



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 10:48 PM UTC

PDB ID : 3BZU / pdb_00003bzu
Title : Crystal structure of human 11-beta-hydroxysteroid dehydrogenase(HSD1) in complex with NADP and thiazolone inhibitor
Authors : Min, X.; Sudom, A.; Xu, H.; Wang, Z.; Walker, N.P.
Deposited on : 2008-01-18
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

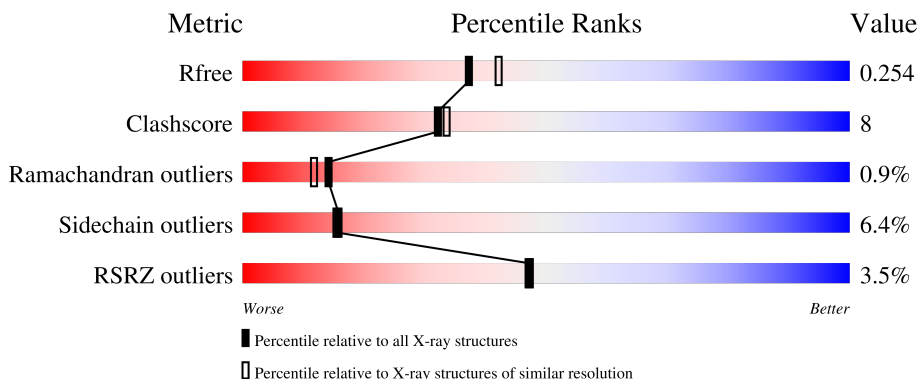
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	286	 2% 72% 18% .. 8%
1	B	286	 2% 74% 17% • 8%
1	C	286	 2% 70% 18% 11%
1	D	286	 6% 71% 15% .. 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8581 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	6	0
			2039	1299	341	383	16			
1	B	262	Total	C	N	O	S	0	3	0
			2011	1283	339	374	15			
1	C	254	Total	C	N	O	S	0	3	0
			1964	1254	330	365	15			
1	D	254	Total	C	N	O	S	0	1	0
			1946	1244	329	358	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP P28845
A	8	LYS	-	expression tag	UNP P28845
A	9	HIS	-	expression tag	UNP P28845
A	10	GLN	-	expression tag	UNP P28845
A	11	HIS	-	expression tag	UNP P28845
A	12	GLN	-	expression tag	UNP P28845
A	13	HIS	-	expression tag	UNP P28845
A	14	GLN	-	expression tag	UNP P28845
A	15	HIS	-	expression tag	UNP P28845
A	16	GLN	-	expression tag	UNP P28845
A	17	HIS	-	expression tag	UNP P28845
A	18	GLN	-	expression tag	UNP P28845
A	19	HIS	-	expression tag	UNP P28845
A	20	GLN	-	expression tag	UNP P28845
A	21	GLN	-	expression tag	UNP P28845
A	22	PRO	-	expression tag	UNP P28845
A	23	LEU	-	expression tag	UNP P28845
A	272	SER	CYS	engineered mutation	UNP P28845
B	7	MET	-	expression tag	UNP P28845
B	8	LYS	-	expression tag	UNP P28845
B	9	HIS	-	expression tag	UNP P28845

