



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:10 AM UTC

PDB ID : 1W6U / pdb_00001w6u
Title : Structure of human DECR ternary complex
Authors : Alpey, M.S.; Byres, E.; Li, D.; Hunter, W.N.
Deposited on : 2004-08-24
Resolution : 1.75 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

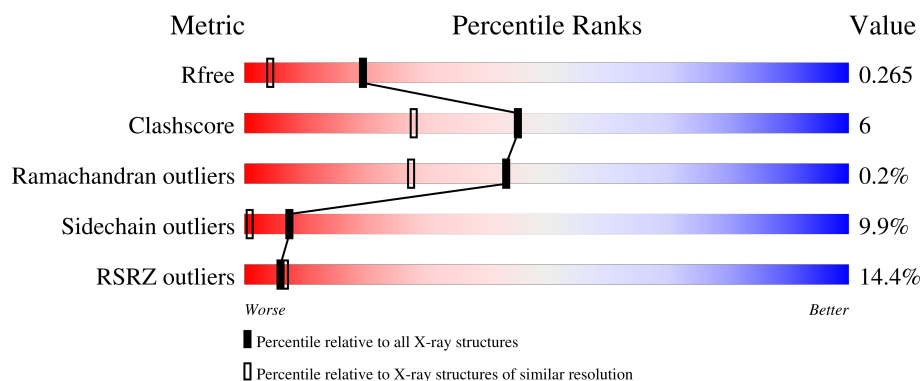
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	302	9% 81% 13% • 5%
1	B	302	10% 81% 12% • 5%
1	C	302	18% 77% 16% • 5%
1	D	302	17% 76% 15% • 7%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HXC	C	1330	-	-	X	-

2 Entry composition [i](#)

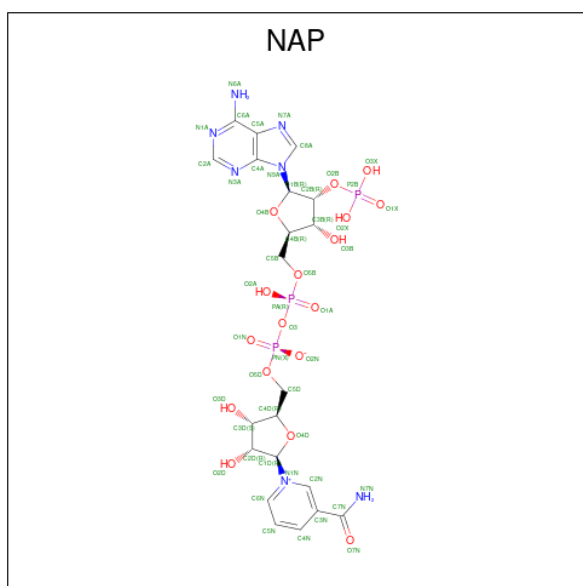
There are 4 unique types of molecules in this entry. The entry contains 9640 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2,4-DIENOYL-COA REDUCTASE, MITOCHONDRIAL PRE-CURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	6	0
			2171	1375	370	415	11			
1	B	286	Total	C	N	O	S	0	6	0
			2162	1368	368	414	12			
1	C	286	Total	C	N	O	S	0	6	0
			2158	1367	365	415	11			
1	D	282	Total	C	N	O	S	0	2	0
			2125	1348	359	406	12			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



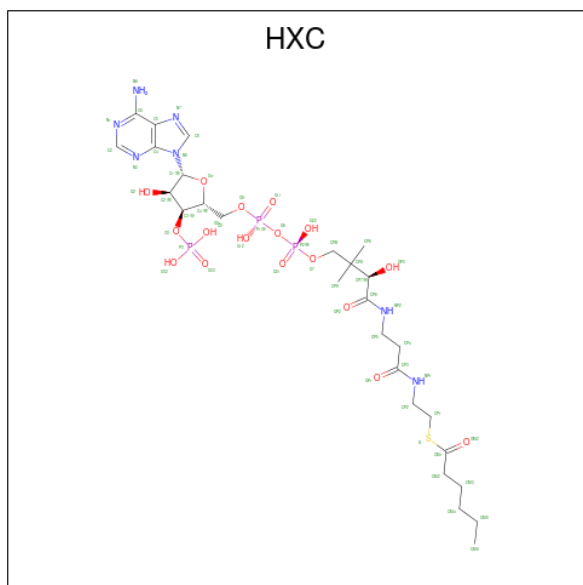
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			56	23	7	21	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	1
			56	23	7	21	5		
2	C	1	Total	C	N	O	P	0	1
			56	23	7	21	5		
2	D	1	Total	C	N	O	P	0	1
			56	23	7	21	5		

- Molecule 3 is HEXANOYL-COENZYME A (CCD ID: HXC) (formula: $C_{27}H_{46}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	138	Total O	0	0
			138 138		
4	B	149	Total O	0	0
			149 149		

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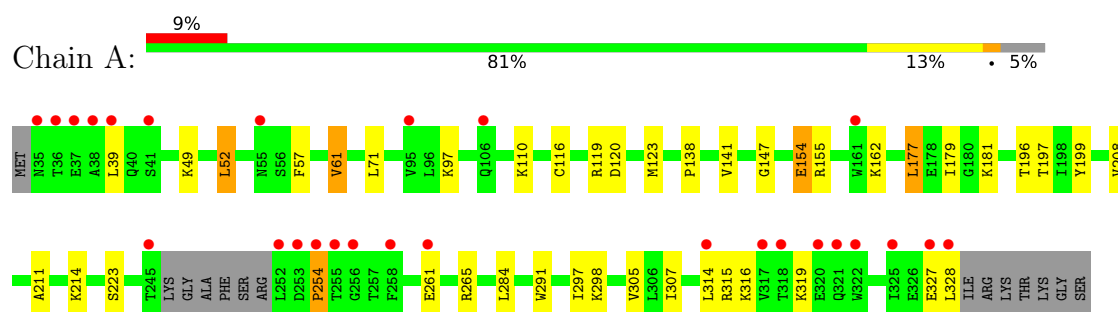
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	131	Total 131	O 131	0	0
4	D	162	Total 162	O 162	0	0

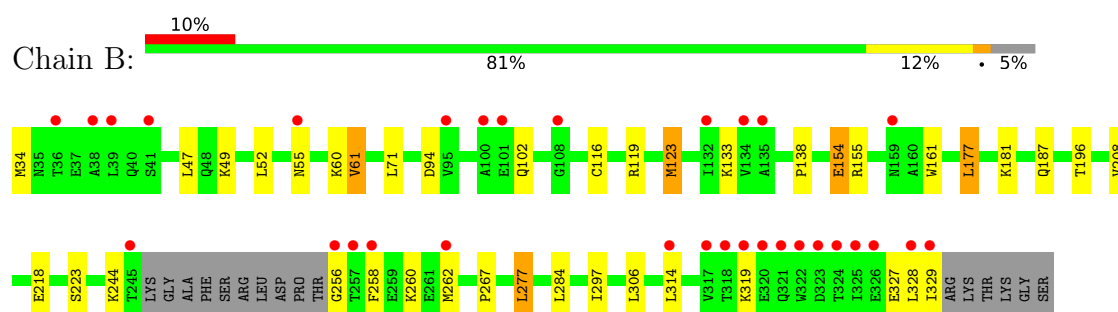
3 Residue-property plots [i](#)

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.

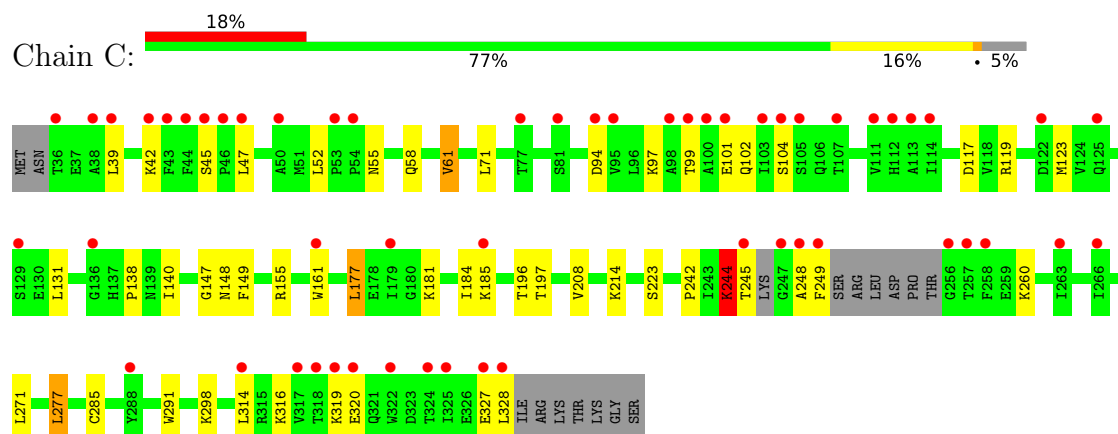
- Molecule 1: 2,4-DIENOYL-COA REDUCTASE, MITOCHONDRIAL PRECURSOR



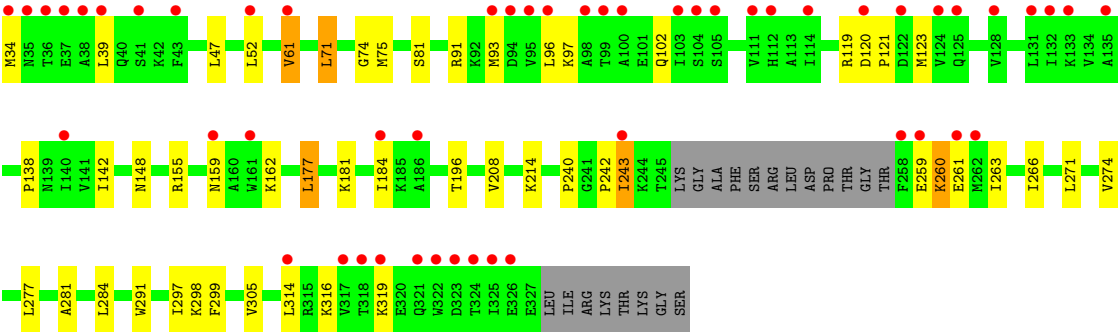
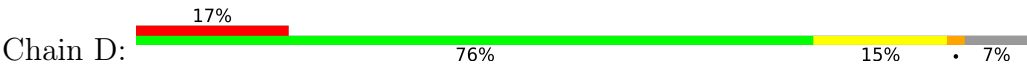
- Molecule 1: 2,4-DIENOYL-COA REDUCTASE, MITOCHONDRIAL PRECURSOR



