



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:55 PM UTC

PDB ID : 5A4D / pdb_00005a4d
Title : Crystal structure of the chloroplastic gamma-ketol reductase from Arabidopsis thaliana bound to 13KOTE and NADP
Authors : Mas-y-mas, S.; Curien, G.; Giustini, C.; Rolland, N.; Ferrer, J.L.; Cobessi, D.
Deposited on : 2015-06-08
Resolution : 2.81 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:

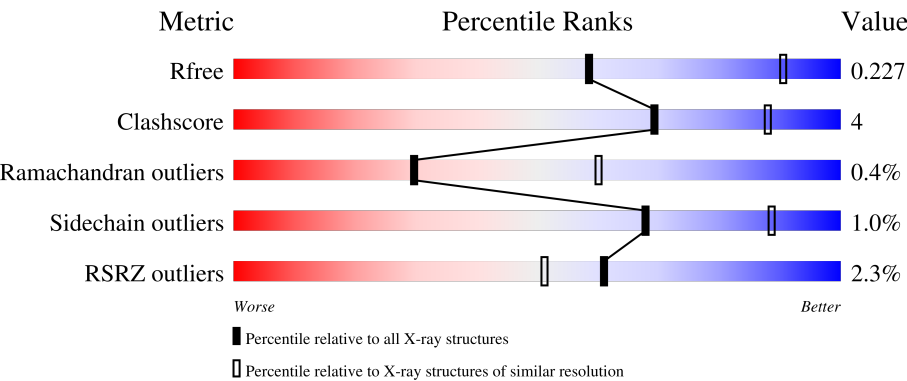
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	329	91%8% ..
1	B	329	3% 90%8% ..
1	C	329	2% 92%7% ..
1	D	329	89%10% ..
1	E	329	9% 86%8% • 5%

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Mol	Chain	Length	Quality of chain
1	F	329	88% 10% ..
1	G	329	% 90% 8% ..
1	H	329	4% 91% 8% ..

2 Entry composition

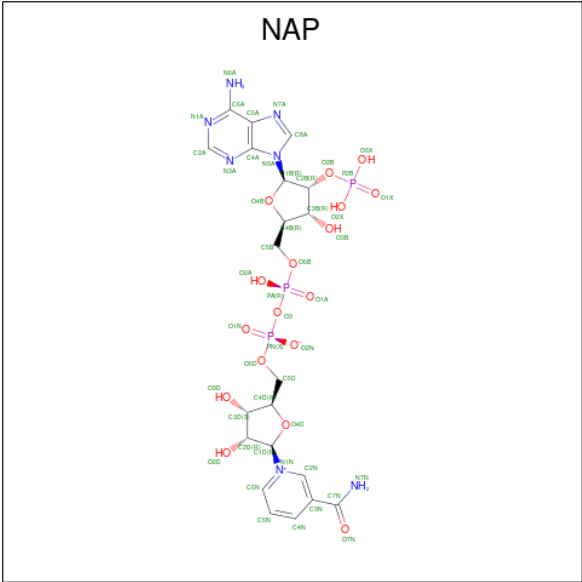
There are 3 unique types of molecules in this entry. The entry contains 19576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC.

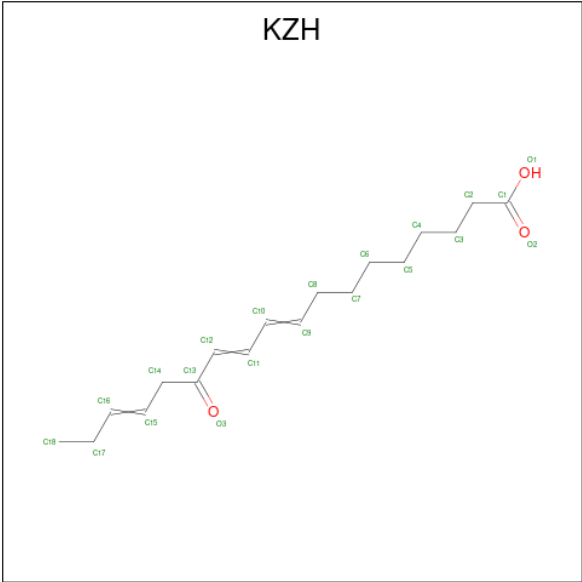
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2400	1535	410	446	9			
1	B	324	Total	C	N	O	S	0	3	0
			2390	1529	406	446	9			
1	C	326	Total	C	N	O	S	0	1	0
			2406	1539	412	446	9			
1	D	327	Total	C	N	O	S	0	3	0
			2417	1547	412	448	10			
1	E	313	Total	C	N	O	S	0	0	0
			2285	1463	391	423	8			
1	F	327	Total	C	N	O	S	0	2	0
			2412	1543	411	449	9			
1	G	327	Total	C	N	O	S	0	4	0
			2422	1550	414	448	10			
1	H	326	Total	C	N	O	S	0	0	0
			2396	1533	409	445	9			

- 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		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is (13-oxo-9(Z),11(E),15(Z)-octadecatrienoic acid) (CCD ID: KZH) (formula: C₁₈H₂₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	11	2		
3	C	1	Total	C	O	0	0
			9	7	2		
3	D	1	Total	C	O	0	0
			10	8	2		
3	F	1	Total	C	O	0	0
			11	9	2		
3	G	1	Total	C	O	0	0
			13	11	2		
3	H	1	Total	C	O	0	0
			8	6	2		

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.

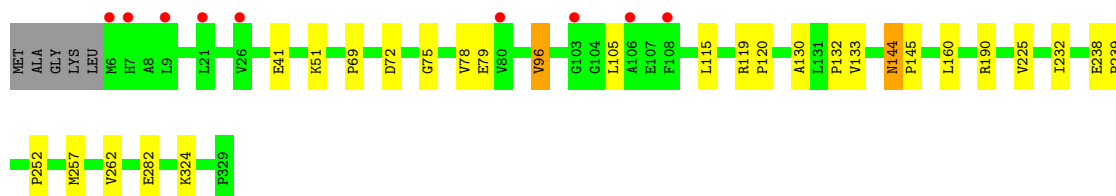
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC

Chain A: 

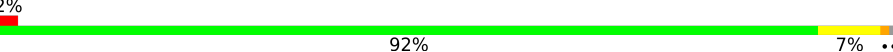


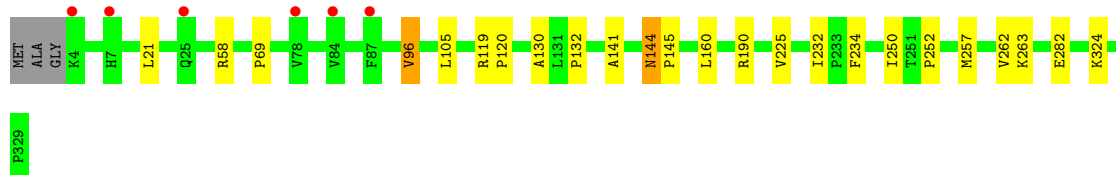
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC

Chain B: 



- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC

Chain C: 



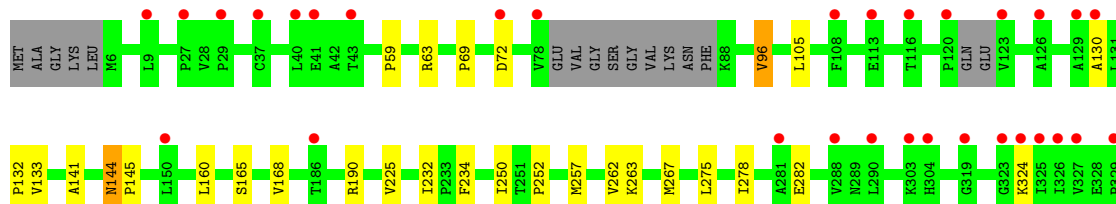
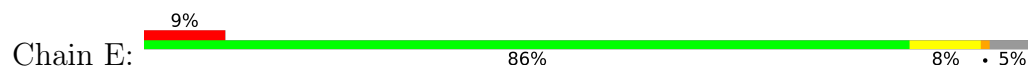
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC

Chain D: 

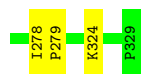
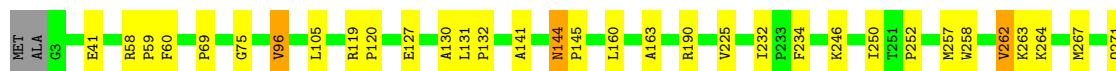
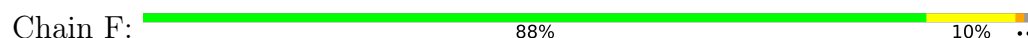




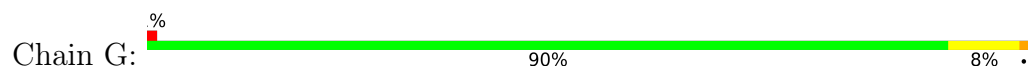
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC



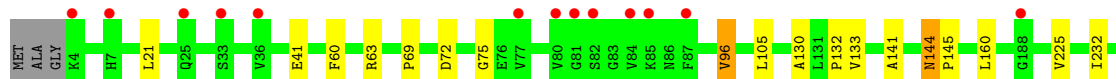
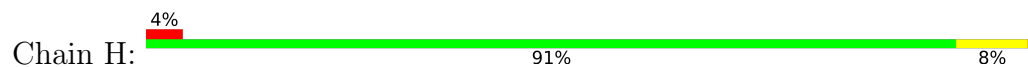
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC



- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC



- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.16Å 128.60Å 150.12Å 90.00° 97.76° 90.00°	Depositor
Resolution (Å)	49.58 – 2.81 49.58 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.58-2.81) 99.5 (49.58-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.188 , 0.225 0.200 , 0.227	Depositor DCC
R_{free} test set	3788 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19576	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: KZH, 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	0.62	0/2448	0.89	2/3326 (0.1%)
1	B	0.47	0/2446	0.81	1/3324 (0.0%)
1	C	0.50	0/2455	0.83	1/3336 (0.0%)
1	D	0.56	0/2474	0.86	4/3360 (0.1%)
1	E	0.49	0/2329	0.81	1/3165 (0.0%)
1	F	0.61	0/2466	0.87	2/3350 (0.1%)
1	G	0.59	0/2483	0.85	2/3373 (0.1%)
1	H	0.48	0/2444	0.83	1/3321 (0.0%)
All	All	0.54	0/19545	0.84	14/26555 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	232	ILE	N-CA-C	7.97	116.70	107.77
1	D	232	ILE	N-CA-C	7.73	116.43	107.77
1	C	232	ILE	N-CA-C	7.47	116.13	107.77
1	D	101	GLY	CA-C-N	-7.41	106.89	121.41
1	D	101	GLY	C-N-CA	-7.41	106.89	121.41
1	A	232	ILE	N-CA-C	7.39	116.16	107.73
1	F	232	ILE	N-CA-C	7.15	115.88	107.73
1	G	232	ILE	N-CA-C	6.98	115.68	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	ILE	N-CA-C	6.82	115.51	107.73
1	H	232	ILE	N-CA-C	6.79	115.37	107.77
1	D	102	GLY	N-CA-C	6.78	129.25	113.18
1	G	131	LEU	N-CA-C	5.34	119.51	112.35
1	A	131	LEU	N-CA-C	5.22	119.35	112.35
1	F	131	LEU	N-CA-C	5.22	119.35	112.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	102	GLY	Peptide

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	2400	0	2476	15	0
1	B	2390	0	2467	16	0
1	C	2406	0	2479	14	0
1	D	2417	0	2501	20	0
1	E	2285	0	2356	22	0
1	F	2412	0	2490	25	0
1	G	2422	0	2504	21	0
1	H	2396	0	2473	18	0
2	A	48	0	25	2	0
2	B	48	0	25	2	0
2	C	48	0	25	2	0
2	D	48	0	25	2	0
2	E	48	0	25	6	0
2	F	48	0	25	3	0
2	G	48	0	25	3	0
2	H	48	0	25	2	0
3	A	13	0	0	0	0
3	C	9	0	0	1	0
3	D	10	0	0	1	0
3	F	11	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	13	0	0	0	0
3	H	8	0	0	0	0
All	All	19576	0	19946	140	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 4.

