



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:17 PM UTC

PDB ID : 7OSN / pdb_00007osn
Title : IRED361 from Micromonospora sp. in complex with NADP+
Authors : Gilio, A.K.; Harawa, V.; Turner, N.; Grogan, G.J.
Deposited on : 2021-06-09
Resolution : 2.55 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

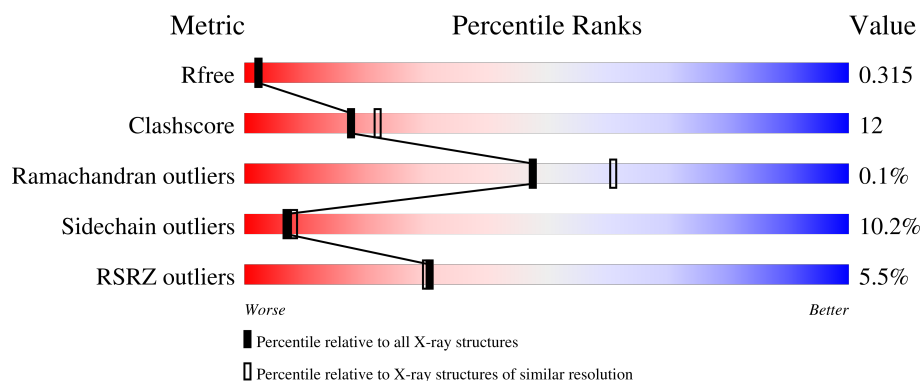
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	297	2% 69% 26% ..
1	B	297	71% 24% ..
1	C	297	2% 72% 21% ..
1	D	297	4% 75% 20% ..
1	E	297	15% 76% 18% ..

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Mol	Chain	Length	Quality of chain
1	F	297	9% 74% 20%

2 Entry composition ⓘ

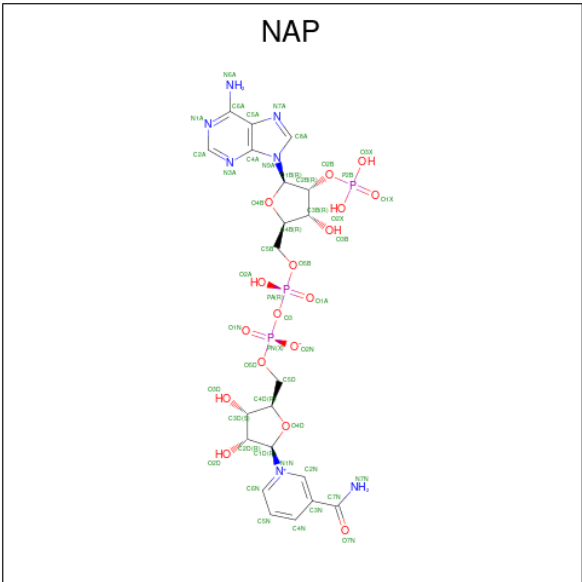
There are 3 unique types of molecules in this entry. The entry contains 12963 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-phosphogluconate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2124	1348	354	413	9			
1	B	291	Total	C	N	O	S	0	0	0
			2112	1346	353	404	9			
1	C	290	Total	C	N	O	S	0	0	0
			2125	1349	356	411	9			
1	D	290	Total	C	N	O	S	0	0	0
			2116	1343	355	409	9			
1	E	289	Total	C	N	O	S	0	0	0
			2002	1254	347	392	9			
1	F	289	Total	C	N	O	S	0	0	0
			2032	1278	350	396	8			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

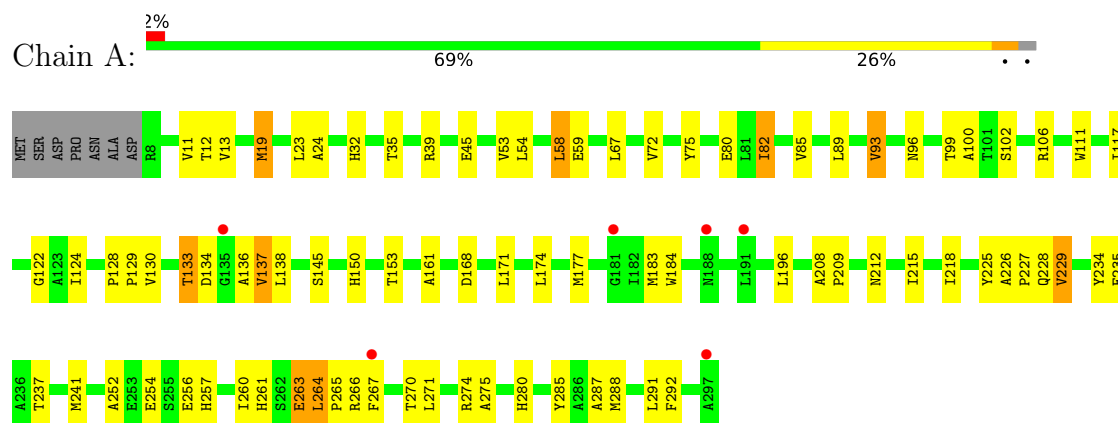
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	41	Total	O	0	0
			41	41		
3	C	43	Total	O	0	0
			43	43		
3	D	30	Total	O	0	0
			30	30		
3	E	10	Total	O	0	0
			10	10		
3	F	11	Total	O	0	0
			11	11		

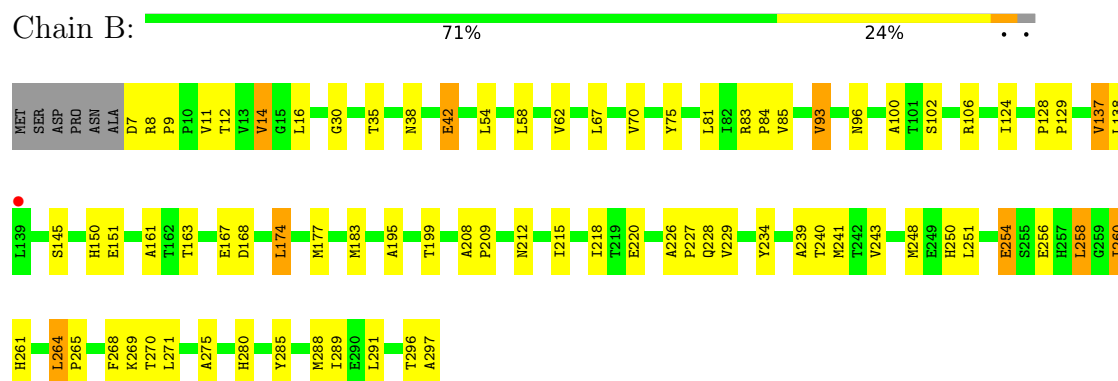
3 Residue-property plots

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.

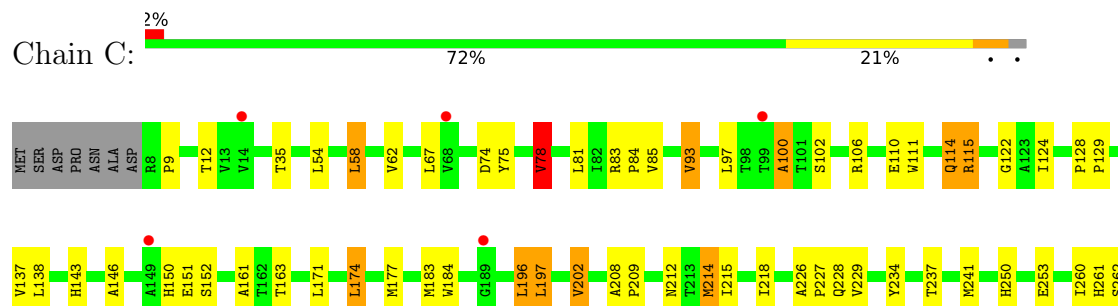
• Molecule 1: 6-phosphogluconate dehydrogenase



• Molecule 1: 6-phosphogluconate dehydrogenase

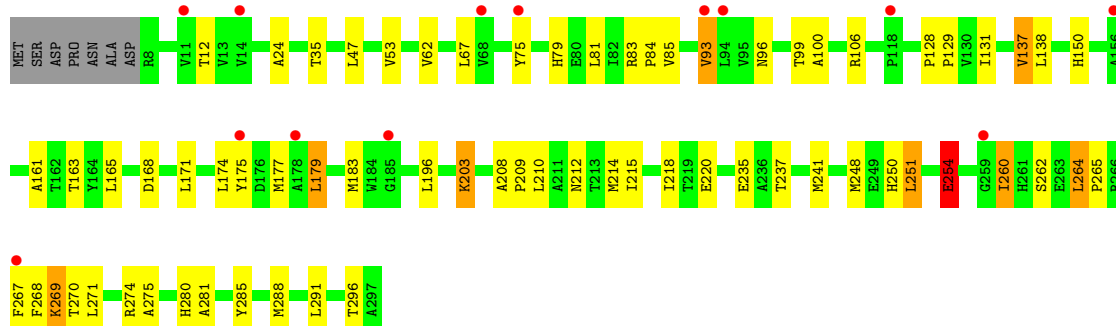
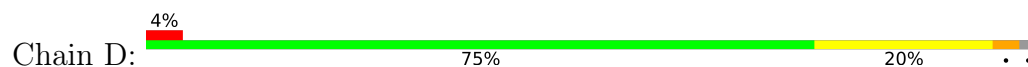


• Molecule 1: 6-phosphogluconate dehydrogenase

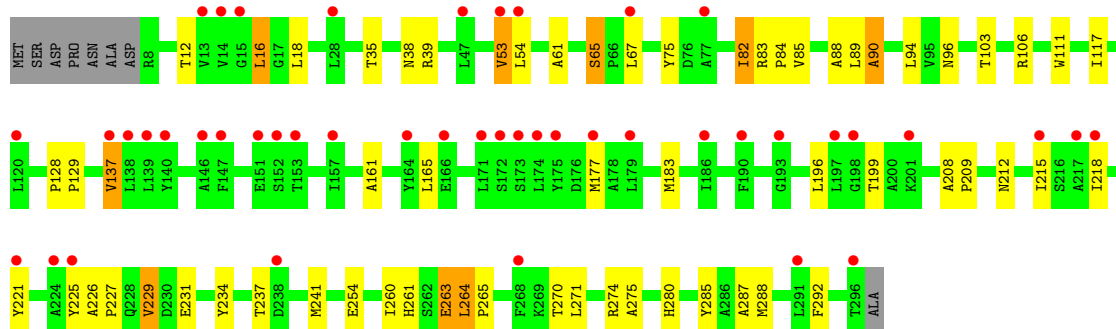
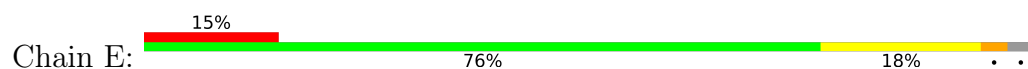