- Molecule 1: 2,4-DIENOYL-COA REDUCTASE, MITOCHONDRIAL PRECURSOR



- Molecule 1: 2,4-DIENOYL-COA REDUCTASE, MITOCHONDRIAL PRECURSOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.28Å 131.66Å 70.85Å 90.00° 92.64° 90.00°	Depositor
Resolution (Å)	70.71 – 1.75 70.71 – 1.75	Depositor EDS
% Data completeness (in resolution range)	95.3 (70.71-1.75) 95.3 (70.71-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.227 , 0.268 0.225 , 0.265	Depositor DCC
R_{free} test set	5590 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.877	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9640	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HXC, 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	0.49	0/2232	0.87	1/3019 (0.0%)
1	B	0.48	0/2224	0.85	0/3006
1	C	0.45	0/2218	0.86	0/2998
1	D	0.43	0/2169	0.85	0/2932
All	All	0.46	0/8843	0.86	1/11955 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	PRO	N-CA-CB	6.72	110.31	103.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2171	0	2181	24	0
1	B	2162	0	2184	15	0
1	C	2158	0	2174	29	0
1	D	2125	0	2151	26	0
2	A	56	0	10	0	0
2	B	56	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	56	0	10	2	0
2	D	56	0	10	0	0
3	A	55	0	42	4	0
3	B	55	0	42	5	0
3	C	55	0	42	21	0
3	D	55	0	42	8	0
4	A	138	0	0	1	0
4	B	149	0	0	2	0
4	C	131	0	0	3	0
4	D	162	0	0	7	0
All	All	9640	0	8898	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (107) 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)
3:D:1329:HXC:HM32	3:D:1329:HXC:HP11	1.12	1.07
3:C:1330:HXC:HP2	3:C:1330:HXC:HP81	1.21	1.05
1:C:148:ASN:H	3:C:1330:HXC:HP52	1.27	0.99
3:D:1329:HXC:HP11	3:D:1329:HXC:CM3	1.96	0.92
1:A:154:GLU:HG2	1:C:184:ILE:HD13	1.50	0.91
3:D:1329:HXC:HM32	3:D:1329:HXC:CP1	2.03	0.86
1:C:197[A]:THR:HG21	3:C:1330:HXC:OM2	1.77	0.83
1:C:148:ASN:HB2	3:C:1330:HXC:HP11	1.64	0.79
1:C:148:ASN:H	3:C:1330:HXC:CP5	1.97	0.78
1:C:55[B]:ASN:ND2	1:C:58[B]:GLN:OE1	2.18	0.75
2:C:1329[B]:NAP:O1A	3:C:1330:HXC:HP21	1.87	0.75
1:C:148:ASN:N	3:C:1330:HXC:HP52	2.03	0.70
1:B:154:GLU:HG2	1:D:184:ILE:HD13	1.74	0.69
1:D:75:MET:SD	4:D:2129:HOH:O	2.50	0.69
1:D:71:LEU:HG	1:D:277:LEU:HD22	1.76	0.68
1:C:147:GLY:HA2	3:C:1330:HXC:HP51	1.76	0.67
1:D:243:ILE:HD13	4:D:2160:HOH:O	1.95	0.67
1:D:148:ASN:N	3:D:1329:HXC:OP1	2.28	0.66
1:B:55:ASN:ND2	4:B:2016:HOH:O	2.30	0.64
1:D:96:LEU:C	4:D:2039:HOH:O	2.40	0.64
1:A:61:VAL:HG22	1:A:138:PRO:HA	1.79	0.64
3:B:1331:HXC:HP11	3:B:1331:HXC:OP1	1.97	0.64
1:B:177:LEU:HD22	1:B:181:LYS:HE3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:CYS:HA	1:B:123:MET:HE2	1.81	0.61
1:D:142:ILE:HD13	4:D:2129:HOH:O	2.00	0.61
3:C:1330:HXC:HP2	3:C:1330:HXC:CP8	2.01	0.61
1:C:148:ASN:CB	3:C:1330:HXC:HP11	2.31	0.61
1:A:177:LEU:HD22	1:A:181:LYS:HE3	1.84	0.59
1:A:211:ALA:HB3	4:A:2074:HOH:O	2.03	0.59
1:C:197[A]:THR:CG2	3:C:1330:HXC:OM2	2.49	0.58
1:B:284:LEU:HD11	1:B:297:ILE:HD12	1.85	0.58
2:B:1330[B]:NAP:O1A	3:B:1331:HXC:HP12	2.05	0.57
1:A:154:GLU:HG2	1:C:184:ILE:CD1	2.30	0.57
1:C:71:LEU:HG	1:C:277:LEU:HD22	1.87	0.56
1:B:71:LEU:HG	1:B:277:LEU:HD22	1.88	0.56
1:D:34:MET:HG3	1:D:39:LEU:HG	1.89	0.55
1:A:284:LEU:HD11	1:A:297:ILE:HD12	1.87	0.55
1:D:61:VAL:HG13	1:D:138:PRO:HA	1.89	0.54
1:A:116:CYS:HA	1:A:123:MET:HE2	1.88	0.54
1:A:52:LEU:HD23	1:A:57:PHE:HE1	1.73	0.54
3:B:1331:HXC:HP2	3:B:1331:HXC:HP1	1.56	0.54
1:C:248:ALA:O	1:C:249:PHE:CB	2.55	0.54
1:C:244:LYS:HG2	1:C:271:LEU:HD12	1.89	0.53
1:D:148:ASN:HD22	3:D:1329:HXC:HM31	1.74	0.53
3:B:1331:HXC:HP83	3:B:1331:HXC:OP2	2.08	0.53
1:A:199:TYR:OH	3:A:1330:HXC:OM2	2.21	0.53
1:C:177:LEU:HD22	1:C:181:LYS:HE3	1.91	0.52
1:D:260:LYS:HA	4:D:2120:HOH:O	2.10	0.52
1:A:265[B]:ARG:HH11	1:A:315:ARG:HH22	1.58	0.51
1:A:147:GLY:HA2	3:A:1330:HXC:OP2	2.11	0.50
3:B:1331:HXC:OP2	3:B:1331:HXC:CP8	2.59	0.50
4:C:2115:HOH:O	1:D:297:ILE:HD11	2.11	0.50
1:D:263:ILE:HA	1:D:266:ILE:HD12	1.95	0.49
1:C:242:PRO:HB2	1:C:271:LEU:HD22	1.94	0.49
1:B:61:VAL:HG13	1:B:138:PRO:HA	1.94	0.49
1:C:148:ASN:HB2	3:C:1330:HXC:CP1	2.40	0.49
1:A:196:THR:HA	1:A:214:LYS:HD2	1.95	0.47
1:A:223:SER:HB3	1:C:208:VAL:HG22	1.97	0.47
1:C:196:THR:HA	1:C:214:LYS:HD2	1.96	0.47
1:A:208:VAL:HG22	1:C:223:SER:HB3	1.97	0.47
1:B:262:MET:HE3	4:B:2115:HOH:O	2.15	0.47
1:C:161:TRP:C	1:C:161:TRP:CD1	2.93	0.46
1:C:148:ASN:N	3:C:1330:HXC:HP1	2.13	0.46
1:C:147:GLY:HA2	3:C:1330:HXC:HP1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ILE:HG12	1:B:297:ILE:HG12	1.99	0.45
1:C:149:PHE:CE2	3:C:1330:HXC:HP83	2.51	0.45
1:A:298:LYS:NZ	1:A:305:VAL:HG13	2.31	0.44
1:B:267:PRO:HG3	1:B:306:LEU:HD12	2.00	0.44
1:D:281:ALA:HB1	4:D:2129:HOH:O	2.16	0.44
1:B:223:SER:HB3	1:D:208:VAL:HG22	1.99	0.44
1:C:147:GLY:C	3:C:1330:HXC:HP1	2.25	0.44
1:C:61:VAL:HG13	1:C:138:PRO:HA	1.99	0.44
1:B:161:TRP:CH2	1:B:208:VAL:HG12	2.52	0.44
1:D:298:LYS:NZ	1:D:305:VAL:HG13	2.33	0.44
1:A:52:LEU:HD23	1:A:57:PHE:CE1	2.54	0.43
1:D:177:LEU:HD22	1:D:181:LYS:HE3	2.00	0.43
1:C:117:ASP:OD1	1:C:119:ARG:HG2	2.19	0.43
3:D:1329:HXC:HP51	3:D:1329:HXC:HP81	2.01	0.42
3:C:1330:HXC:HP81	3:C:1330:HXC:NP2	2.06	0.42
3:C:1330:HXC:S	4:C:2079:HOH:O	2.62	0.42
1:B:196:THR:HG21	1:B:218:GLU:HG2	2.01	0.42
2:C:1329[B]:NAP:O2A	3:C:1330:HXC:OP1	2.37	0.42
1:D:91:ARG:HH12	3:D:1329:HXC:HPB2	1.84	0.42
1:B:256:GLY:C	1:B:258:PHE:H	2.28	0.42
1:D:159:ASN:HB2	4:D:2088:HOH:O	2.18	0.42
1:D:196:THR:HA	1:D:214:LYS:HD2	2.01	0.42
1:A:265[B]:ARG:HG2	1:A:307:ILE:CG2	2.49	0.42
1:A:197[B]:THR:HG21	1:A:199:TYR:CE1	2.55	0.41
1:D:120:ASP:HA	1:D:121:PRO:HD3	1.95	0.41
1:A:162:LYS:HE2	4:C:2059:HOH:O	2.21	0.41
3:A:1330:HXC:HM21	3:A:1330:HXC:HP11	1.90	0.41
1:D:240:PRO:HA	1:D:299:PHE:O	2.21	0.41
1:A:116:CYS:HA	1:A:123:MET:CE	2.51	0.41
1:C:140:ILE:HG12	1:C:285:CYS:HB3	2.02	0.41
1:D:284:LEU:HD11	1:D:297:ILE:HD12	2.01	0.41
1:A:141:VAL:HG21	1:A:179:ILE:HG21	2.02	0.41
1:A:120:ASP:HB3	1:A:123:MET:HB2	2.04	0.40
1:D:74:GLY:HA3	1:D:274:VAL:CG1	2.52	0.40
1:D:242:PRO:HB2	1:D:271:LEU:HD22	2.03	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	290/302 (96%)	281 (97%)	8 (3%)	1 (0%)	36	21
1	B	288/302 (95%)	281 (98%)	7 (2%)	0	100	100
1	C	286/302 (95%)	279 (98%)	6 (2%)	1 (0%)	36	21
1	D	280/302 (93%)	272 (97%)	8 (3%)	0	100	100
All	All	1144/1208 (95%)	1113 (97%)	29 (2%)	2 (0%)	43	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	PRO
1	C	244	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/243 (96%)	216 (93%)	17 (7%)	13	2
1	B	234/243 (96%)	210 (90%)	24 (10%)	7	0
1	C	233/243 (96%)	203 (87%)	30 (13%)	4	0
1	D	229/243 (94%)	208 (91%)	21 (9%)	8	1
All	All	929/972 (96%)	837 (90%)	92 (10%)	7	1

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	49	LYS
1	A	52	LEU
1	A	61	VAL
1	A	97	LYS
1	A	110	LYS
1	A	119	ARG
1	A	154	GLU
1	A	155	ARG
1	A	177	LEU
1	A	261	GLU
1	A	291	TRP
1	A	314	LEU
1	A	316	LYS
1	A	319	LYS
1	A	327	GLU
1	A	328	LEU
1	B	34	MET
1	B	47	LEU
1	B	49	LYS
1	B	52	LEU
1	B	60	LYS
1	B	61	VAL
1	B	94[A]	ASP
1	B	94[B]	ASP
1	B	102	GLN
1	B	119	ARG
1	B	123	MET
1	B	133	LYS
1	B	154	GLU
1	B	155	ARG
1	B	177	LEU
1	B	187	GLN
1	B	244	LYS
1	B	260	LYS
1	B	277	LEU
1	B	314	LEU
1	B	319	LYS
1	B	327	GLU
1	B	328	LEU
1	B	329	ILE
1	C	39	LEU
1	C	42	LYS

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Mol	Chain	Res	Type
1	C	45	SER
1	C	47	LEU
1	C	52	LEU
1	C	61	VAL
1	C	94[A]	ASP
1	C	94[B]	ASP
1	C	97	LYS
1	C	99	THR
1	C	101	GLU
1	C	102	GLN
1	C	104	SER
1	C	123	MET
1	C	131	LEU
1	C	155	ARG
1	C	177	LEU
1	C	185	LYS
1	C	244	LYS
1	C	245	THR
1	C	260	LYS
1	C	277	LEU
1	C	291	TRP
1	C	298	LYS
1	C	314	LEU
1	C	316	LYS
1	C	319	LYS
1	C	320	GLU
1	C	327	GLU
1	C	328	LEU
1	D	47	LEU
1	D	52	LEU
1	D	61	VAL
1	D	71	LEU
1	D	81	SER
1	D	93	MET
1	D	97	LYS
1	D	102	GLN
1	D	119	ARG
1	D	123	MET
1	D	155	ARG
1	D	162	LYS
1	D	177	LEU
1	D	243	ILE

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Mol	Chain	Res	Type
1	D	259	GLU
1	D	260	LYS
1	D	261	GLU
1	D	291	TRP
1	D	314	LEU
1	D	316	LYS
1	D	319	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	126	ASN
1	A	143	ASN
1	A	321	GLN
1	B	55	ASN
1	B	102	GLN
1	B	126	ASN
1	B	137	HIS
1	B	143	ASN
1	C	106	GLN
1	C	126	ASN
1	C	137	HIS
1	C	143	ASN
1	C	321	GLN
1	D	48	GLN
1	D	85	GLN
1	D	126	ASN
1	D	137	HIS
1	D	143	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HXC	B	1331	-	55,57,57	2.46	13 (23%)	77,83,83	2.30	20 (25%)
2	NAP	C	1329[A]	-	50,52,52	1.63	5 (10%)	71,80,80	1.49	7 (9%)
2	NAP	B	1330[B]	-	50,52,52	1.68	7 (14%)	71,80,80	1.45	8 (11%)
3	HXC	C	1330	-	55,57,57	2.42	13 (23%)	77,83,83	2.13	16 (20%)
3	HXC	D	1329	-	55,57,57	2.41	11 (20%)	77,83,83	2.39	19 (24%)
2	NAP	D	1328[B]	-	50,52,52	1.69	8 (16%)	71,80,80	1.46	9 (12%)
2	NAP	A	1329[B]	-	50,52,52	1.67	7 (14%)	71,80,80	1.43	8 (11%)
2	NAP	B	1330[A]	-	50,52,52	1.64	5 (10%)	71,80,80	1.52	10 (14%)
3	HXC	A	1330	-	55,57,57	2.45	13 (23%)	77,83,83	2.05	17 (22%)
2	NAP	C	1329[B]	-	50,52,52	1.63	5 (10%)	71,80,80	1.49	7 (9%)
2	NAP	D	1328[A]	-	50,52,52	1.65	6 (12%)	71,80,80	1.54	10 (14%)
2	NAP	A	1329[A]	-	50,52,52	1.66	7 (14%)	71,80,80	1.46	8 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HXC	B	1331	-	-	27/56/72/72	0/3/3/3
2	NAP	C	1329[A]	-	-	6/35/67/67	0/5/5/5
2	NAP	B	1330[B]	-	-	7/35/67/67	0/5/5/5
3	HXC	C	1330	-	-	19/56/72/72	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HXC	D	1329	-	-	14/56/72/72	0/3/3/3
2	NAP	D	1328[B]	-	-	10/35/67/67	0/5/5/5
2	NAP	A	1329[B]	-	-	1/35/67/67	0/5/5/5
2	NAP	B	1330[A]	-	-	3/35/67/67	0/5/5/5
3	HXC	A	1330	-	-	16/56/72/72	0/3/3/3
2	NAP	C	1329[B]	-	-	1/35/67/67	0/5/5/5
2	NAP	D	1328[A]	-	-	6/35/67/67	0/5/5/5
2	NAP	A	1329[A]	-	-	6/35/67/67	0/5/5/5