All (140) 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:190:ARG:NH2	2:B:1330:NAP:O1X	2.15	0.79
1:E:267:MET:HE3	1:F:278:ILE:HG23	1.64	0.78
1:F:190:ARG:NH2	2:F:1330:NAP:O1X	2.16	0.77
1:B:144:ASN:HB2	1:B:145:PRO:HD3	1.67	0.76
1:A:144:ASN:HB2	1:A:145:PRO:HD3	1.69	0.74
1:D:58:ARG:NH2	3:D:1331:KZH:O2	2.20	0.74
1:E:130:ALA:HB1	1:E:324:LYS:HG3	1.70	0.74
1:C:144:ASN:HB2	1:C:145:PRO:HD3	1.69	0.73
1:F:144:ASN:HB2	1:F:145:PRO:HD3	1.68	0.73
1:E:144:ASN:HB2	1:E:145:PRO:HD3	1.69	0.73
1:H:144:ASN:HB2	1:H:145:PRO:HD3	1.71	0.73
1:D:144:ASN:HB2	1:D:145:PRO:HD3	1.70	0.73
1:G:144:ASN:HB2	1:G:145:PRO:HD3	1.71	0.71
1:E:168:VAL:N	2:E:1330:NAP:O1N	2.19	0.70
1:G:278:ILE:HG23	1:H:267:MET:HE3	1.73	0.70
1:B:130:ALA:HB1	1:B:324:LYS:HG3	1.73	0.70
1:D:130:ALA:HB1	1:D:324:LYS:HG3	1.74	0.70
1:C:130:ALA:HB1	1:C:324:LYS:HG3	1.73	0.69
1:A:190:ARG:NH2	2:A:1330:NAP:O1X	2.26	0.69
1:G:267:MET:HE3	1:H:278:ILE:HG23	1.73	0.68
1:F:130:ALA:HB1	1:F:324:LYS:HG3	1.74	0.68
1:G:130:ALA:HB1	1:G:324:LYS:HG3	1.75	0.67
1:H:96:VAL:HG22	1:H:132:PRO:HB3	1.77	0.66
1:D:96:VAL:HG22	1:D:132:PRO:HB3	1.76	0.66
1:A:130:ALA:HB1	1:A:324:LYS:HG3	1.78	0.65
1:H:130:ALA:HB1	1:H:324:LYS:HG3	1.78	0.64
1:G:96:VAL:HG22	1:G:132:PRO:HB3	1.81	0.63
1:E:96:VAL:HG22	1:E:132:PRO:HB3	1.81	0.62
1:F:96:VAL:HG22	1:F:132:PRO:HB3	1.82	0.62
1:B:96:VAL:HG22	1:B:132:PRO:HB3	1.81	0.62
1:C:96:VAL:HG22	1:C:132:PRO:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:SER:OG	2:E:1330:NAP:O3B	2.18	0.61
1:C:190:ARG:NH2	2:C:1330:NAP:O1X	2.34	0.60
1:A:96:VAL:HG22	1:A:132:PRO:HB3	1.84	0.59
1:D:190:ARG:NH2	2:D:1330:NAP:O1X	2.35	0.58
1:H:250:ILE:O	2:H:1330:NAP:H2N	2.04	0.58
1:F:60:PHE:CE1	1:G:59:PRO:HG2	2.38	0.57
1:F:69:PRO:HG2	1:F:105:LEU:HD12	1.87	0.57
1:E:278:ILE:HG23	1:F:267:MET:HE3	1.86	0.57
1:D:250:ILE:O	2:D:1330:NAP:H2N	2.05	0.56
1:E:63:ARG:HH21	1:H:63:ARG:HA	1.70	0.56
1:F:59:PRO:HG2	1:G:60:PHE:CE1	2.41	0.56
1:E:165:SER:HG	2:E:1330:NAP:HO3A	1.52	0.55
1:E:252:PRO:HB2	1:E:257:MET:HE2	1.88	0.55
1:F:252:PRO:HB2	1:F:257:MET:HE2	1.89	0.53
1:G:250:ILE:O	2:G:1330:NAP:H2N	2.08	0.53
1:G:69:PRO:HG2	1:G:105:LEU:HD12	1.91	0.51
1:E:275:LEU:O	2:E:1330:NAP:N7N	2.43	0.51
1:E:63:ARG:HA	1:H:63:ARG:HH21	1.76	0.50
1:B:252:PRO:HB2	1:B:257:MET:HE2	1.94	0.50
1:C:250:ILE:O	2:C:1330:NAP:H2N	2.12	0.50
1:G:141:ALA:O	1:G:145:PRO:HD2	2.11	0.50
1:A:69:PRO:HG2	1:A:105:LEU:HD12	1.93	0.49
1:C:58:ARG:NH2	3:C:1331:KZH:O2	2.42	0.49
1:A:252:PRO:HB2	1:A:257:MET:HE2	1.94	0.49
1:D:68:ILE:CG2	1:D:103:GLY:HA2	2.42	0.49
1:D:68:ILE:HG22	1:D:103:GLY:HA2	1.95	0.49
1:F:58:ARG:NH2	3:F:1331:KZH:O2	2.43	0.48
1:F:163:ALA:HA	2:F:1330:NAP:N3A	2.29	0.48
1:A:41:GLU:HG3	1:A:75:GLY:HA2	1.96	0.47
1:D:69:PRO:HG2	1:D:105:LEU:HD12	1.96	0.47
1:H:69:PRO:HG2	1:H:105:LEU:HD12	1.96	0.47
1:A:72:ASP:OD1	1:A:133:VAL:HG23	2.13	0.47
1:C:252:PRO:HB2	1:C:257:MET:HE2	1.96	0.47
1:E:160:LEU:HB3	1:E:225:VAL:HG22	1.96	0.47
1:F:250:ILE:O	2:F:1330:NAP:H2N	2.14	0.47
1:D:97:LEU:HD13	1:D:102:GLY:O	2.14	0.47
1:F:160:LEU:HB3	1:F:225:VAL:HG22	1.97	0.47
1:A:234:PHE:CE2	1:A:263:LYS:HE3	2.50	0.46
1:F:264:LYS:HE2	1:F:271[A]:GLN:NE2	2.30	0.46
1:D:252:PRO:HB2	1:D:257:MET:HE2	1.97	0.46
1:E:282:GLU:CD	1:E:282:GLU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ASP:OD1	1:D:133:VAL:HG23	2.15	0.46
1:A:141:ALA:O	1:A:145:PRO:HD2	2.15	0.46
1:D:282:GLU:H	1:D:282:GLU:CD	2.24	0.46
1:B:51:LYS:NZ	2:B:1330:NAP:O3D	2.42	0.45
1:E:267:MET:HE1	1:F:279:PRO:HD2	1.99	0.45
1:B:160:LEU:HB3	1:B:225:VAL:HG22	1.98	0.45
1:B:282:GLU:H	1:B:282:GLU:CD	2.24	0.45
1:C:282:GLU:H	1:C:282:GLU:CD	2.24	0.45
1:D:160:LEU:HB3	1:D:225:VAL:HG22	1.99	0.45
1:A:282:GLU:H	1:A:282:GLU:CD	2.25	0.45
1:E:69:PRO:HG2	1:E:105:LEU:HD12	1.99	0.45
1:B:69:PRO:HG2	1:B:105:LEU:HD12	1.99	0.44
1:C:21:LEU:HD12	1:C:21:LEU:HA	1.90	0.44
1:D:21:LEU:HD12	1:D:21:LEU:HA	1.86	0.44
1:G:234:PHE:CE2	1:G:263:LYS:HE3	2.53	0.44
1:H:282:GLU:H	1:H:282:GLU:CD	2.26	0.44
1:C:69:PRO:HG2	1:C:105:LEU:HD12	2.00	0.44
1:H:252:PRO:HB2	1:H:257:MET:HE2	1.99	0.44
1:G:190:ARG:NH2	2:G:1330:NAP:O1X	2.50	0.44
1:F:59:PRO:HG2	1:G:60:PHE:HE1	1.83	0.43
1:F:41:GLU:HG3	1:F:75:GLY:HA2	2.00	0.43
1:B:78:VAL:O	1:B:79[B]:GLU:HG3	2.18	0.43
1:G:160:LEU:HB3	1:G:225:VAL:HG22	1.99	0.43
1:H:72:ASP:OD1	1:H:133:VAL:HG23	2.19	0.43
1:G:282:GLU:H	1:G:282:GLU:CD	2.26	0.43
1:E:250:ILE:O	2:E:1330:NAP:H2N	2.19	0.42
1:F:141:ALA:O	1:F:145:PRO:HD2	2.19	0.42
1:B:238:GLU:HB3	1:B:239:PRO:HD3	2.01	0.42
1:H:160:LEU:HB3	1:H:225:VAL:HG22	2.01	0.42
1:A:21:LEU:HD12	1:A:21:LEU:HA	1.87	0.42
1:A:252:PRO:HB3	1:A:274:PRO:HB3	2.02	0.42
1:H:141:ALA:O	1:H:145:PRO:HD2	2.19	0.42
1:B:119:ARG:HA	1:B:120:PRO:HD2	1.94	0.42
1:C:234:PHE:CE2	1:C:263:LYS:HE3	2.55	0.42
1:F:246:LYS:HG2	1:F:271[B]:GLN:HG3	2.01	0.42
1:E:72:ASP:OD1	1:E:133:VAL:HG23	2.20	0.42
1:B:41:GLU:HG3	1:B:75:GLY:HA2	2.02	0.42
1:G:238:GLU:HB3	1:G:239:PRO:HD3	2.01	0.42
1:B:72:ASP:OD1	1:B:133:VAL:HG23	2.19	0.42
1:D:41:GLU:HG3	1:D:75:GLY:HA2	2.01	0.42
1:G:252:PRO:HB2	1:G:257:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:LEU:HD12	1:H:21:LEU:HA	1.89	0.42
1:E:234:PHE:CE2	1:E:263:LYS:HE3	2.55	0.41
1:F:60:PHE:CD1	1:G:59:PRO:HG2	2.55	0.41
1:D:177:LYS:HA	1:D:177:LYS:HD2	1.86	0.41
1:E:190:ARG:NH2	2:E:1330:NAP:O1X	2.53	0.41
1:G:163:ALA:HA	2:G:1330:NAP:N3A	2.34	0.41
1:A:163:ALA:HA	2:A:1330:NAP:N3A	2.35	0.41
1:G:21:LEU:HD12	1:G:21:LEU:HA	1.83	0.41
1:B:144:ASN:HB2	1:B:145:PRO:CD	2.45	0.41
1:E:59:PRO:HG2	1:H:60:PHE:CE1	2.55	0.41
1:E:141:ALA:O	1:E:145:PRO:HD2	2.20	0.41
1:A:234:PHE:CD2	1:A:263:LYS:HE3	2.56	0.41
1:D:141:ALA:O	1:D:145:PRO:HD2	2.21	0.41
1:D:238:GLU:HB3	1:D:239:PRO:HD3	2.02	0.41
1:F:119:ARG:HA	1:F:120:PRO:HD2	1.96	0.41
1:G:69:PRO:O	1:G:70:ALA:HB3	2.21	0.41
1:C:141:ALA:O	1:C:145:PRO:HD2	2.21	0.40
1:F:234:PHE:CE2	1:F:263:LYS:HE3	2.55	0.40
1:F:258:TRP:O	1:F:262:VAL:HG13	2.21	0.40
1:D:234:PHE:CE2	1:D:263:LYS:HE3	2.56	0.40
1:F:234:PHE:CD2	1:F:263:LYS:HE3	2.57	0.40
1:H:252:PRO:HB3	1:H:274:PRO:HB3	2.03	0.40
1:C:119:ARG:HA	1:C:120:PRO:HD2	1.94	0.40
1:C:160:LEU:HB3	1:C:225:VAL:HG22	2.02	0.40
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.92	0.40
1:H:41:GLU:HG3	1:H:75:GLY:HA2	2.02	0.40
2:H:1330:NAP:H6N	2:H:1330:NAP:H2D	1.84	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	325/329 (99%)	318 (98%)	5 (2%)	2 (1%)	21	51
1	B	325/329 (99%)	319 (98%)	5 (2%)	1 (0%)	36	66
1	C	325/329 (99%)	317 (98%)	7 (2%)	1 (0%)	36	66
1	D	328/329 (100%)	320 (98%)	6 (2%)	2 (1%)	21	51
1	E	307/329 (93%)	301 (98%)	5 (2%)	1 (0%)	36	66
1	F	327/329 (99%)	320 (98%)	6 (2%)	1 (0%)	36	66
1	G	329/329 (100%)	322 (98%)	5 (2%)	2 (1%)	21	51
1	H	324/329 (98%)	316 (98%)	7 (2%)	1 (0%)	36	66
All	All	2590/2632 (98%)	2533 (98%)	46 (2%)	11 (0%)	30	60

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	144	ASN
1	A	144	ASN
1	B	144	ASN
1	C	144	ASN
1	D	144	ASN
1	E	144	ASN
1	F	144	ASN
1	G	70	ALA
1	H	144	ASN
1	A	70	ALA
1	D	70	ALA

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	252/255 (99%)	248 (98%)	4 (2%)	55	83
1	B	252/255 (99%)	250 (99%)	2 (1%)	73	90
1	C	253/255 (99%)	251 (99%)	2 (1%)	73	90
1	D	255/255 (100%)	253 (99%)	2 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	238/255 (93%)	236 (99%)	2 (1%)	73	90
1	F	254/255 (100%)	250 (98%)	4 (2%)	55	83
1	G	256/255 (100%)	254 (99%)	2 (1%)	73	90
1	H	252/255 (99%)	250 (99%)	2 (1%)	73	90
All	All	2012/2040 (99%)	1992 (99%)	20 (1%)	68	88

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	VAL
1	A	96	VAL
1	A	143	THR
1	A	262	VAL
1	B	96	VAL
1	B	262	VAL
1	C	96	VAL
1	C	262	VAL
1	D	96	VAL
1	D	262	VAL
1	E	96	VAL
1	E	262	VAL
1	F	96	VAL
1	F	127[A]	GLU
1	F	127[B]	GLU
1	F	262	VAL
1	G	96	VAL
1	G	262	VAL
1	H	96	VAL
1	H	262	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	E	244	ASN

5.3.3 RNA ⓘ

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](#)

14 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	F	1330	-	50,52,52	2.26	15 (30%)	71,80,80	2.04	18 (25%)
2	NAP	D	1330	-	50,52,52	2.24	14 (28%)	71,80,80	1.87	13 (18%)
2	NAP	G	1330	-	50,52,52	2.16	13 (26%)	71,80,80	1.92	15 (21%)
2	NAP	H	1330	-	50,52,52	2.05	11 (22%)	71,80,80	1.85	15 (21%)
3	KZH	H	1331	-	7,7,20	0.83	0	7,7,21	1.17	1 (14%)
3	KZH	D	1331	-	9,9,20	0.54	0	9,9,21	1.22	1 (11%)
2	NAP	A	1330	-	50,52,52	2.11	13 (26%)	71,80,80	1.91	18 (25%)
2	NAP	E	1330	-	50,52,52	2.28	17 (34%)	71,80,80	2.08	15 (21%)
3	KZH	F	1331	-	10,10,20	0.73	0	10,10,21	1.03	0
3	KZH	C	1331	-	8,8,20	0.76	0	8,8,21	1.07	1 (12%)
2	NAP	C	1330	-	50,52,52	2.05	14 (28%)	71,80,80	1.80	13 (18%)
2	NAP	B	1330	-	50,52,52	2.29	13 (26%)	71,80,80	1.98	18 (25%)
3	KZH	A	1331	-	12,12,20	0.70	0	12,12,21	1.17	1 (8%)
3	KZH	G	1331	-	12,12,20	0.75	0	12,12,21	1.18	2 (16%)

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	F	1330	-	-	5/35/67/67	0/5/5/5
2	NAP	D	1330	-	-	7/35/67/67	0/5/5/5
2	NAP	G	1330	-	-	4/35/67/67	0/5/5/5
2	NAP	H	1330	-	-	6/35/67/67	0/5/5/5
3	KZH	H	1331	-	-	4/5/5/19	-
3	KZH	D	1331	-	-	3/7/7/19	-
2	NAP	A	1330	-	-	9/35/67/67	0/5/5/5
2	NAP	E	1330	-	-	11/35/67/67	0/5/5/5
3	KZH	F	1331	-	-	4/8/8/19	-
3	KZH	C	1331	-	-	3/6/6/19	-
2	NAP	C	1330	-	-	7/35/67/67	0/5/5/5
2	NAP	B	1330	-	-	12/35/67/67	0/5/5/5
3	KZH	A	1331	-	-	6/10/10/19	-
3	KZH	G	1331	-	-	4/10/10/19	-