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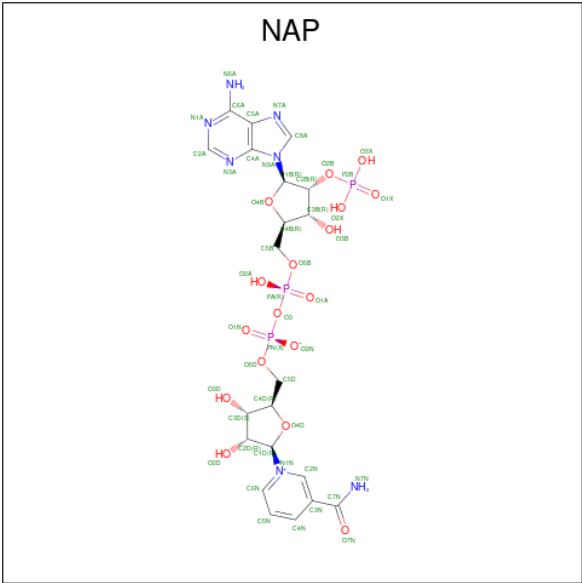
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	expression tag	UNP P28845
B	11	HIS	-	expression tag	UNP P28845
B	12	GLN	-	expression tag	UNP P28845
B	13	HIS	-	expression tag	UNP P28845
B	14	GLN	-	expression tag	UNP P28845
B	15	HIS	-	expression tag	UNP P28845
B	16	GLN	-	expression tag	UNP P28845
B	17	HIS	-	expression tag	UNP P28845
B	18	GLN	-	expression tag	UNP P28845
B	19	HIS	-	expression tag	UNP P28845
B	20	GLN	-	expression tag	UNP P28845
B	21	GLN	-	expression tag	UNP P28845
B	22	PRO	-	expression tag	UNP P28845
B	23	LEU	-	expression tag	UNP P28845
B	272	SER	CYS	engineered mutation	UNP P28845
C	7	MET	-	expression tag	UNP P28845
C	8	LYS	-	expression tag	UNP P28845
C	9	HIS	-	expression tag	UNP P28845
C	10	GLN	-	expression tag	UNP P28845
C	11	HIS	-	expression tag	UNP P28845
C	12	GLN	-	expression tag	UNP P28845
C	13	HIS	-	expression tag	UNP P28845
C	14	GLN	-	expression tag	UNP P28845
C	15	HIS	-	expression tag	UNP P28845
C	16	GLN	-	expression tag	UNP P28845
C	17	HIS	-	expression tag	UNP P28845
C	18	GLN	-	expression tag	UNP P28845
C	19	HIS	-	expression tag	UNP P28845
C	20	GLN	-	expression tag	UNP P28845
C	21	GLN	-	expression tag	UNP P28845
C	22	PRO	-	expression tag	UNP P28845
C	23	LEU	-	expression tag	UNP P28845
C	272	SER	CYS	engineered mutation	UNP P28845
D	7	MET	-	expression tag	UNP P28845
D	8	LYS	-	expression tag	UNP P28845
D	9	HIS	-	expression tag	UNP P28845
D	10	GLN	-	expression tag	UNP P28845
D	11	HIS	-	expression tag	UNP P28845
D	12	GLN	-	expression tag	UNP P28845
D	13	HIS	-	expression tag	UNP P28845
D	14	GLN	-	expression tag	UNP P28845
D	15	HIS	-	expression tag	UNP P28845

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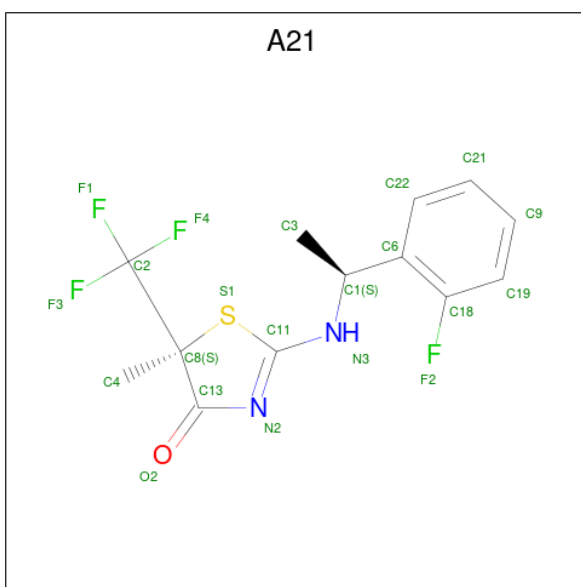
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	expression tag	UNP P28845
D	17	HIS	-	expression tag	UNP P28845
D	18	GLN	-	expression tag	UNP P28845
D	19	HIS	-	expression tag	UNP P28845
D	20	GLN	-	expression tag	UNP P28845
D	21	GLN	-	expression tag	UNP P28845
D	22	PRO	-	expression tag	UNP P28845
D	23	LEU	-	expression tag	UNP P28845
D	272	SER	CYS	engineered mutation	UNP P28845

- 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		

- Molecule 3 is (5S)-2-[[[(1S)-1-(2-fluorophenyl)ethyl]amino}-5-methyl-5-(trifluoromethyl)-1,3-thiazol-4(5H)-one (CCD ID: A21) (formula: C₁₃H₁₂F₄N₂OS).

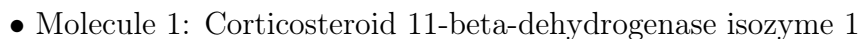
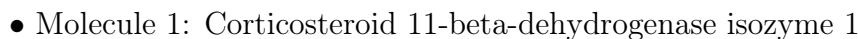


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			21	13	4	2	1	1		
3	B	1	Total	C	F	N	O	S	0	0
			21	13	4	2	1	1		
3	C	1	Total	C	F	N	O	S	0	0
			21	13	4	2	1	1		
3	D	1	Total	C	F	N	O	S	0	0
			21	13	4	2	1	1		