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1330	HXC	CM2-CM1	-11.24	1.39	1.50
3	B	1331	HXC	CM2-CM1	-10.98	1.40	1.50
3	D	1329	HXC	CM2-CM1	-10.64	1.40	1.50
3	C	1330	HXC	CM2-CM1	-10.35	1.40	1.50
2	D	1328[A]	NAP	O7N-C7N	9.17	1.41	1.24
2	D	1328[B]	NAP	O7N-C7N	9.17	1.41	1.24
2	C	1329[A]	NAP	O7N-C7N	8.99	1.40	1.24
2	C	1329[B]	NAP	O7N-C7N	8.99	1.40	1.24
2	A	1329[A]	NAP	O7N-C7N	8.92	1.40	1.24
2	A	1329[B]	NAP	O7N-C7N	8.92	1.40	1.24
2	B	1330[A]	NAP	O7N-C7N	8.88	1.40	1.24
2	B	1330[B]	NAP	O7N-C7N	8.88	1.40	1.24
3	B	1331	HXC	OP2-CP6	7.02	1.36	1.23
3	C	1330	HXC	OP2-CP6	6.89	1.36	1.23
3	A	1330	HXC	OP2-CP6	6.79	1.36	1.23
3	D	1329	HXC	OP2-CP6	6.75	1.36	1.23
3	C	1330	HXC	CP5-NP2	-6.02	1.32	1.46
3	B	1331	HXC	CP5-NP2	-5.91	1.32	1.46
3	C	1330	HXC	CP4-CP3	-5.79	1.39	1.51
3	D	1329	HXC	CP5-NP2	-5.79	1.33	1.46
3	A	1330	HXC	CP5-NP2	-5.58	1.33	1.46
3	A	1330	HXC	CP4-CP3	-5.56	1.40	1.51
3	D	1329	HXC	CP4-CP3	-5.55	1.40	1.51
3	B	1331	HXC	CP4-CP3	-5.55	1.40	1.51
3	C	1330	HXC	CP5-CP4	-3.63	1.39	1.51
3	D	1329	HXC	CM3-CM2	-3.46	1.39	1.52
3	A	1330	HXC	CM3-CM2	-3.44	1.39	1.52
3	B	1331	HXC	CM3-CM2	-3.43	1.39	1.52
3	B	1331	HXC	CP5-CP4	-3.39	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1329	HXC	CP5-CP4	-3.38	1.40	1.51
3	A	1330	HXC	CP5-CP4	-3.35	1.40	1.51
3	C	1330	HXC	CM3-CM2	-3.35	1.39	1.52
3	B	1331	HXC	C5-N7	-3.21	1.33	1.39
3	A	1330	HXC	C5-N7	-3.20	1.33	1.39
3	C	1330	HXC	C5-N7	-3.19	1.33	1.39
3	D	1329	HXC	P2-O6	3.18	1.62	1.59
3	D	1329	HXC	C5-N7	-3.15	1.33	1.39
2	D	1328[A]	NAP	C2A-N1A	2.76	1.38	1.33
2	D	1328[B]	NAP	C2A-N1A	2.76	1.38	1.33
3	A	1330	HXC	P2-O6	2.70	1.62	1.59
2	B	1330[A]	NAP	C2A-N1A	2.69	1.38	1.33
2	B	1330[B]	NAP	C2A-N1A	2.69	1.38	1.33
3	C	1330	HXC	P2-O6	2.68	1.62	1.59
2	B	1330[B]	NAP	PN-O3	2.65	1.62	1.59
2	B	1330[A]	NAP	C2A-N3A	2.65	1.38	1.33
2	B	1330[B]	NAP	C2A-N3A	2.65	1.38	1.33
2	A	1329[A]	NAP	C2A-N1A	2.63	1.38	1.33
2	A	1329[B]	NAP	C2A-N1A	2.63	1.38	1.33
3	C	1330	HXC	CM4-CM3	-2.61	1.38	1.51
2	D	1328[A]	NAP	C2N-N1N	2.60	1.37	1.35
2	D	1328[B]	NAP	C2N-N1N	2.60	1.37	1.35
3	B	1331	HXC	P2-O6	2.60	1.62	1.59
2	B	1330[A]	NAP	C2N-N1N	2.58	1.37	1.35
2	B	1330[B]	NAP	C2N-N1N	2.58	1.37	1.35
2	C	1329[A]	NAP	C2N-N1N	2.53	1.37	1.35
2	C	1329[B]	NAP	C2N-N1N	2.53	1.37	1.35
3	A	1330	HXC	P1-O6	2.51	1.62	1.59
3	D	1329	HXC	CM4-CM3	-2.51	1.39	1.51
2	A	1329[A]	NAP	C2A-N3A	2.51	1.38	1.33
2	A	1329[B]	NAP	C2A-N3A	2.51	1.38	1.33
3	A	1330	HXC	CM4-CM3	-2.49	1.39	1.51
3	B	1331	HXC	CM4-CM3	-2.47	1.39	1.51
2	C	1329[A]	NAP	C2A-N1A	2.43	1.38	1.33
2	C	1329[B]	NAP	C2A-N1A	2.43	1.38	1.33
2	C	1329[A]	NAP	C2A-N3A	2.43	1.38	1.33
2	C	1329[B]	NAP	C2A-N3A	2.43	1.38	1.33
2	A	1329[A]	NAP	PA-O3	2.41	1.62	1.59
2	D	1328[A]	NAP	C2A-N3A	2.40	1.38	1.33
2	D	1328[B]	NAP	C2A-N3A	2.40	1.38	1.33
2	A	1329[B]	NAP	PA-O3	2.40	1.62	1.59
2	A	1329[B]	NAP	PN-O3	2.36	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1330	HXC	P1-O6	2.27	1.62	1.59
2	A	1329[A]	NAP	C2N-N1N	2.25	1.37	1.35
2	A	1329[B]	NAP	C2N-N1N	2.25	1.37	1.35
2	B	1330[B]	NAP	PA-O3	2.23	1.61	1.59
2	D	1328[B]	NAP	PA-O3	2.22	1.61	1.59
3	B	1331	HXC	P1-O6	2.20	1.61	1.59
2	A	1329[A]	NAP	PN-O3	2.15	1.61	1.59
3	A	1330	HXC	C8-N9	-2.11	1.34	1.37
3	B	1331	HXC	C8-N9	-2.11	1.34	1.37
3	C	1330	HXC	P3-O31	2.10	1.62	1.54
3	A	1330	HXC	P3-O31	2.08	1.62	1.54
3	D	1329	HXC	C4-N9	-2.08	1.33	1.37
2	B	1330[A]	NAP	C8A-N7A	2.07	1.35	1.31
2	B	1330[B]	NAP	C8A-N7A	2.07	1.35	1.31
2	D	1328[B]	NAP	PN-O3	2.06	1.61	1.59
3	C	1330	HXC	C8-N9	-2.06	1.34	1.37
2	C	1329[A]	NAP	C8A-N7A	2.04	1.35	1.31
2	C	1329[B]	NAP	C8A-N7A	2.04	1.35	1.31
2	A	1329[A]	NAP	C8A-N7A	2.04	1.35	1.31
2	A	1329[B]	NAP	C8A-N7A	2.04	1.35	1.31
3	C	1330	HXC	CM5-CM4	-2.04	1.39	1.51
3	D	1329	HXC	C8-N9	-2.04	1.34	1.37
3	B	1331	HXC	P3-O32	2.04	1.62	1.54
2	D	1328[A]	NAP	C5A-N7A	-2.03	1.35	1.39
2	D	1328[B]	NAP	C5A-N7A	-2.03	1.35	1.39
3	A	1330	HXC	C4-N9	-2.02	1.33	1.37
3	B	1331	HXC	C4-N9	-2.02	1.33	1.37
2	D	1328[A]	NAP	C8A-N7A	2.00	1.35	1.31
2	D	1328[B]	NAP	C8A-N7A	2.00	1.35	1.31

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1329	HXC	CM2-CM1-S	10.35	125.74	113.40
3	B	1331	HXC	CP5-CP4-CP3	9.92	128.91	112.39
3	C	1330	HXC	CM2-CM1-S	8.30	123.29	113.40
3	C	1330	HXC	CP4-CP5-NP2	7.87	128.74	112.00
3	B	1331	HXC	CP4-CP5-NP2	7.11	127.13	112.00
3	D	1329	HXC	CP5-CP4-CP3	6.68	123.52	112.39
3	A	1330	HXC	CP4-CP5-NP2	6.43	125.69	112.00
3	D	1329	HXC	OM2-CM1-CM2	-6.07	116.98	123.98
3	A	1330	HXC	CM2-CM1-S	6.06	120.63	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1329[A]	NAP	N3A-C2A-N1A	-5.85	119.72	128.58
2	A	1329[B]	NAP	N3A-C2A-N1A	-5.85	119.72	128.58
2	C	1329[A]	NAP	N3A-C2A-N1A	-5.83	119.76	128.58
2	C	1329[B]	NAP	N3A-C2A-N1A	-5.83	119.76	128.58
2	B	1330[A]	NAP	N3A-C2A-N1A	-5.74	119.89	128.58
2	B	1330[B]	NAP	N3A-C2A-N1A	-5.74	119.89	128.58
2	D	1328[A]	NAP	N3A-C2A-N1A	-5.65	120.04	128.58
2	D	1328[B]	NAP	N3A-C2A-N1A	-5.65	120.04	128.58
3	C	1330	HXC	C5-C4-N3	-5.37	119.33	126.72
3	B	1331	HXC	C5-C4-N3	-5.36	119.33	126.72
3	A	1330	HXC	C5-C4-N3	-5.36	119.34	126.72
3	D	1329	HXC	C5-C4-N3	-5.26	119.47	126.72
3	B	1331	HXC	CM2-CM1-S	5.26	119.67	113.40
3	B	1331	HXC	CM3-CM2-CM1	5.23	123.81	112.27
3	D	1329	HXC	CM3-CM2-CM1	5.15	123.63	112.27
3	D	1329	HXC	N1-C2-N3	-4.82	121.29	128.58
3	A	1330	HXC	CM3-CM2-CM1	4.80	122.86	112.27
3	A	1330	HXC	CP5-CP4-CP3	4.80	120.39	112.39
3	A	1330	HXC	N1-C2-N3	-4.78	121.34	128.58
3	B	1331	HXC	N1-C2-N3	-4.65	121.55	128.58
3	C	1330	HXC	N1-C2-N3	-4.58	121.65	128.58
3	D	1329	HXC	CP4-CP5-NP2	4.43	121.42	112.00
2	C	1329[A]	NAP	C5A-C4A-N3A	-4.40	120.65	126.72
2	C	1329[B]	NAP	C5A-C4A-N3A	-4.40	120.65	126.72
2	D	1328[A]	NAP	N9A-C8A-N7A	-4.25	107.91	113.94
2	D	1328[B]	NAP	N9A-C8A-N7A	-4.25	107.91	113.94
3	D	1329	HXC	OM2-CM1-S	-4.25	117.28	122.68
3	C	1330	HXC	OM2-CM1-S	-4.16	117.39	122.68
2	A	1329[A]	NAP	C5A-C4A-N3A	-4.08	121.10	126.72
2	A	1329[B]	NAP	C5A-C4A-N3A	-4.08	121.10	126.72
3	C	1330	HXC	OM2-CM1-CM2	-4.04	119.32	123.98
3	B	1331	HXC	OP1-CP3-CP4	-3.94	114.88	122.02
2	B	1330[A]	NAP	C5A-C4A-N3A	-3.92	121.32	126.72
2	B	1330[B]	NAP	C5A-C4A-N3A	-3.92	121.32	126.72
2	D	1328[A]	NAP	C5A-C4A-N3A	-3.92	121.32	126.72
2	D	1328[B]	NAP	C5A-C4A-N3A	-3.92	121.32	126.72
2	C	1329[A]	NAP	N9A-C8A-N7A	-3.89	108.42	113.94
2	C	1329[B]	NAP	N9A-C8A-N7A	-3.89	108.42	113.94
2	B	1330[A]	NAP	N9A-C8A-N7A	-3.82	108.51	113.94
2	B	1330[B]	NAP	N9A-C8A-N7A	-3.82	108.51	113.94
3	A	1330	HXC	N3-C4-N9	3.72	133.49	127.17
3	C	1330	HXC	CP5-NP2-CP6	3.71	129.21	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1330	HXC	N3-C4-N9	3.68	133.43	127.17
3	B	1331	HXC	N3-C4-N9	3.68	133.42	127.17
3	A	1330	HXC	C2-N3-C4	3.64	120.72	111.83
3	D	1329	HXC	C2-N3-C4	3.63	120.70	111.83
3	D	1329	HXC	N3-C4-N9	3.62	133.33	127.17
3	B	1331	HXC	C2-N3-C4	3.60	120.63	111.83
3	C	1330	HXC	C2-N3-C4	3.58	120.58	111.83
2	C	1329[A]	NAP	C2A-N3A-C4A	3.50	120.37	111.83
2	C	1329[B]	NAP	C2A-N3A-C4A	3.50	120.37	111.83
2	D	1328[A]	NAP	C5A-N7A-C8A	3.50	108.94	103.45
2	D	1328[B]	NAP	C5A-N7A-C8A	3.50	108.94	103.45
2	A	1329[A]	NAP	N9A-C8A-N7A	-3.42	109.09	113.94
2	A	1329[B]	NAP	N9A-C8A-N7A	-3.42	109.09	113.94
3	A	1330	HXC	OM2-CM1-CM2	-3.42	120.04	123.98
2	C	1329[A]	NAP	C5A-N7A-C8A	3.38	108.77	103.45
2	C	1329[B]	NAP	C5A-N7A-C8A	3.38	108.77	103.45
2	A	1329[A]	NAP	C2A-N3A-C4A	3.28	119.83	111.83
2	A	1329[B]	NAP	C2A-N3A-C4A	3.28	119.83	111.83
3	D	1329	HXC	N9-C8-N7	-3.25	109.32	113.94
2	D	1328[A]	NAP	C2A-N3A-C4A	3.21	119.68	111.83
2	D	1328[B]	NAP	C2A-N3A-C4A	3.21	119.68	111.83
3	A	1330	HXC	N9-C8-N7	-3.19	109.41	113.94
3	D	1329	HXC	CP5-NP2-CP6	3.18	128.26	122.55
3	B	1331	HXC	CP8-CPA-CP7	3.17	114.16	108.77
2	B	1330[A]	NAP	C2A-N3A-C4A	3.16	119.56	111.83
2	B	1330[B]	NAP	C2A-N3A-C4A	3.16	119.56	111.83
3	D	1329	HXC	CP7-CP6-NP2	3.16	122.48	116.48
3	C	1330	HXC	N9-C8-N7	-3.13	109.50	113.94
2	B	1330[A]	NAP	C5A-N7A-C8A	3.12	108.35	103.45
2	B	1330[B]	NAP	C5A-N7A-C8A	3.12	108.35	103.45
3	B	1331	HXC	N9-C8-N7	-3.12	109.52	113.94
2	A	1329[A]	NAP	C5A-N7A-C8A	3.11	108.34	103.45
2	A	1329[B]	NAP	C5A-N7A-C8A	3.11	108.34	103.45
2	C	1329[A]	NAP	N3A-C4A-N9A	2.88	132.07	127.17
2	C	1329[B]	NAP	N3A-C4A-N9A	2.88	132.07	127.17
3	D	1329	HXC	C5-N7-C8	2.83	107.89	103.45
3	A	1330	HXC	C5-N7-C8	2.82	107.88	103.45
3	B	1331	HXC	C5-N7-C8	2.81	107.87	103.45
3	A	1330	HXC	CP4-CP3-NP1	2.80	121.45	116.34
3	C	1330	HXC	C5-N7-C8	2.80	107.85	103.45
3	C	1330	HXC	CM3-CM2-CM1	2.73	118.30	112.27
2	B	1330[A]	NAP	N3A-C4A-N9A	2.72	131.80	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1330[B]	NAP	N3A-C4A-N9A	2.72	131.80	127.17
2	D	1328[A]	NAP	N3A-C4A-N9A	2.69	131.74	127.17
2	D	1328[B]	NAP	N3A-C4A-N9A	2.69	131.74	127.17
3	B	1331	HXC	C4-C5-N7	-2.69	107.51	110.58
3	D	1329	HXC	C4-C5-N7	-2.66	107.54	110.58
3	B	1331	HXC	OM2-CM1-S	-2.64	119.32	122.68
3	A	1330	HXC	C4-C5-N7	-2.64	107.56	110.58
3	C	1330	HXC	C4-C5-N7	-2.64	107.57	110.58
3	B	1331	HXC	CP4-CP3-NP1	2.64	121.15	116.34
3	A	1330	HXC	OM2-CM1-S	-2.63	119.33	122.68
2	A	1329[A]	NAP	N3A-C4A-N9A	2.63	131.64	127.17
2	A	1329[B]	NAP	N3A-C4A-N9A	2.63	131.64	127.17
3	C	1330	HXC	CM4-CM3-CM2	2.61	122.73	113.13
3	B	1331	HXC	OM2-CM1-CM2	-2.57	121.01	123.98
3	C	1330	HXC	CP5-CP4-CP3	2.55	116.64	112.39
3	A	1330	HXC	OP1-CP3-CP4	-2.50	117.49	122.02
3	B	1331	HXC	CP2-NP1-CP3	2.45	127.38	122.82
2	B	1330[A]	NAP	O2A-PA-O3	2.45	113.89	107.27
3	D	1329	HXC	CM4-CM3-CM2	2.43	122.04	113.13
2	D	1328[A]	NAP	C4A-N9A-C8A	2.37	108.22	105.74
2	D	1328[B]	NAP	C4A-N9A-C8A	2.37	108.22	105.74
3	B	1331	HXC	CP5-NP2-CP6	-2.35	118.32	122.55
2	C	1329[A]	NAP	C4A-C5A-N7A	-2.32	107.93	110.58
2	C	1329[B]	NAP	C4A-C5A-N7A	-2.32	107.93	110.58
2	D	1328[A]	NAP	C4A-C5A-N7A	-2.28	107.98	110.58
2	D	1328[B]	NAP	C4A-C5A-N7A	-2.28	107.98	110.58
3	D	1329	HXC	C4'-O4'-C1'	-2.24	104.52	109.47
2	B	1330[A]	NAP	O3B-C3B-C4B	-2.24	104.64	111.08
2	A	1329[A]	NAP	C4A-C5A-N7A	-2.23	108.03	110.58
2	A	1329[B]	NAP	C4A-C5A-N7A	-2.23	108.03	110.58
2	A	1329[A]	NAP	C3N-C7N-N7N	2.23	120.48	117.74
2	A	1329[B]	NAP	C3N-C7N-N7N	2.23	120.48	117.74
3	D	1329	HXC	C4-N9-C8	2.20	108.05	105.74
3	B	1331	HXC	O7-CPB-CPA	2.18	114.06	110.55
3	D	1329	HXC	O4'-C1'-C2'	-2.15	102.01	106.62
2	B	1330[A]	NAP	C4A-N9A-C8A	2.14	107.99	105.74
2	B	1330[B]	NAP	C4A-N9A-C8A	2.14	107.99	105.74
3	A	1330	HXC	C4-N9-C8	2.13	107.98	105.74
2	D	1328[A]	NAP	C6N-N1N-C2N	-2.10	120.09	121.88
2	D	1328[B]	NAP	C6N-N1N-C2N	-2.10	120.09	121.88
3	A	1330	HXC	C4'-O4'-C1'	-2.09	104.86	109.47
3	C	1330	HXC	CP8-CPA-CP7	2.05	112.27	108.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1328[A]	NAP	O3B-C3B-C4B	-2.04	105.23	111.08
2	B	1330[A]	NAP	C4A-C5A-N7A	-2.03	108.27	110.58
2	B	1330[B]	NAP	C4A-C5A-N7A	-2.03	108.27	110.58
3	B	1331	HXC	C4-N9-C8	2.02	107.86	105.74