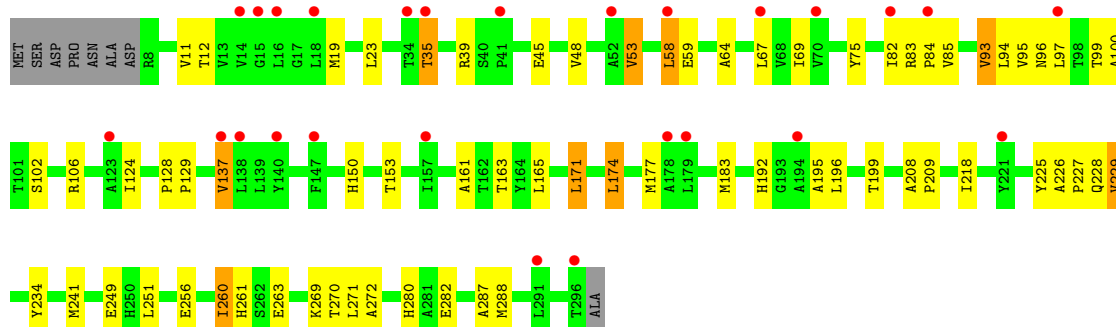
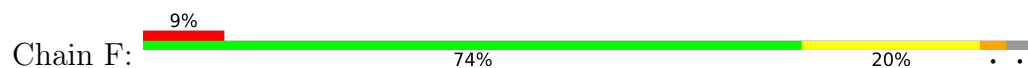
• Molecule 1: 6-phosphogluconate dehydrogenase



• Molecule 1: 6-phosphogluconate dehydrogenase



• Molecule 1: 6-phosphogluconate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	50.00Å 142.00Å 266.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.55 50.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.55) 99.5 (50.00-2.55)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.260 , 0.307 0.279 , 0.315	Depositor DCC
R_{free} test set	3270 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.976	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12963	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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: NAP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	1/2170 (0.0%)	1.54	0/2973
1	B	1.06	0/2158	1.57	1/2959 (0.0%)
1	C	1.05	1/2171 (0.0%)	1.54	3/2975 (0.1%)
1	D	1.06	0/2161	1.54	1/2961 (0.0%)
1	E	1.08	0/2046	1.58	1/2811 (0.0%)
1	F	1.09	0/2077	1.58	1/2854 (0.0%)
All	All	1.07	2/12783 (0.0%)	1.56	7/17533 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	9	PRO	C-O	-5.34	1.20	1.24
1	A	117	ILE	N-CA	5.10	1.50	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	GLU	CB-CG-CD	8.50	127.06	112.60
1	C	9	PRO	N-CA-C	7.46	118.56	110.58
1	E	117	ILE	CA-C-O	-5.95	116.83	120.88
1	C	78	VAL	N-CA-CB	5.47	116.95	110.55
1	C	100	ALA	N-CA-C	5.37	117.01	108.79
1	F	99	THR	CB-CA-C	5.19	119.10	109.54
1	D	254	GLU	CB-CG-CD	5.02	121.14	112.60

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	2124	0	2058	61	0
1	B	2112	0	2044	66	0
1	C	2125	0	2064	54	0
1	D	2116	0	2062	59	0
1	E	2002	0	1800	47	0
1	F	2032	0	1865	54	0
2	A	48	0	25	5	0
2	B	48	0	25	2	0
2	C	48	0	25	1	0
2	D	48	0	25	0	0
2	E	48	0	25	0	0
2	F	48	0	25	2	0
3	A	29	0	0	3	0
3	B	41	0	0	2	0
3	C	43	0	0	1	0
3	D	30	0	0	1	0
3	E	10	0	0	1	0
3	F	11	0	0	0	0
All	All	12963	0	12043	309	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 12.

