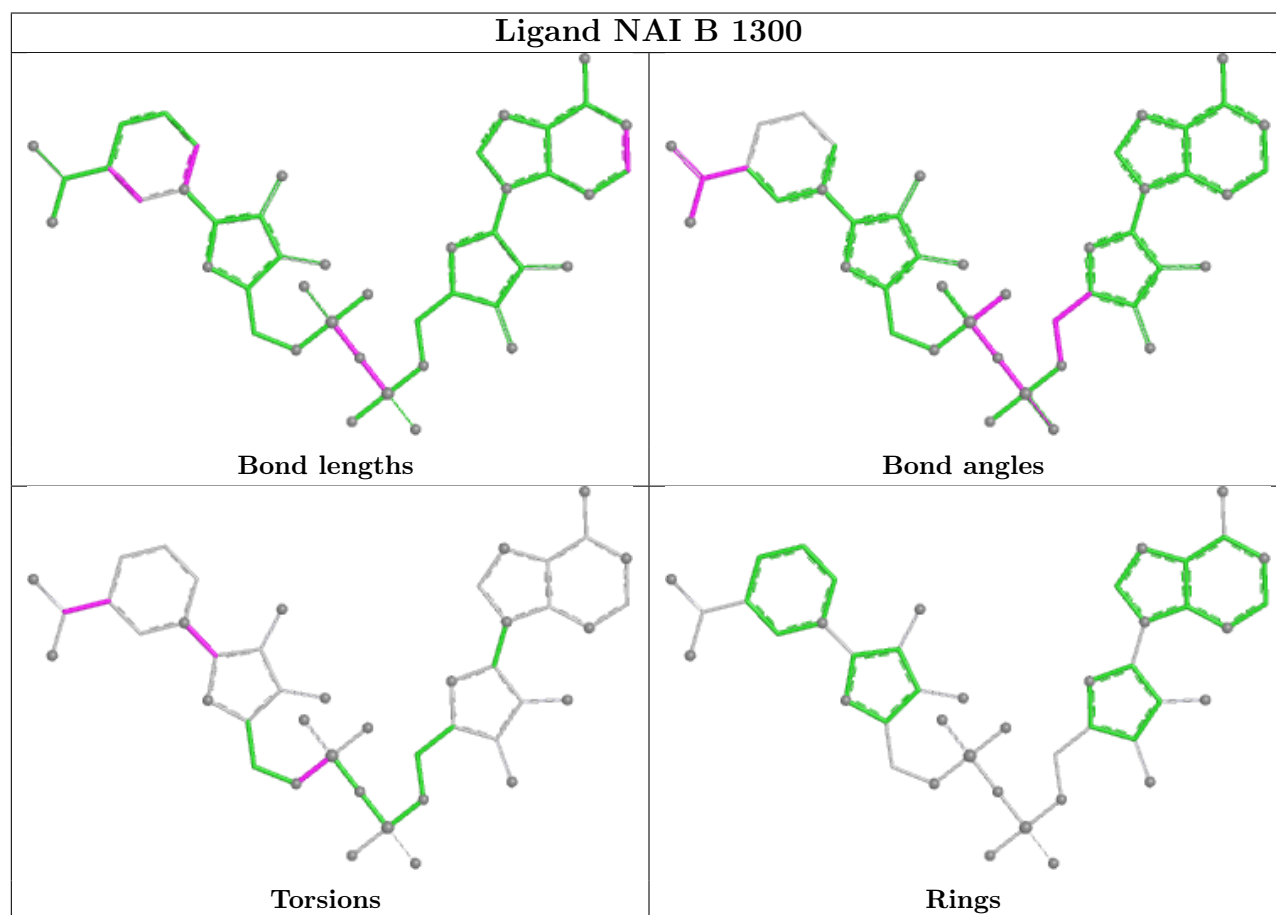
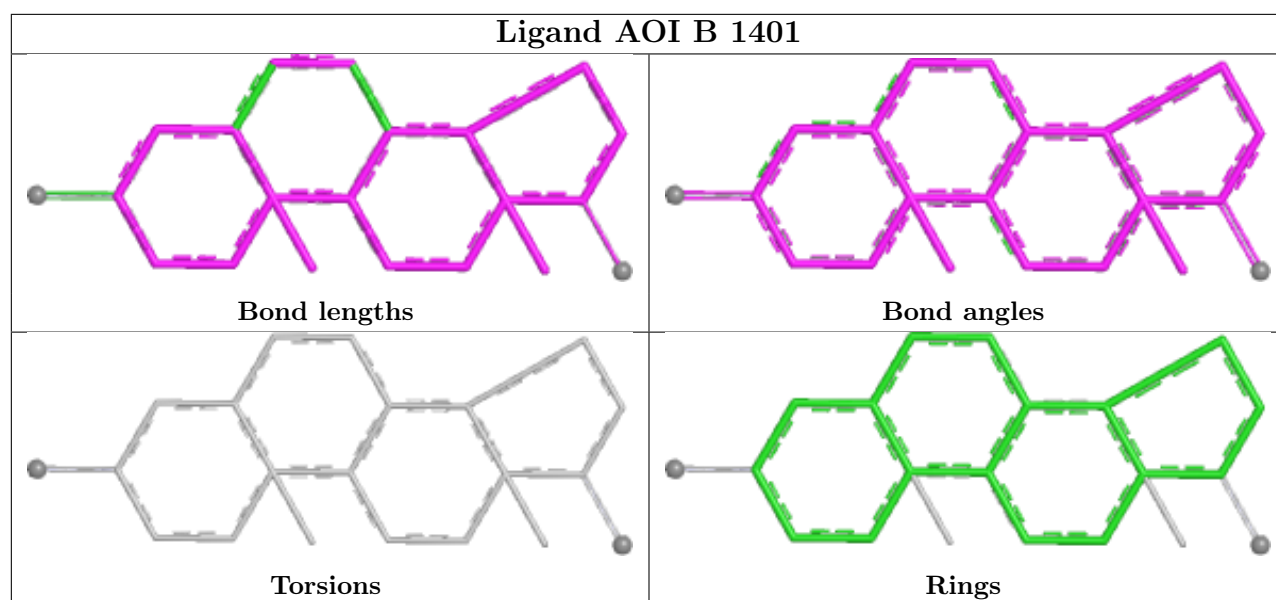
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