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1329[A]	NAP	C5B-O5B-PA-O1A
2	A	1329[A]	NAP	C5B-O5B-PA-O2A
2	A	1329[A]	NAP	C5B-O5B-PA-O3
2	A	1329[B]	NAP	PA-O3-PN-O5D
2	B	1330[A]	NAP	C5D-O5D-PN-O3
2	B	1330[A]	NAP	C5D-O5D-PN-O2N
2	B	1330[B]	NAP	C5D-O5D-PN-O3
2	B	1330[B]	NAP	C5D-O5D-PN-O2N
2	C	1329[A]	NAP	C5B-O5B-PA-O1A
2	C	1329[A]	NAP	C5B-O5B-PA-O2A
2	D	1328[A]	NAP	C5D-O5D-PN-O3
2	D	1328[A]	NAP	C5D-O5D-PN-O2N
2	D	1328[B]	NAP	C5B-O5B-PA-O2A
2	D	1328[B]	NAP	C5D-O5D-PN-O3
2	D	1328[B]	NAP	C5D-O5D-PN-O2N
3	A	1330	HXC	C5'-O5'-P1-O12
3	A	1330	HXC	C5'-O5'-P1-O6
3	A	1330	HXC	P1-O6-P2-O7
3	A	1330	HXC	CP4-CP3-NP1-CP2
3	A	1330	HXC	OP1-CP3-NP1-CP2
3	A	1330	HXC	S-CP1-CP2-NP1
3	A	1330	HXC	CP2-CP1-S-CM1
3	A	1330	HXC	CM2-CM1-S-CP1
3	A	1330	HXC	OM2-CM1-S-CP1
3	B	1331	HXC	CP7-CPA-CPB-O7
3	B	1331	HXC	CP9-CPA-CPB-O7
3	B	1331	HXC	CP8-CPA-CPB-O7
3	B	1331	HXC	OP3-CP7-CPA-CPB
3	B	1331	HXC	CP6-CP7-CPA-CPB
3	B	1331	HXC	OP3-CP7-CPA-CP9
3	B	1331	HXC	CP6-CP7-CPA-CP9
3	B	1331	HXC	OP3-CP7-CPA-CP8
3	B	1331	HXC	CP6-CP7-CPA-CP8

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Mol	Chain	Res	Type	Atoms
3	B	1331	HXC	OP2-CP6-CP7-OP3
3	B	1331	HXC	CP3-CP4-CP5-NP2
3	B	1331	HXC	CP1-CP2-NP1-CP3
3	B	1331	HXC	S-CP1-CP2-NP1
3	B	1331	HXC	CP2-CP1-S-CM1
3	B	1331	HXC	CM2-CM1-S-CP1
3	B	1331	HXC	OM2-CM1-S-CP1
3	C	1330	HXC	O4'-C4'-C5'-O5'
3	C	1330	HXC	C5'-O5'-P1-O6
3	C	1330	HXC	P1-O6-P2-O7
3	C	1330	HXC	OP2-CP6-CP7-CPA
3	C	1330	HXC	NP2-CP6-CP7-CPA
3	C	1330	HXC	CM2-CM1-S-CP1
3	C	1330	HXC	OM2-CM1-S-CP1
3	C	1330	HXC	CM1-CM2-CM3-CM4
3	D	1329	HXC	O4'-C4'-C5'-O5'
3	D	1329	HXC	C5'-O5'-P1-O12
3	D	1329	HXC	C5'-O5'-P1-O6
3	D	1329	HXC	CP7-CP6-NP2-CP5
3	D	1329	HXC	CP3-CP4-CP5-NP2
3	D	1329	HXC	CP2-CP1-S-CM1
3	D	1329	HXC	CM2-CM1-S-CP1
3	D	1329	HXC	OM2-CM1-S-CP1
3	D	1329	HXC	S-CM1-CM2-CM3
3	A	1330	HXC	CP4-CP5-NP2-CP6
3	C	1330	HXC	CP4-CP5-NP2-CP6
2	D	1328[B]	NAP	C3B-C4B-C5B-O5B
3	B	1331	HXC	C3'-C4'-C5'-O5'
3	B	1331	HXC	O4'-C4'-C5'-O5'
3	D	1329	HXC	OP2-CP6-NP2-CP5
3	B	1331	HXC	OP1-CP3-CP4-CP5
3	C	1330	HXC	OP1-CP3-CP4-CP5
3	B	1331	HXC	NP1-CP3-CP4-CP5
3	C	1330	HXC	NP1-CP3-CP4-CP5
3	D	1329	HXC	C3'-C4'-C5'-O5'
2	A	1329[A]	NAP	O4B-C4B-C5B-O5B
2	C	1329[A]	NAP	O4B-C4B-C5B-O5B
3	C	1330	HXC	C3'-C4'-C5'-O5'
2	D	1328[B]	NAP	O4B-C4B-C5B-O5B
3	C	1330	HXC	OP2-CP6-CP7-OP3
3	C	1330	HXC	C4'-C5'-O5'-P1
3	C	1330	HXC	S-CP1-CP2-NP1

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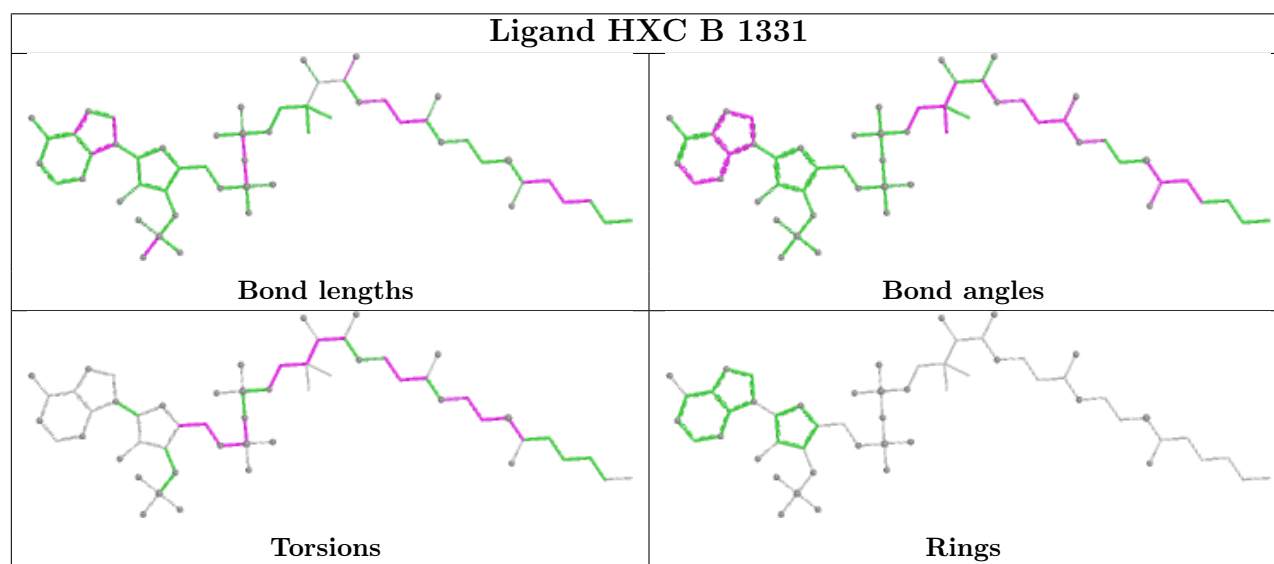
Mol	Chain	Res	Type	Atoms
3	A	1330	HXC	NP2-CP6-CP7-OP3
3	B	1331	HXC	NP2-CP6-CP7-OP3
3	D	1329	HXC	OM2-CM1-CM2-CM3
3	A	1330	HXC	CM2-CM3-CM4-CM5
2	B	1330[B]	NAP	PA-O3-PN-O5D
2	D	1328[B]	NAP	PA-O3-PN-O5D
3	C	1330	HXC	CP8-CPA-CPB-O7
2	B	1330[A]	NAP	C5D-O5D-PN-O1N
2	B	1330[B]	NAP	C5D-O5D-PN-O1N
2	C	1329[A]	NAP	C5B-O5B-PA-O3
2	D	1328[A]	NAP	C5D-O5D-PN-O1N
2	D	1328[B]	NAP	C5B-O5B-PA-O1A
2	D	1328[B]	NAP	C5B-O5B-PA-O3
2	D	1328[B]	NAP	C5D-O5D-PN-O1N
3	A	1330	HXC	CPB-O7-P2-O21
3	B	1331	HXC	C5'-O5'-P1-O11
3	C	1330	HXC	C5'-O5'-P1-O11
3	C	1330	HXC	C5'-O5'-P1-O12
3	A	1330	HXC	C4'-C5'-O5'-P1
2	A	1329[A]	NAP	C3B-C4B-C5B-O5B
3	B	1331	HXC	OP2-CP6-CP7-CPA
3	B	1331	HXC	NP2-CP6-CP7-CPA
2	C	1329[A]	NAP	C4B-C5B-O5B-PA
3	A	1330	HXC	OP2-CP6-CP7-OP3
3	B	1331	HXC	C4'-C5'-O5'-P1
2	C	1329[B]	NAP	C3B-C4B-C5B-O5B
2	B	1330[B]	NAP	C3B-C4B-C5B-O5B
2	C	1329[A]	NAP	C3B-C4B-C5B-O5B
2	B	1330[B]	NAP	PN-O3-PA-O2A
2	B	1330[B]	NAP	PA-O3-PN-O2N
2	D	1328[A]	NAP	PA-O3-PN-O2N
3	D	1329	HXC	P1-O6-P2-O22
2	D	1328[A]	NAP	C2B-O2B-P2B-O3X
2	D	1328[B]	NAP	C2B-O2B-P2B-O3X
3	B	1331	HXC	CPA-CPB-O7-P2
2	A	1329[A]	NAP	C4B-C5B-O5B-PA
3	C	1330	HXC	NP2-CP6-CP7-OP3
2	D	1328[A]	NAP	PA-O3-PN-O1N
3	B	1331	HXC	P2-O6-P1-O12
3	D	1329	HXC	P1-O6-P2-O21
3	A	1330	HXC	C3'-C4'-C5'-O5'

There are no ring outliers.

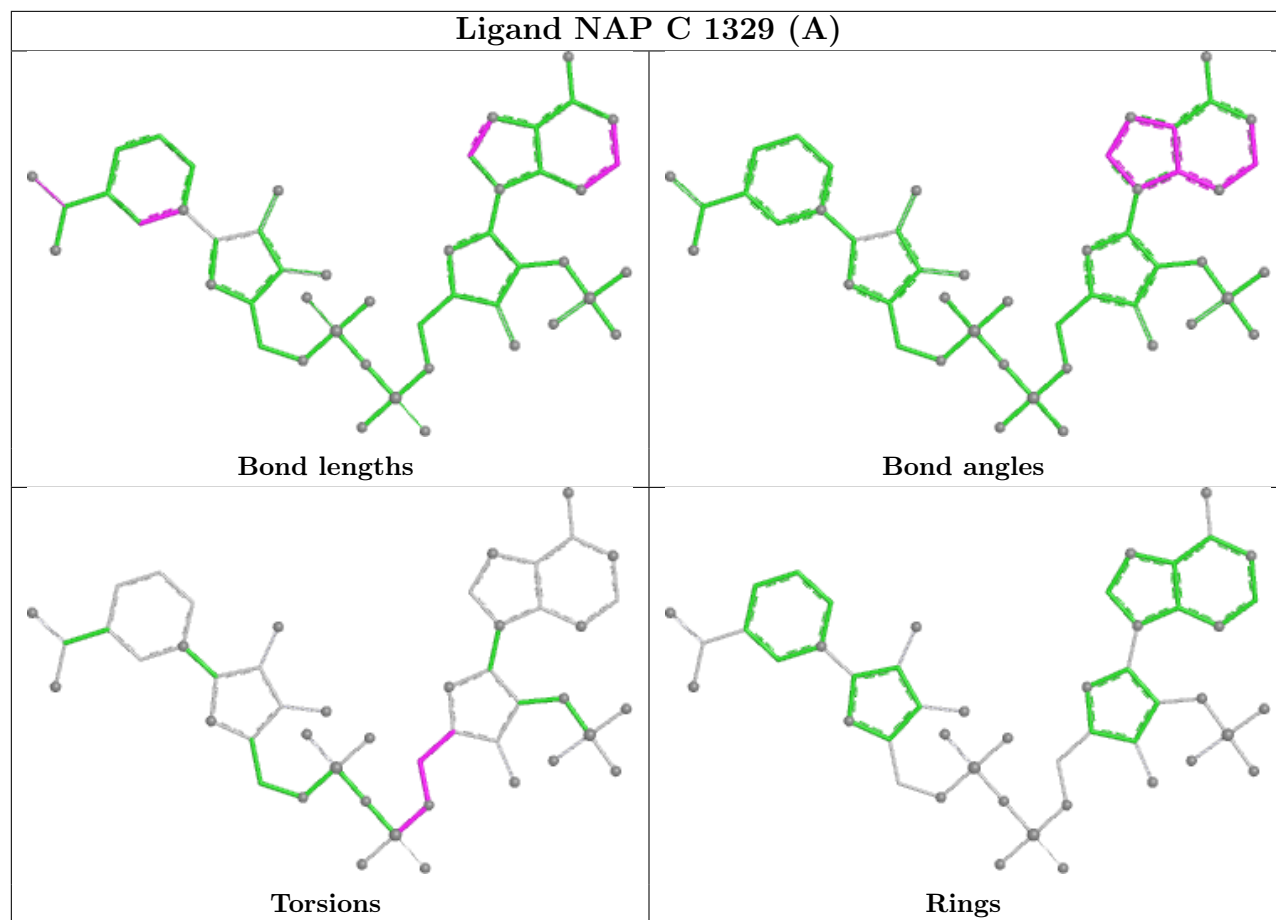
6 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1331	HXC	5	0
2	B	1330[B]	NAP	1	0
3	C	1330	HXC	21	0
3	D	1329	HXC	8	0
3	A	1330	HXC	4	0
2	C	1329[B]	NAP	2	0