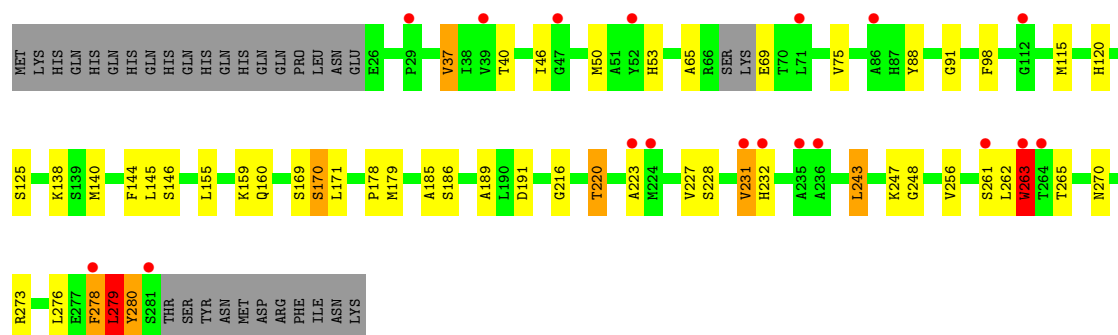
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	104	Total	O	0	0
			104	104		
4	B	99	Total	O	0	0
			99	99		
4	C	97	Total	O	0	0
			97	97		
4	D	45	Total	O	0	0
			45	45		

- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



Chain D: 6% 71% 15% .. 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.02Å 153.01Å 73.72Å 90.00° 92.16° 90.00°	Depositor
Resolution (Å)	31.33 – 2.25 31.33 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.5 (31.33-2.25) 96.5 (31.33-2.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.3.0026	Depositor
R, R_{free}	0.201 , 0.263 0.196 , 0.254	Depositor DCC
R_{free} test set	2862 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8581	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, A21

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	0.80	0/2099	0.93	1/2835 (0.0%)
1	B	0.78	0/2058	0.99	0/2779
1	C	0.78	0/2008	0.93	0/2710
1	D	0.70	0/1982	0.99	2/2675 (0.1%)
All	All	0.77	0/8147	0.96	3/10999 (0.0%)

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	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	232	HIS	N-CA-C	6.72	118.60	108.46
1	D	279	LEU	CA-CB-CG	5.20	134.50	116.30
1	D	37	VAL	N-CA-C	5.12	115.27	108.11

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	D	278	PHE	Peptide

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	2039	0	2069	34	0
1	B	2011	0	2063	35	0
1	C	1964	0	2006	31	0
1	D	1946	0	1992	42	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
3	A	21	0	12	0	0
3	B	21	0	12	0	0
3	C	21	0	12	0	0
3	D	21	0	12	0	0
4	A	104	0	0	1	0
4	B	99	0	0	8	0
4	C	97	0	0	4	0
4	D	45	0	0	1	0
All	All	8581	0	8278	132	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 8.