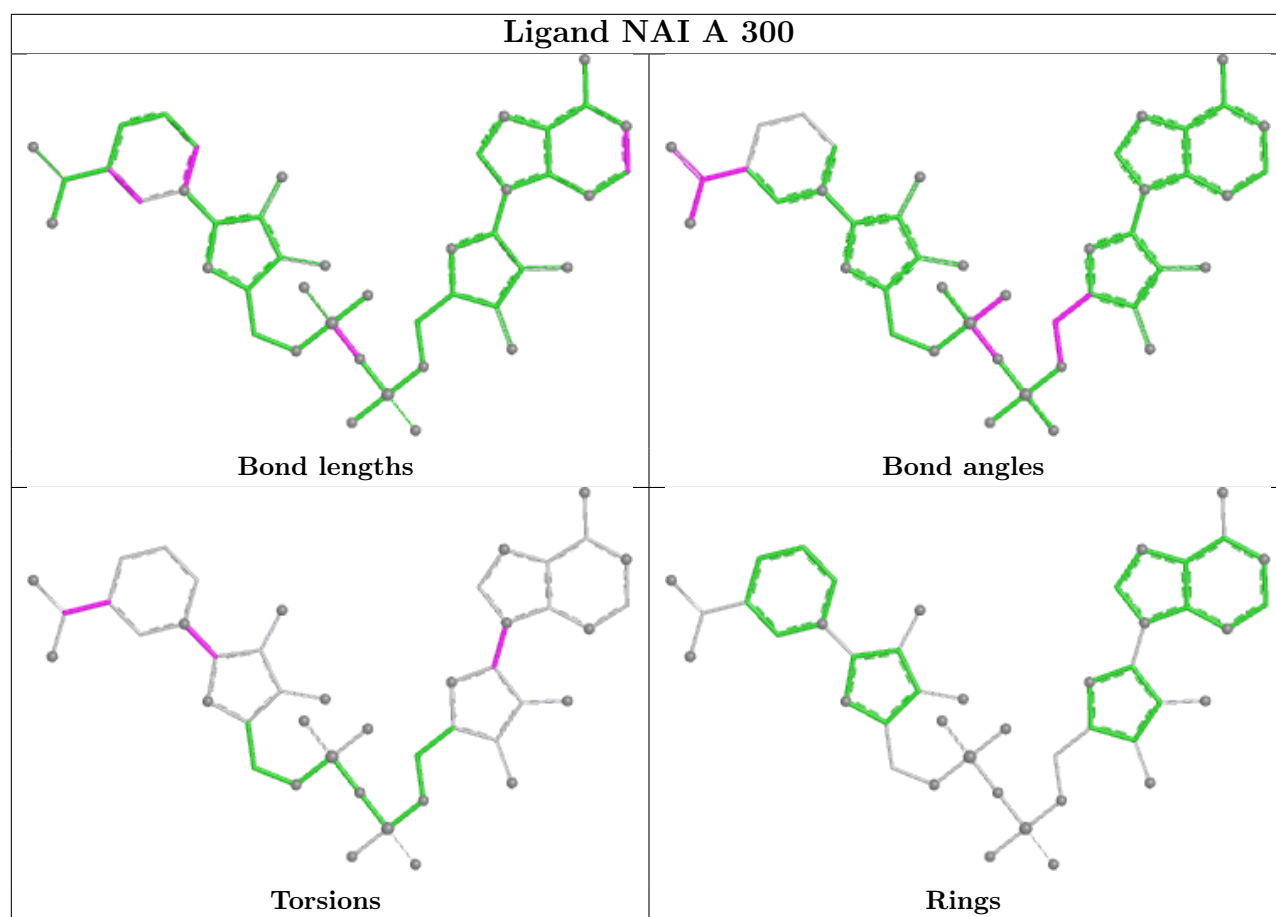
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1300	NAI	2	0
2	A	300	NAI	1	0
2	D	3300	NAI	2	0
3	C	2401	AOI	3	0