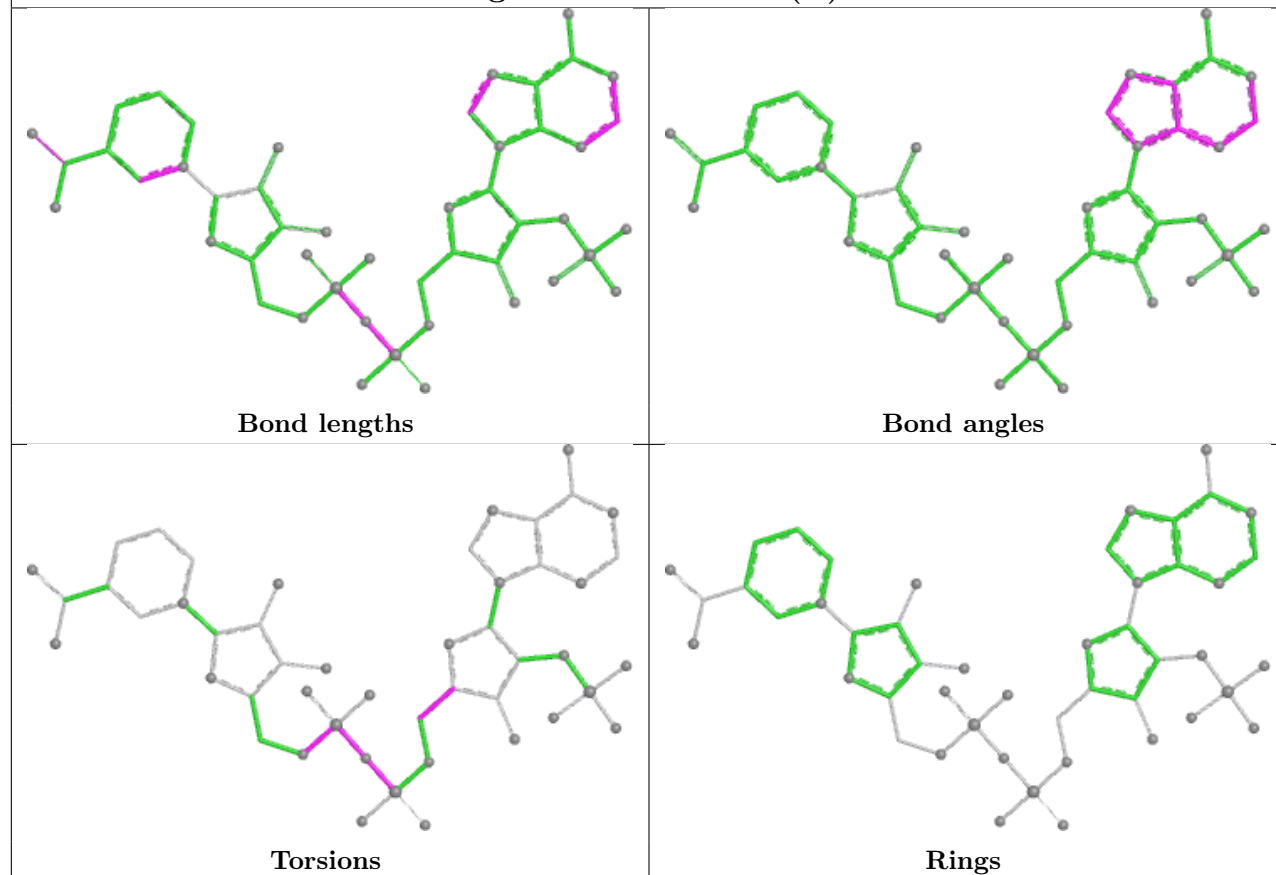
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



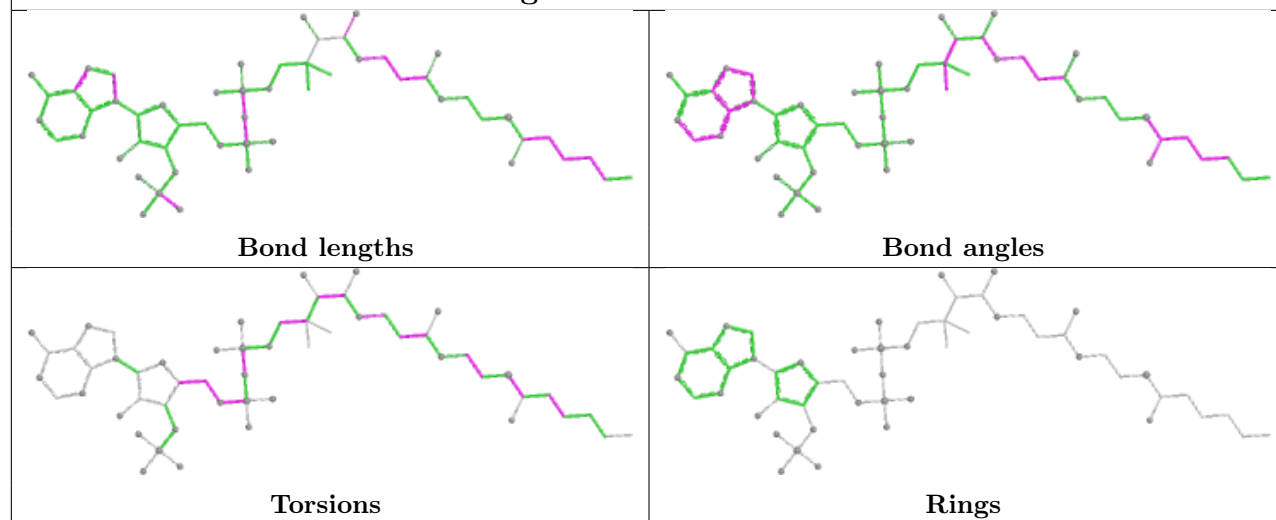
Ligand NAP C 1329 (A)



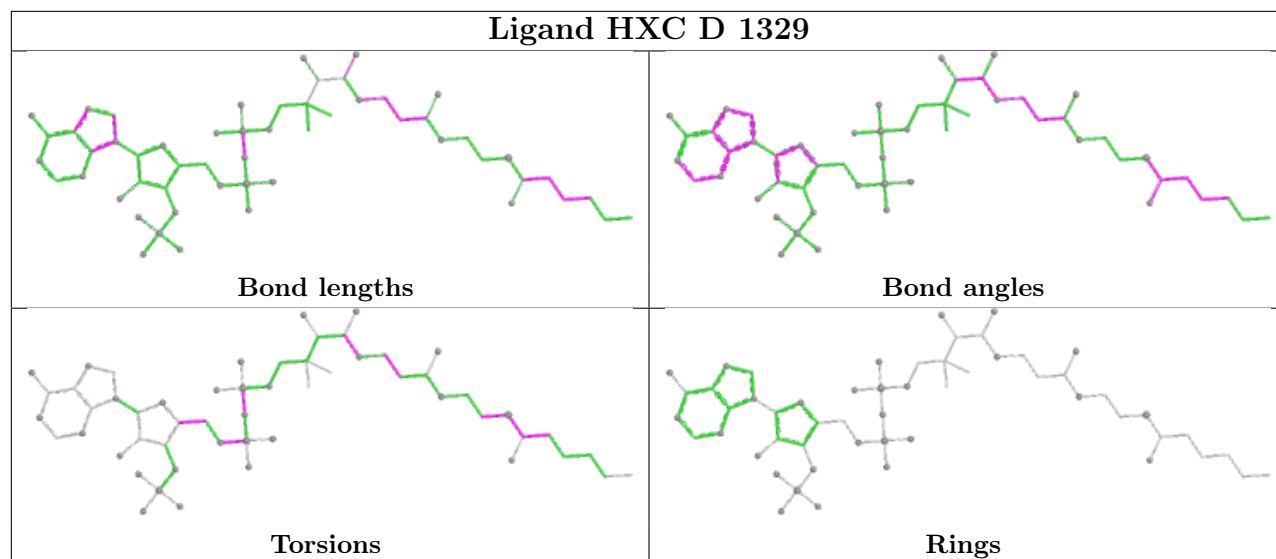
Ligand NAP B 1330 (B)