All (132) 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:227:VAL:HB	1:B:231:VAL:CG1	1.90	1.02
1:D:140:MET:HE1	1:D:186:SER:HA	1.57	0.85
1:D:243:LEU:O	1:D:247:LYS:HG3	1.81	0.79
1:A:178:PRO:O	1:A:179:MET:HB2	1.83	0.78
1:B:227:VAL:HB	1:B:231:VAL:HG12	1.64	0.77
1:B:224:MET:HA	1:B:224:MET:HE2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:HIS:HB3	4:C:477:HOH:O	1.88	0.73
1:B:130:HIS:HB3	4:B:358:HOH:O	1.87	0.73
1:B:274:LYS:O	1:B:278:PHE:CD1	2.42	0.73
1:A:203:VAL:HG21	1:A:286:MET:HE2	1.71	0.72
1:B:140:MET:HE3	1:B:140:MET:HA	1.72	0.71
1:C:92:THR:OG1	1:C:94:GLU:HG3	1.91	0.70
1:C:72[B]:GLN:HG2	1:C:88:TYR:CE2	2.27	0.70
1:A:224:MET:HA	1:A:224:MET:CE	2.23	0.69
1:D:276:LEU:O	1:D:279:LEU:HD13	1.96	0.66
1:A:275:ILE:HD12	1:C:266:LEU:HD12	1.77	0.65
1:D:140:MET:CE	1:D:144:PHE:HB3	2.27	0.65
1:D:220:THR:HG22	1:D:223:ALA:H	1.63	0.63
1:D:270:ASN:C	1:D:270:ASN:HD22	2.07	0.63
1:D:220:THR:HG21	2:D:4:NAP:O2N	1.99	0.62
1:D:140:MET:HE2	1:D:144:PHE:CD2	2.36	0.61
1:A:216:GLY:HA3	1:A:259:ASP:OD2	2.01	0.60
1:D:140:MET:HA	1:D:140:MET:HE3	1.84	0.60
1:D:37:VAL:HG13	1:D:115:MET:HB3	1.82	0.60
1:A:164:SER:HB2	4:A:352:HOH:O	2.02	0.60
1:C:140:MET:HE3	1:D:144:PHE:CE2	2.37	0.60
1:C:120:HIS:HE1	1:C:146:SER:OG	1.85	0.59
1:A:231:VAL:O	1:A:232:HIS:HB2	2.02	0.59
1:D:278:PHE:C	1:D:280:TYR:H	2.09	0.59
1:C:270:ASN:C	1:C:270:ASN:HD22	2.11	0.59
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.85	0.58
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.86	0.58
1:D:140:MET:HE3	1:D:144:PHE:HB3	1.84	0.58
1:C:270:ASN:ND2	1:C:273:ARG:H	2.02	0.58
1:D:263:TRP:HE3	1:D:263:TRP:C	2.11	0.58
1:C:126:LEU:HB3	1:C:179:MET:HE2	1.86	0.57
1:B:87:HIS:HD2	4:B:384:HOH:O	1.87	0.57
1:B:243:LEU:HG	1:B:247:LYS:HE3	1.87	0.57
1:D:140:MET:CE	1:D:186:SER:HA	2.31	0.56
1:A:172:ALA:HB2	1:A:177[A]:TYR:HD2	1.70	0.56
1:A:224:MET:HE1	1:A:232:HIS:NE2	2.22	0.55
1:B:42:ALA:HB3	1:B:63:VAL:HB	1.88	0.55
1:A:60:HIS:HD2	1:A:85:SER:OG	1.89	0.55
1:D:140:MET:CE	1:D:144:PHE:CB	2.86	0.54
1:D:279:LEU:HD22	1:D:279:LEU:O	2.08	0.54
1:A:224:MET:HA	1:A:224:MET:HE3	1.89	0.54
1:C:120:HIS:CE1	1:C:146:SER:OG	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:HE2	1:B:176:ALA:HB3	1.91	0.53
1:C:97:THR:HG22	1:C:101:GLN:NE2	2.23	0.53
1:D:178:PRO:O	1:D:179:MET:HB2	2.09	0.53
1:A:224:MET:O	1:A:228:SER:HB2	2.09	0.52
1:B:227:VAL:HB	1:B:231:VAL:HG13	1.84	0.52
1:D:223:ALA:O	1:D:227:VAL:HG22	2.09	0.52
1:B:171:LEU:HD22	1:B:175:VAL:HG22	1.92	0.52
1:A:164:SER:HB3	1:A:209:SER:OG	2.10	0.52
1:B:140:MET:HE3	1:B:144:PHE:HB3	1.92	0.52
1:B:205:ARG:NH1	4:B:380:HOH:O	2.42	0.52
1:B:27:PHE:CD2	1:B:247:LYS:HG2	2.46	0.51
1:A:170:SER:O	1:A:214:VAL:HG13	2.11	0.51
1:C:193:PHE:HB2	1:D:185:ALA:HB2	1.92	0.51
1:B:140:MET:HE3	1:B:140:MET:CA	2.40	0.51
1:A:280:TYR:OH	1:B:264:THR:HG21	2.11	0.51
1:A:257:TYR:CD2	1:A:268:ILE:HG23	2.46	0.51
1:B:26:GLU:HG2	4:B:364:HOH:O	2.10	0.50
1:B:262:LEU:HG	4:B:349:HOH:O	2.11	0.50
1:C:257:TYR:CE1	1:C:269:ARG:HG2	2.47	0.49
1:D:276:LEU:O	1:D:279:LEU:CD1	2.60	0.49
1:D:53:HIS:CE1	1:D:243:LEU:HD22	2.47	0.49
1:B:263:TRP:HA	1:B:266:LEU:HD13	1.93	0.49
1:A:224:MET:HA	1:A:224:MET:HE2	1.94	0.49
1:C:87:HIS:HD2	4:C:394:HOH:O	1.95	0.49
1:C:214:VAL:HG11	1:C:268:ILE:HG12	1.95	0.49