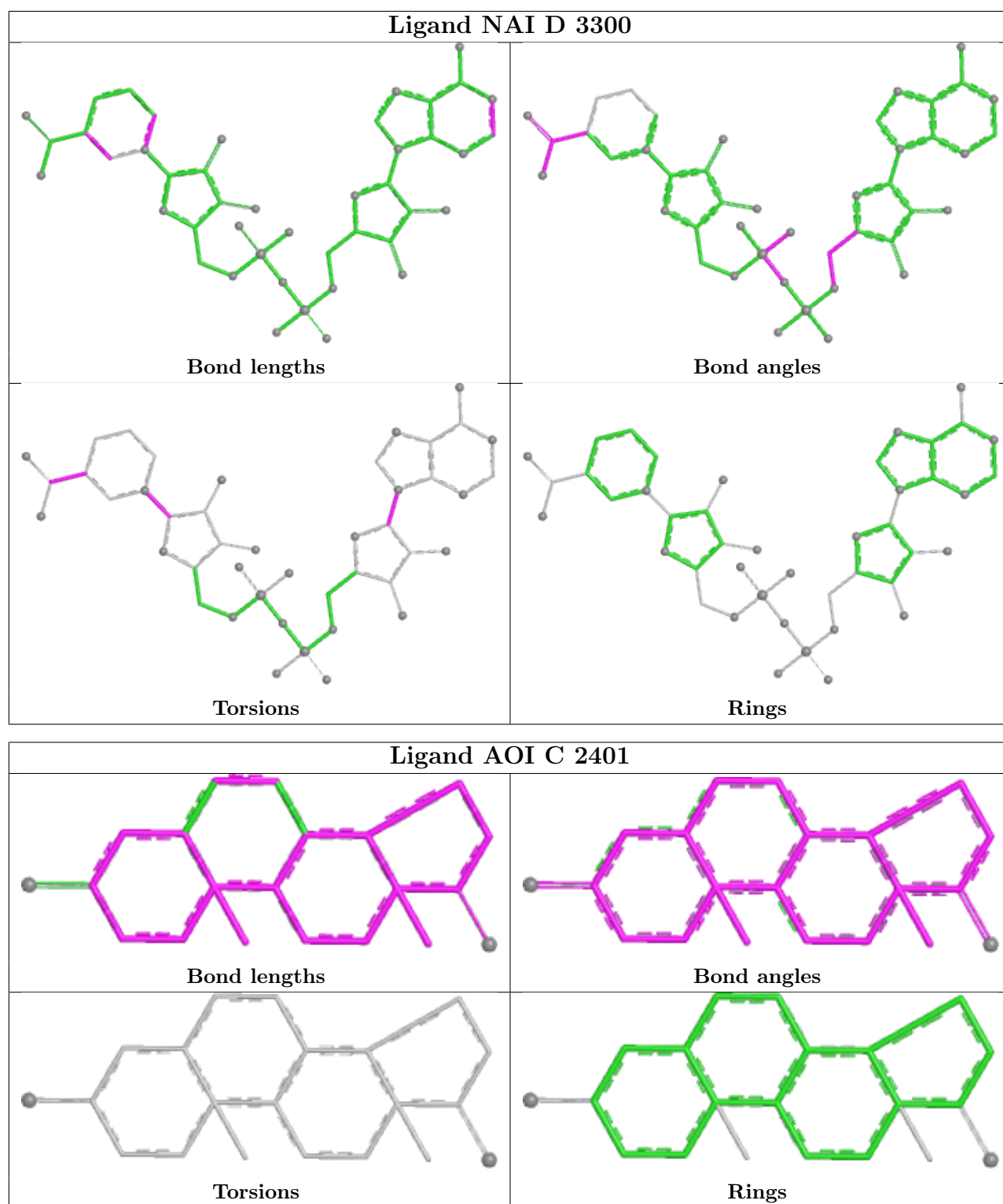
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	244/260 (93%)	-0.37	1 (0%) 88 86	24, 35, 60, 80	0
1	B	244/260 (93%)	-0.61	2 (0%) 82 80	20, 30, 53, 68	0
1	C	244/260 (93%)	-0.51	1 (0%) 88 86	22, 34, 55, 68	0
1	D	244/260 (93%)	-0.43	1 (0%) 88 86	24, 36, 59, 72	0
All	All	976/1040 (93%)	-0.48	5 (0%) 87 85	20, 34, 59, 80	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	SER	3.1
1	A	132	ARG	2.9
1	C	2	SER	2.8
1	B	42	GLU	2.4
1	D	2	SER	2.2