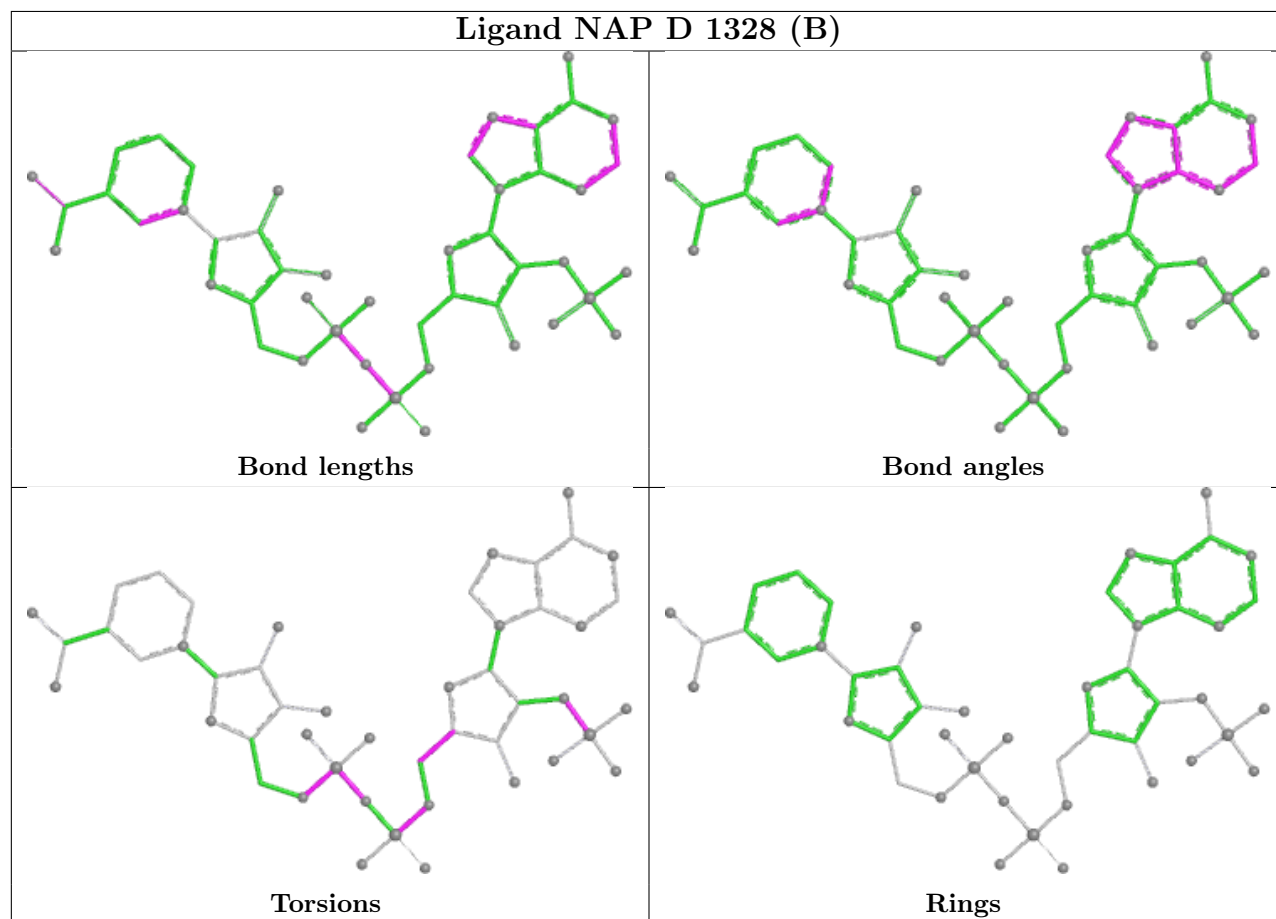
Ligand HXC C 1330



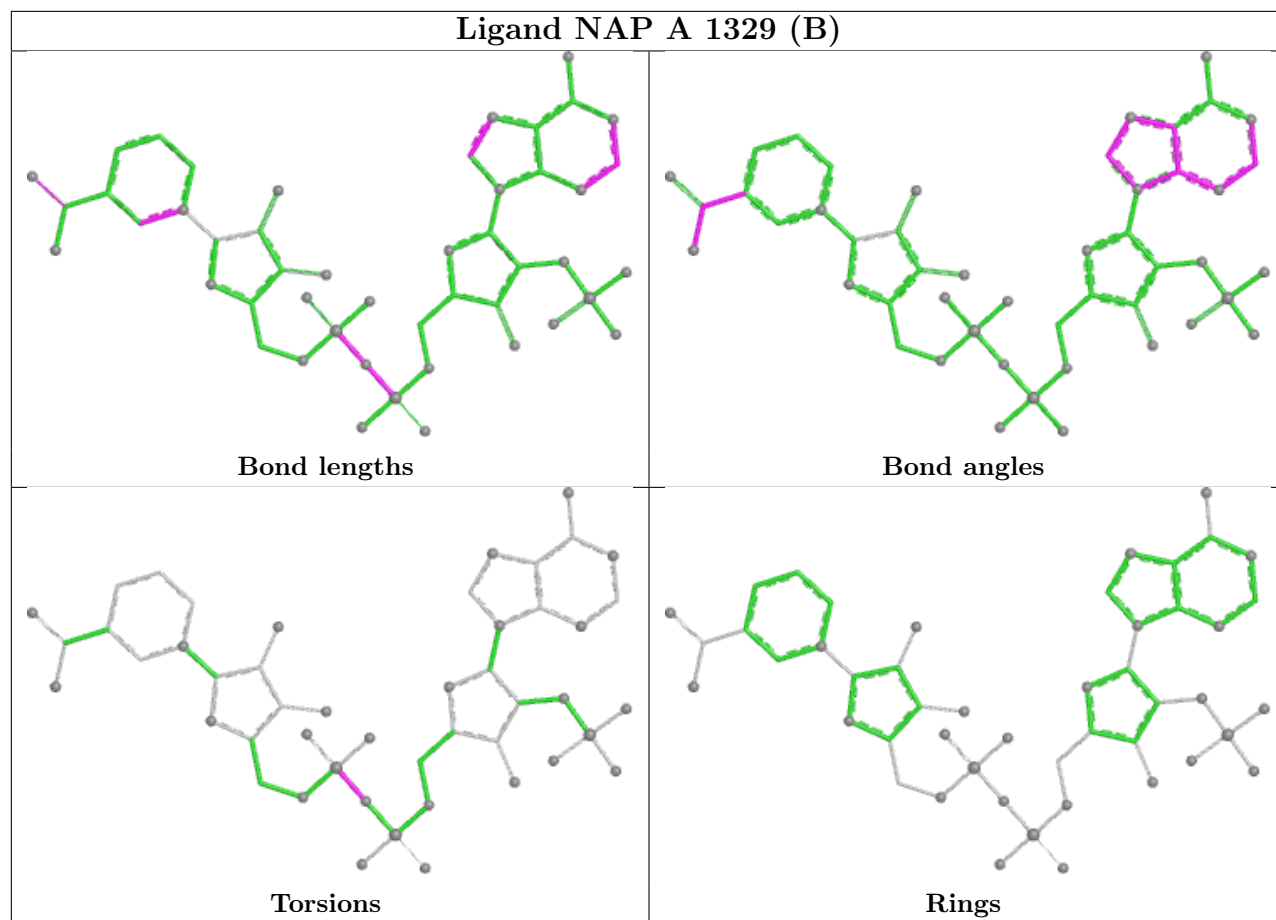
Ligand HXC D 1329



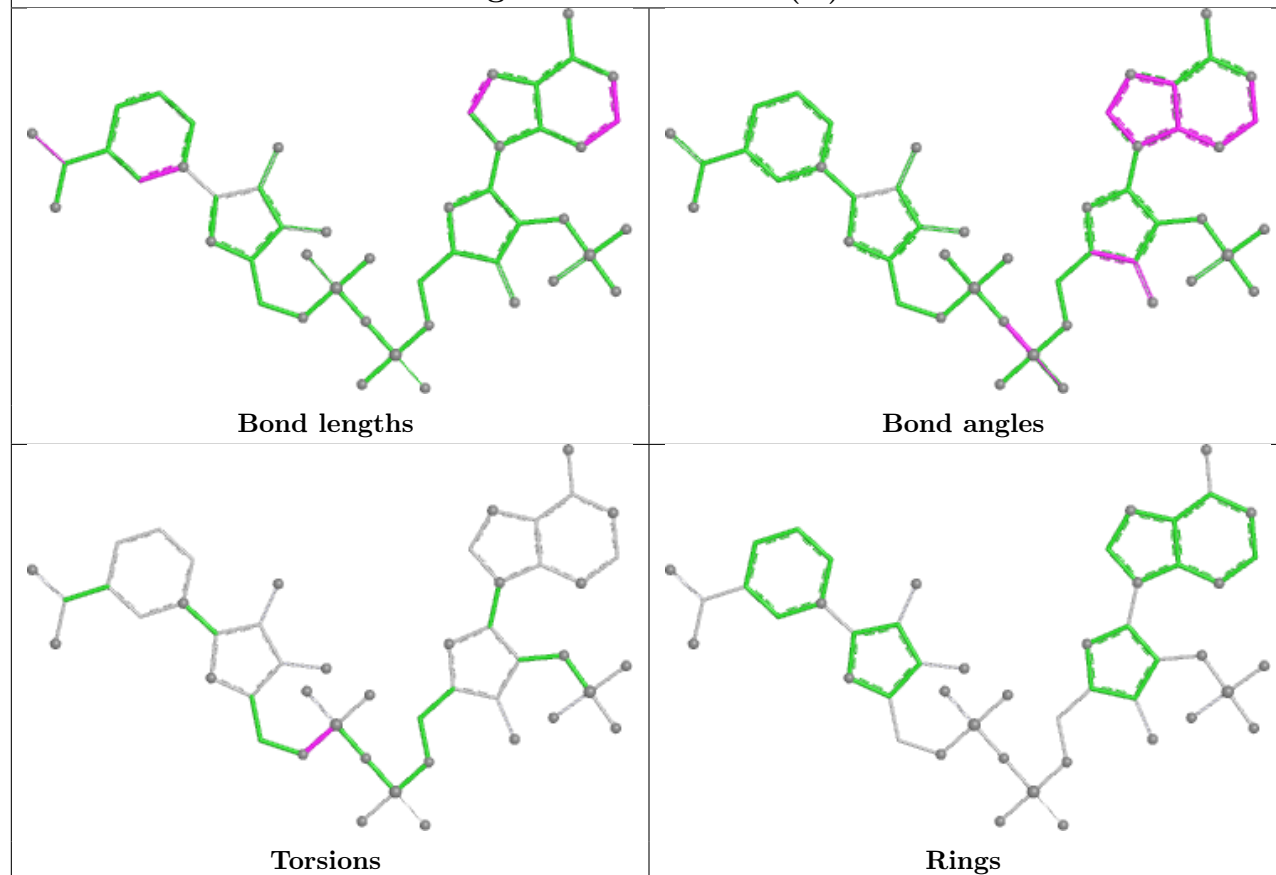
Ligand NAP D 1328 (B)



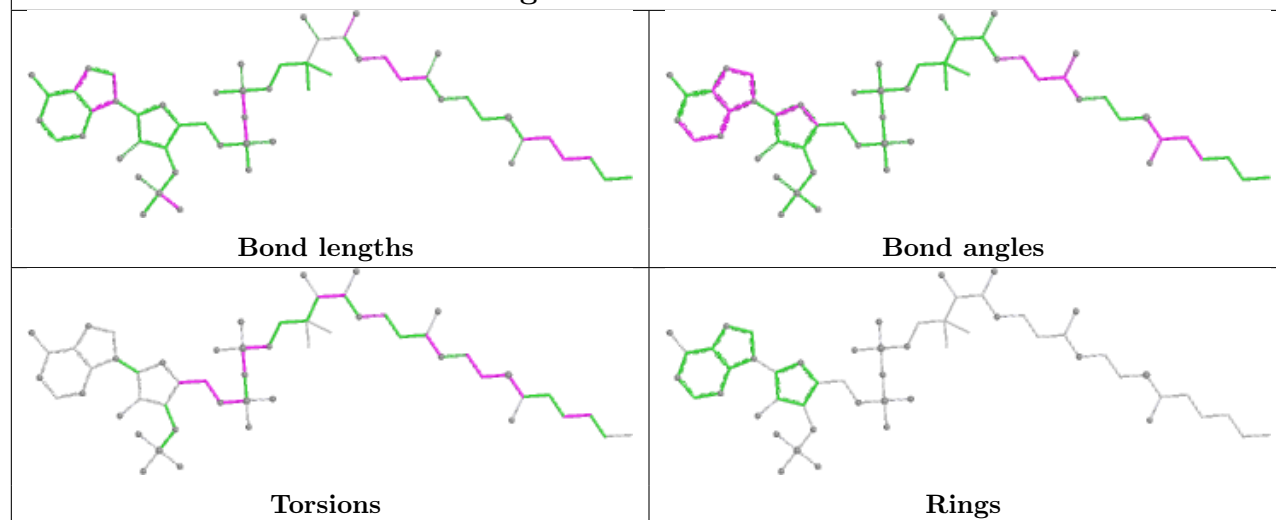
Ligand NAP A 1329 (B)



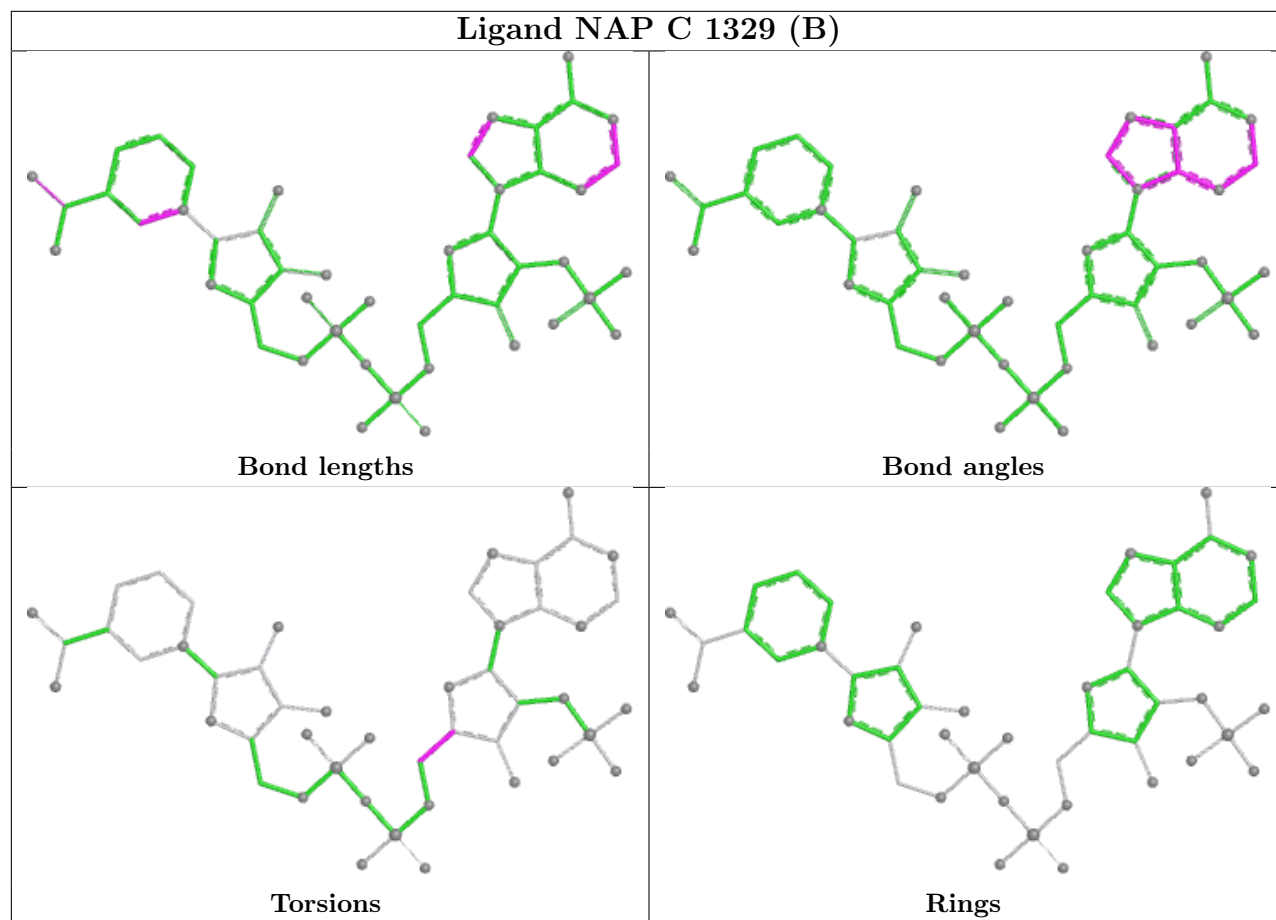
Ligand NAP B 1330 (A)