1:A:132[A]:ASP:OD1	1:A:134:HIS:CE1	2.66	0.48
1:C:223:ALA:O	1:C:227:VAL:HG22	2.13	0.48
1:D:248:GLY:HA3	1:D:256:VAL:HG21	1.96	0.48
1:B:52:TYR:O	1:B:56:LYS:HG3	2.14	0.47
1:A:275:ILE:CD1	1:C:266:LEU:HD12	2.42	0.47
1:B:76:SER:O	1:B:80:GLU:HG2	2.14	0.47
1:D:261:SER:OG	1:D:263:TRP:HB3	2.14	0.47
1:B:178:PRO:O	1:B:179:MET:HB2	2.14	0.47
1:A:132[A]:ASP:OD1	1:A:134:HIS:NE2	2.48	0.46
1:D:46:ILE:HG22	1:D:50:MET:HE2	1.97	0.46
1:D:263:TRP:C	1:D:263:TRP:CE3	2.92	0.46
1:A:36:LYS:HE2	1:A:110:MET:O	2.16	0.46
1:D:120:HIS:HE1	1:D:146:SER:OG	1.99	0.46
1:D:155:LEU:HG	1:D:159:LYS:HE3	1.98	0.46
1:C:279:LEU:HD11	1:D:263:TRP:CH2	2.50	0.46
1:D:270:ASN:C	1:D:270:ASN:ND2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ALA:HB2	1:B:193:PHE:HB2	1.97	0.45
1:A:60:HIS:CD2	1:A:85:SER:OG	2.68	0.45
1:B:278:PHE:O	1:B:281:SER:HB3	2.17	0.45
1:A:180:VAL:O	1:A:184[A]:SER:OG	2.30	0.45
1:C:217:LEU:HD22	1:C:233:MET:HB2	1.99	0.44
1:D:170:SER:HB3	2:D:4:NAP:H5N	1.98	0.44
1:B:164:SER:HB3	4:B:310:HOH:O	2.18	0.44
1:A:140:MET:HE3	1:A:144:PHE:HB3	2.00	0.44
1:D:191:ASP:HB2	4:D:306:HOH:O	2.18	0.44
1:D:278:PHE:C	1:D:280:TYR:N	2.76	0.44
1:B:263:TRP:HA	1:B:266:LEU:CD1	2.47	0.44
1:A:49:GLU:HG3	1:A:238:LYS:HG3	2.00	0.44
1:A:255:GLU:OE2	1:A:257:TYR:OH	2.34	0.43
1:C:224:MET:HA	1:C:224:MET:HE2	2.00	0.43
1:A:172:ALA:O	1:A:184[B]:SER:HB2	2.18	0.43
1:B:50:MET:CE	1:B:117:ILE:HG21	2.48	0.43
1:D:75:VAL:HG21	1:D:88:TYR:HB3	2.00	0.43
1:B:233:MET:HE3	4:B:353:HOH:O	2.19	0.42
1:C:68:LYS:NZ	4:C:463:HOH:O	2.52	0.42
1:B:170:SER:OG	2:B:2:NAP:H6N	2.20	0.42
1:C:169:SER:OG	1:C:170:SER:N	2.51	0.42
1:B:40:THR:OG1	1:B:120:HIS:HD2	2.03	0.42
1:D:171:LEU:HG	1:D:216:GLY:HA2	2.01	0.42
1:C:123:ASN:N	1:C:123:ASN:HD22	2.18	0.42
1:A:41:GLY:O	1:A:47:GLY:HA3	2.19	0.42
1:C:215:LEU:HD11	1:C:245:ILE:HD11	2.01	0.41
1:D:270:ASN:ND2	1:D:273:ARG:H	2.18	0.41
1:D:227:VAL:HB	1:D:231:VAL:HG22	2.01	0.41
1:A:189:ALA:HB2	1:B:189:ALA:HB2	2.01	0.41
1:C:31:MET:HE1	1:C:251:LEU:HD23	2.03	0.41
1:D:91:GLY:HA3	1:D:98:PHE:CZ	2.55	0.41
1:A:248:GLY:HA3	1:A:256:VAL:CG2	2.50	0.41
1:C:212:LEU:O	1:C:255:GLU:HA	2.20	0.41
1:D:169:SER:OG	1:D:170:SER:N	2.53	0.41
1:C:119:ASN:OD1	2:C:3:NAP:H4D	2.21	0.41
1:B:140:MET:CE	1:B:144:PHE:HB3	2.51	0.40
1:C:189:ALA:HB2	1:D:189:ALA:HB2	2.03	0.40
1:A:42:ALA:HB3	1:A:63:VAL:HB	2.03	0.40
1:C:233:MET:HG2	4:C:467:HOH:O	2.21	0.40
1:D:140:MET:HE2	1:D:144:PHE:CG	2.56	0.40
1:A:212:LEU:HB3	1:A:255:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ASN:ND2	4:B:295:HOH:O	2.54	0.40
1:C:88:TYR:CD1	1:C:88:TYR:C	3.00	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	267/286 (93%)	248 (93%)	16 (6%)	3 (1%)	11	8
1	B	263/286 (92%)	246 (94%)	16 (6%)	1 (0%)	30	31
1	C	253/286 (88%)	238 (94%)	13 (5%)	2 (1%)	16	14
1	D	251/286 (88%)	232 (92%)	16 (6%)	3 (1%)	10	7
All	All	1034/1144 (90%)	964 (93%)	61 (6%)	9 (1%)	14	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	ILE
1	D	263	TRP
1	A	228	SER
1	D	280	TYR
1	C	202	SER
1	C	279	LEU
1	D	65	ALA
1	A	231	VAL
1	B	65	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	226/243 (93%)	211 (93%)	15 (7%)	15	14
1	B	222/243 (91%)	210 (95%)	12 (5%)	20	21
1	C	215/243 (88%)	202 (94%)	13 (6%)	17	18
1	D	211/243 (87%)	196 (93%)	15 (7%)	13	12
All	All	874/972 (90%)	819 (94%)	55 (6%)	16	16