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1330	NAP	O4D-C1D	9.10	1.52	1.40
2	F	1330	NAP	O4D-C1D	8.41	1.51	1.40
2	H	1330	NAP	O4D-C1D	8.26	1.51	1.40
2	E	1330	NAP	O4D-C1D	8.08	1.51	1.40
2	A	1330	NAP	O4D-C1D	7.87	1.51	1.40
2	D	1330	NAP	O4D-C1D	7.68	1.51	1.40
2	G	1330	NAP	O4D-C1D	7.66	1.50	1.40
2	C	1330	NAP	O4D-C1D	7.57	1.50	1.40
2	D	1330	NAP	C7N-N7N	6.63	1.45	1.33
2	G	1330	NAP	C7N-N7N	6.08	1.44	1.33
2	E	1330	NAP	C7N-N7N	6.01	1.44	1.33
2	C	1330	NAP	C7N-N7N	5.95	1.43	1.33
2	B	1330	NAP	C7N-N7N	5.92	1.43	1.33
2	F	1330	NAP	C7N-N7N	5.72	1.43	1.33
2	A	1330	NAP	C7N-N7N	5.60	1.43	1.33
2	H	1330	NAP	C7N-N7N	5.39	1.42	1.33
2	D	1330	NAP	C3N-C7N	4.44	1.57	1.50
2	F	1330	NAP	PN-O3	4.15	1.64	1.59
2	A	1330	NAP	C3N-C7N	3.98	1.56	1.50
2	D	1330	NAP	C2N-N1N	3.89	1.39	1.35
2	E	1330	NAP	C2N-N1N	3.80	1.39	1.35
2	B	1330	NAP	C3N-C7N	3.79	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1330	NAP	C3N-C7N	3.74	1.56	1.50
2	D	1330	NAP	C6A-N6A	3.68	1.43	1.34
2	E	1330	NAP	C6A-N6A	3.67	1.43	1.34
2	F	1330	NAP	O4B-C1B	3.64	1.50	1.42
2	H	1330	NAP	C3N-C7N	3.62	1.56	1.50
2	B	1330	NAP	C6A-N6A	3.60	1.43	1.34
2	C	1330	NAP	C6A-N6A	3.58	1.43	1.34
2	F	1330	NAP	PA-O3	3.58	1.63	1.59
2	E	1330	NAP	C3N-C7N	3.55	1.55	1.50
2	B	1330	NAP	C2N-N1N	3.53	1.38	1.35
2	G	1330	NAP	O4B-C1B	3.51	1.50	1.42
2	D	1330	NAP	O4B-C1B	3.46	1.50	1.42
2	F	1330	NAP	C2N-N1N	3.45	1.38	1.35
2	E	1330	NAP	PA-O3	3.43	1.63	1.59
2	G	1330	NAP	C3B-C2B	-3.43	1.45	1.53
2	F	1330	NAP	C3N-C7N	3.34	1.55	1.50
2	G	1330	NAP	C2N-N1N	3.34	1.38	1.35
2	E	1330	NAP	O4B-C1B	3.33	1.49	1.42
2	B	1330	NAP	O4B-C1B	3.33	1.49	1.42
2	C	1330	NAP	O4B-C1B	3.33	1.49	1.42
2	F	1330	NAP	C6A-N6A	3.32	1.42	1.34
2	E	1330	NAP	PN-O3	3.22	1.63	1.59
2	B	1330	NAP	PA-O3	3.19	1.62	1.59
2	A	1330	NAP	O4B-C1B	3.18	1.49	1.42
2	E	1330	NAP	C3B-C2B	-3.16	1.46	1.53
2	A	1330	NAP	C6A-N6A	3.11	1.42	1.34
2	A	1330	NAP	C2N-N1N	3.11	1.38	1.35
2	D	1330	NAP	C5A-N7A	-3.06	1.33	1.39
2	G	1330	NAP	C5A-N7A	-2.96	1.33	1.39
2	H	1330	NAP	O4B-C1B	2.96	1.48	1.42
2	H	1330	NAP	C2D-C3D	-2.95	1.45	1.53
2	G	1330	NAP	C2B-C1B	-2.90	1.46	1.53
2	C	1330	NAP	C3N-C7N	2.89	1.54	1.50
2	C	1330	NAP	C5A-N7A	-2.85	1.33	1.39
2	F	1330	NAP	C2D-C3D	-2.84	1.45	1.53
2	H	1330	NAP	C5A-N7A	-2.81	1.33	1.39
2	B	1330	NAP	C5A-N7A	-2.81	1.34	1.39
2	A	1330	NAP	C5A-N7A	-2.80	1.34	1.39
2	B	1330	NAP	PN-O3	2.75	1.62	1.59
2	B	1330	NAP	C3B-C2B	-2.74	1.47	1.53
2	G	1330	NAP	C6A-N6A	2.74	1.41	1.34
2	H	1330	NAP	C6A-N6A	2.74	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1330	NAP	C2N-N1N	2.73	1.38	1.35
2	E	1330	NAP	C5A-N7A	-2.72	1.34	1.39
2	A	1330	NAP	C3B-C2B	-2.69	1.47	1.53
2	G	1330	NAP	C1B-N9A	-2.60	1.39	1.46
2	F	1330	NAP	C3D-C4D	-2.59	1.46	1.53
2	D	1330	NAP	O4D-C4D	2.51	1.50	1.45
2	C	1330	NAP	C2N-N1N	2.48	1.37	1.35
2	F	1330	NAP	C3B-C2B	-2.47	1.47	1.53
2	G	1330	NAP	C2D-C3D	-2.46	1.46	1.53
2	C	1330	NAP	C2B-C1B	-2.46	1.47	1.53
2	D	1330	NAP	C8A-N9A	-2.42	1.33	1.37
2	C	1330	NAP	C3B-C2B	-2.41	1.47	1.53
2	E	1330	NAP	C2D-C3D	-2.37	1.47	1.53
2	C	1330	NAP	C2D-C3D	-2.34	1.47	1.53
2	B	1330	NAP	O4D-C4D	2.32	1.50	1.45
2	H	1330	NAP	C3B-C2B	-2.31	1.47	1.53
2	H	1330	NAP	C3D-C4D	-2.30	1.47	1.53
2	A	1330	NAP	O4D-C4D	2.30	1.50	1.45
2	G	1330	NAP	O4D-C4D	2.29	1.50	1.45
2	A	1330	NAP	C2B-C1B	-2.28	1.47	1.53
2	F	1330	NAP	C5A-N7A	-2.28	1.34	1.39
2	D	1330	NAP	C2D-C3D	-2.28	1.47	1.53
2	C	1330	NAP	C1B-N9A	-2.26	1.40	1.46
2	D	1330	NAP	C2A-N3A	2.26	1.37	1.33
2	A	1330	NAP	C1B-N9A	-2.23	1.40	1.46
2	E	1330	NAP	O4B-C4B	2.23	1.49	1.45
2	D	1330	NAP	C1B-N9A	-2.22	1.40	1.46
2	B	1330	NAP	C1B-N9A	-2.22	1.40	1.46
2	C	1330	NAP	C8A-N9A	-2.22	1.33	1.37
2	D	1330	NAP	C3D-C4D	-2.21	1.47	1.53
2	C	1330	NAP	C3D-C4D	-2.15	1.47	1.53
2	A	1330	NAP	C3D-C4D	-2.14	1.47	1.53
2	F	1330	NAP	O2D-C2D	2.14	1.48	1.43
2	B	1330	NAP	C8A-N9A	-2.14	1.33	1.37
2	E	1330	NAP	C8A-N9A	-2.13	1.33	1.37
2	E	1330	NAP	C3D-C4D	-2.13	1.47	1.53
2	F	1330	NAP	O4B-C4B	2.12	1.49	1.45
2	E	1330	NAP	O4D-C4D	2.11	1.49	1.45
2	G	1330	NAP	O3D-C3D	2.11	1.48	1.43
2	F	1330	NAP	O4D-C4D	2.09	1.49	1.45
2	C	1330	NAP	O4D-C4D	2.05	1.49	1.45
2	A	1330	NAP	C8A-N9A	-2.05	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1330	NAP	C1B-N9A	-2.03	1.40	1.46
2	H	1330	NAP	O4D-C4D	2.02	1.49	1.45
2	D	1330	NAP	C2B-C1B	-2.01	1.48	1.53
2	E	1330	NAP	O2D-C2D	2.01	1.47	1.43

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1330	NAP	C4D-O4D-C1D	-7.65	102.92	109.92
2	G	1330	NAP	C4D-O4D-C1D	-6.91	103.59	109.92
2	E	1330	NAP	C5A-C4A-N3A	-6.76	117.40	126.72
2	D	1330	NAP	C5A-C4A-N3A	-6.52	117.74	126.72
2	G	1330	NAP	N3A-C2A-N1A	-6.50	118.75	128.58
2	B	1330	NAP	C5A-C4A-N3A	-6.32	118.01	126.72
2	H	1330	NAP	C5A-C4A-N3A	-5.74	118.81	126.72
2	F	1330	NAP	N3A-C2A-N1A	-5.71	119.94	128.58
2	C	1330	NAP	C4D-O4D-C1D	-5.71	104.70	109.92
2	D	1330	NAP	C4D-O4D-C1D	-5.70	104.71	109.92
2	C	1330	NAP	C5A-C4A-N3A	-5.65	118.94	126.72
2	H	1330	NAP	C4D-O4D-C1D	-5.65	104.75	109.92
2	A	1330	NAP	C5A-C4A-N3A	-5.64	118.95	126.72
2	A	1330	NAP	N3A-C2A-N1A	-5.61	120.08	128.58
2	B	1330	NAP	C4D-O4D-C1D	-5.57	104.83	109.92
2	F	1330	NAP	C4D-O4D-C1D	-5.43	104.95	109.92
2	E	1330	NAP	N3A-C4A-N9A	5.43	136.41	127.17
2	E	1330	NAP	N3A-C2A-N1A	-5.31	120.55	128.58
2	H	1330	NAP	N3A-C2A-N1A	-5.27	120.61	128.58
2	B	1330	NAP	N3A-C2A-N1A	-5.21	120.69	128.58
2	F	1330	NAP	C5A-C4A-N3A	-5.21	119.55	126.72
2	G	1330	NAP	C5A-C4A-N3A	-5.19	119.57	126.72
2	D	1330	NAP	N3A-C4A-N9A	5.07	135.79	127.17
2	B	1330	NAP	N3A-C4A-N9A	5.07	135.78	127.17
2	C	1330	NAP	N3A-C2A-N1A	-4.91	121.16	128.58
2	C	1330	NAP	N3A-C4A-N9A	4.23	134.36	127.17
2	B	1330	NAP	C5A-N7A-C8A	4.21	110.06	103.45
2	G	1330	NAP	N3A-C4A-N9A	4.17	134.26	127.17
2	E	1330	NAP	C2A-N3A-C4A	4.15	121.96	111.83
2	D	1330	NAP	N3A-C2A-N1A	-4.13	122.33	128.58
2	F	1330	NAP	C5A-N7A-C8A	4.10	109.90	103.45
2	B	1330	NAP	C6N-N1N-C2N	-4.06	118.42	121.88
2	A	1330	NAP	N3A-C4A-N9A	4.06	134.07	127.17
2	A	1330	NAP	O7N-C7N-N7N	-3.94	116.93	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1330	NAP	C5A-N7A-C8A	3.90	109.58	103.45
2	B	1330	NAP	C2A-N3A-C4A	3.88	121.31	111.83
2	F	1330	NAP	C4A-C5A-N7A	-3.86	106.16	110.58
2	H	1330	NAP	C4A-C5A-N7A	-3.83	106.20	110.58
2	G	1330	NAP	C2A-N3A-C4A	3.81	121.14	111.83
2	H	1330	NAP	N3A-C4A-N9A	3.79	133.62	127.17
2	F	1330	NAP	C2A-N3A-C4A	3.78	121.06	111.83
2	A	1330	NAP	C2A-N3A-C4A	3.76	121.02	111.83
2	E	1330	NAP	C5A-N7A-C8A	3.76	109.36	103.45
2	C	1330	NAP	C6N-N1N-C2N	-3.76	118.68	121.88
2	C	1330	NAP	C5A-N7A-C8A	3.76	109.35	103.45
2	G	1330	NAP	C4B-O4B-C1B	-3.75	101.18	109.47
2	F	1330	NAP	O7N-C7N-C3N	3.73	124.16	119.60
2	D	1330	NAP	C5A-N7A-C8A	3.71	109.28	103.45
2	F	1330	NAP	N3A-C4A-N9A	3.71	133.47	127.17
2	E	1330	NAP	C6N-N1N-C2N	-3.62	118.80	121.88
2	A	1330	NAP	C5A-N7A-C8A	3.59	109.09	103.45
2	H	1330	NAP	C2A-N3A-C4A	3.58	120.58	111.83
2	A	1330	NAP	C4D-O4D-C1D	-3.58	106.64	109.92
2	B	1330	NAP	C4A-C5A-N7A	-3.49	106.59	110.58
2	C	1330	NAP	C4A-C5A-N7A	-3.46	106.62	110.58
2	D	1330	NAP	C4A-C5A-N7A	-3.45	106.64	110.58
2	C	1330	NAP	C2A-N3A-C4A	3.44	120.23	111.83
2	F	1330	NAP	O4B-C1B-N9A	3.42	114.66	108.09
2	A	1330	NAP	C4A-C5A-N7A	-3.36	106.74	110.58
2	A	1330	NAP	C6N-N1N-C2N	-3.32	119.05	121.88
2	D	1330	NAP	C6N-N1N-C2N	-3.31	119.06	121.88
2	D	1330	NAP	C2A-N3A-C4A	3.30	119.89	111.83
2	F	1330	NAP	C6N-N1N-C2N	-3.29	119.08	121.88
2	G	1330	NAP	C6N-N1N-C2N	-3.25	119.11	121.88
2	E	1330	NAP	C4A-C5A-N7A	-3.24	106.88	110.58
2	F	1330	NAP	C4B-O4B-C1B	-3.22	102.35	109.47
2	G	1330	NAP	C5A-N7A-C8A	3.21	108.49	103.45
2	E	1330	NAP	C3N-C7N-N7N	3.18	121.65	117.74
2	E	1330	NAP	O4B-C1B-N9A	3.06	113.96	108.09
2	A	1330	NAP	C4B-O4B-C1B	-3.02	102.81	109.47
2	F	1330	NAP	N9A-C8A-N7A	-2.95	109.75	113.94
2	B	1330	NAP	N9A-C8A-N7A	-2.90	109.82	113.94
2	F	1330	NAP	O2N-PN-O3	2.88	115.06	107.27
2	H	1330	NAP	C6N-N1N-C2N	-2.87	119.43	121.88
2	B	1330	NAP	O7N-C7N-C3N	2.80	123.02	119.60
2	A	1330	NAP	O7N-C7N-C3N	2.78	123.00	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1331	KZH	O1-C1-C2	2.76	122.72	114.00
2	H	1330	NAP	C2D-C3D-C4D	2.65	107.73	102.61
3	A	1331	KZH	O1-C1-C2	2.64	122.35	114.00
2	F	1330	NAP	C2D-C3D-C4D	2.60	107.64	102.61
2	E	1330	NAP	O7N-C7N-N7N	-2.58	118.88	122.62
2	G	1330	NAP	N9A-C8A-N7A	-2.58	110.28	113.94
2	D	1330	NAP	C4B-O4B-C1B	-2.54	103.85	109.47
2	C	1330	NAP	C4B-O4B-C1B	-2.54	103.87	109.47
2	F	1330	NAP	C2B-C3B-C4B	2.53	107.43	101.99
2	F	1330	NAP	O3D-C3D-C4D	-2.50	103.89	111.08
2	H	1330	NAP	P2B-O2B-C2B	-2.50	116.76	123.43
2	A	1330	NAP	O4B-C1B-N9A	2.50	112.88	108.09
2	D	1330	NAP	O7N-C7N-N7N	-2.45	119.07	122.62
2	C	1330	NAP	P2B-O2B-C2B	-2.43	116.94	123.43
2	D	1330	NAP	C6A-C5A-C4A	2.40	120.46	117.18
2	G	1330	NAP	O2N-PN-O3	2.40	113.76	107.27
2	G	1330	NAP	C4A-C5A-N7A	-2.39	107.85	110.58
3	G	1331	KZH	O1-C1-C2	2.39	121.56	114.00
2	A	1330	NAP	C2D-C3D-C4D	2.38	107.20	102.61
2	E	1330	NAP	C2B-C1B-N9A	-2.36	109.87	113.75
2	A	1330	NAP	N9A-C8A-N7A	-2.35	110.61	113.94
2	C	1330	NAP	N9A-C8A-N7A	-2.34	110.61	113.94
2	C	1330	NAP	O3X-P2B-O2B	2.34	114.97	105.85
2	H	1330	NAP	N9A-C8A-N7A	-2.34	110.62	113.94
2	G	1330	NAP	C2B-C3B-C4B	2.33	107.01	101.99
2	H	1330	NAP	O7N-C7N-C3N	2.33	122.45	119.60
2	H	1330	NAP	O7N-C7N-N7N	-2.29	119.30	122.62
2	C	1330	NAP	C2B-C3B-C4B	2.28	106.90	101.99
2	A	1330	NAP	O3D-C3D-C4D	-2.28	104.53	111.08
3	C	1331	KZH	O1-C1-C2	2.26	121.15	114.00
2	F	1330	NAP	C6A-C5A-N7A	2.25	136.44	132.09
2	G	1330	NAP	C2A-N1A-C6A	2.24	122.41	118.73
2	B	1330	NAP	O2A-PA-O3	2.23	113.30	107.27
2	A	1330	NAP	O3X-P2B-O2X	2.22	116.12	107.80
2	F	1330	NAP	O7N-C7N-N7N	-2.22	119.41	122.62
2	B	1330	NAP	C2B-C3B-C4B	2.18	106.67	101.99
2	A	1330	NAP	C5B-C4B-C3B	-2.17	107.42	115.21
2	G	1330	NAP	P2B-O2B-C2B	-2.16	117.65	123.43
2	B	1330	NAP	C4B-O4B-C1B	-2.16	104.70	109.47
2	A	1330	NAP	C2B-C3B-C4B	2.16	106.63	101.99
3	G	1331	KZH	C3-C2-C1	2.15	120.12	114.51
2	D	1330	NAP	C2B-C3B-C4B	2.15	106.62	101.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1330	NAP	N9A-C8A-N7A	-2.13	110.91	113.94
2	B	1330	NAP	O3X-P2B-O2B	2.13	114.16	105.85
2	B	1330	NAP	O7N-C7N-N7N	-2.12	119.55	122.62
2	H	1330	NAP	C4B-O4B-C1B	-2.11	104.81	109.47
3	H	1331	KZH	O1-C1-C2	2.11	120.65	114.00
2	D	1330	NAP	C2D-C3D-C4D	2.10	106.66	102.61
2	H	1330	NAP	C3B-C2B-C1B	2.09	106.80	102.81
2	G	1330	NAP	O7N-C7N-N7N	-2.08	119.61	122.62
2	B	1330	NAP	C3B-C2B-C1B	2.07	106.78	102.81
2	B	1330	NAP	C2D-C3D-C4D	2.07	106.61	102.61
2	E	1330	NAP	C2D-C3D-C4D	2.07	106.60	102.61
2	E	1330	NAP	O3X-P2B-O2B	2.04	113.79	105.85
2	B	1330	NAP	O3-PA-O1A	-2.02	104.64	110.70