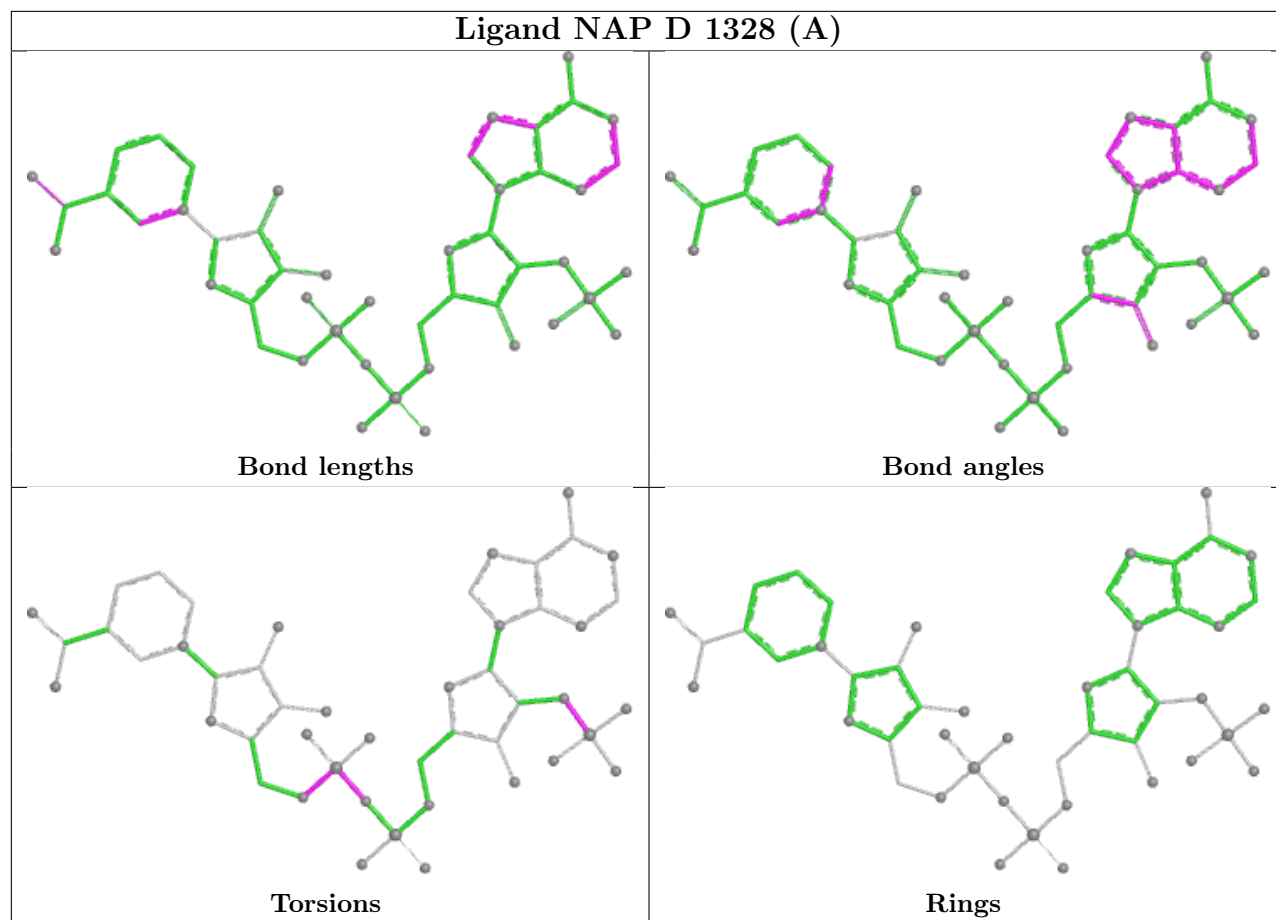
Ligand HXC A 1330

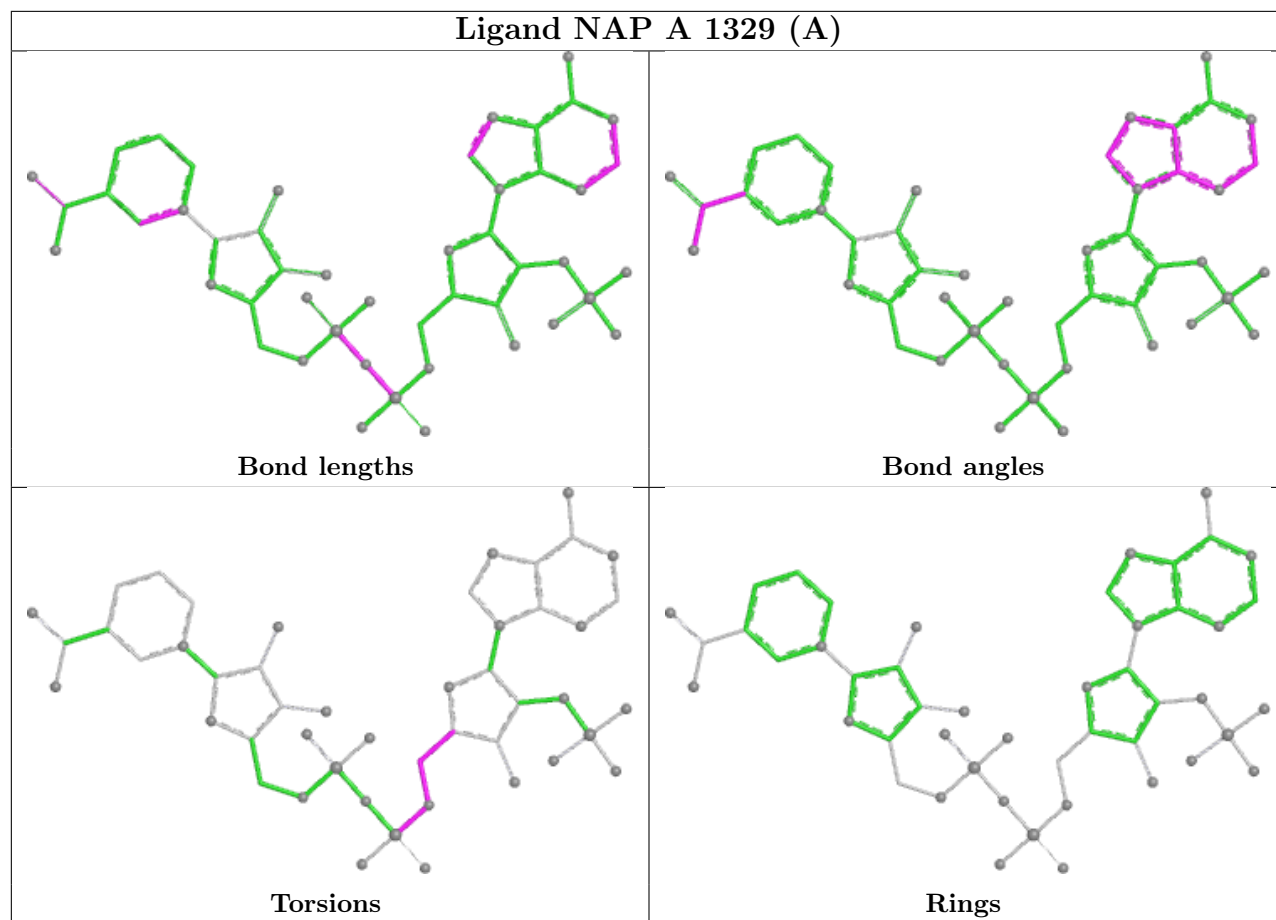


Ligand NAP C 1329 (B)



Ligand NAP D 1328 (A)





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	288/302 (95%)	0.61	27 (9%) 14 17	14, 26, 59, 77	6 (2%)
1	B	286/302 (94%)	0.74	31 (10%) 11 12	15, 27, 56, 74	6 (2%)
1	C	286/302 (94%)	1.04	55 (19%) 3 3	16, 32, 63, 82	6 (2%)
1	D	282/302 (93%)	1.14	52 (18%) 3 3	17, 33, 56, 75	2 (0%)
All	All	1142/1208 (94%)	0.88	165 (14%) 6 7	14, 30, 59, 82	20 (1%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	PHE	7.1
1	A	39	LEU	5.8
1	C	39	LEU	5.6
1	B	257	THR	5.0
1	D	258	PHE	5.0
1	B	245	THR	4.8
1	D	317	VAL	4.8
1	A	254	PRO	4.7
1	B	322	TRP	4.7
1	D	98	ALA	4.7
1	B	317	VAL	4.6
1	D	322	TRP	4.6
1	D	100	ALA	4.5
1	D	36	THR	4.5
1	A	258	PHE	4.4
1	D	325	ILE	4.4
1	B	329	ILE	4.3
1	A	322	TRP	4.3
1	D	324	THR	4.2
1	C	38	ALA	4.1
1	D	318	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	324	THR	4.1
1	A	245	THR	4.0
1	C	322	TRP	4.0
1	C	247	GLY	3.7
1	C	107	THR	3.7
1	C	43	PHE	3.6
1	C	318	THR	3.5
1	A	320	GLU	3.5
1	C	47	LEU	3.4
1	A	317	VAL	3.4
1	C	257	THR	3.3
1	A	37	GLU	3.3
1	C	98	ALA	3.3
1	B	318	THR	3.2
1	C	161	TRP	3.2
1	C	258	PHE	3.2
1	C	245	THR	3.2
1	D	132	ILE	3.1
1	A	328	LEU	3.1
1	B	39	LEU	3.1
1	B	314	LEU	3.1
1	D	38	ALA	3.1
1	A	252	LEU	3.1
1	C	101	GLU	3.1
1	C	249	PHE	3.1
1	A	255	THR	3.0
1	D	323	ASP	3.0
1	C	320	GLU	3.0
1	C	100	ALA	3.0
1	A	253	ASP	2.9
1	C	317	VAL	2.9
1	B	328	LEU	2.9
1	D	114	ILE	2.9
1	C	36	THR	2.9
1	D	95	VAL	2.9
1	A	327	GLU	2.9
1	D	35	ASN	2.9
1	C	50	ALA	2.8
1	C	325	ILE	2.8
1	B	36	THR	2.8
1	D	186	ALA	2.8
1	B	321	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	261	GLU	2.8
1	C	125	GLN	2.8
1	D	103	ILE	2.8
1	C	95	VAL	2.7
1	B	320	GLU	2.7
1	C	327	GLU	2.7
1	C	53	PRO	2.7
1	C	122	ASP	2.7
1	B	326	GLU	2.7
1	D	43	PHE	2.6
1	A	36	THR	2.6
1	C	324	THR	2.6
1	C	314	LEU	2.6
1	D	321	GLN	2.6
1	D	104	SER	2.6
1	B	95	VAL	2.6
1	C	248	ALA	2.6
1	B	108	GLY	2.6
1	D	94	ASP	2.6
1	C	111	VAL	2.6
1	D	124	VAL	2.6
1	D	262	MET	2.6
1	A	35	ASN	2.6
1	A	38	ALA	2.6
1	C	81	SER	2.5
1	C	112[A]	HIS	2.5
1	A	261	GLU	2.5
1	B	101	GLU	2.5
1	C	328	LEU	2.5
1	C	54	PRO	2.5
1	C	103	ILE	2.5
1	D	243	ILE	2.5
1	A	321	GLN	2.5
1	B	323	ASP	2.5
1	B	325	ILE	2.5
1	D	133	LYS	2.5
1	C	105	SER	2.5
1	D	161	TRP	2.4
1	D	96	LEU	2.4
1	D	326	GLU	2.4
1	A	256	GLY	2.4
1	A	325	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	184	ILE	2.4
1	D	120	ASP	2.4
1	B	319	LYS	2.4
1	B	41	SER	2.4
1	B	134	VAL	2.4
1	B	262	MET	2.4
1	B	256	GLY	2.4
1	C	256	GLY	2.4
1	B	135	ALA	2.3
1	C	319	LYS	2.3
1	B	132	ILE	2.3
1	D	61	VAL	2.3
1	A	41	SER	2.3
1	C	136	GLY	2.3
1	C	46	PRO	2.3
1	C	185	LYS	2.3
1	B	38	ALA	2.3
1	D	39	LEU	2.3
1	C	129	SER	2.3
1	D	259	GLU	2.3
1	D	125	GLN	2.3
1	C	266	ILE	2.3
1	D	111	VAL	2.3
1	C	99	THR	2.2
1	B	100	ALA	2.2
1	D	105	SER	2.2
1	D	122	ASP	2.2
1	D	93	MET	2.2
1	D	37	GLU	2.2
1	D	128	VAL	2.2
1	A	161	TRP	2.2
1	C	104	SER	2.2
1	A	314	LEU	2.2
1	A	318	THR	2.2
1	C	42	LYS	2.2
1	D	159	ASN	2.2
1	C	45	SER	2.1
1	C	44	PHE	2.1
1	C	114	ILE	2.1
1	A	95	VAL	2.1
1	D	112[A]	HIS	2.1
1	B	159	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	106	GLN	2.1
1	C	288	TYR	2.1
1	C	113	ALA	2.1
1	D	135	ALA	2.1
1	D	319	LYS	2.1
1	A	55	ASN	2.1
1	B	55	ASN	2.1
1	D	131	LEU	2.1
1	C	77	THR	2.1
1	D	99	THR	2.1
1	D	52	LEU	2.0
1	D	314	LEU	2.0
1	D	34	MET	2.0
1	C	179	ILE	2.0
1	C	263	ILE	2.0
1	D	140	ILE	2.0
1	C	94[A]	ASP	2.0
1	D	41	SER	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(Å ²)	Q<0.9
3	HXC	C	1330	55/55	0.63	0.23	78,84,86,86	45
3	HXC	D	1329	55/55	0.63	0.20	75,77,79,79	45
3	HXC	B	1331	55/55	0.66	0.20	77,79,82,82	45
3	HXC	A	1330	55/55	0.68	0.21	81,83,84,84	45
2	NAP	D	1328[A]	48/48	0.89	0.12	34,37,41,42	8

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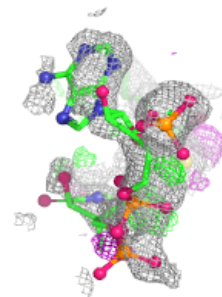
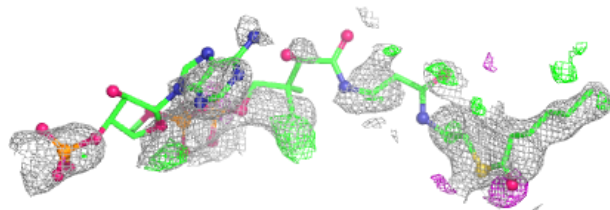
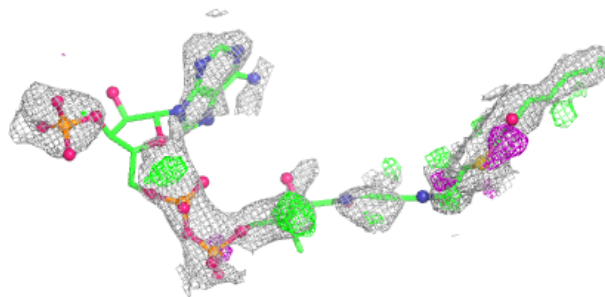
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	D	1328[B]	48/48	0.89	0.12	34,37,41,42	8
2	NAP	C	1329[A]	48/48	0.93	0.10	37,39,43,43	8
2	NAP	C	1329[B]	48/48	0.93	0.10	37,39,41,42	8
2	NAP	B	1330[A]	48/48	0.93	0.10	29,33,36,37	8
2	NAP	B	1330[B]	48/48	0.93	0.10	29,33,36,37	8
2	NAP	A	1329[A]	48/48	0.94	0.10	27,30,34,36	8
2	NAP	A	1329[B]	48/48	0.94	0.10	27,30,32,34	8

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.