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	61	VAL
1	A	81	LEU
1	A	117	ILE
1	A	127	ASN
1	A	130	HIS
1	A	179	MET
1	A	221	GLU
1	A	224	MET
1	A	232	HIS
1	A	233	MET
1	A	239	GLU
1	A	265	THR
1	A	279	LEU
1	A	287	ASP
1	B	70	THR
1	B	80	GLU
1	B	108	LYS
1	B	109	LEU
1	B	119	ASN
1	B	145	LEU
1	B	171	LEU
1	B	231	VAL
1	B	234	GLN

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Mol	Chain	Res	Type
1	B	267	LEU
1	B	269	ARG
1	B	279	LEU
1	C	24	ASN
1	C	28	ARG
1	C	44	LYS
1	C	127	ASN
1	C	155	LEU
1	C	199	LYS
1	C	203	VAL
1	C	205	ARG
1	C	222	THR
1	C	233	MET
1	C	262	LEU
1	C	265	THR
1	C	279	LEU
1	D	69	GLU
1	D	125	SER
1	D	138	LYS
1	D	145	LEU
1	D	160	GLN
1	D	170	SER
1	D	220	THR
1	D	228	SER
1	D	231	VAL
1	D	232	HIS
1	D	243	LEU
1	D	262	LEU
1	D	263	TRP
1	D	265	THR
1	D	279	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	123	ASN
1	A	270	ASN
1	B	119	ASN
1	B	120	HIS
1	B	135	HIS
1	B	207	ASN

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Mol	Chain	Res	Type
1	C	24	ASN
1	C	101	GLN
1	C	105	GLN
1	C	120	HIS
1	C	123	ASN
1	C	234	GLN
1	C	253	GLN
1	C	270	ASN
1	D	53	HIS
1	D	120	HIS
1	D	135	HIS
1	D	232	HIS
1	D	234	GLN
1	D	270	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A21	A	293	-	22,22,22	1.69	4 (18%)	27,34,34	1.85	9 (33%)
3	A21	B	293	-	22,22,22	2.05	6 (27%)	27,34,34	1.81	8 (29%)
2	NAP	D	4	-	50,52,52	1.69	6 (12%)	71,80,80	1.54	9 (12%)
2	NAP	A	1	-	50,52,52	1.70	3 (6%)	71,80,80	1.61	13 (18%)
2	NAP	C	3	-	50,52,52	1.69	4 (8%)	71,80,80	1.65	14 (19%)
3	A21	D	293	-	22,22,22	2.28	6 (27%)	27,34,34	1.99	11 (40%)
2	NAP	B	2	-	50,52,52	1.76	7 (14%)	71,80,80	1.79	12 (16%)
3	A21	C	293	-	22,22,22	1.72	5 (22%)	27,34,34	1.96	9 (33%)

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	A21	A	293	-	-	0/17/32/32	0/2/2/2
3	A21	B	293	-	-	0/17/32/32	0/2/2/2
2	NAP	D	4	-	-	4/35/67/67	0/5/5/5
2	NAP	A	1	-	-	6/35/67/67	0/5/5/5
2	NAP	C	3	-	-	4/35/67/67	0/5/5/5
3	A21	D	293	-	-	0/17/32/32	0/2/2/2
2	NAP	B	2	-	-	8/35/67/67	0/5/5/5
3	A21	C	293	-	-	0/17/32/32	0/2/2/2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAP	O7N-C7N	9.16	1.41	1.24
2	D	4	NAP	O7N-C7N	9.10	1.41	1.24
2	C	3	NAP	O7N-C7N	8.66	1.40	1.24
3	D	293	A21	C11-S1	-8.06	1.67	1.75
2	B	2	NAP	O7N-C7N	7.87	1.38	1.24
3	B	293	A21	C11-S1	-7.27	1.68	1.75
3	A	293	A21	C11-S1	-5.38	1.70	1.75
3	C	293	A21	C11-S1	-5.10	1.70	1.75
2	C	3	NAP	C2N-N1N	5.01	1.40	1.35
2	A	1	NAP	C2N-N1N	3.83	1.39	1.35
2	B	2	NAP	PA-O3	3.70	1.63	1.59
2	B	2	NAP	C2N-N1N	3.64	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	293	A21	C13-N2	-3.60	1.32	1.38
3	D	293	A21	C8-C13	-3.27	1.51	1.54
3	B	293	A21	C13-N2	-3.25	1.33	1.38
2	D	4	NAP	PA-O3	3.15	1.62	1.59
3	A	293	A21	C13-N2	-3.12	1.33	1.38
3	C	293	A21	C11-N2	-2.87	1.27	1.31
3	C	293	A21	C8-C13	-2.86	1.51	1.54
3	D	293	A21	C11-N2	-2.84	1.27	1.31
2	A	1	NAP	C8A-N7A	2.83	1.37	1.31
3	B	293	A21	C8-C13	-2.78	1.51	1.54
3	B	293	A21	C6-C1	-2.77	1.48	1.52
2	B	2	NAP	C3N-C7N	2.63	1.54	1.50
3	C	293	A21	C8-S1	-2.62	1.76	1.84
3	D	293	A21	C8-S1	-2.61	1.76	1.84
2	B	2	NAP	PN-O5D	2.58	1.69	1.59
3	C	293	A21	C13-N2	-2.56	1.34	1.38
2	B	2	NAP	C2A-N1A	2.34	1.38	1.33
3	B	293	A21	C8-S1	-2.31	1.77	1.84
3	A	293	A21	C8-S1	-2.31	1.77	1.84
2	B	2	NAP	C2A-N3A	2.25	1.37	1.33
2	D	4	NAP	C2A-N3A	2.24	1.37	1.33
2	D	4	NAP	C8A-N7A	2.22	1.36	1.31
3	D	293	A21	C6-C1	-2.20	1.49	1.52
2	D	4	NAP	C2A-N1A	2.17	1.37	1.33
2	C	3	NAP	C2A-N1A	2.13	1.37	1.33
3	A	293	A21	C11-N2	-2.06	1.28	1.31
3	B	293	A21	C11-N2	-2.04	1.28	1.31
2	D	4	NAP	C5A-N7A	-2.02	1.35	1.39
2	C	3	NAP	C8A-N7A	2.02	1.35	1.31