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1330	NAP	C5B-O5B-PA-O1A
2	A	1330	NAP	C5B-O5B-PA-O3
2	A	1330	NAP	C5D-O5D-PN-O1N
2	A	1330	NAP	O4D-C1D-N1N-C6N
2	B	1330	NAP	C5B-O5B-PA-O1A
2	B	1330	NAP	C5B-O5B-PA-O2A
2	B	1330	NAP	C5B-O5B-PA-O3
2	B	1330	NAP	C5D-O5D-PN-O3
2	B	1330	NAP	C5D-O5D-PN-O1N
2	C	1330	NAP	C5D-O5D-PN-O3
2	C	1330	NAP	C5D-O5D-PN-O1N
2	C	1330	NAP	O4D-C1D-N1N-C2N
2	C	1330	NAP	O4D-C1D-N1N-C6N
2	C	1330	NAP	C2D-C1D-N1N-C2N
2	C	1330	NAP	C2D-C1D-N1N-C6N
2	D	1330	NAP	C5D-O5D-PN-O1N
2	D	1330	NAP	O4D-C1D-N1N-C2N
2	D	1330	NAP	O4D-C1D-N1N-C6N
2	D	1330	NAP	C2D-C1D-N1N-C2N
2	D	1330	NAP	C2D-C1D-N1N-C6N
2	E	1330	NAP	C5B-O5B-PA-O2A
2	E	1330	NAP	C5B-O5B-PA-O3
2	E	1330	NAP	C5D-O5D-PN-O3
2	E	1330	NAP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	F	1330	NAP	C5D-O5D-PN-O1N
2	F	1330	NAP	O4D-C1D-N1N-C6N
2	G	1330	NAP	C5D-O5D-PN-O1N
2	G	1330	NAP	O4D-C1D-N1N-C6N
2	H	1330	NAP	O4D-C1D-N1N-C2N
2	H	1330	NAP	O4D-C1D-N1N-C6N
2	H	1330	NAP	C2D-C1D-N1N-C2N
2	H	1330	NAP	C2D-C1D-N1N-C6N
3	A	1331	KZH	C11-C10-C9-C8
2	A	1330	NAP	O4B-C4B-C5B-O5B
2	A	1330	NAP	C3B-C4B-C5B-O5B
2	E	1330	NAP	O4D-C4D-C5D-O5D
3	H	1331	KZH	C1-C2-C3-C4
2	B	1330	NAP	C3B-C4B-C5B-O5B
2	E	1330	NAP	C3D-C4D-C5D-O5D
3	D	1331	KZH	C3-C4-C5-C6
3	A	1331	KZH	C1-C2-C3-C4
2	B	1330	NAP	O4D-C4D-C5D-O5D
3	F	1331	KZH	C3-C4-C5-C6
3	C	1331	KZH	C2-C3-C4-C5
3	G	1331	KZH	C3-C4-C5-C6
2	E	1330	NAP	PA-O3-PN-O1N
3	G	1331	KZH	C11-C10-C9-C8
3	C	1331	KZH	C4-C5-C6-C7
2	B	1330	NAP	C3D-C4D-C5D-O5D
2	C	1330	NAP	PN-O3-PA-O1A
2	G	1330	NAP	PN-O3-PA-O2A
3	A	1331	KZH	C5-C6-C7-C8
3	A	1331	KZH	C3-C4-C5-C6
2	B	1330	NAP	C2B-O2B-P2B-O1X
2	E	1330	NAP	C5B-O5B-PA-O1A
2	E	1330	NAP	C5D-O5D-PN-O2N
3	H	1331	KZH	C2-C3-C4-C5
2	D	1330	NAP	PN-O3-PA-O2A
2	B	1330	NAP	O4B-C4B-C5B-O5B
2	A	1330	NAP	C2D-C1D-N1N-C2N
3	D	1331	KZH	O2-C1-C2-C3
3	G	1331	KZH	O2-C1-C2-C3
3	H	1331	KZH	O2-C1-C2-C3
3	D	1331	KZH	O1-C1-C2-C3
3	G	1331	KZH	O1-C1-C2-C3
3	A	1331	KZH	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	H	1331	KZH	O1-C1-C2-C3
2	A	1330	NAP	O4D-C1D-N1N-C2N
2	B	1330	NAP	O4D-C1D-N1N-C2N
2	B	1330	NAP	O4D-C1D-N1N-C6N
2	E	1330	NAP	O4D-C1D-N1N-C2N
2	F	1330	NAP	O4D-C1D-N1N-C2N
2	G	1330	NAP	O4D-C1D-N1N-C2N
3	A	1331	KZH	O2-C1-C2-C3
3	F	1331	KZH	O1-C1-C2-C3
3	F	1331	KZH	O2-C1-C2-C3
2	A	1330	NAP	PN-O3-PA-O2A
2	F	1330	NAP	PN-O3-PA-O1A
2	F	1330	NAP	PN-O3-PA-O2A
2	H	1330	NAP	PN-O3-PA-O2A
3	F	1331	KZH	C5-C6-C7-C8
3	C	1331	KZH	O1-C1-C2-C3
2	D	1330	NAP	PN-O3-PA-O1A
2	H	1330	NAP	PN-O3-PA-O1A
2	E	1330	NAP	C3B-C4B-C5B-O5B

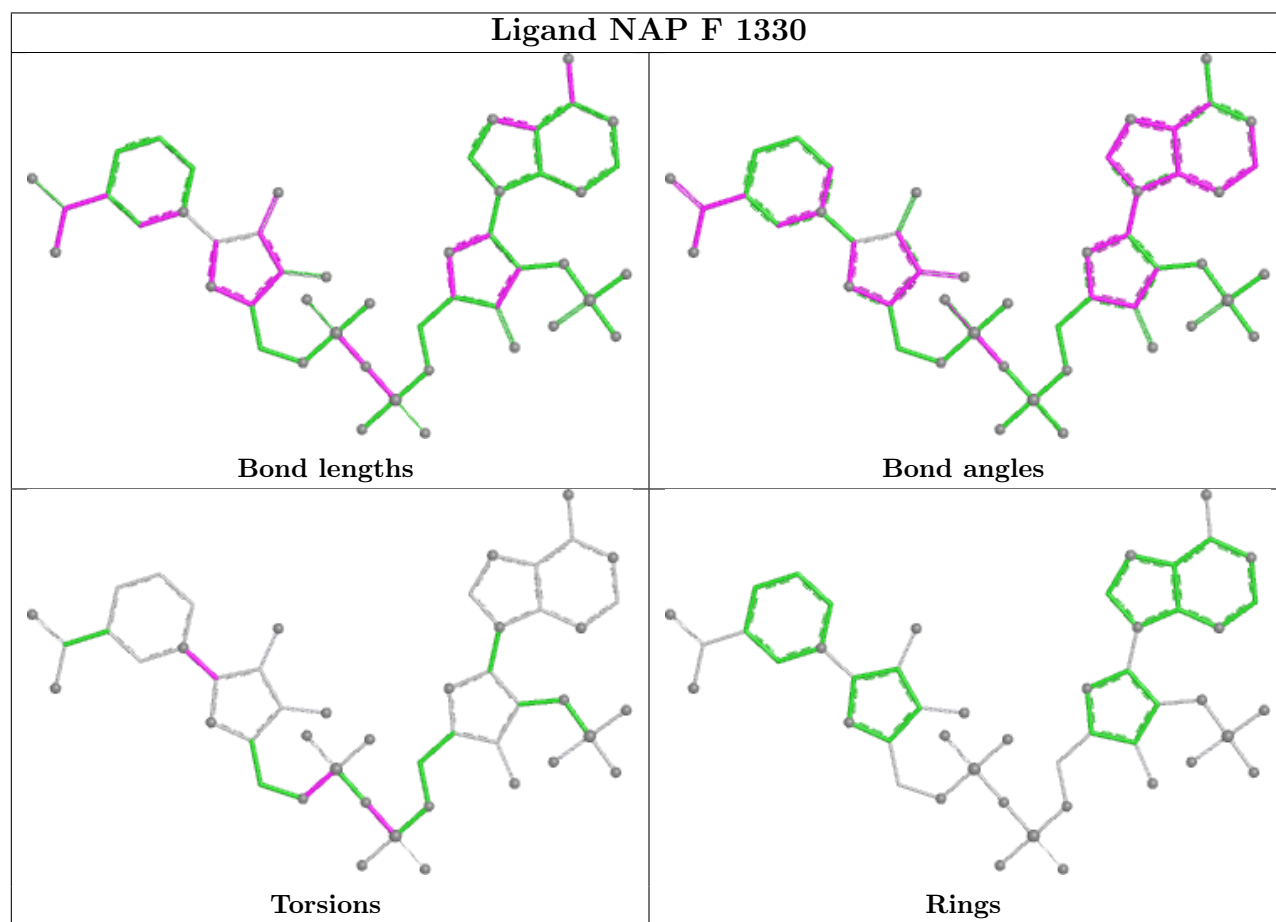
There are no ring outliers.