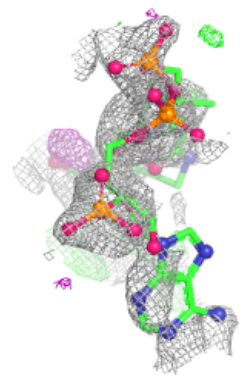
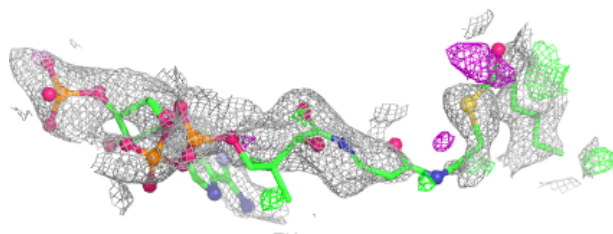
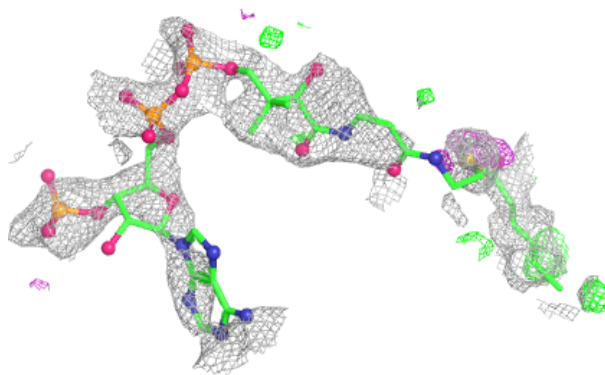
Electron density around HXC C 1330:

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

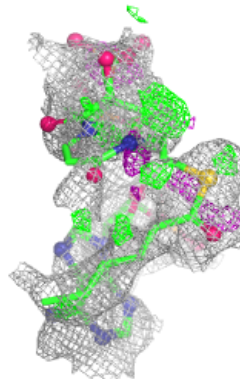
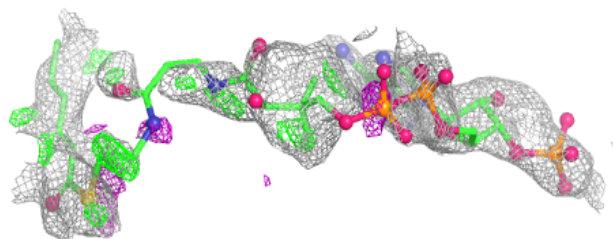
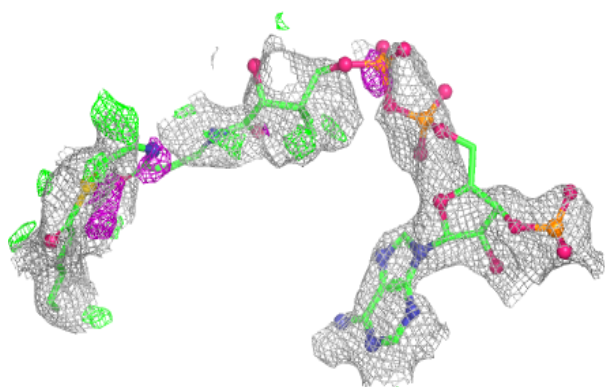


Electron density around HXC D 1329:

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

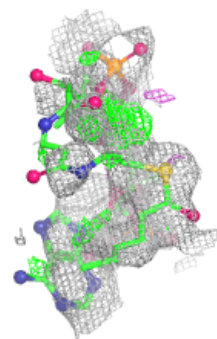
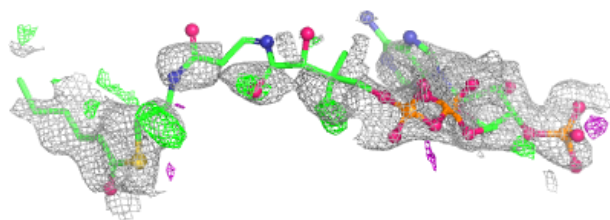
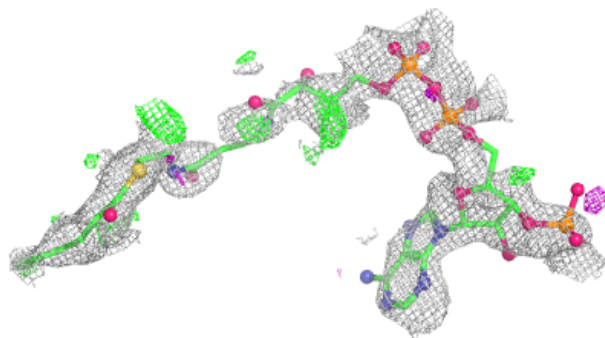
**Electron density around HXC B 1331:**

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and green (positive)

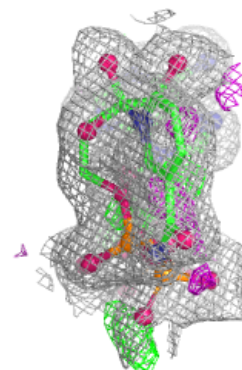
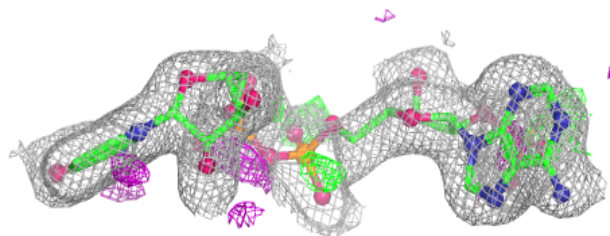
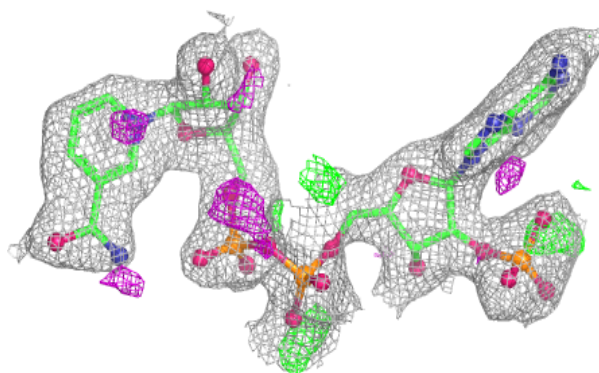


Electron density around HXC A 1330:

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and green (positive)

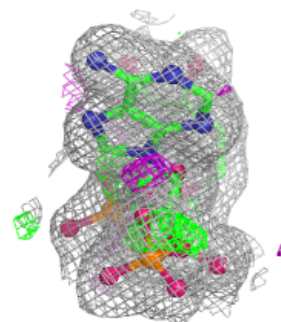
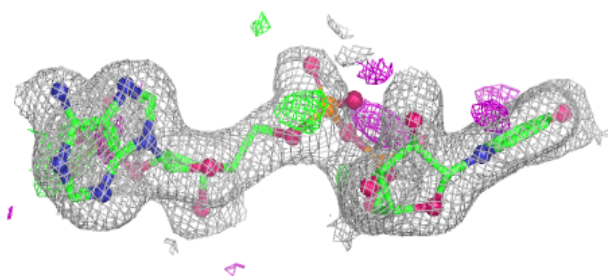
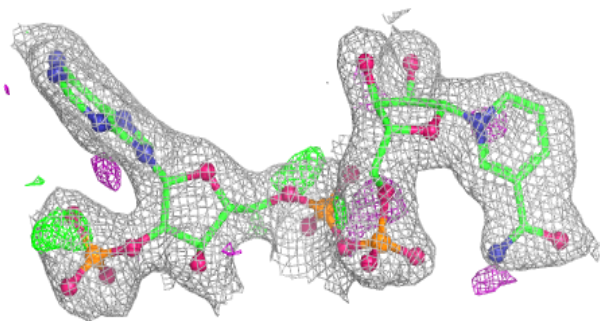
**Electron density around NAP D 1328 (A):**

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

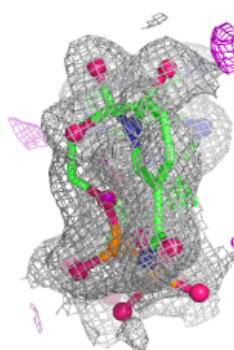
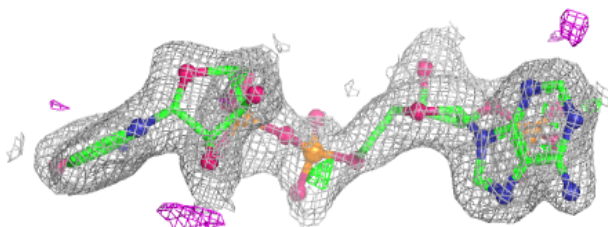
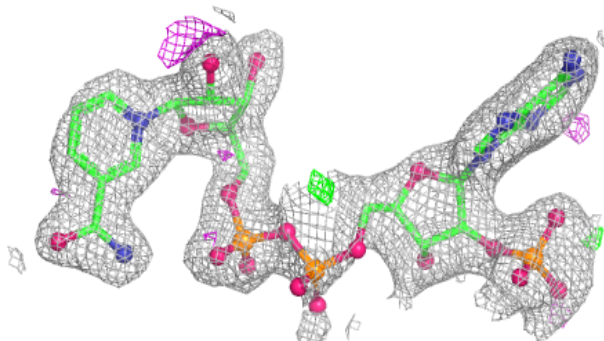


Electron density around NAP D 1328 (B):

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

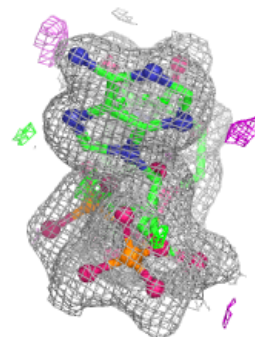
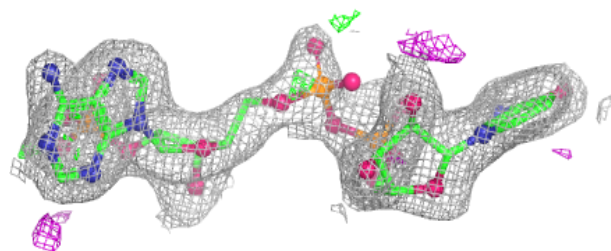
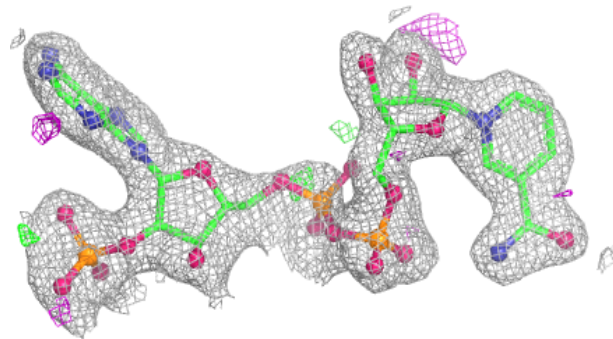
**Electron density around NAP C 1329 (A):**

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and green (positive)

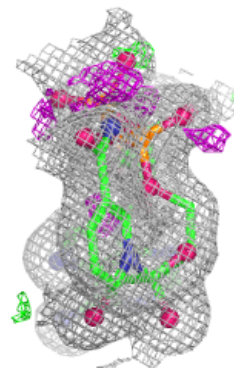
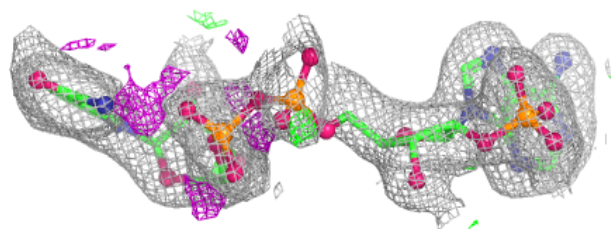
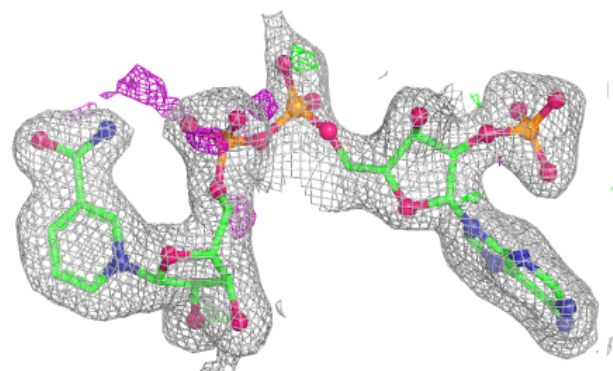


Electron density around NAP C 1329 (B):

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

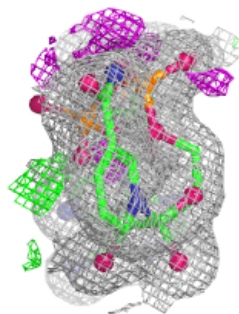
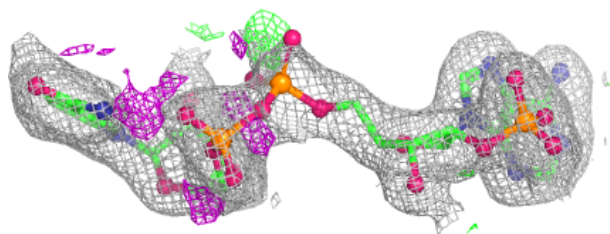
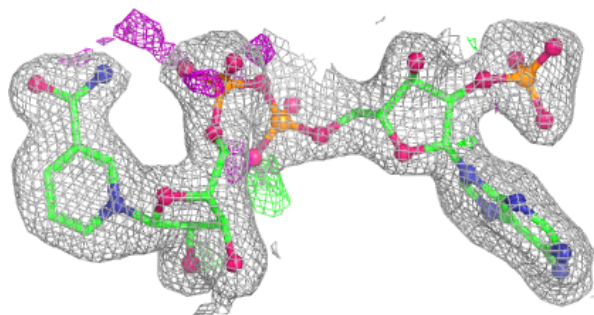
**Electron density around NAP B 1330 (A):**

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and green (positive)

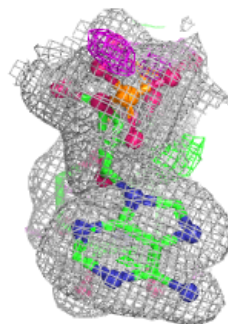
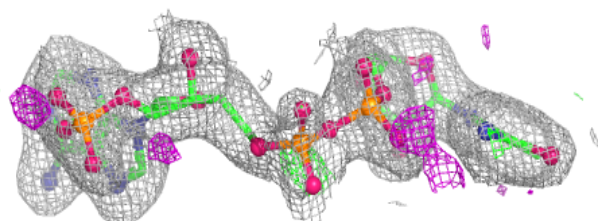
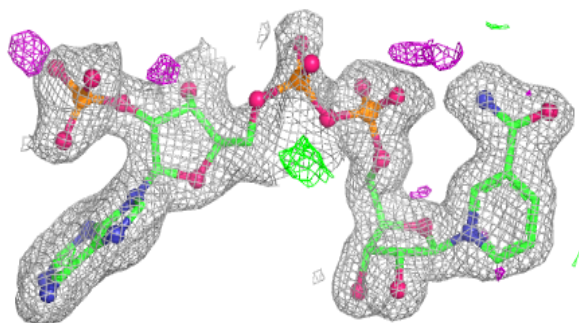


Electron density around NAP B 1330 (B):

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and green (positive)

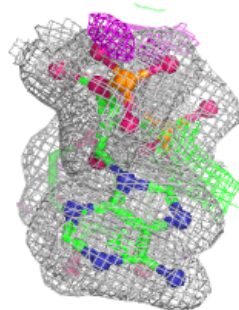
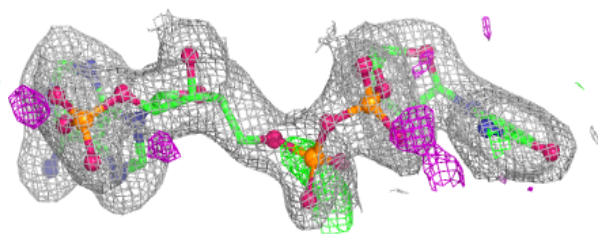
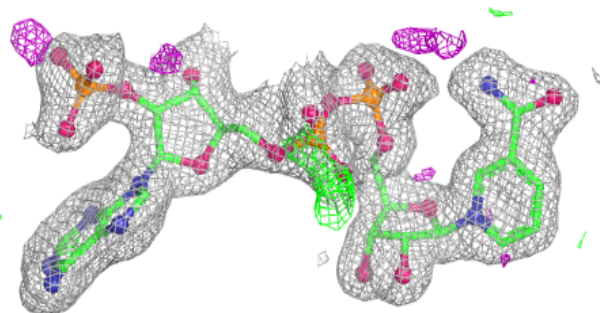
**Electron density around NAP A 1329 (A):**

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and green (positive)



Electron density around NAP A 1329 (B):

$2mF_o-DF_c$ (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.