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAP	N3A-C2A-N1A	-7.87	116.67	128.58
2	D	4	NAP	N3A-C2A-N1A	-5.85	119.73	128.58
2	C	3	NAP	N3A-C2A-N1A	-5.49	120.28	128.58
2	A	1	NAP	N3A-C2A-N1A	-5.25	120.64	128.58
3	D	293	A21	C8-C13-N2	-5.03	111.11	115.42
2	C	3	NAP	C5A-C4A-N3A	-4.94	119.92	126.72
2	A	1	NAP	O4B-C1B-N9A	4.79	117.30	108.09
2	D	4	NAP	C5A-C4A-N3A	-4.47	120.56	126.72
2	B	2	NAP	N9A-C8A-N7A	-4.45	107.62	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	293	A21	N3-C11-N2	-4.41	119.17	124.26
3	C	293	A21	F3-C2-C8	-4.29	107.24	112.39
3	B	293	A21	C13-C8-S1	4.26	106.34	104.16
2	B	2	NAP	C2A-N3A-C4A	4.18	122.05	111.83
3	B	293	A21	C8-C13-N2	-4.14	111.87	115.42
2	C	3	NAP	C3N-C7N-N7N	4.09	122.78	117.74
3	A	293	A21	F1-C2-C8	-3.86	107.76	112.39
2	B	2	NAP	C3N-C7N-N7N	3.81	122.44	117.74
2	C	3	NAP	C2A-N3A-C4A	3.80	121.12	111.83
3	C	293	A21	C8-C13-N2	-3.80	112.17	115.42
3	B	293	A21	C2-C8-S1	3.76	111.53	107.49
2	B	2	NAP	C5A-N7A-C8A	3.70	109.26	103.45
2	A	1	NAP	C5A-C4A-N3A	-3.70	121.62	126.72
3	A	293	A21	F3-C2-C8	-3.69	107.96	112.39
3	D	293	A21	C13-C8-S1	3.65	106.02	104.16
3	C	293	A21	C13-C8-S1	3.62	106.01	104.16
2	D	4	NAP	N9A-C8A-N7A	-3.54	108.91	113.94
2	B	2	NAP	C5A-C4A-N3A	-3.51	121.89	126.72
2	D	4	NAP	C2A-N3A-C4A	3.49	120.35	111.83
2	C	3	NAP	N9A-C8A-N7A	-3.41	109.09	113.94
2	C	3	NAP	C5A-N7A-C8A	3.35	108.71	103.45
2	A	1	NAP	N9A-C8A-N7A	-3.30	109.25	113.94
3	C	293	A21	C2-C8-S1	3.20	110.93	107.49
2	B	2	NAP	O4B-C1B-N9A	3.11	114.07	108.09
2	A	1	NAP	C5A-N7A-C8A	3.10	108.32	103.45
3	A	293	A21	C8-C13-N2	-3.09	112.77	115.42
3	D	293	A21	F4-C2-C8	-3.06	108.72	112.39
3	D	293	A21	O2-C13-C8	3.05	124.27	120.83
2	D	4	NAP	C5A-N7A-C8A	3.02	108.20	103.45
2	D	4	NAP	N3A-C4A-N9A	2.95	132.18	127.17
2	C	3	NAP	N3A-C4A-N9A	2.93	132.15	127.17
3	C	293	A21	N3-C11-N2	-2.93	120.89	124.26
3	D	293	A21	F3-C2-C8	-2.89	108.92	112.39
2	B	2	NAP	C4A-C5A-N7A	-2.88	107.28	110.58
2	A	1	NAP	O2N-PN-O1N	2.87	125.81	112.44
3	B	293	A21	C19-C18-C6	-2.86	120.54	123.68
2	A	1	NAP	C4A-C5A-N7A	-2.84	107.34	110.58
2	C	3	NAP	O2B-P2B-O1X	-2.81	99.32	109.33
2	A	1	NAP	C2A-N3A-C4A	2.80	118.67	111.83
2	A	1	NAP	C5A-C4A-N9A	2.74	108.80	105.81
2	C	3	NAP	C4A-C5A-N7A	-2.69	107.50	110.58
3	C	293	A21	C3-C1-N3	2.61	113.76	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	293	A21	C4-C8-C13	2.59	112.43	108.76
2	C	3	NAP	O7N-C7N-C3N	-2.59	116.43	119.60
3	B	293	A21	C22-C6-C18	2.58	119.48	116.22
2	D	4	NAP	O3B-C3B-C2B	-2.58	103.98	111.19
3	C	293	A21	C22-C6-C18	2.54	119.42	116.22
2	D	4	NAP	O4B-C1B-N9A	2.51	112.90	108.09
3	B	293	A21	C3-C1-C6	-2.50	108.05	111.58
3	A	293	A21	C22-C6-C18	2.47	119.34	116.22
3	C	293	A21	C19-C18-C6	-2.47	120.97	123.68
2	C	3	NAP	O3B-C3B-C2B	-2.45	104.32	111.19
3	C	293	A21	C4-C8-C13	2.42	112.19	108.76
3	D	293	A21	N3-C11-N2	-2.40	121.50	124.26
2	B	2	NAP	O2N-PN-O1N	2.37	123.48	112.44
3	A	293	A21	C18-C6-C1	-2.36	118.06	121.02
3	D	293	A21	F1-C2-C8	-2.32	109.60	112.39
3	A	293	A21	C4-C8-C13	2.32	112.04	108.76
3	D	293	A21	C22-C6-C18	2.28	119.10	116.22
2	A	1	NAP	O3-PN-O1N	-2.28	103.86	110.70
2	C	3	NAP	C6N-N1N-C2N	-2.27	119.95	121.88
2	D	4	NAP	O2N-PN-O1N	2.25	122.89	112.44
3	A	293	A21	C13-C8-S1	2.24	105.30	104.16
3	D	293	A21	C19-C18-C6	-2.22	121.24	123.68
3	B	293	A21	N3-C11-N2	-2.20	121.72	124.26
3	A	293	A21	C19-C18-C6	-2.19	121.27	123.68
2	B	2	NAP	C2A-N1A-C6A	2.19	122.32	118.73
3	B	293	A21	F1-C2-C8	-2.17	109.78	112.39
2	A	1	NAP	C2A-N1A-C6A	2.15	122.26	118.73
2	B	2	NAP	C4A-N9A-C1B	-2.13	121.66	126.63
3	D	293	A21	C3-C1-C6	-2.07	108.65	111.58
2	A	1	NAP	C1B-N9A-C8A	2.07	131.68	127.09
2	B	2	NAP	C5A-C4A-N9A	2.02	108.02	105.81
2	C	3	NAP	O2X-P2B-O2B	2.02	113.71	105.85
2	C	3	NAP	C4D-O4D-C1D	2.01	111.77	109.92
2	A	1	NAP	C4A-N9A-C1B	-2.01	121.94	126.63