All (309) 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:A:19:MET:HE2	1:A:124:ILE:HD13	1.31	1.08
1:F:19:MET:O	1:F:23:LEU:HD12	1.69	0.93
1:F:69:ILE:HD13	1:F:95:VAL:HB	1.54	0.87
1:A:82:ILE:HG13	1:A:89:LEU:HD11	1.58	0.84
1:B:241:MET:HE1	1:B:285:TYR:HA	1.59	0.84
1:B:240:THR:O	1:B:243:VAL:HG22	1.78	0.83
1:B:271:LEU:HB3	1:B:288:MET:HE1	1.61	0.82
1:E:241:MET:HE1	1:E:285:TYR:HA	1.61	0.82
1:B:248:MET:CE	1:B:269:LYS:HA	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:PHE:CD2	1:F:192:HIS:HB2	2.14	0.82
1:E:12:THR:HG21	1:E:61:ALA:O	1.80	0.81
1:D:288:MET:CE	1:D:291:LEU:HD23	2.11	0.81
1:E:12:THR:HG22	1:E:35:THR:HB	1.61	0.81
1:C:241:MET:HE1	1:C:285:TYR:HA	1.63	0.80
1:D:274:ARG:NH2	1:D:291:LEU:HD11	1.96	0.80
1:D:241:MET:HE1	1:D:285:TYR:HA	1.65	0.79
1:D:248:MET:CE	1:D:269:LYS:HA	2.14	0.78
1:D:214:MET:HE2	1:D:214:MET:HA	1.64	0.78
1:F:124:ILE:O	2:F:301:NAP:H5N	1.83	0.78
1:C:196:LEU:HD12	1:C:260:ILE:HD11	1.65	0.78
1:A:13:VAL:HG21	1:A:24:ALA:HB2	1.66	0.77
1:A:274:ARG:CZ	1:A:291:LEU:HD11	2.14	0.77
1:A:241:MET:HE1	1:A:285:TYR:HA	1.65	0.77
1:C:214:MET:HG3	1:D:179:LEU:HG	1.65	0.76
1:F:196:LEU:O	1:F:199:THR:HG22	1.85	0.76
1:E:218:ILE:HD12	1:F:183:MET:HG3	1.68	0.76
1:E:226:ALA:HB3	1:E:227:PRO:HD3	1.67	0.76
1:B:264:LEU:HB3	1:B:265:PRO:HD3	1.68	0.75
1:C:75:TYR:HA	1:C:78:VAL:HG13	1.68	0.74
1:A:274:ARG:NH2	1:A:291:LEU:HD11	2.03	0.74
1:B:226:ALA:HB3	1:B:227:PRO:HD3	1.70	0.73
1:A:271:LEU:HB3	1:A:288:MET:HE1	1.72	0.72
1:F:82:ILE:CD1	1:F:94:LEU:HD22	2.20	0.72
1:F:82:ILE:HD11	1:F:94:LEU:HD22	1.69	0.71
1:E:177:MET:HA	1:E:177:MET:HE2	1.71	0.71
1:D:271:LEU:O	1:D:288:MET:HE1	1.90	0.71
1:A:130:VAL:O	1:A:136:ALA:HB2	1.91	0.71
1:F:271:LEU:HB3	1:F:288:MET:HE1	1.74	0.70
1:B:75:TYR:CE1	1:B:100:ALA:HB2	2.27	0.70
1:B:199:THR:OG1	1:B:258:LEU:HD13	1.91	0.69
1:B:177:MET:HE2	1:B:177:MET:HA	1.73	0.69
1:C:197:LEU:HB3	1:C:202:VAL:HG22	1.74	0.69
1:D:288:MET:HE2	1:D:291:LEU:HD23	1.74	0.69
1:F:75:TYR:CE1	1:F:100:ALA:HB2	2.28	0.69
1:F:177:MET:HE2	1:F:177:MET:HA	1.73	0.69
1:A:75:TYR:CE1	1:A:100:ALA:HB2	2.28	0.69
1:A:177:MET:HE2	1:A:177:MET:HA	1.75	0.69
1:D:75:TYR:CE1	1:D:100:ALA:HB2	2.27	0.69
1:D:248:MET:HE3	1:D:269:LYS:HA	1.75	0.68
1:C:197:LEU:O	1:C:202:VAL:HG13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:MET:HE2	1:D:177:MET:HA	1.75	0.68
1:B:85:VAL:HG12	1:B:85:VAL:O	1.94	0.68
1:E:12:THR:HG23	1:E:65:SER:HB3	1.74	0.68
1:A:19:MET:HE3	1:A:23:LEU:HG	1.75	0.68
1:C:85:VAL:HG12	1:C:85:VAL:O	1.94	0.67
1:F:11:VAL:HG12	1:F:67:LEU:HD23	1.76	0.67
1:F:82:ILE:CD1	1:F:94:LEU:CD2	2.74	0.66
1:A:150:HIS:ND1	3:A:403:HOH:O	2.30	0.65
1:A:19:MET:CE	1:A:124:ILE:HD13	2.19	0.64
1:D:85:VAL:HG12	1:D:85:VAL:O	1.95	0.64
1:A:102:SER:HB2	1:B:254:GLU:OE1	1.98	0.63
1:F:82:ILE:HD12	1:F:94:LEU:HD21	1.79	0.63
1:A:82:ILE:HG23	1:A:111:TRP:CH2	2.34	0.63
1:E:271:LEU:HB3	1:E:288:MET:HE2	1.80	0.63
1:E:82:ILE:HG23	1:E:111:TRP:CH2	2.33	0.63
1:E:292:PHE:HD2	1:F:192:HIS:HB2	1.63	0.63
1:C:114:GLN:HE21	1:C:114:GLN:HA	1.64	0.63
1:F:19:MET:HG3	1:F:23:LEU:HD11	1.81	0.62
1:F:82:ILE:HD12	1:F:94:LEU:CD2	2.31	0.61
1:A:252:ALA:O	1:A:256:GLU:HG3	2.01	0.60
1:D:288:MET:CE	1:D:291:LEU:CD2	2.79	0.59
1:A:196:LEU:HD12	1:A:260:ILE:HD11	1.83	0.59
1:C:114:GLN:HA	1:C:114:GLN:NE2	2.17	0.59
1:E:82:ILE:CD1	1:E:94:LEU:HD21	2.32	0.59
1:E:82:ILE:HD11	1:E:94:LEU:HD11	1.84	0.59
1:E:225:TYR:O	1:E:229:VAL:HG13	2.03	0.58
1:B:261:HIS:HE1	1:B:264:LEU:HB2	1.66	0.58
1:D:274:ARG:NH1	3:D:401:HOH:O	2.36	0.58
1:B:38:ASN:ND2	2:B:301:NAP:O3B	2.32	0.58
1:F:228:GLN:HE21	1:F:234:TYR:HA	1.67	0.58
1:D:214:MET:HE2	1:D:214:MET:CA	2.34	0.58
1:E:292:PHE:HD2	1:F:192:HIS:CA	2.16	0.57
1:C:228:GLN:HE21	1:C:234:TYR:HA	1.69	0.57
1:E:82:ILE:HD13	1:E:94:LEU:HD21	1.86	0.57
1:A:228:GLN:HE21	1:A:234:TYR:HA	1.70	0.57
1:B:248:MET:HE3	1:B:269:LYS:HA	1.83	0.56
1:E:208:ALA:HB3	1:E:209:PRO:HD3	1.88	0.56
1:B:296:THR:HG22	1:B:297:ALA:N	2.21	0.56
1:C:218:ILE:HD13	1:D:183:MET:HA	1.87	0.55
1:C:262:SER:OG	1:D:296:THR:HB	2.06	0.55
1:F:19:MET:O	1:F:23:LEU:CD1	2.50	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:SER:HB3	1:C:174:LEU:HD13	1.88	0.55
1:D:248:MET:HE3	1:D:269:LYS:CA	2.35	0.55
1:E:196:LEU:HD12	1:E:260:ILE:HD11	1.89	0.55
1:B:228:GLN:HE21	1:B:234:TYR:HA	1.70	0.55
1:C:264:LEU:HB3	1:C:265:PRO:HD3	1.88	0.55
1:F:45:GLU:O	1:F:48:VAL:HG22	2.06	0.55
1:B:208:ALA:HB3	1:B:209:PRO:HD3	1.89	0.55
1:C:97:LEU:HD23	1:C:122:GLY:HA3	1.89	0.55
1:B:102:SER:HB3	1:B:174:LEU:HD13	1.90	0.54
1:D:214:MET:HA	1:D:214:MET:CE	2.37	0.54
1:F:102:SER:HB3	1:F:174:LEU:HD13	1.89	0.54
1:A:19:MET:CE	1:A:23:LEU:HG	2.38	0.54
1:B:93:VAL:HG11	1:B:150:HIS:CD2	2.42	0.54
1:F:208:ALA:HB3	1:F:209:PRO:HD3	1.88	0.54
1:D:251:LEU:HD13	1:D:265:PRO:HB3	1.90	0.54
1:C:261:HIS:HE1	1:C:264:LEU:HB2	1.72	0.54
1:E:226:ALA:O	1:E:229:VAL:HG22	2.08	0.54
1:C:75:TYR:CE1	1:C:100:ALA:HB2	2.43	0.54
1:C:111:TRP:O	1:C:115:ARG:HG2	2.08	0.54
1:E:271:LEU:C	1:E:288:MET:HE1	2.33	0.54
1:B:248:MET:HE1	1:B:268:PHE:O	2.07	0.53
1:A:264:LEU:HB3	1:A:265:PRO:HD3	1.90	0.53
1:D:264:LEU:HB3	1:D:265:PRO:HD3	1.89	0.53
1:A:208:ALA:HB3	1:A:209:PRO:HD3	1.89	0.53
1:A:292:PHE:O	1:B:260:ILE:HG12	2.09	0.53
1:D:274:ARG:CZ	1:D:291:LEU:HD11	2.39	0.52
1:E:271:LEU:O	1:E:288:MET:HE1	2.09	0.52
1:B:239:ALA:HB1	1:B:243:VAL:HG21	1.90	0.52
1:C:183:MET:HA	1:D:218:ILE:HD13	1.91	0.52
1:C:93:VAL:HG11	1:C:150:HIS:NE2	2.24	0.52
1:D:208:ALA:HB3	1:D:209:PRO:HD3	1.91	0.52
1:E:264:LEU:HB3	1:E:265:PRO:HD3	1.91	0.52
1:E:292:PHE:HD2	1:F:192:HIS:CB	2.22	0.52
1:F:59:GLU:HG2	1:F:85:VAL:HG23	1.92	0.52
1:C:208:ALA:HB3	1:C:209:PRO:HD3	1.91	0.52
1:C:229:VAL:HG13	1:C:289:ILE:HG12	1.92	0.52
1:D:93:VAL:HG11	1:D:150:HIS:NE2	2.25	0.52
1:A:218:ILE:HD13	1:B:183:MET:HA	1.92	0.51
1:D:248:MET:HE1	1:D:268:PHE:O	2.10	0.51
1:A:184:TRP:CZ2	1:B:248:MET:HG3	2.46	0.51
1:B:93:VAL:HG11	1:B:150:HIS:NE2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:THR:HB	1:D:262:SER:OG	2.11	0.51
1:D:288:MET:HE3	1:D:291:LEU:HD23	1.90	0.51
1:D:93:VAL:HG11	1:D:150:HIS:CD2	2.46	0.51
1:A:93:VAL:HG11	1:A:150:HIS:CD2	2.46	0.50
1:C:143:HIS:CD2	3:C:408:HOH:O	2.65	0.50
1:D:264:LEU:HB3	1:D:265:PRO:CD	2.42	0.50
1:F:19:MET:HG3	1:F:23:LEU:CD1	2.42	0.50
1:C:264:LEU:HB3	1:C:265:PRO:CD	2.41	0.50
1:E:183:MET:HA	1:F:218:ILE:HD13	1.92	0.50
1:F:39:ARG:NH2	2:F:301:NAP:O3X	2.40	0.50
1:D:85:VAL:O	1:D:85:VAL:CG1	2.60	0.50
1:A:59:GLU:HG3	1:A:85:VAL:HG12	1.94	0.49
1:A:252:ALA:O	1:A:256:GLU:CG	2.59	0.49
1:A:264:LEU:HB3	1:A:265:PRO:CD	2.42	0.49
1:B:229:VAL:HG13	1:B:289:ILE:HG12	1.95	0.49
1:F:69:ILE:HD13	1:F:95:VAL:CB	2.33	0.49
1:B:75:TYR:CZ	1:B:96:ASN:ND2	2.80	0.49
1:B:291:LEU:HD13	3:B:439:HOH:O	2.12	0.49
1:F:67:LEU:HD13	1:F:150:HIS:ND1	2.27	0.49
1:B:239:ALA:HB1	1:B:243:VAL:CG2	2.42	0.49
1:C:93:VAL:HG11	1:C:150:HIS:CD2	2.47	0.49
1:D:75:TYR:CZ	1:D:96:ASN:ND2	2.80	0.49
1:A:106:ARG:HD3	1:A:168:ASP:OD1	2.13	0.49
1:A:183:MET:HA	1:B:218:ILE:HD13	1.93	0.49
1:B:85:VAL:O	1:B:85:VAL:CG1	2.61	0.49
1:B:8:ARG:NE	1:B:30:GLY:O	2.45	0.49
1:A:39:ARG:HH11	2:A:301:NAP:C4A	2.26	0.49
1:E:264:LEU:HB3	1:E:265:PRO:CD	2.43	0.48
1:B:106:ARG:HD3	1:B:168:ASP:OD1	2.13	0.48
1:B:248:MET:HE3	1:B:269:LYS:CA	2.42	0.48
1:E:75:TYR:CZ	1:E:96:ASN:ND2	2.81	0.48
1:B:195:ALA:HB3	1:B:260:ILE:HD11	1.95	0.48
1:A:261:HIS:CE1	1:A:263:GLU:HB2	2.48	0.48
1:A:19:MET:HE2	1:A:124:ILE:HG21	1.96	0.48
1:B:261:HIS:CE1	1:B:264:LEU:H	2.30	0.48
1:C:261:HIS:CE1	1:C:264:LEU:H	2.31	0.48
1:D:288:MET:HE3	1:D:291:LEU:CD2	2.43	0.48
1:A:124:ILE:O	2:A:301:NAP:H5N	2.14	0.48
1:A:267:PHE:O	1:A:270:THR:OG1	2.27	0.48
1:D:106:ARG:HD3	1:D:168:ASP:OD1	2.13	0.47
1:D:248:MET:HE3	1:D:268:PHE:C	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:MET:HE3	1:D:269:LYS:N	2.29	0.47
1:A:257:HIS:NE2	3:A:402:HOH:O	2.24	0.47
1:B:296:THR:CG2	1:B:297:ALA:N	2.77	0.47
1:C:85:VAL:O	1:C:85:VAL:CG1	2.59	0.47
1:A:122:GLY:O	3:A:401:HOH:O	2.20	0.47
1:B:12:THR:HA	1:B:35:THR:O	2.15	0.47
1:B:261:HIS:CE1	1:B:264:LEU:HB2	2.47	0.47
1:E:177:MET:HB3	1:F:251:LEU:HD13	1.97	0.47
1:C:288:MET:HE3	1:C:288:MET:HA	1.96	0.47
1:A:12:THR:HA	1:A:35:THR:O	2.15	0.47
1:A:67:LEU:HD12	1:A:93:VAL:HG13	1.96	0.47
1:B:67:LEU:HD12	1:B:93:VAL:HG13	1.96	0.47
1:C:58:LEU:HD13	1:C:85:VAL:HG21	1.97	0.47
1:C:137:VAL:HA	1:C:161:ALA:HB3	1.97	0.47
1:D:12:THR:HA	1:D:35:THR:O	2.15	0.47
1:D:24:ALA:HB3	1:D:47:LEU:HD21	1.96	0.47
1:E:12:THR:HA	1:E:35:THR:O	2.15	0.47
1:B:128:PRO:HB2	1:B:129:PRO:HD3	1.97	0.47
1:E:16:LEU:H	1:E:38:ASN:ND2	2.13	0.47
1:A:75:TYR:CZ	1:A:96:ASN:ND2	2.83	0.46
1:B:248:MET:HE3	1:B:268:PHE:C	2.40	0.46
1:F:171:LEU:HD23	1:F:171:LEU:HA	1.84	0.46
1:C:184:TRP:CZ2	1:D:248:MET:HG3	2.51	0.46
1:F:75:TYR:CZ	1:F:96:ASN:ND2	2.83	0.46
1:B:240:THR:O	1:B:243:VAL:CG2	2.59	0.46
1:B:248:MET:HE2	1:B:269:LYS:HA	1.95	0.46
1:C:12:THR:HA	1:C:35:THR:O	2.15	0.46
1:F:35:THR:HB	1:F:53:VAL:HG13	1.98	0.46
1:A:72:VAL:O	2:A:301:NAP:H4D	2.14	0.46
1:B:248:MET:HE3	1:B:269:LYS:N	2.31	0.46
1:F:12:THR:HA	1:F:35:THR:O	2.15	0.46
1:A:58:LEU:HD13	1:A:85:VAL:HG21	1.96	0.46
1:C:67:LEU:HD12	1:C:93:VAL:HG13	1.97	0.46
1:D:274:ARG:HG2	1:E:84:PRO:HB3	1.98	0.46
1:F:35:THR:HA	1:F:53:VAL:HG13	1.98	0.46
1:E:254:GLU:CD	1:F:102:SER:HG	2.23	0.46
1:C:143:HIS:HD2	1:C:146:ALA:H	1.64	0.46
1:A:254:GLU:OE1	1:B:102:SER:OG	2.32	0.45
1:D:128:PRO:HB2	1:D:129:PRO:HD3	1.98	0.45
1:E:35:THR:HA	1:E:53:VAL:HG13	1.98	0.45
1:A:99:THR:HG22	1:B:250:HIS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LEU:HG	1:D:175:TYR:CE1	2.52	0.45
1:C:292:PHE:O	1:D:260:ILE:HG13	2.15	0.45
1:E:83:ARG:N	1:E:84:PRO:HD2	2.31	0.45
1:F:137:VAL:HA	1:F:161:ALA:HB3	1.99	0.45
1:A:93:VAL:HG11	1:A:150:HIS:NE2	2.31	0.45
1:D:175:TYR:O	1:D:179:LEU:HD22	2.15	0.45
1:F:93:VAL:HG21	1:F:150:HIS:ND1	2.31	0.45
1:A:226:ALA:HB3	1:A:227:PRO:CD	2.47	0.45
1:B:42:GLU:CD	1:B:42:GLU:H	2.25	0.45
1:A:128:PRO:HB2	1:A:129:PRO:HD3	1.98	0.45
1:E:16:LEU:HB2	1:E:38:ASN:HB2	1.99	0.45
1:F:249:GLU:HB2	1:F:269:LYS:NZ	2.31	0.45
1:B:229:VAL:O	3:B:401:HOH:O	2.21	0.45
1:D:137:VAL:HA	1:D:161:ALA:HB3	1.99	0.45
1:A:32:HIS:CE1	1:A:153:THR:HG23	2.52	0.44
1:C:212:ASN:HD22	1:C:215:ILE:HD12	1.82	0.44
1:F:83:ARG:N	1:F:84:PRO:HD2	2.32	0.44
1:B:250:HIS:O	1:B:254:GLU:HB2	2.18	0.44
1:A:137:VAL:HA	1:A:161:ALA:HB3	1.98	0.44
1:D:79:HIS:CD2	1:D:83:ARG:NH1	2.85	0.44
1:B:212:ASN:HD22	1:B:215:ILE:HD12	1.83	0.44
1:C:197:LEU:HB3	1:C:202:VAL:CG2	2.45	0.44
1:E:128:PRO:HB2	1:E:129:PRO:HD3	1.99	0.44
1:A:82:ILE:HG13	1:A:89:LEU:CD1	2.38	0.44
1:D:83:ARG:N	1:D:84:PRO:HD2	2.32	0.44
1:B:83:ARG:N	1:B:84:PRO:HD2	2.32	0.44
1:B:137:VAL:HA	1:B:161:ALA:HB3	2.00	0.44
1:E:137:VAL:HA	1:E:161:ALA:HB3	2.00	0.44
1:A:212:ASN:HD22	1:A:215:ILE:HD12	1.83	0.44
1:B:16:LEU:H	1:B:38:ASN:ND2	2.15	0.44
1:C:83:ARG:N	1:C:84:PRO:HD2	2.32	0.44
1:F:128:PRO:HB2	1:F:129:PRO:HD3	1.99	0.44
1:F:195:ALA:CB	1:F:260:ILE:HD11	2.48	0.44
1:F:226:ALA:HB3	1:F:227:PRO:CD	2.48	0.44
1:D:67:LEU:HD12	1:D:93:VAL:HG13	1.99	0.43
1:D:281:ALA:HB2	1:E:39:ARG:HG3	2.00	0.43
1:E:261:HIS:CE1	1:E:263:GLU:HB2	2.53	0.43
1:B:199:THR:OG1	1:B:258:LEU:CD1	2.64	0.43
1:C:124:ILE:O	2:C:301:NAP:H5N	2.17	0.43
1:B:124:ILE:O	2:B:301:NAP:H5N	2.18	0.43
1:C:128:PRO:HB2	1:C:129:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:ASN:HD22	1:E:215:ILE:HD12	1.83	0.43
1:C:226:ALA:HB3	1:C:227:PRO:CD	2.48	0.43
1:E:82:ILE:HD11	1:E:94:LEU:HD21	2.00	0.43
1:A:275:ALA:O	1:A:280:HIS:HB2	2.19	0.43
1:B:62:VAL:HG21	1:B:85:VAL:HG11	1.99	0.43
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.79	0.43
1:D:267:PHE:O	1:D:270:THR:OG1	2.27	0.43
1:D:212:ASN:HD22	1:D:215:ILE:HD12	1.82	0.43
1:A:274:ARG:NH1	1:A:291:LEU:HD11	2.34	0.43
1:A:280:HIS:CD2	1:A:287:ALA:HB1	2.54	0.43
1:A:39:ARG:HB3	2:A:301:NAP:O2X	2.19	0.43
1:A:75:TYR:CZ	1:A:100:ALA:HB2	2.53	0.43
1:C:197:LEU:HD12	1:D:174:LEU:HB3	2.01	0.43
1:D:62:VAL:HG21	1:D:85:VAL:HG11	2.01	0.43
1:D:250:HIS:O	1:D:254:GLU:HB2	2.19	0.43
1:E:89:LEU:O	1:E:90:ALA:C	2.62	0.43
1:D:203:LYS:HA	1:D:203:LYS:HE2	2.01	0.42
1:B:58:LEU:HD23	1:B:85:VAL:HG21	2.02	0.42
1:C:280:HIS:CD2	1:C:287:ALA:HB1	2.54	0.42
1:E:85:VAL:HG22	1:E:88:ALA:HB3	2.00	0.42
1:A:263:GLU:OE2	1:B:296:THR:HG23	2.19	0.42
1:E:280:HIS:CD2	1:E:287:ALA:HB1	2.55	0.42
1:A:225:TYR:O	1:A:229:VAL:HG13	2.19	0.42
1:B:14:VAL:HG13	1:B:70:VAL:HB	2.00	0.42
1:B:275:ALA:O	1:B:280:HIS:HB2	2.19	0.42
1:D:275:ALA:O	1:D:280:HIS:HB2	2.20	0.42
1:F:58:LEU:HG	1:F:59:GLU:N	2.35	0.42
1:F:261:HIS:CE1	1:F:263:GLU:HB2	2.55	0.42
1:C:174:LEU:CD1	1:D:254:GLU:OE1	2.68	0.42
1:F:280:HIS:CD2	1:F:287:ALA:HB1	2.55	0.42
1:A:39:ARG:NH1	2:A:301:NAP:C4A	2.83	0.41
1:C:275:ALA:O	1:C:280:HIS:HB2	2.20	0.41
1:F:23:LEU:CD2	1:F:97:LEU:HD12	2.50	0.41
1:A:133:THR:OG1	1:A:134:ASP:N	2.53	0.41
1:B:174:LEU:HD12	1:B:174:LEU:HA	1.83	0.41
1:F:241:MET:CE	1:F:272:ALA:HA	2.51	0.41
1:E:275:ALA:O	1:E:280:HIS:HB2	2.20	0.41
1:F:75:TYR:CZ	1:F:100:ALA:HB2	2.55	0.41
1:C:150:HIS:O	1:C:151:GLU:C	2.64	0.41
1:E:199:THR:HG22	3:E:407:HOH:O	2.19	0.41
1:E:218:ILE:HD13	1:E:221:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:GLN:NE2	1:C:114:GLN:CA	2.85	0.41
1:C:174:LEU:HD11	1:D:254:GLU:OE1	2.20	0.41
1:C:261:HIS:CE1	1:C:264:LEU:HB2	2.53	0.41
1:F:225:TYR:O	1:F:229:VAL:HG13	2.22	0.40
1:A:102:SER:CB	1:B:254:GLU:OE1	2.66	0.40
1:C:62:VAL:HG21	1:C:85:VAL:HG11	2.03	0.40
1:F:35:THR:HG21	1:F:64:ALA:CB	2.52	0.40
1:F:249:GLU:HB2	1:F:269:LYS:HZ3	1.86	0.40
1:B:8:ARG:HA	1:B:9:PRO:HD3	1.94	0.40
1:C:250:HIS:HD2	1:D:99:THR:HG22	1.87	0.40
1:C:274:ARG:HB2	1:C:291:LEU:CD1	2.52	0.40
1:B:150:HIS:O	1:B:151:GLU:C	2.65	0.40
1:E:254:GLU:OE1	1:F:102:SER:OG	2.35	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	288/297 (97%)	272 (94%)	16 (6%)	0	100	100
1	B	289/297 (97%)	273 (94%)	16 (6%)	0	100	100
1	C	288/297 (97%)	274 (95%)	14 (5%)	0	100	100
1	D	288/297 (97%)	275 (96%)	13 (4%)	0	100	100
1	E	287/297 (97%)	271 (94%)	14 (5%)	2 (1%)	18	25
1	F	287/297 (97%)	270 (94%)	17 (6%)	0	100	100
All	All	1727/1782 (97%)	1635 (95%)	90 (5%)	2 (0%)	48	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	90	ALA
1	E	165	LEU