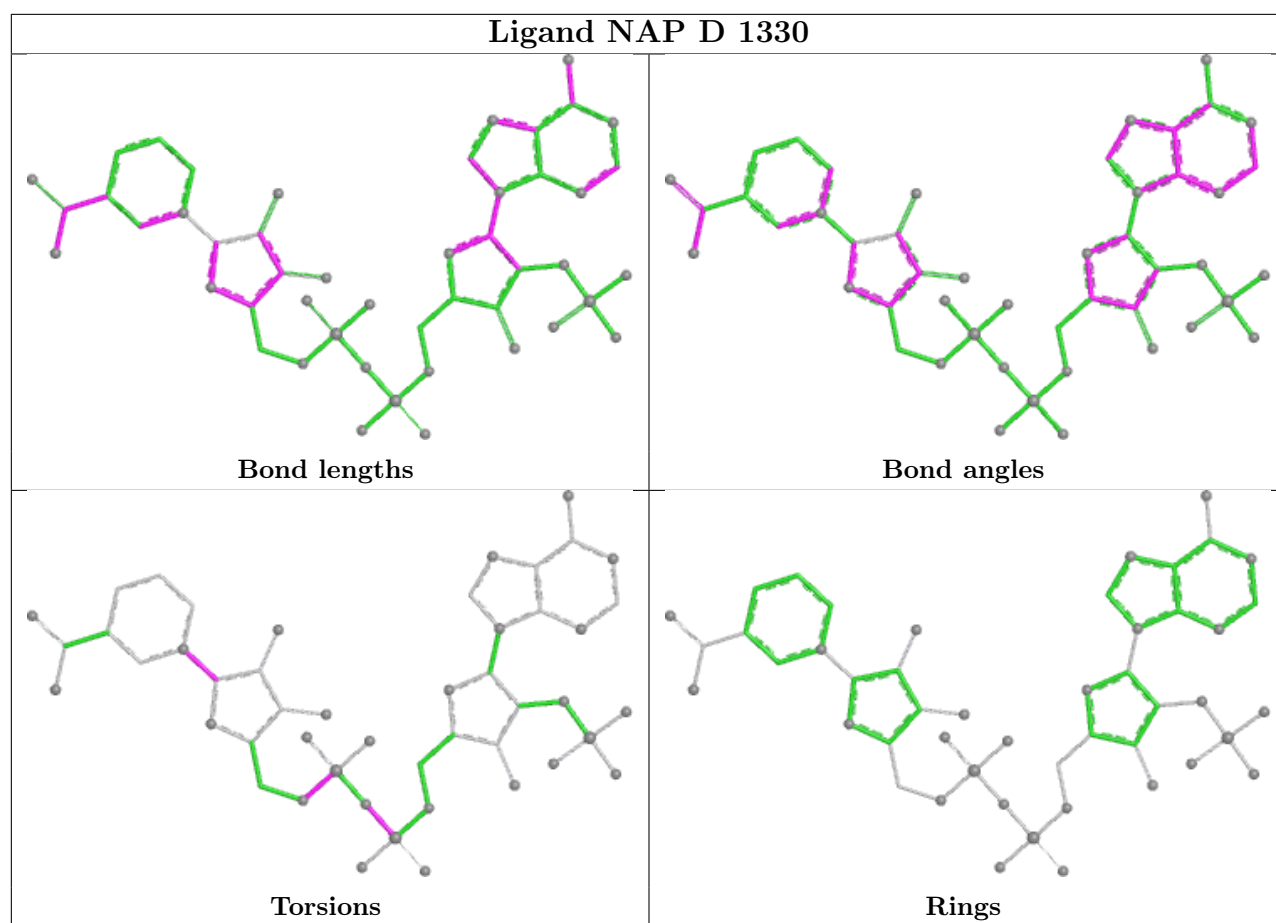
11 monomers are involved in 25 short contacts:

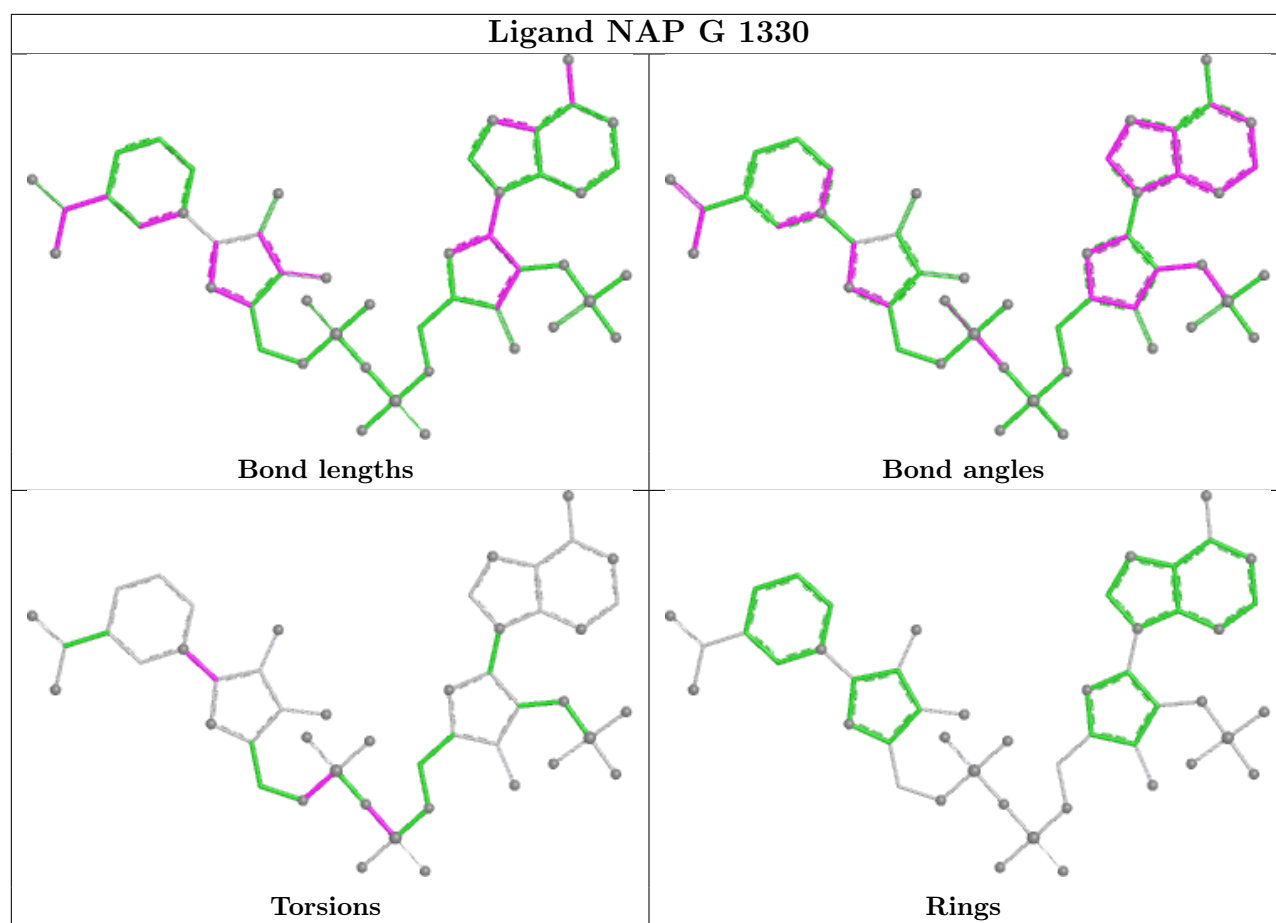
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1330	NAP	3	0
2	D	1330	NAP	2	0
2	G	1330	NAP	3	0
2	H	1330	NAP	2	0
3	D	1331	KZH	1	0
2	A	1330	NAP	2	0
2	E	1330	NAP	6	0
3	F	1331	KZH	1	0
3	C	1331	KZH	1	0
2	C	1330	NAP	2	0
2	B	1330	NAP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

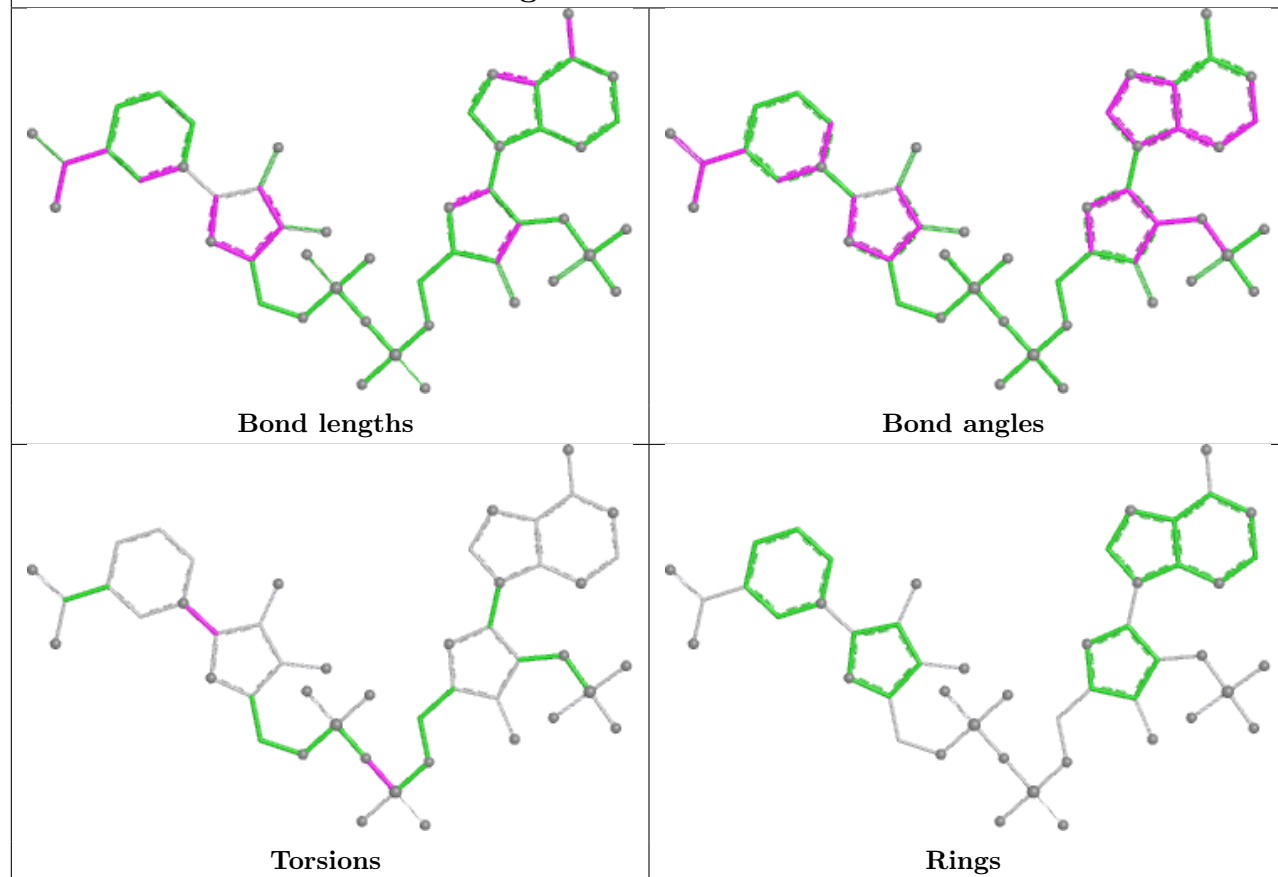
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



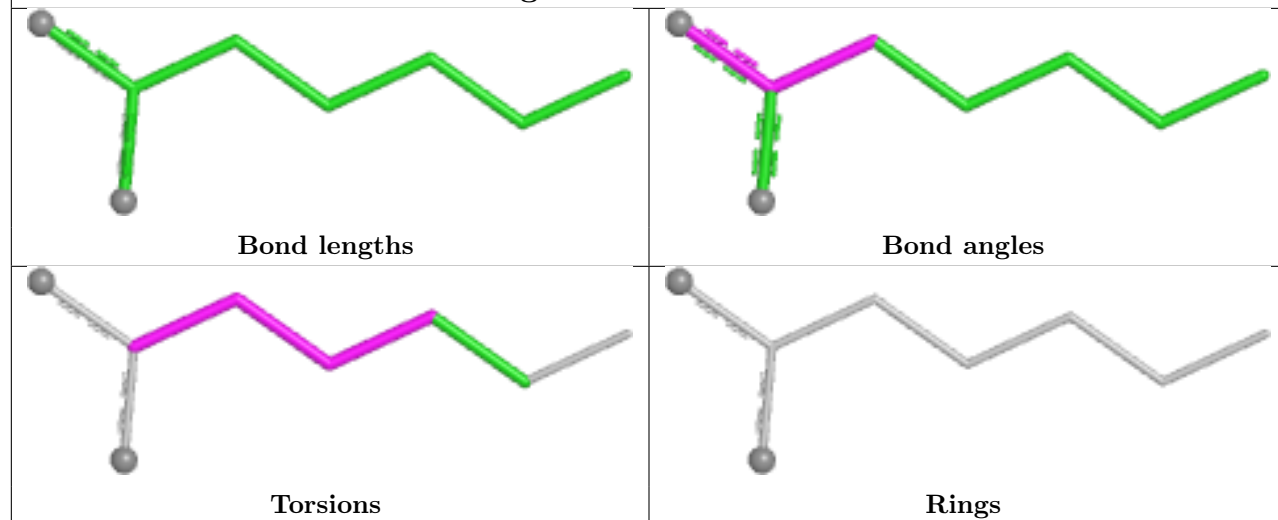


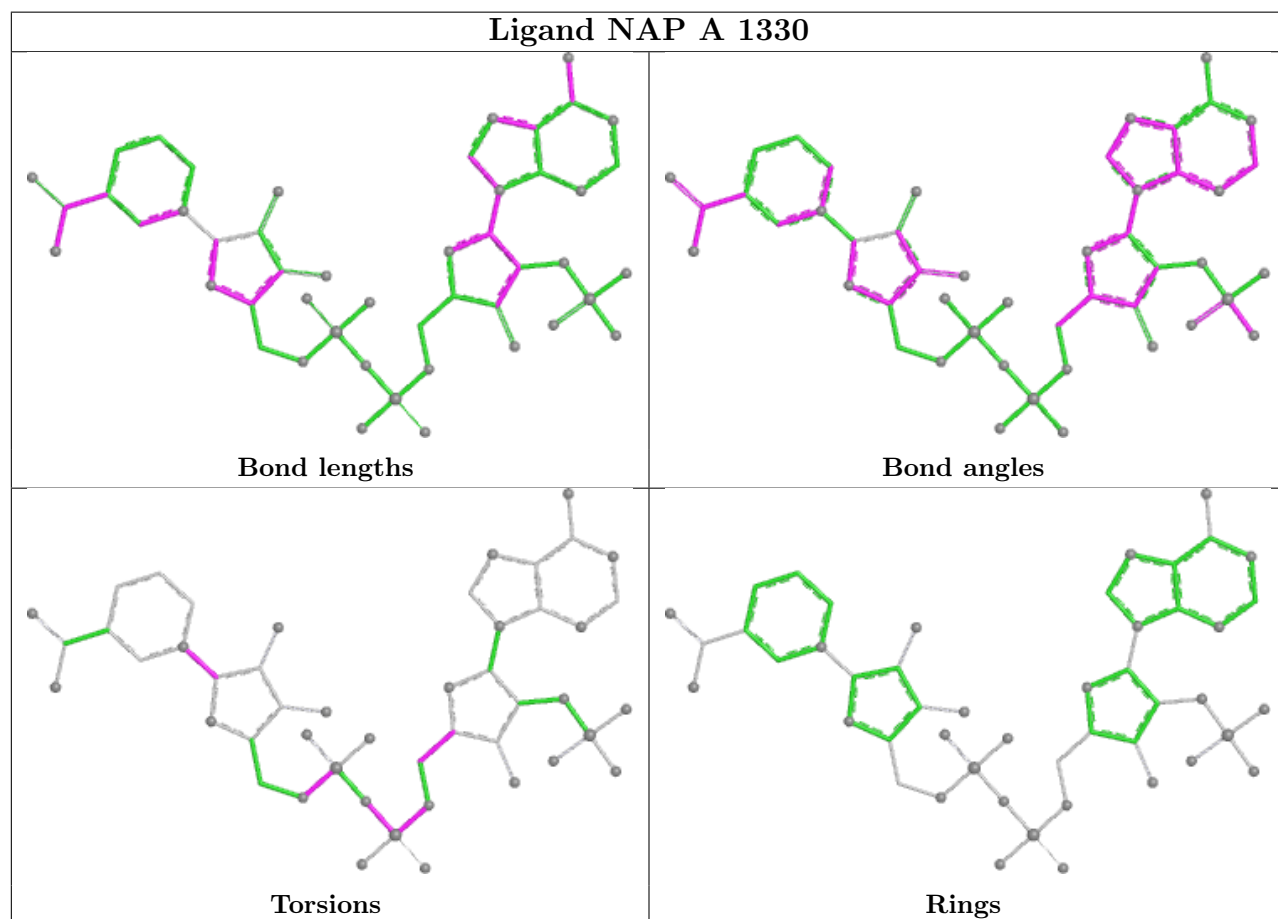
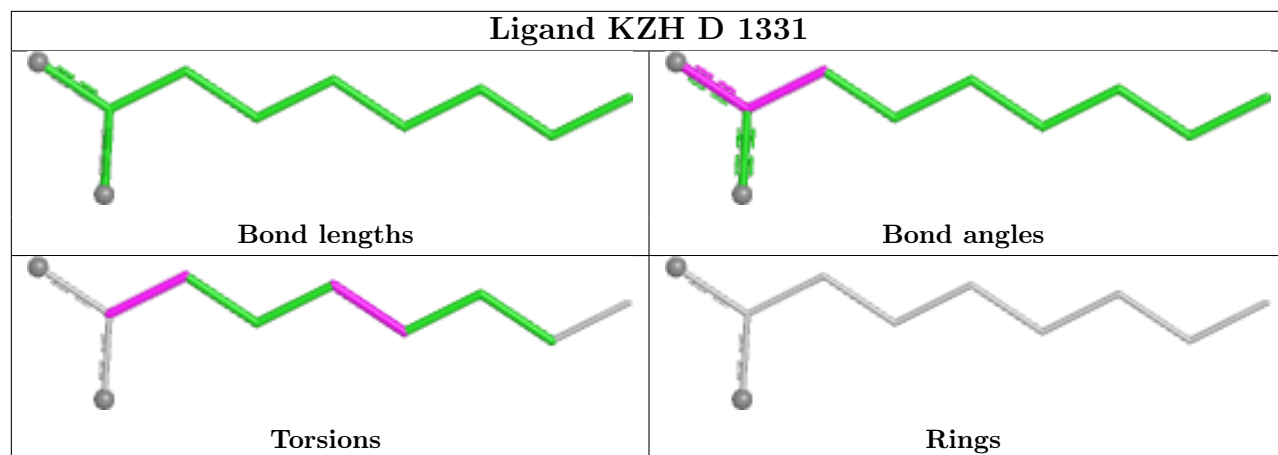