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.

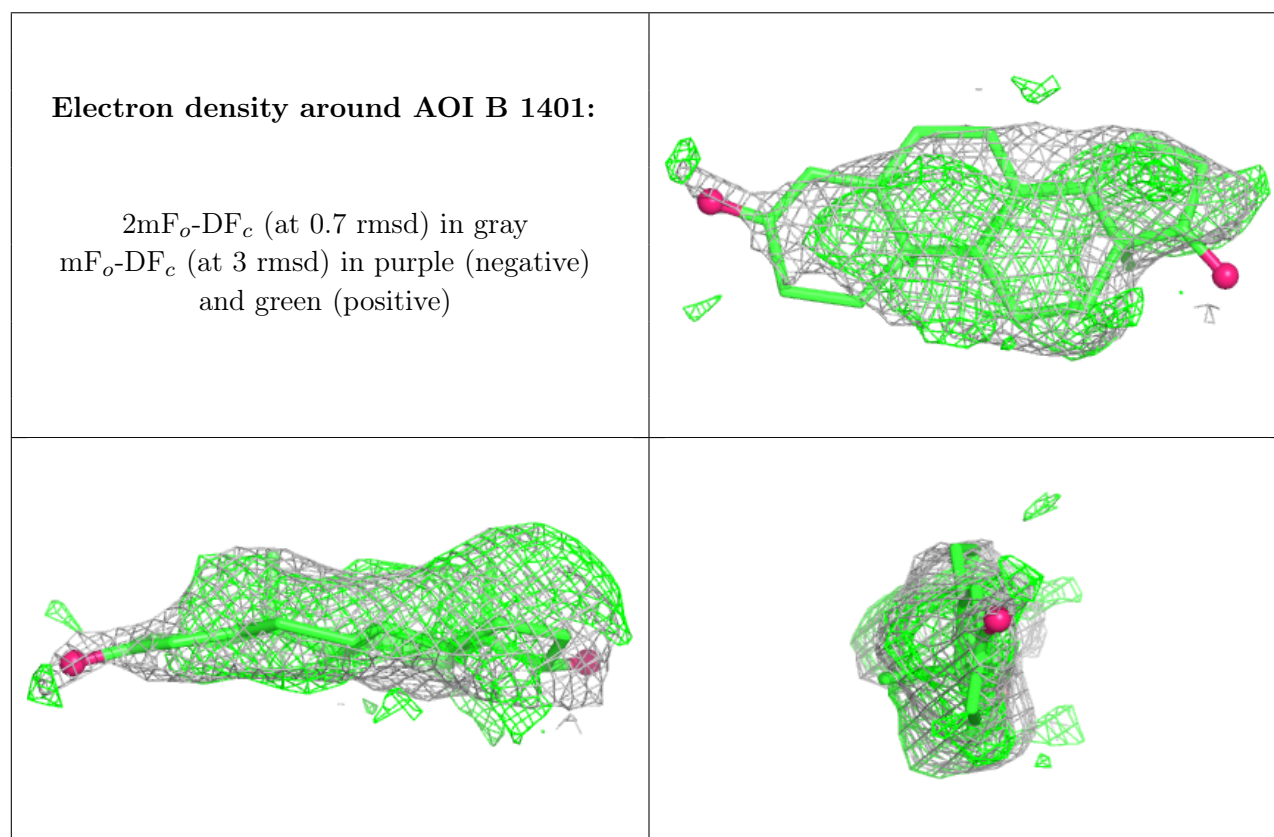
6.4 Ligands [i](#)