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	210/227 (92%)	189 (90%)	21 (10%)	7	9
1	B	205/227 (90%)	186 (91%)	19 (9%)	8	10
1	C	211/227 (93%)	184 (87%)	27 (13%)	4	4
1	D	210/227 (92%)	189 (90%)	21 (10%)	7	9
1	E	176/227 (78%)	158 (90%)	18 (10%)	7	8
1	F	184/227 (81%)	168 (91%)	16 (9%)	9	13
All	All	1196/1362 (88%)	1074 (90%)	122 (10%)	7	8

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	19	MET
1	A	45	GLU
1	A	53	VAL
1	A	54	LEU
1	A	58	LEU
1	A	80	GLU
1	A	82	ILE
1	A	93	VAL
1	A	133	THR
1	A	137	VAL
1	A	138	LEU
1	A	145	SER
1	A	171	LEU
1	A	174	LEU
1	A	229	VAL
1	A	235	GLU

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Mol	Chain	Res	Type
1	A	237	THR
1	A	263	GLU
1	A	264	LEU
1	A	266	ARG
1	B	7	ASP
1	B	11	VAL
1	B	14	VAL
1	B	54	LEU
1	B	93	VAL
1	B	137	VAL
1	B	138	LEU
1	B	145	SER
1	B	163	THR
1	B	167	GLU
1	B	174	LEU
1	B	220	GLU
1	B	251	LEU
1	B	254	GLU
1	B	256	GLU
1	B	258	LEU
1	B	260	ILE
1	B	264	LEU
1	B	270	THR
1	C	54	LEU
1	C	58	LEU
1	C	74	ASP
1	C	78	VAL
1	C	81	LEU
1	C	93	VAL
1	C	106	ARG
1	C	110	GLU
1	C	114	GLN
1	C	115	ARG
1	C	138	LEU
1	C	152	SER
1	C	163	THR
1	C	171	LEU
1	C	174	LEU
1	C	177	MET
1	C	196	LEU
1	C	197	LEU
1	C	202	VAL

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Mol	Chain	Res	Type
1	C	214	MET
1	C	237	THR
1	C	253	GLU
1	C	264	LEU
1	C	270	THR
1	C	274	ARG
1	C	288	MET
1	C	293	ARG
1	D	53	VAL
1	D	81	LEU
1	D	93	VAL
1	D	131	ILE
1	D	137	VAL
1	D	138	LEU
1	D	163	THR
1	D	165	LEU
1	D	171	LEU
1	D	179	LEU
1	D	196	LEU
1	D	203	LYS
1	D	210	LEU
1	D	220	GLU
1	D	235	GLU
1	D	237	THR
1	D	251	LEU
1	D	254	GLU
1	D	260	ILE
1	D	264	LEU
1	D	269	LYS
1	E	16	LEU
1	E	18	LEU
1	E	53	VAL
1	E	54	LEU
1	E	65	SER
1	E	67	LEU
1	E	82	ILE
1	E	103	THR
1	E	106	ARG
1	E	137	VAL
1	E	229	VAL
1	E	231	GLU
1	E	234	TYR

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Mol	Chain	Res	Type
1	E	237	THR
1	E	263	GLU
1	E	264	LEU
1	E	270	THR
1	E	274	ARG
1	F	35	THR
1	F	53	VAL
1	F	58	LEU
1	F	93	VAL
1	F	106	ARG
1	F	137	VAL
1	F	153	THR
1	F	163	THR
1	F	165	LEU
1	F	171	LEU
1	F	174	LEU
1	F	229	VAL
1	F	256	GLU
1	F	260	ILE
1	F	270	THR
1	F	282	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	32	HIS
1	A	212	ASN
1	A	228	GLN
1	A	280	HIS
1	B	21	GLN
1	B	38	ASN
1	B	212	ASN
1	B	228	GLN
1	B	250	HIS
1	B	261	HIS
1	C	21	GLN
1	C	32	HIS
1	C	114	GLN
1	C	143	HIS
1	C	212	ASN
1	C	228	GLN

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Mol	Chain	Res	Type
1	C	245	GLN
1	C	250	HIS
1	C	261	HIS
1	C	280	HIS
1	D	21	GLN
1	D	212	ASN
1	D	250	HIS
1	E	21	GLN
1	E	38	ASN
1	E	143	HIS
1	E	212	ASN
1	E	280	HIS
1	F	32	HIS
1	F	228	GLN
1	F	280	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](#)