Ligand NAP H 1330

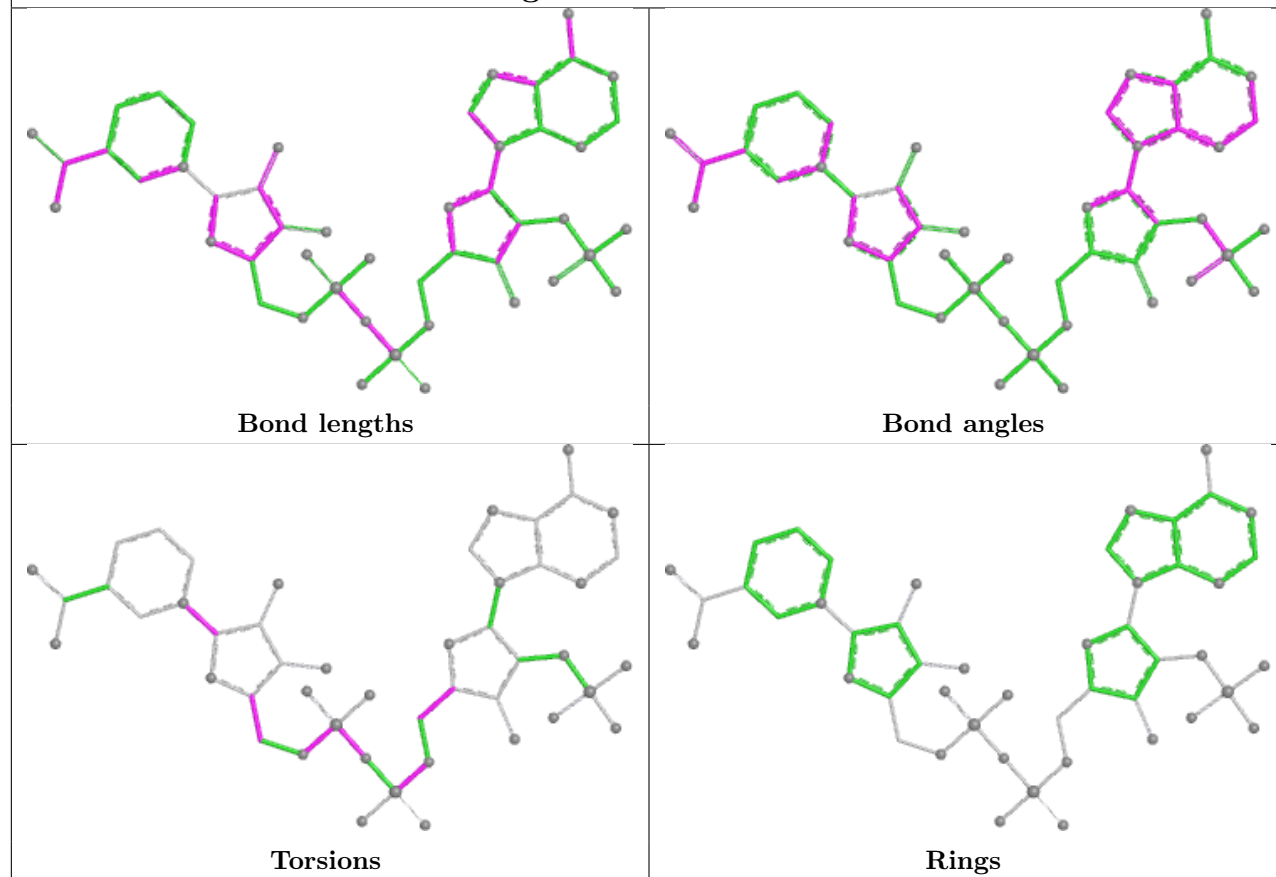


Ligand KZH H 1331

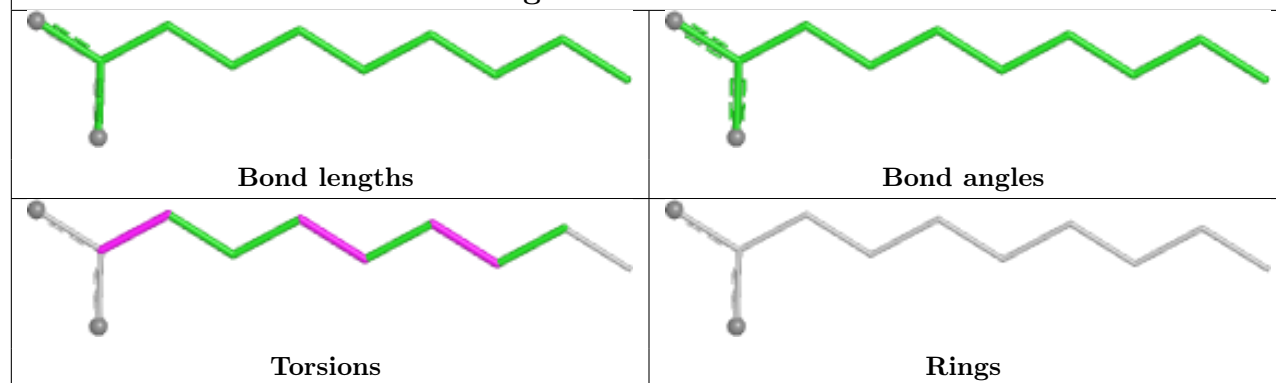




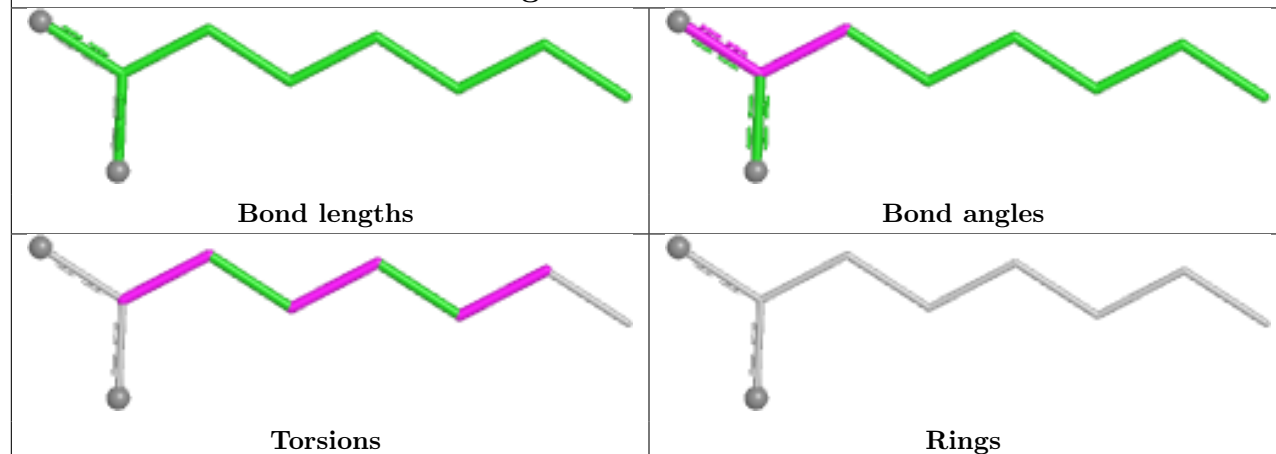
Ligand NAP E 1330



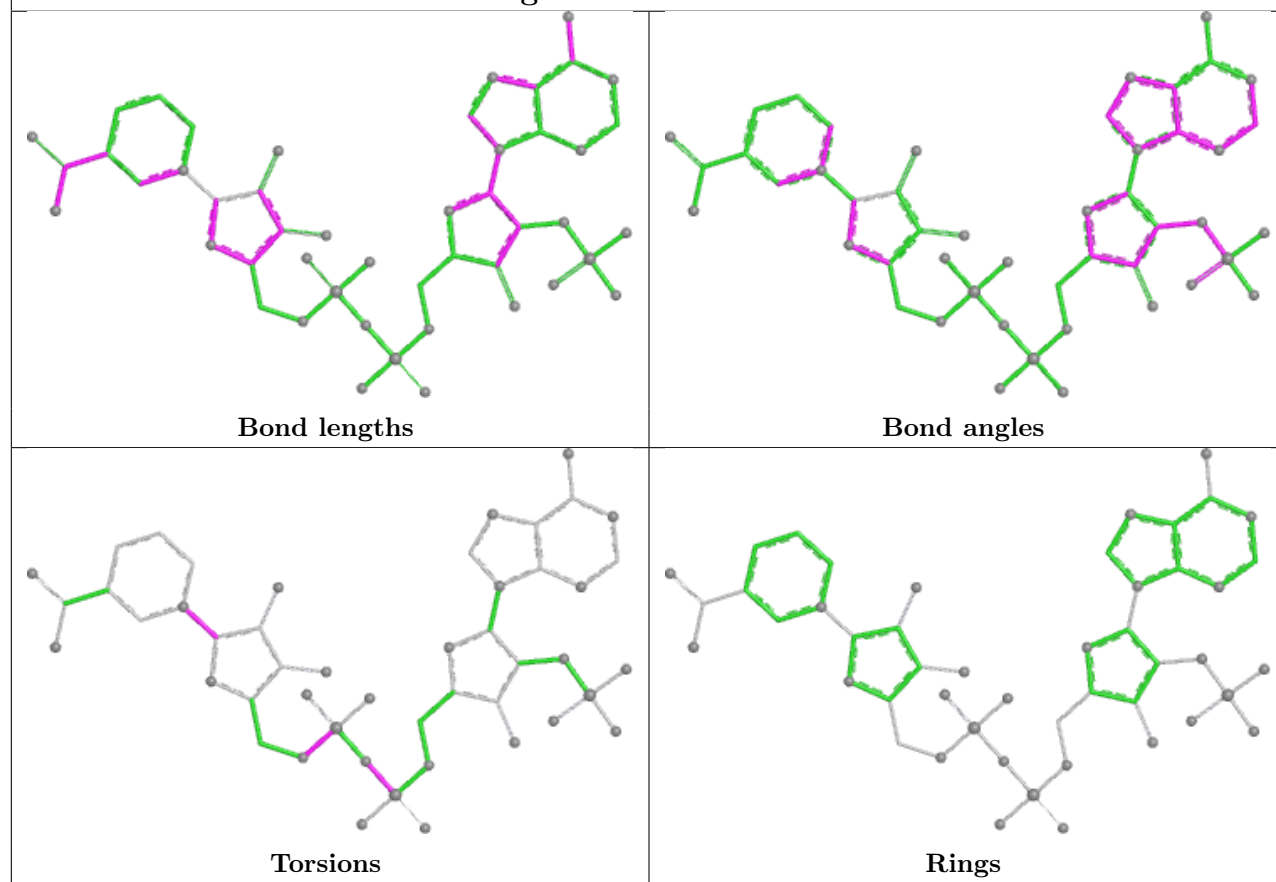
Ligand KZH F 1331

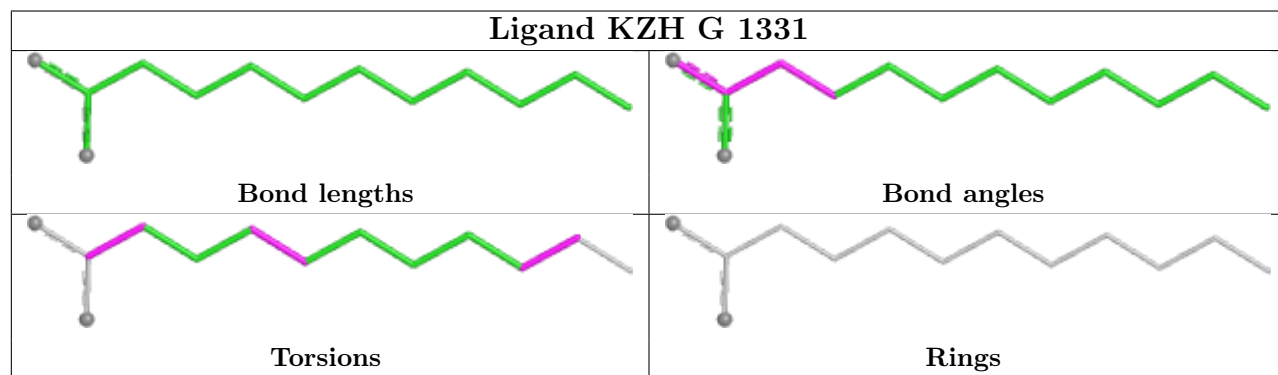
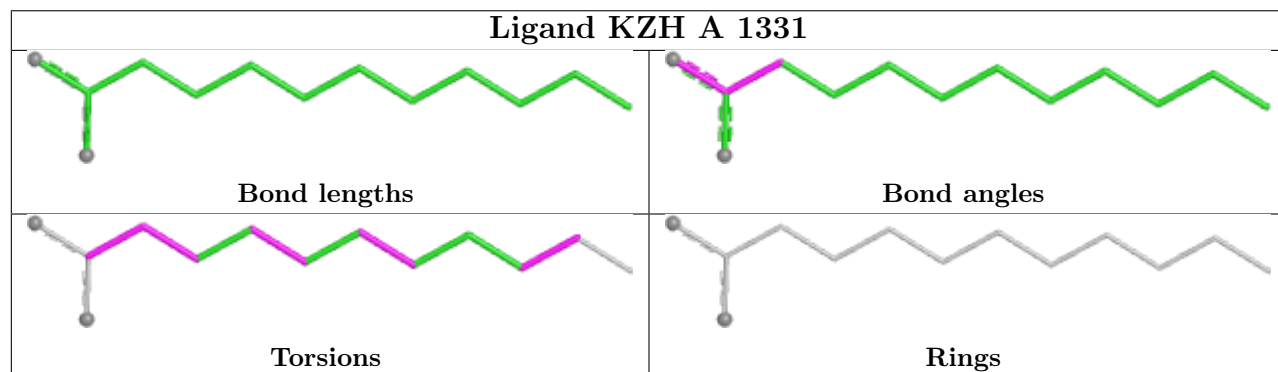
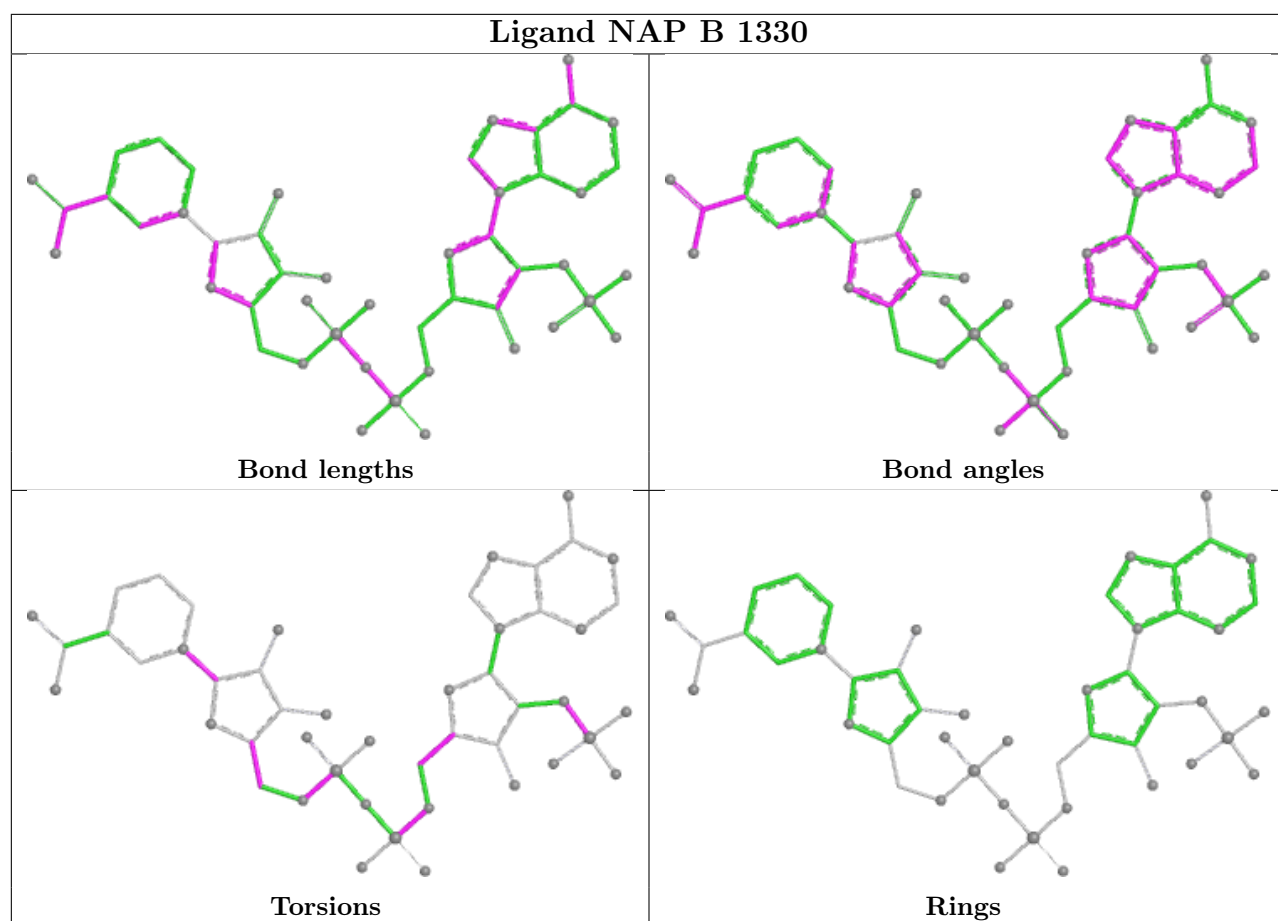


Ligand KZH C 1331



Ligand NAP C 1330





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	327/329 (99%)	-0.66	0 100 100	26, 46, 70, 88	0
1	B	324/329 (98%)	0.19	9 (2%) 55 45	32, 86, 128, 142	3 (0%)
1	C	326/329 (99%)	0.13	6 (1%) 67 58	35, 78, 125, 145	1 (0%)
1	D	327/329 (99%)	-0.34	0 100 100	34, 61, 95, 113	3 (0%)
1	E	313/329 (95%)	0.81	31 (9%) 13 9	40, 110, 173, 197	0
1	F	327/329 (99%)	-0.58	0 100 100	28, 46, 68, 89	2 (0%)
1	G	327/329 (99%)	-0.54	2 (0%) 85 80	26, 51, 79, 114	4 (1%)
1	H	326/329 (99%)	0.29	13 (3%) 42 33	43, 81, 148, 195	0
All	All	2597/2632 (98%)	-0.09	61 (2%) 61 51	26, 65, 134, 197	13 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	120	PRO	4.0
1	C	87	PHE	3.8
1	C	4	LYS	3.7
1	E	41	GLU	3.6
1	E	113	GLU	3.4
1	H	4	LYS	3.3
1	H	82	SER	3.1
1	E	29	PRO	3.1
1	H	80	VAL	3.0
1	E	329	PRO	3.0
1	H	84	VAL	3.0
1	E	108	PHE	3.0
1	H	81	GLY	3.0
1	E	40	LEU	2.9
1	C	25	GLN	2.9
1	E	37	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	78	VAL	2.8
1	C	84	VAL	2.8
1	E	327	VAL	2.7
1	B	108	PHE	2.7
1	H	87	PHE	2.6
1	G	152	GLY	2.6
1	E	72	ASP	2.6
1	B	21	LEU	2.6
1	B	6	MET	2.5
1	H	25	GLN	2.5
1	E	326	ILE	2.5
1	H	36	VAL	2.5
1	E	304	HIS	2.4
1	E	126	ALA	2.4
1	E	43	THR	2.4
1	E	324	LYS	2.4
1	H	7	HIS	2.4
1	E	123	VAL	2.4
1	E	288	VAL	2.4
1	G	153	THR	2.4
1	B	7	HIS	2.4
1	H	77	VAL	2.3
1	B	9	LEU	2.3
1	H	188	GLY	2.3
1	E	9	LEU	2.3
1	C	78	VAL	2.3
1	B	106	ALA	2.3