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.

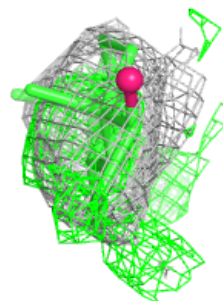
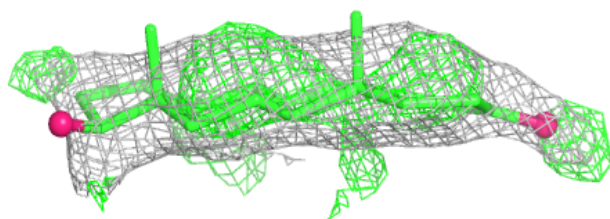
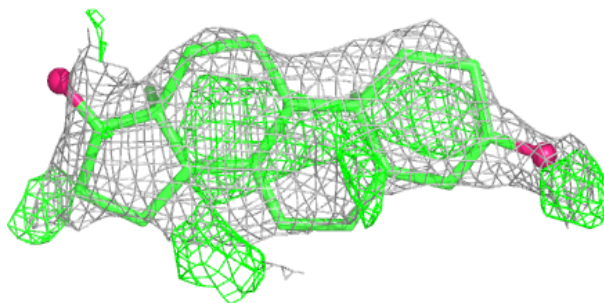
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AOI	B	1401	21/21	0.78	0.30	52,53,54,58	21
3	AOI	A	401	21/21	0.80	0.25	49,52,54,54	21
3	AOI	D	3401	21/21	0.84	0.26	51,53,54,54	21
3	AOI	C	2401	21/21	0.86	0.28	51,52,54,54	21
2	NAI	A	300	44/44	0.93	0.08	38,45,48,52	0
2	NAI	D	3300	44/44	0.94	0.08	37,46,50,51	0
2	NAI	C	2300	44/44	0.96	0.06	34,39,44,46	0
2	NAI	B	1300	44/44	0.97	0.05	25,30,35,37	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.

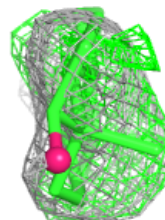
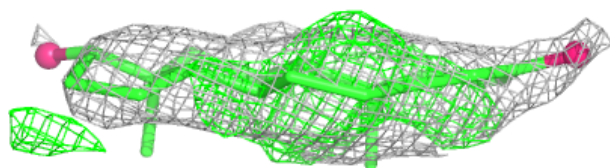
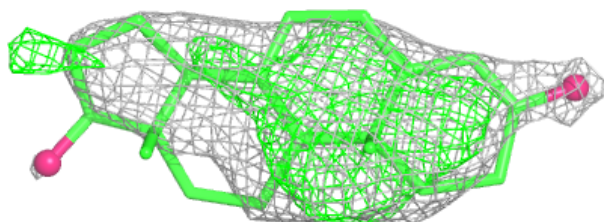


Electron density around AOI A 401:

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

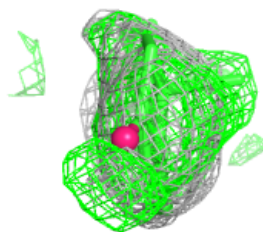
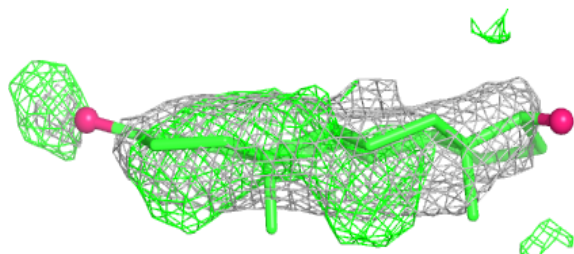
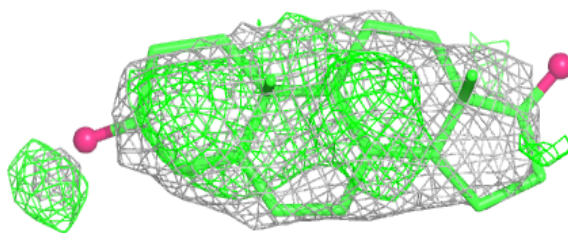
**Electron density around AOI D 3401:**

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

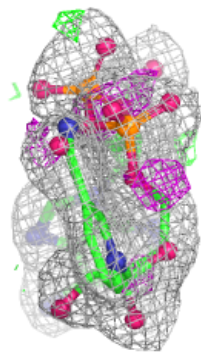
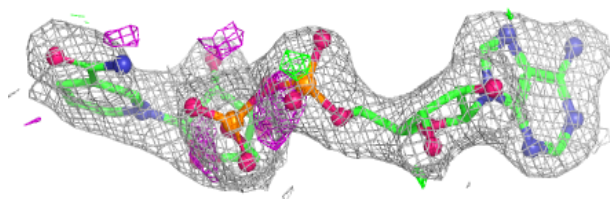
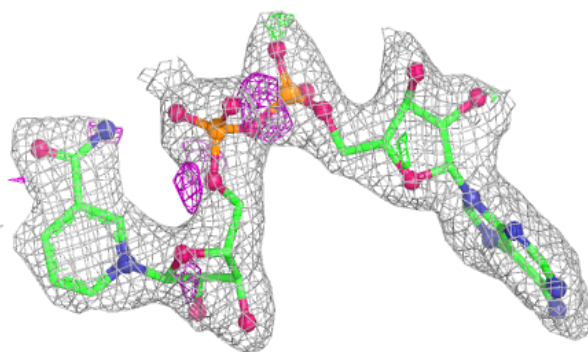


Electron density around AOI C 2401:

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

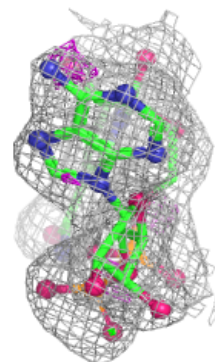
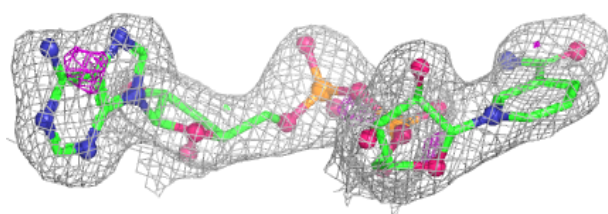
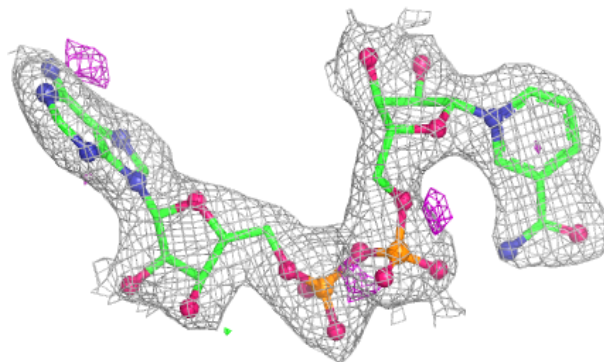
**Electron density around NAI A 300:**