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	NAP	B	301	-	50,52,52	0.72	0	71,80,80	1.10	3 (4%)
2	NAP	F	301	-	50,52,52	0.90	3 (6%)	71,80,80	0.92	2 (2%)
2	NAP	A	301	-	50,52,52	0.57	1 (2%)	71,80,80	0.79	2 (2%)
2	NAP	C	301	-	50,52,52	0.59	0	71,80,80	0.85	2 (2%)
2	NAP	E	301	-	50,52,52	0.90	3 (6%)	71,80,80	1.03	3 (4%)
2	NAP	D	301	-	50,52,52	0.54	0	71,80,80	0.84	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	B	301	-	-	3/35/67/67	0/5/5/5
2	NAP	F	301	-	-	13/35/67/67	0/5/5/5
2	NAP	A	301	-	-	10/35/67/67	0/5/5/5
2	NAP	C	301	-	-	11/35/67/67	0/5/5/5
2	NAP	E	301	-	-	9/35/67/67	0/5/5/5
2	NAP	D	301	-	-	12/35/67/67	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NAP	C2N-N1N	3.82	1.39	1.35
2	E	301	NAP	C2N-N1N	3.63	1.39	1.35
2	E	301	NAP	O4D-C1D	2.82	1.44	1.40
2	F	301	NAP	PA-O3	2.32	1.62	1.59
2	A	301	NAP	C2N-N1N	2.20	1.37	1.35
2	F	301	NAP	P2B-O2B	2.09	1.63	1.59
2	E	301	NAP	PA-O3	2.02	1.61	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAP	P2B-O2B-C2B	-5.15	109.67	123.43
2	D	301	NAP	P2B-O2B-C2B	-5.03	110.01	123.43
2	A	301	NAP	P2B-O2B-C2B	-4.81	110.59	123.43
2	F	301	NAP	P2B-O2B-C2B	-4.77	110.70	123.43
2	C	301	NAP	P2B-O2B-C2B	-4.64	111.05	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	NAP	C6N-N1N-C2N	-4.46	118.08	121.88
2	B	301	NAP	C6N-N1N-C2N	-3.98	118.49	121.88
2	E	301	NAP	P2B-O2B-C2B	-3.39	114.37	123.43
2	F	301	NAP	C6N-N1N-C2N	-3.36	119.02	121.88
2	E	301	NAP	C3B-C2B-C1B	-3.03	97.00	102.81
2	C	301	NAP	C6N-N1N-C2N	-2.69	119.59	121.88
2	D	301	NAP	C6N-N1N-C2N	-2.51	119.74	121.88
2	A	301	NAP	C6N-N1N-C2N	-2.45	119.79	121.88
2	B	301	NAP	C5N-C4N-C3N	-2.21	118.20	120.36

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C5D-O5D-PN-O3
2	A	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	C5D-O5D-PN-O2N
2	A	301	NAP	O4D-C4D-C5D-O5D
2	A	301	NAP	O4D-C1D-N1N-C2N
2	B	301	NAP	O4D-C1D-N1N-C2N
2	B	301	NAP	O4D-C1D-N1N-C6N
2	C	301	NAP	C5B-O5B-PA-O3
2	C	301	NAP	O4D-C1D-N1N-C2N
2	C	301	NAP	O4D-C1D-N1N-C6N
2	C	301	NAP	C2D-C1D-N1N-C2N
2	C	301	NAP	C2D-C1D-N1N-C6N
2	D	301	NAP	C5B-O5B-PA-O2A
2	D	301	NAP	O4D-C1D-N1N-C2N
2	E	301	NAP	O4D-C1D-N1N-C2N
2	F	301	NAP	C5B-O5B-PA-O3
2	F	301	NAP	C5D-O5D-PN-O1N
2	F	301	NAP	O4D-C1D-N1N-C2N
2	A	301	NAP	C3D-C4D-C5D-O5D
2	E	301	NAP	O4D-C4D-C5D-O5D
2	E	301	NAP	C3D-C4D-C5D-O5D
2	F	301	NAP	C3D-C4D-C5D-O5D
2	C	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	O4B-C4B-C5B-O5B
2	F	301	NAP	O4D-C4D-C5D-O5D
2	C	301	NAP	C3B-C4B-C5B-O5B
2	D	301	NAP	C3B-C4B-C5B-O5B
2	F	301	NAP	PA-O3-PN-O5D

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Mol	Chain	Res	Type	Atoms
2	E	301	NAP	C1B-C2B-O2B-P2B
2	F	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	C5B-O5B-PA-O1A
2	D	301	NAP	C5B-O5B-PA-O3
2	E	301	NAP	C5D-O5D-PN-O1N
2	F	301	NAP	C5B-O5B-PA-O1A
2	F	301	NAP	C5D-O5D-PN-O3
2	F	301	NAP	C5D-O5D-PN-O2N
2	C	301	NAP	C2B-O2B-P2B-O2X
2	B	301	NAP	C2D-C1D-N1N-C6N
2	A	301	NAP	O4D-C1D-N1N-C6N
2	D	301	NAP	O4D-C1D-N1N-C6N
2	E	301	NAP	O4D-C1D-N1N-C6N
2	F	301	NAP	C3B-C4B-C5B-O5B
2	F	301	NAP	O4D-C1D-N1N-C6N
2	A	301	NAP	C2B-O2B-P2B-O1X
2	C	301	NAP	C2B-O2B-P2B-O1X
2	D	301	NAP	C2B-O2B-P2B-O1X
2	D	301	NAP	PN-O3-PA-O1A
2	A	301	NAP	O4B-C4B-C5B-O5B
2	C	301	NAP	PN-O3-PA-O2A
2	D	301	NAP	PN-O3-PA-O2A
2	E	301	NAP	PA-O3-PN-O1N
2	E	301	NAP	PA-O3-PN-O2N
2	C	301	NAP	C2B-O2B-P2B-O3X
2	D	301	NAP	C2B-O2B-P2B-O2X
2	D	301	NAP	C2B-O2B-P2B-O3X
2	E	301	NAP	C3B-C2B-O2B-P2B
2	A	301	NAP	PN-O3-PA-O2A
2	F	301	NAP	PA-O3-PN-O1N

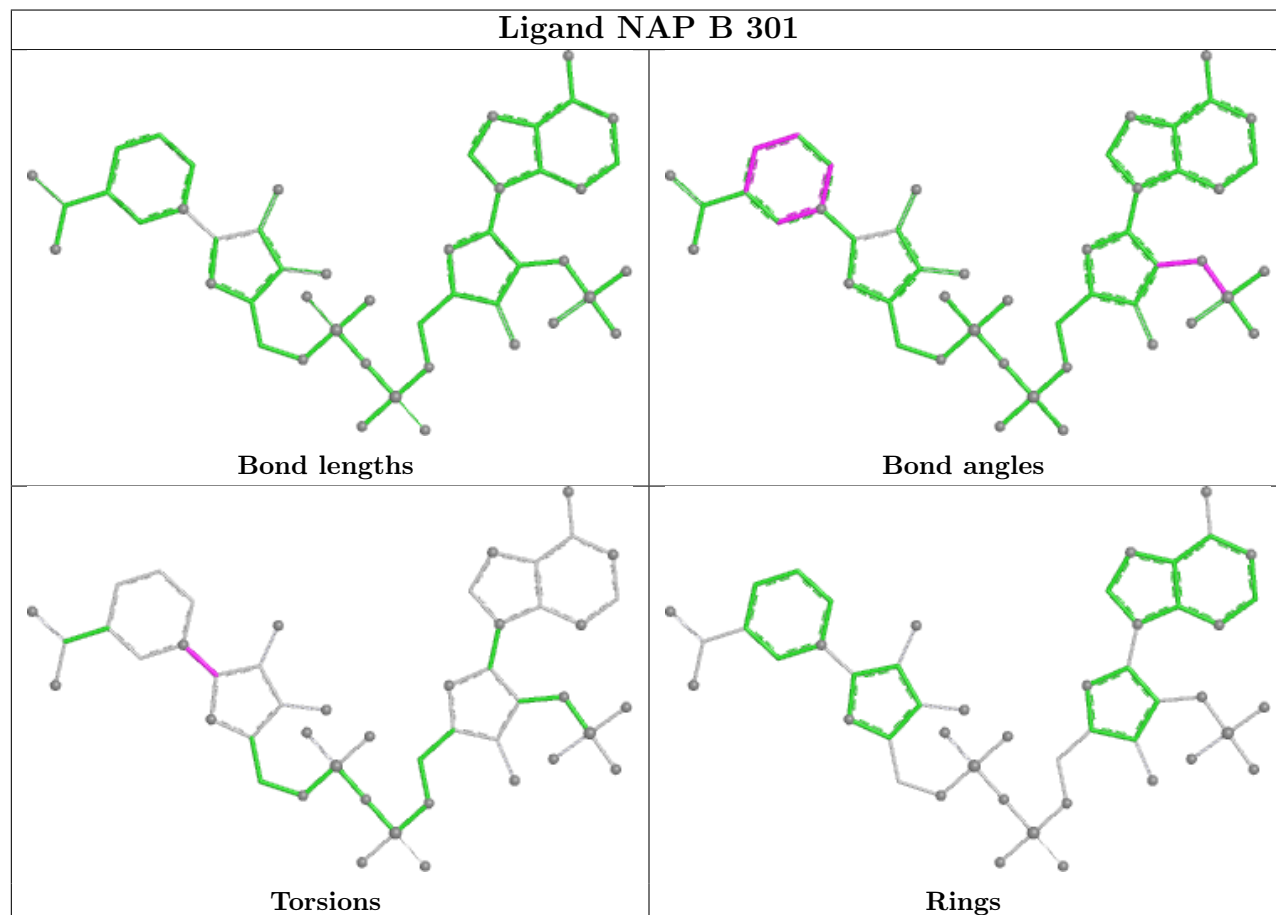
There are no ring outliers.

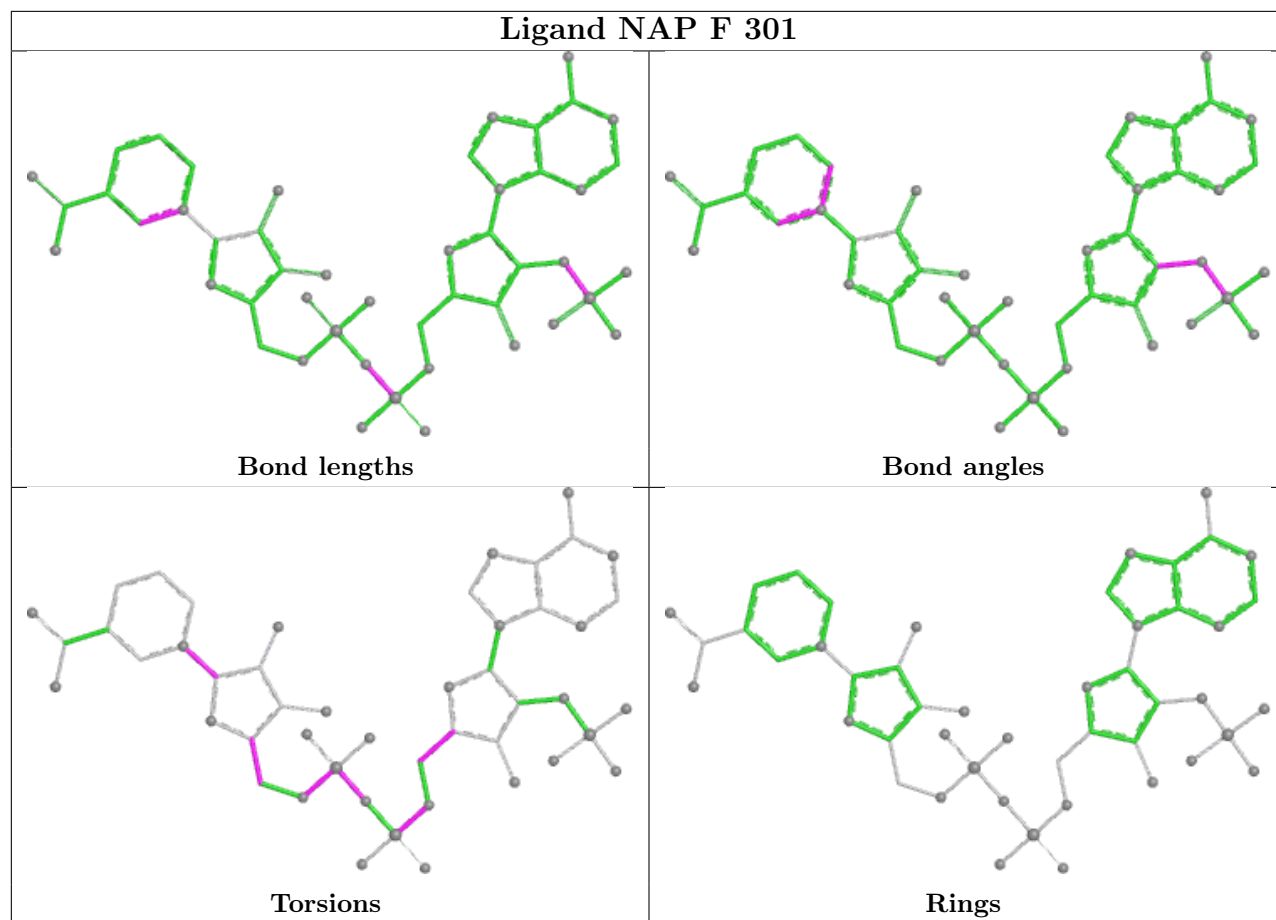
4 monomers are involved in 10 short contacts:

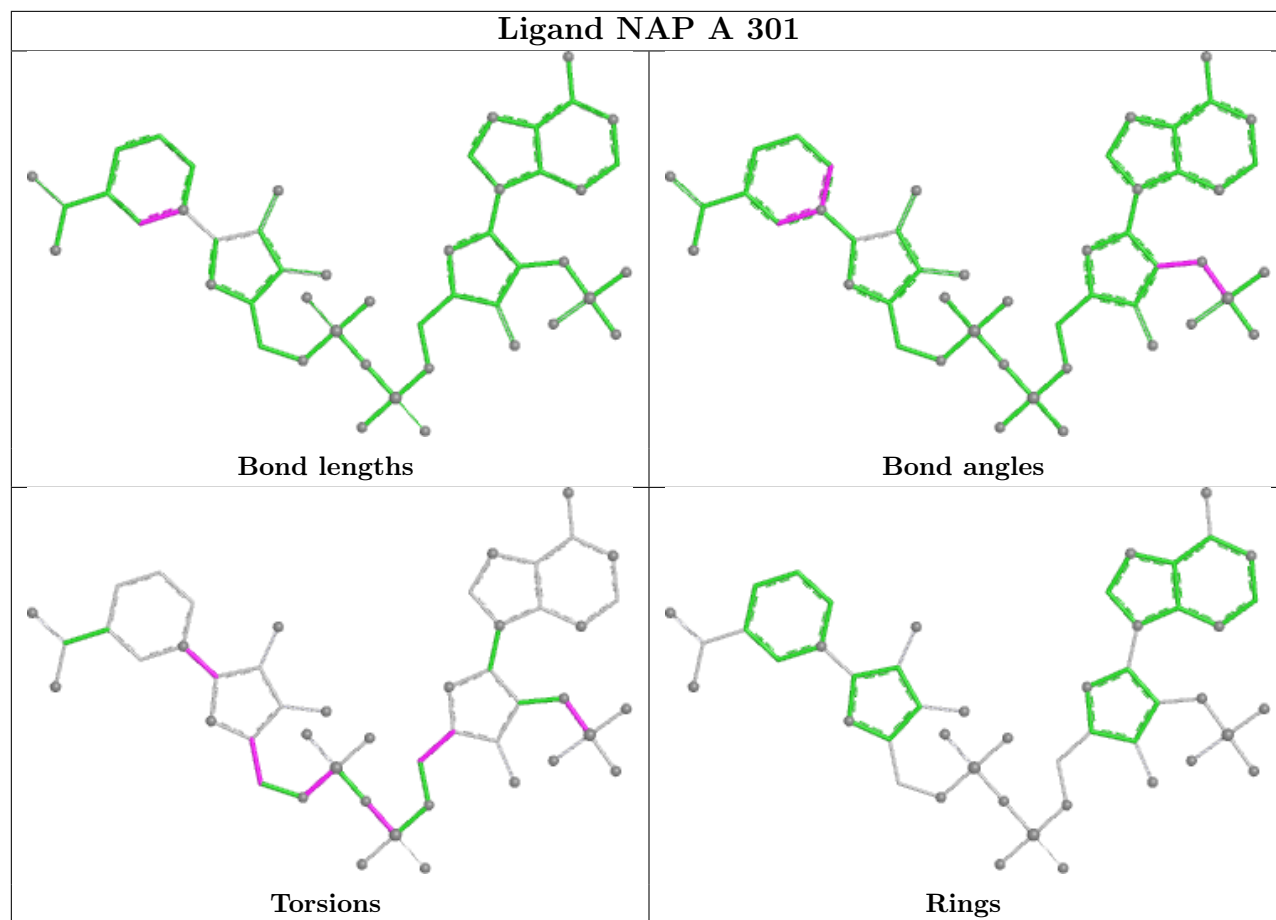
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NAP	2	0
2	F	301	NAP	2	0
2	A	301	NAP	5	0
2	C	301	NAP	1	0

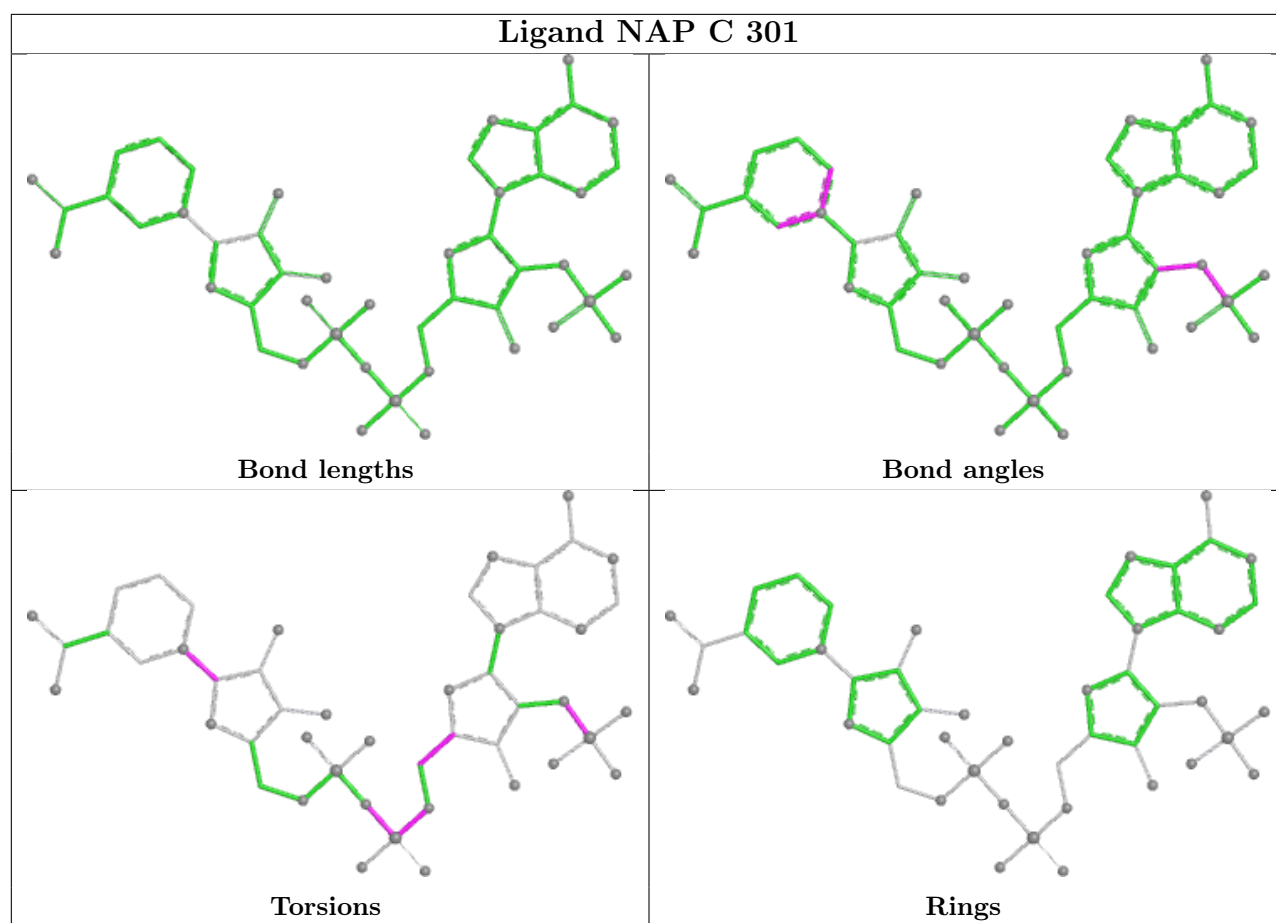
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

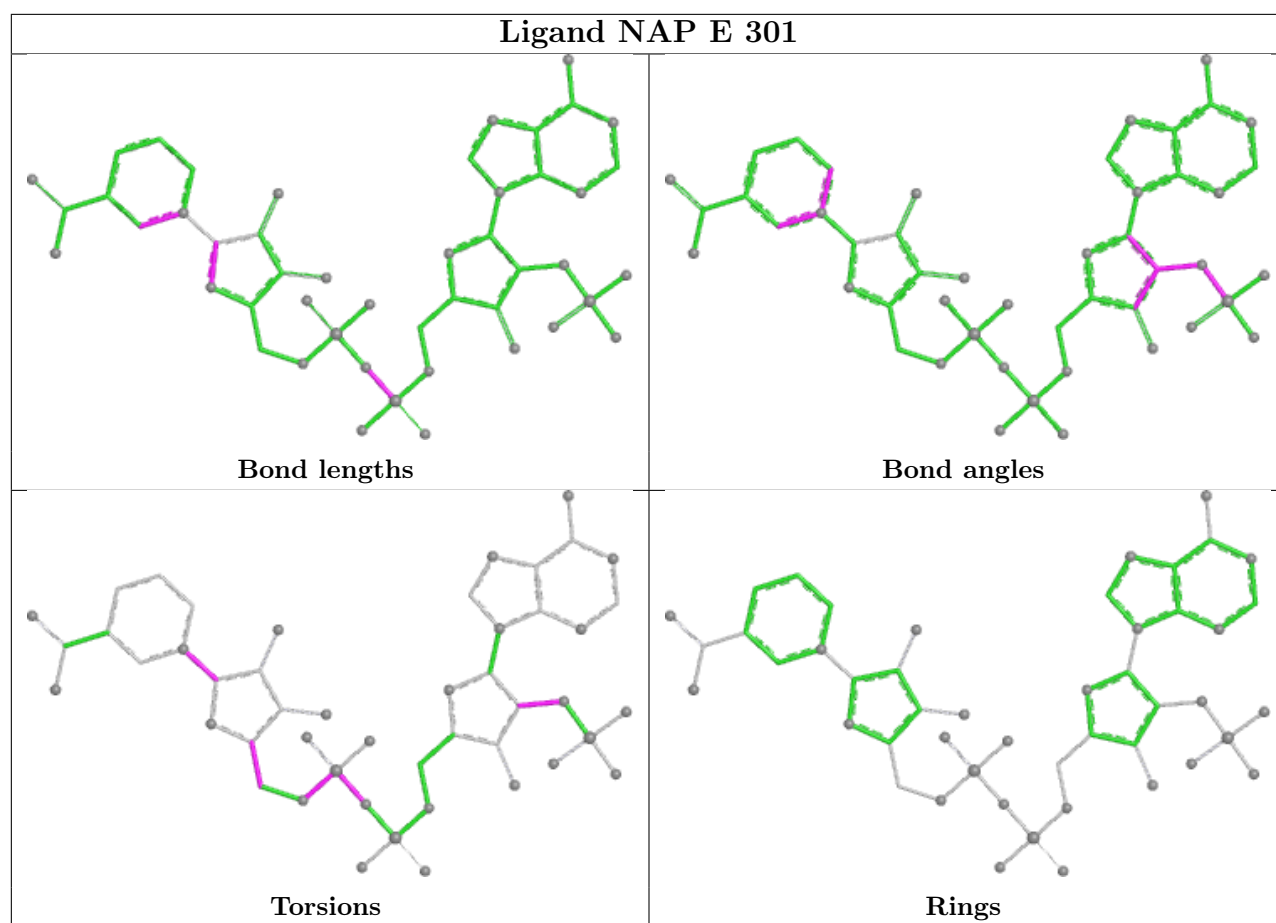
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