1	E	281	ALA	2.3
1	E	130	ALA	2.3
1	E	129	ALA	2.2
1	E	290	LEU	2.2
1	H	33	SER	2.2
1	E	325	ILE	2.2
1	E	116	THR	2.2
1	E	323	GLY	2.2
1	E	27	PRO	2.2
1	E	319	GLY	2.2
1	E	303	LYS	2.1
1	B	80	VAL	2.1
1	H	85	LYS	2.1
1	E	186	THR	2.0
1	C	7	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	150	LEU	2.0
1	B	103	GLY	2.0
1	B	26	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

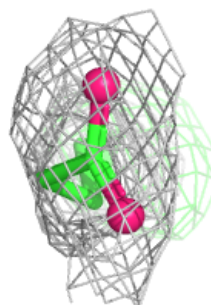
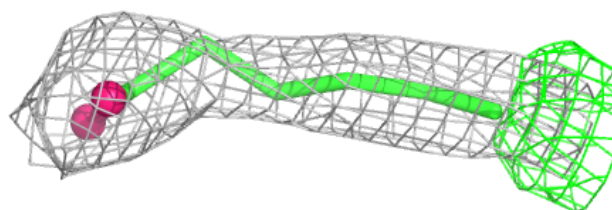
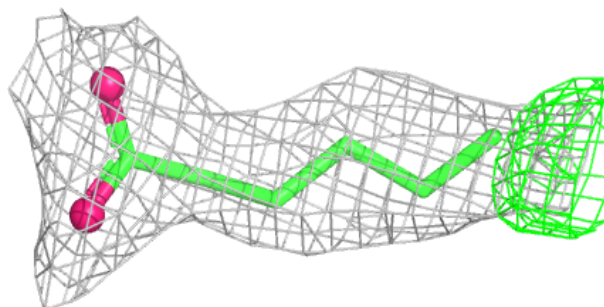
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	KZH	H	1331	8/21	0.76	0.19	67,70,76,79	0
2	NAP	E	1330	48/48	0.81	0.14	76,102,124,195	0
3	KZH	C	1331	9/21	0.84	0.14	55,62,78,81	0
3	KZH	A	1331	13/21	0.84	0.16	39,56,73,74	0
3	KZH	D	1331	10/21	0.87	0.13	32,46,68,77	0
3	KZH	F	1331	11/21	0.90	0.11	35,46,66,73	0
2	NAP	B	1330	48/48	0.90	0.10	59,79,90,99	0
3	KZH	G	1331	13/21	0.91	0.12	39,53,61,63	0
2	NAP	D	1330	48/48	0.95	0.07	33,48,63,78	0
2	NAP	H	1330	48/48	0.95	0.10	37,54,87,121	0
2	NAP	F	1330	48/48	0.96	0.06	25,50,65,69	0
2	NAP	C	1330	48/48	0.96	0.07	36,55,69,75	0
2	NAP	A	1330	48/48	0.97	0.06	31,47,53,58	0
2	NAP	G	1330	48/48	0.98	0.05	25,34,44,54	0

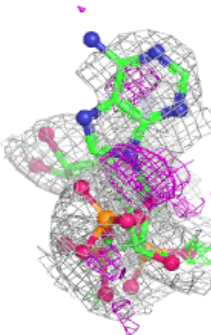
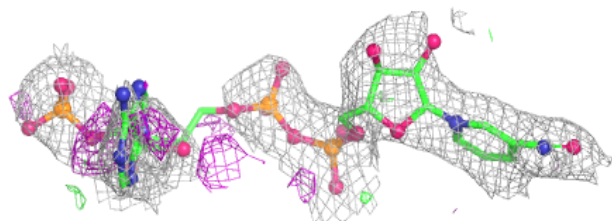
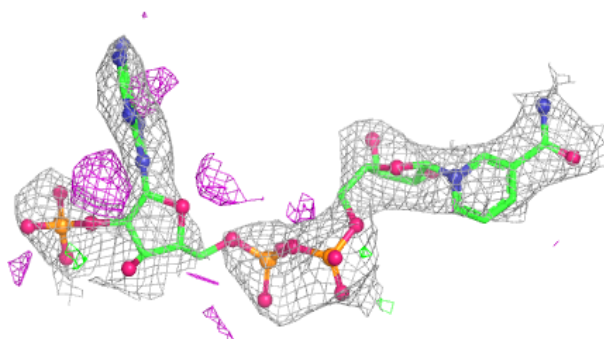
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KZH H 1331:

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

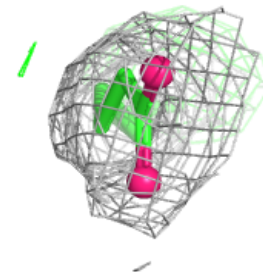
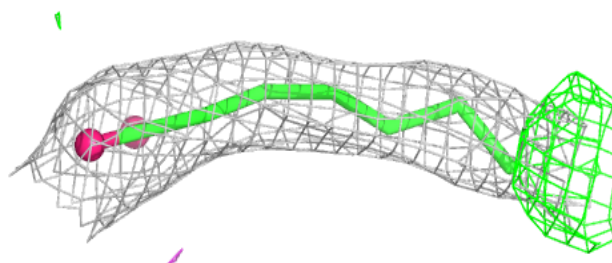
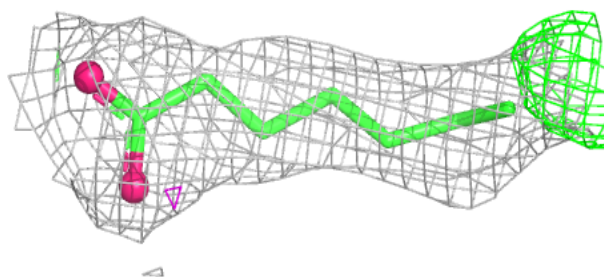
**Electron density around NAP E 1330:**

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

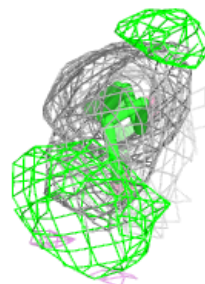
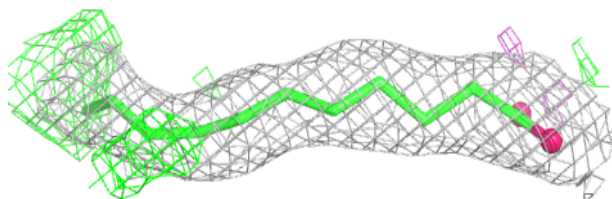
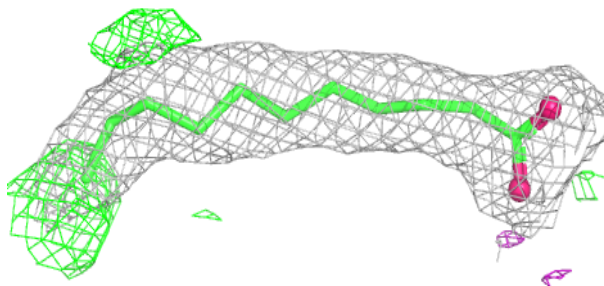