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

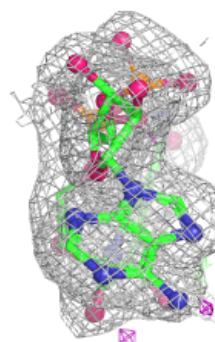
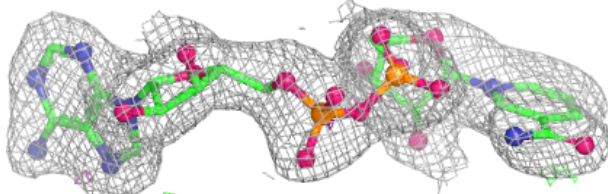
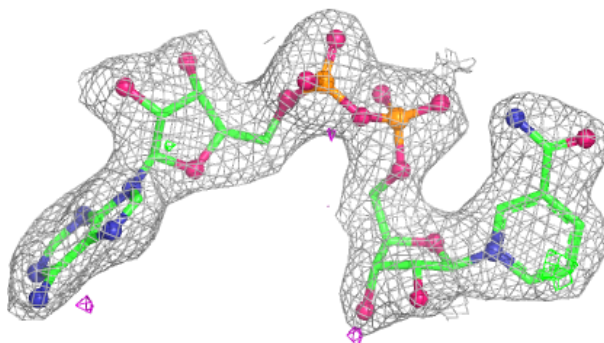


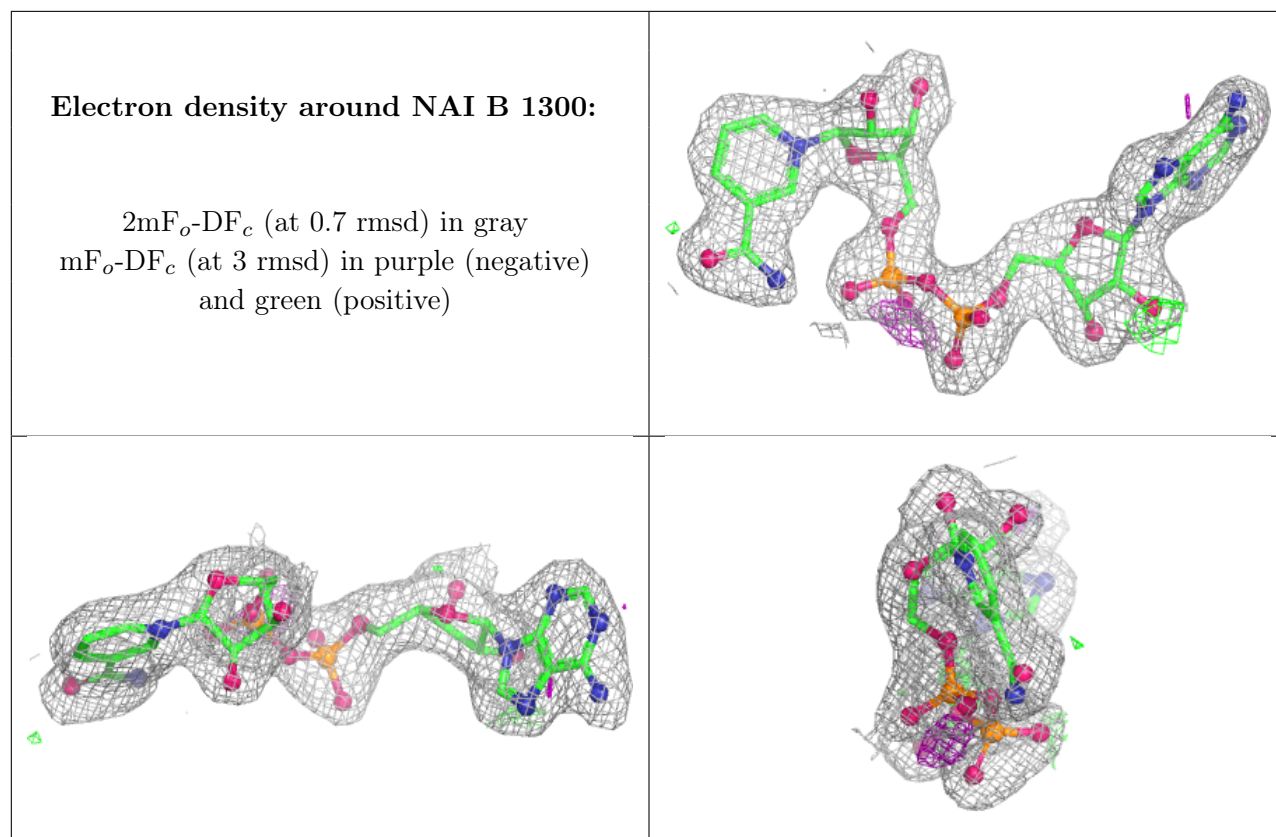
Electron density around NAI D 3300:

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

**Electron density around NAI C 2300:**

$2mF_o-DF_c$ (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.