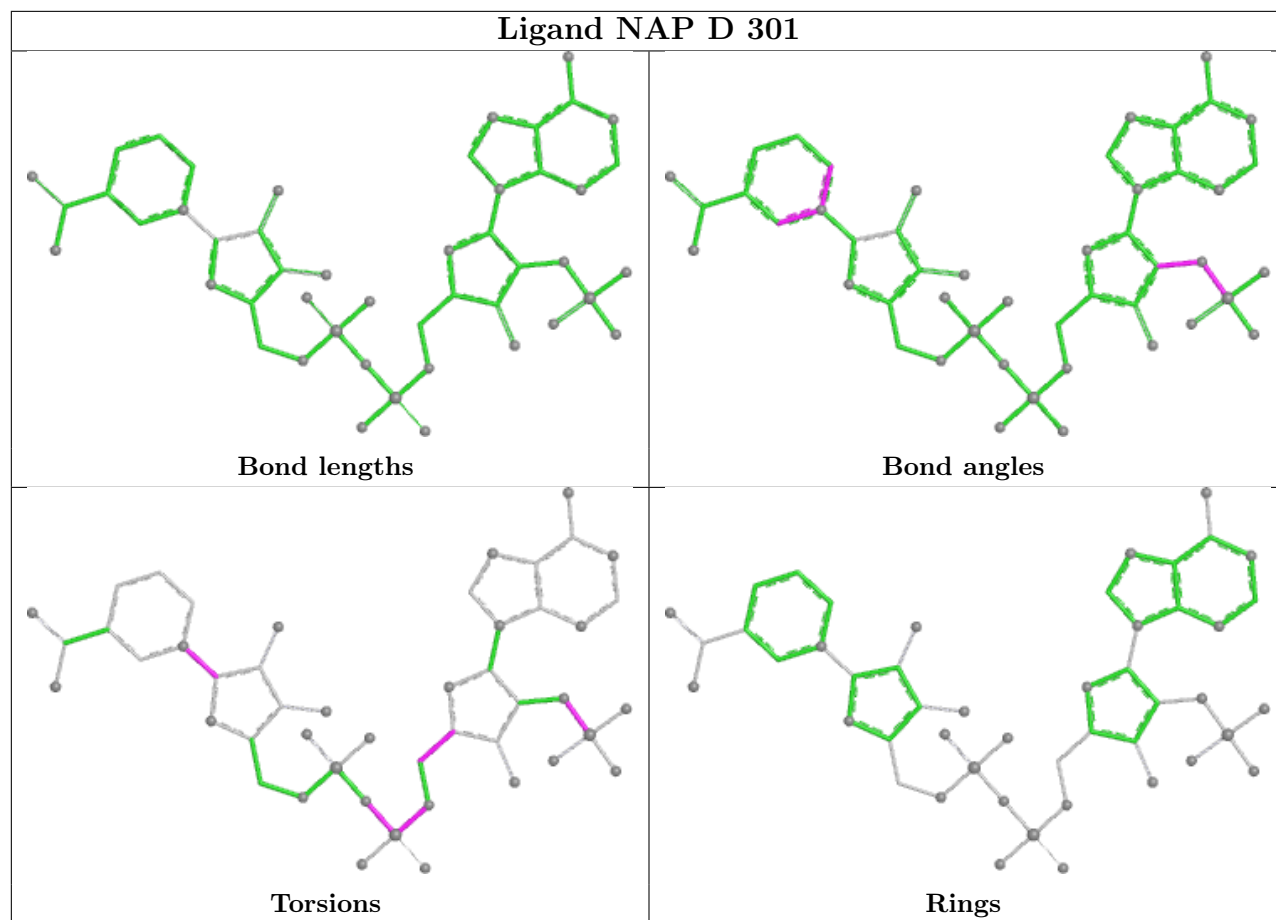












5.7 Other polymers [i](#)

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	290/297 (97%)	0.52	6 (2%) 63 64	50, 74, 99, 114	0
1	B	291/297 (97%)	0.46	1 (0%) 90 92	45, 69, 94, 120	0
1	C	290/297 (97%)	0.42	5 (1%) 69 69	43, 61, 81, 117	0
1	D	290/297 (97%)	0.62	13 (4%) 38 38	30, 71, 97, 113	0
1	E	289/297 (97%)	1.17	45 (15%) 5 4	64, 106, 131, 146	0
1	F	289/297 (97%)	1.03	26 (8%) 15 14	55, 102, 129, 147	0
All	All	1739/1782 (97%)	0.70	96 (5%) 30 30	30, 76, 122, 147	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	175	TYR	6.4
1	A	267	PHE	4.3
1	C	68	VAL	4.2
1	E	47	LEU	4.1
1	F	41	PRO	4.0
1	E	221	TYR	3.8
1	E	177	MET	3.7
1	F	82	ILE	3.6
1	F	178	ALA	3.5
1	E	174	LEU	3.4
1	F	221	TYR	3.3
1	D	267	PHE	3.1
1	E	291	LEU	3.1
1	D	178	ALA	3.1
1	E	77	ALA	3.1
1	E	296	THR	3.0
1	F	123	ALA	3.0
1	D	93	VAL	3.0
1	E	224	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	54	LEU	2.9
1	E	193	GLY	2.9
1	F	194	ALA	2.9
1	E	238	ASP	2.9
1	E	225	TYR	2.9
1	F	179	LEU	2.8
1	F	147	PHE	2.7
1	D	118	PRO	2.7
1	C	189	GLY	2.6
1	D	259	GLY	2.6
1	E	179	LEU	2.6
1	F	14	VAL	2.6
1	A	297	ALA	2.6
1	E	190	PHE	2.6
1	E	138	LEU	2.6
1	F	157	ILE	2.6
1	D	94	LEU	2.6
1	D	185	GLY	2.5
1	D	14	VAL	2.5
1	E	137	VAL	2.5
1	E	166	GLU	2.5
1	D	68	VAL	2.5
1	E	67	LEU	2.5
1	E	171	LEU	2.5
1	F	138	LEU	2.5
1	E	152	SER	2.4
1	E	201	LYS	2.4
1	F	67	LEU	2.4
1	F	137	VAL	2.4
1	F	58	LEU	2.3
1	E	268	PHE	2.3
1	E	140	TYR	2.3
1	F	35	THR	2.3
1	F	296	THR	2.3
1	A	191	LEU	2.3
1	F	97	LEU	2.3
1	E	14	VAL	2.3
1	D	75	TYR	2.3
1	A	181	GLY	2.2
1	E	172	SER	2.2
1	E	215	ILE	2.2
1	F	16	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	135	GLY	2.2
1	E	157	ILE	2.2
1	C	14	VAL	2.2
1	D	11	VAL	2.2
1	B	139	LEU	2.2
1	F	15	GLY	2.2
1	E	173	SER	2.2
1	E	53	VAL	2.2
1	D	156	ALA	2.2
1	E	146	ALA	2.2
1	E	28	LEU	2.2
1	E	197	LEU	2.2
1	E	198	GLY	2.2
1	F	291	LEU	2.2
1	C	99	THR	2.1
1	D	175	TYR	2.1
1	E	164	TYR	2.1
1	E	217	ALA	2.1
1	E	153	THR	2.1
1	E	151	GLU	2.1
1	E	13	VAL	2.1
1	A	188	ASN	2.1
1	E	139	LEU	2.1
1	E	186	ILE	2.1
1	F	140	TYR	2.1
1	F	70	VAL	2.1
1	C	149	ALA	2.1
1	E	147	PHE	2.0
1	F	52	ALA	2.0
1	F	18	LEU	2.0
1	E	218	ILE	2.0
1	F	34	THR	2.0
1	F	84	PRO	2.0
1	E	120	LEU	2.0
1	E	15	GLY	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 ⓘ

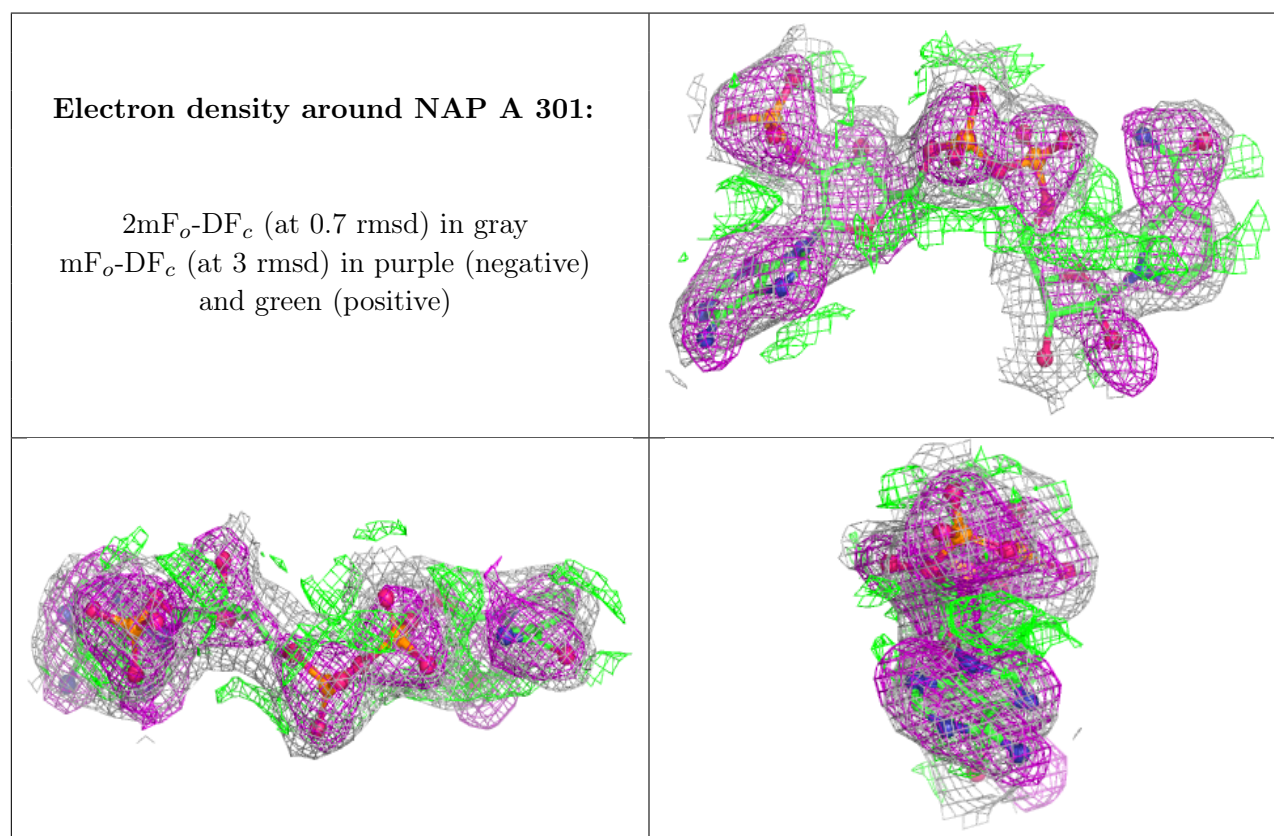
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