Electron density around KZH C 1331:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

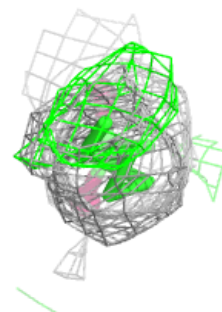
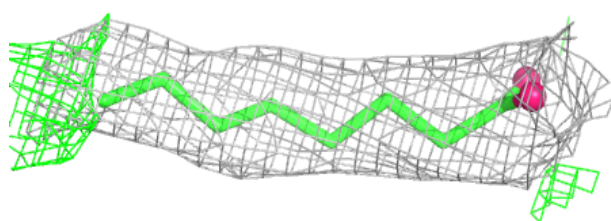
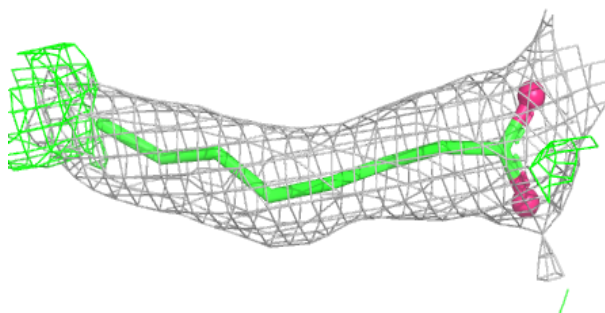
**Electron density around KZH A 1331:**

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and green (positive)

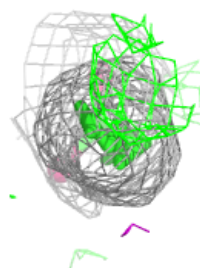
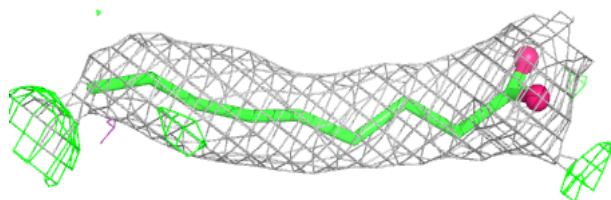
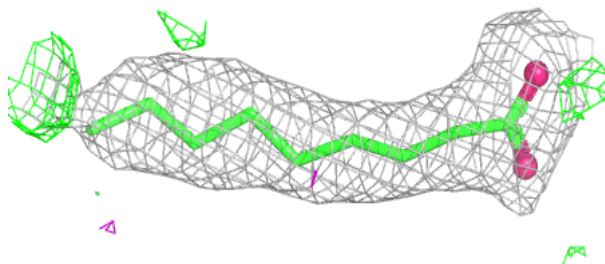


Electron density around KZH D 1331:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

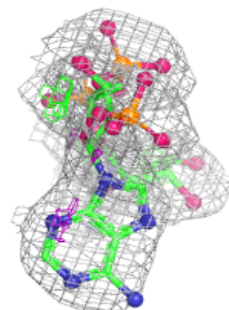
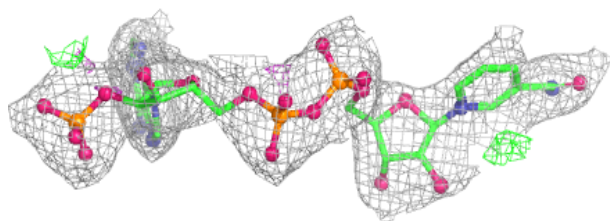
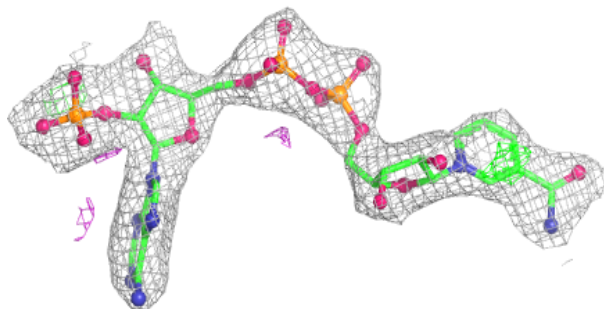
**Electron density around KZH F 1331:**

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and green (positive)

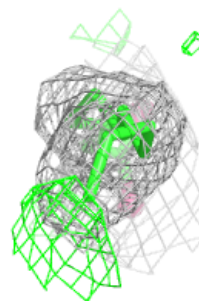
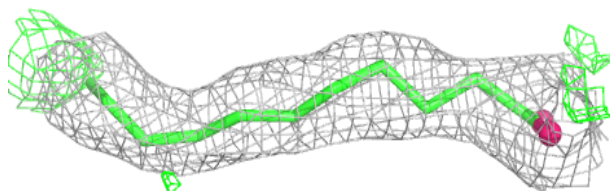
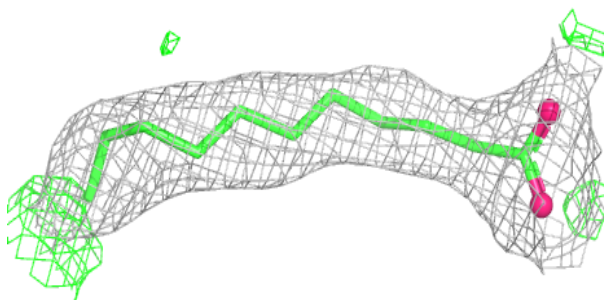


Electron density around NAP B 1330:

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

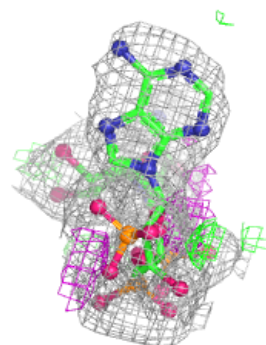
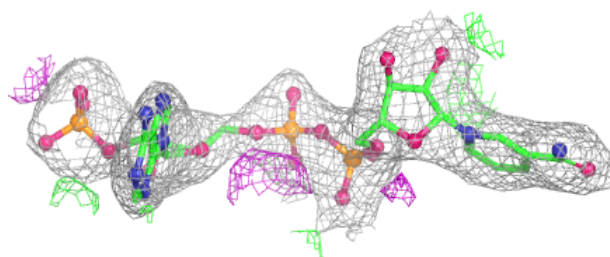
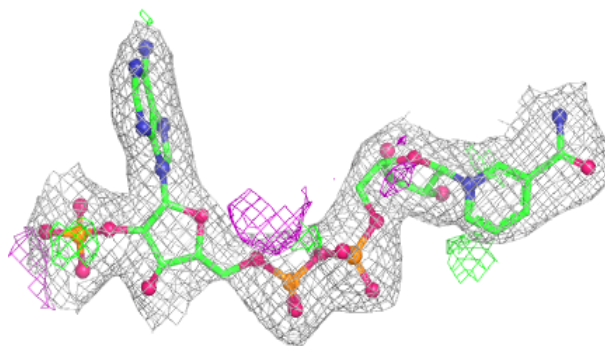
**Electron density around KZH G 1331:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

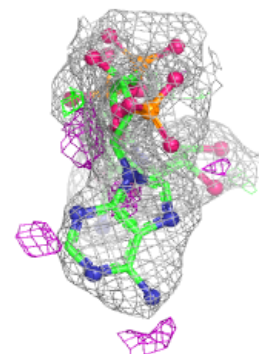
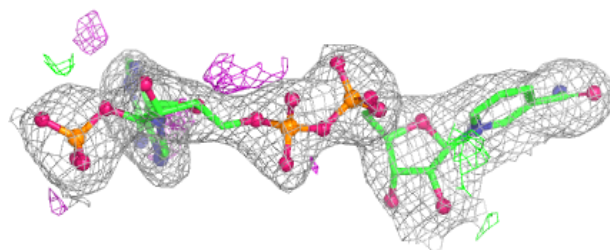
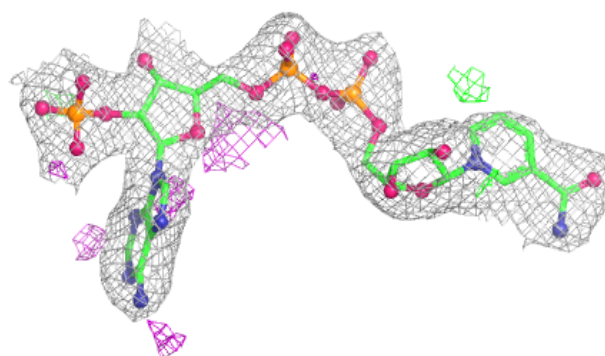


Electron density around NAP D 1330:

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

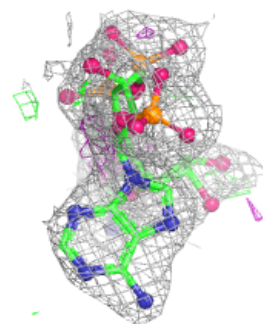
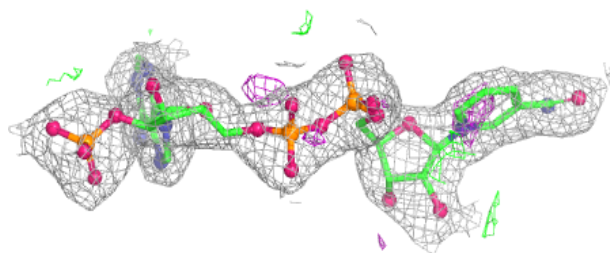
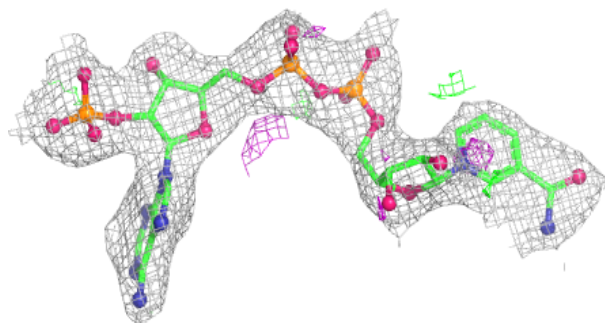
**Electron density around NAP H 1330:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

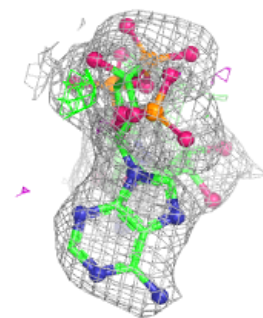
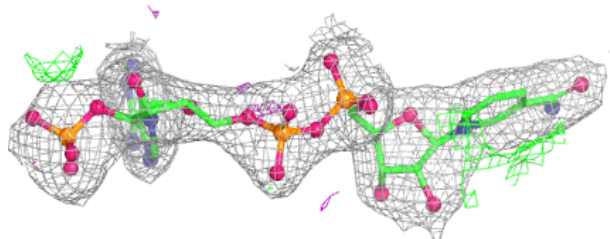
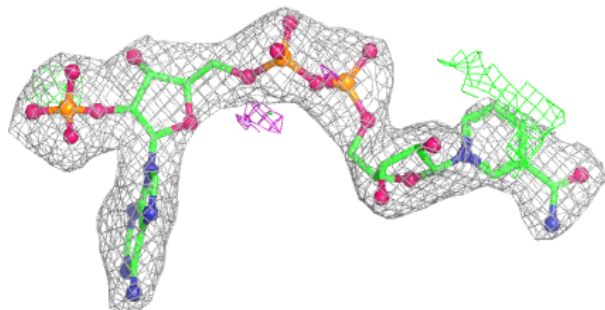


Electron density around NAP F 1330:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

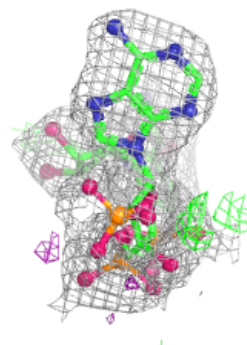
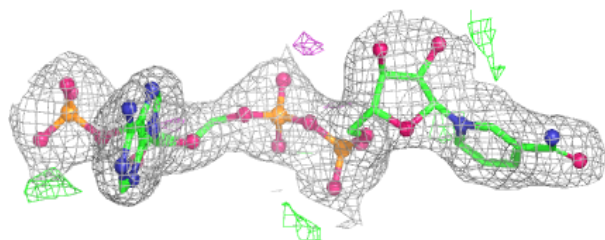
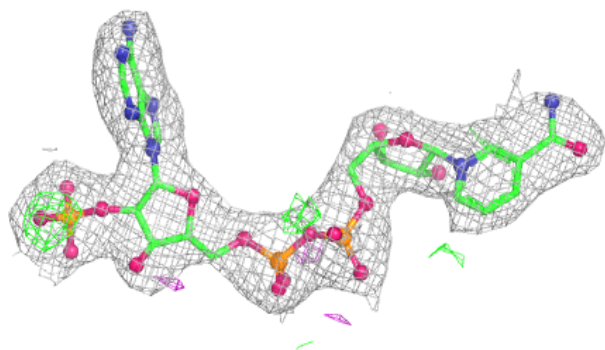
**Electron density around NAP C 1330:**

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

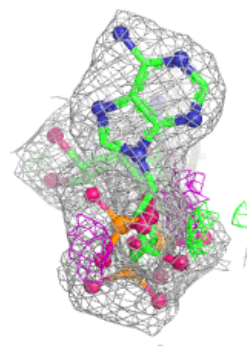
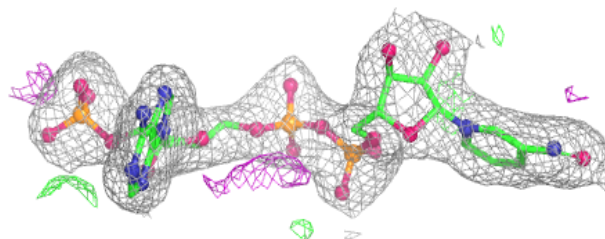
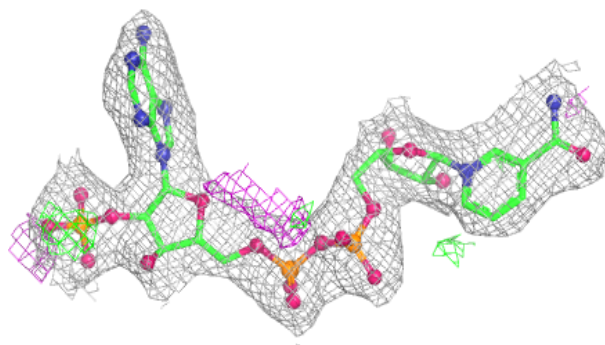


Electron density around NAP A 1330:

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

**Electron density around NAP G 1330:**

$2mF_o-DF_c$ (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.