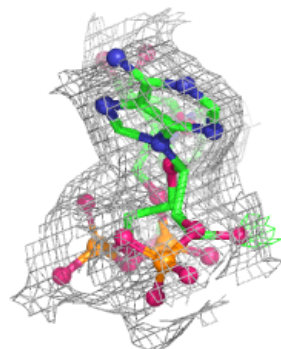
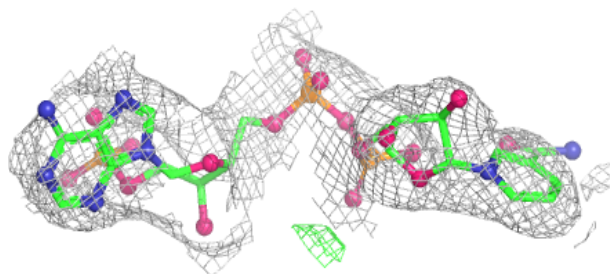
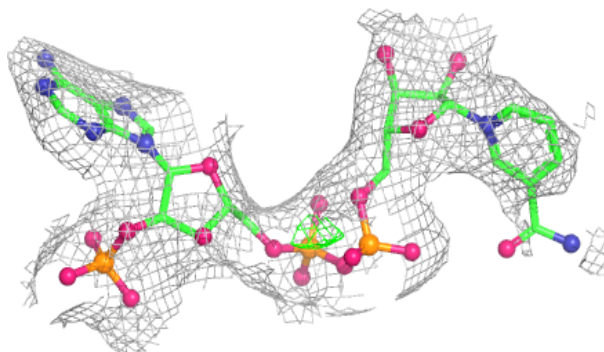
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	A	301	48/48	0.84	0.12	12,15,18,20	0
2	NAP	F	301	48/48	0.86	0.09	79,103,116,119	0
2	NAP	C	301	48/48	0.89	0.10	12,15,18,20	0
2	NAP	D	301	48/48	0.90	0.10	12,15,18,20	0
2	NAP	E	301	48/48	0.93	0.08	58,74,105,110	0
2	NAP	B	301	48/48	0.96	0.07	35,45,52,56	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.

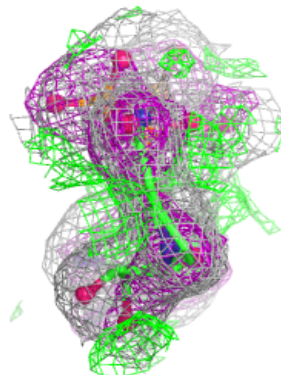
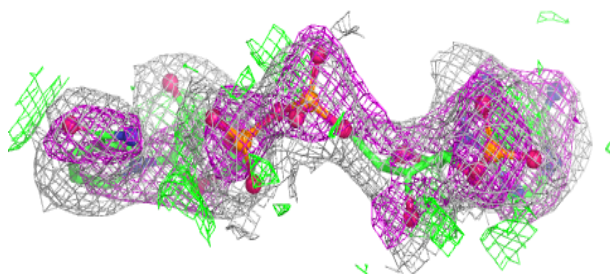
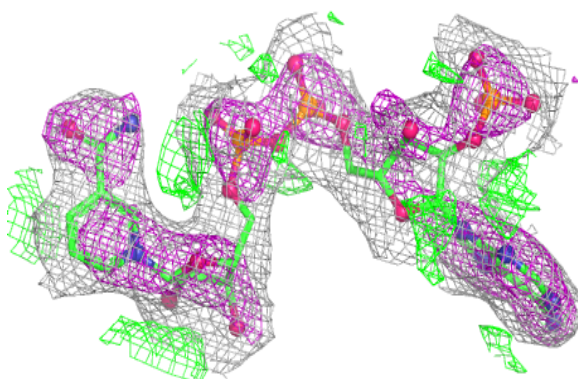


Electron density around NAP F 301:

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

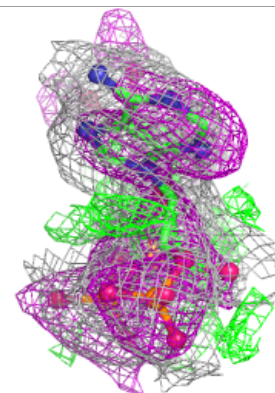
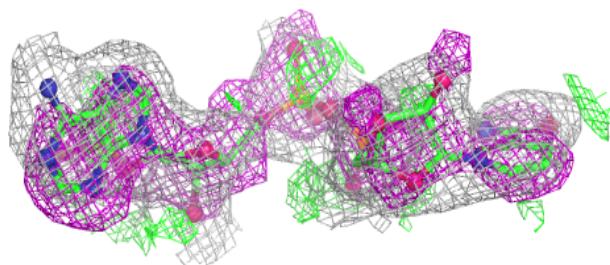
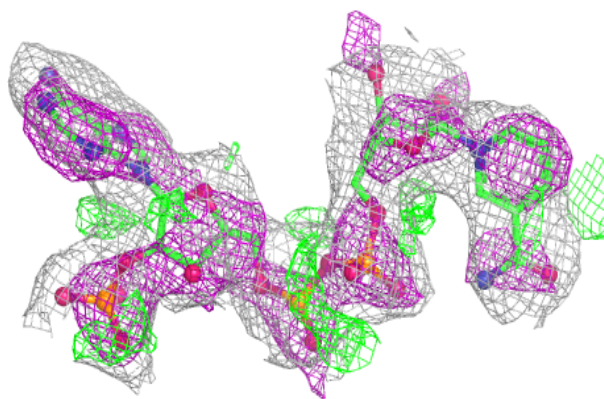
**Electron density around NAP C 301:**

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

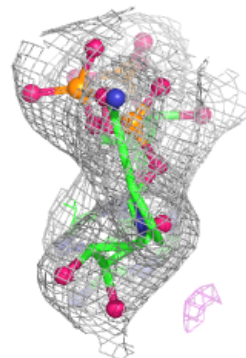
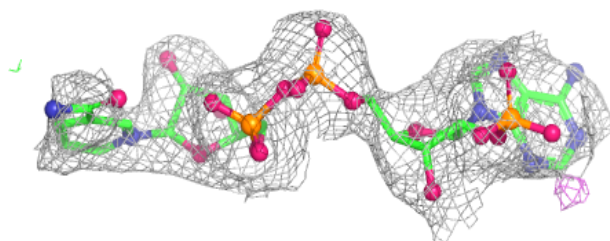
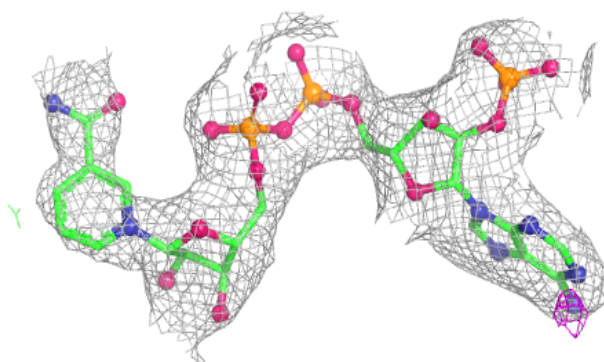


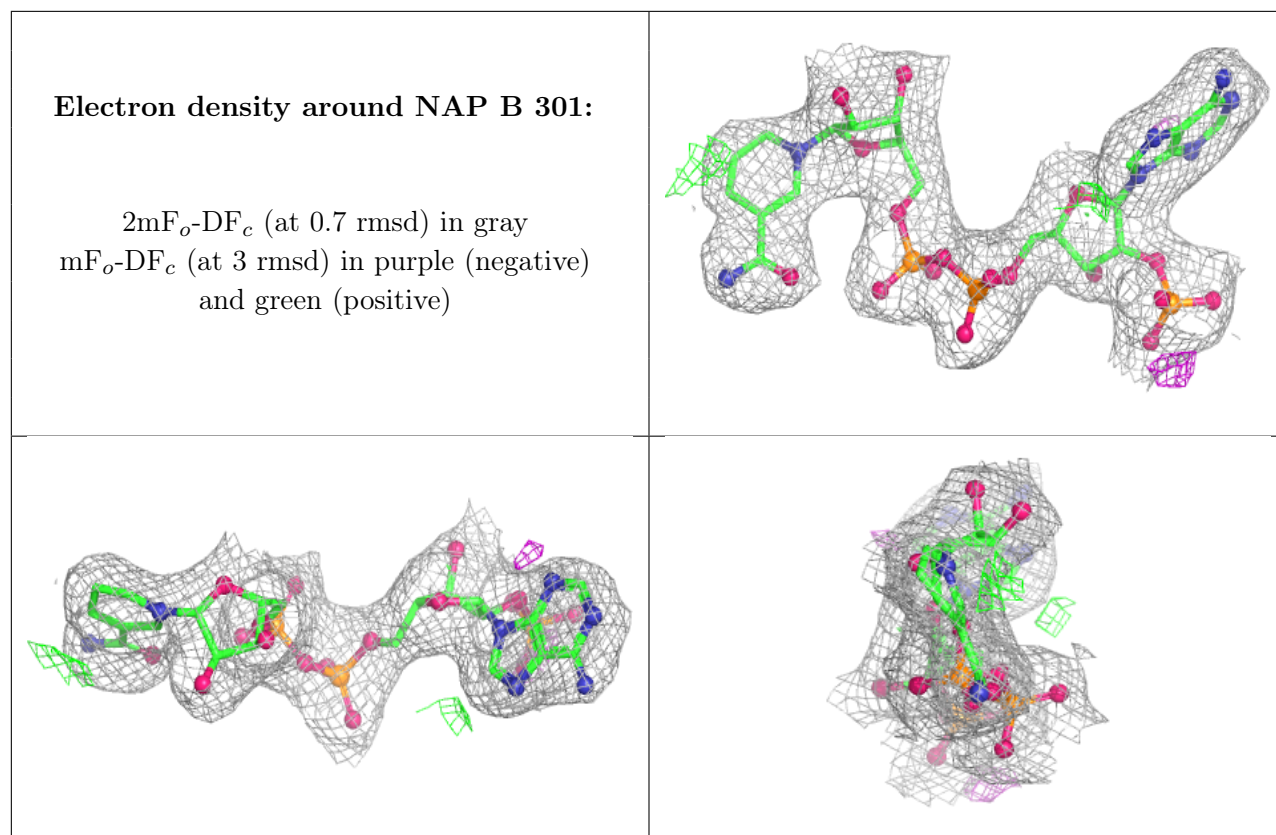
Electron density around NAP D 301:

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

**Electron density around NAP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.