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAP	C5D-O5D-PN-O1N
2	B	2	NAP	C5D-O5D-PN-O3
2	B	2	NAP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	C	3	NAP	C5D-O5D-PN-O3
2	C	3	NAP	C5D-O5D-PN-O1N
2	A	1	NAP	C5D-O5D-PN-O3
2	B	2	NAP	C5D-O5D-PN-O2N
2	C	3	NAP	C5D-O5D-PN-O2N
2	B	2	NAP	C3B-C2B-O2B-P2B
2	B	2	NAP	C2B-O2B-P2B-O2X
2	B	2	NAP	C1B-C2B-O2B-P2B
2	A	1	NAP	PN-O3-PA-O1A
2	B	2	NAP	O4B-C4B-C5B-O5B
2	A	1	NAP	C2B-O2B-P2B-O2X
2	D	4	NAP	C2B-O2B-P2B-O3X
2	C	3	NAP	O4B-C4B-C5B-O5B
2	D	4	NAP	O4B-C4B-C5B-O5B
2	D	4	NAP	C2B-O2B-P2B-O1X
2	A	1	NAP	C1B-C2B-O2B-P2B
2	A	1	NAP	PN-O3-PA-O2A
2	B	2	NAP	PN-O3-PA-O2A
2	D	4	NAP	PN-O3-PA-O2A

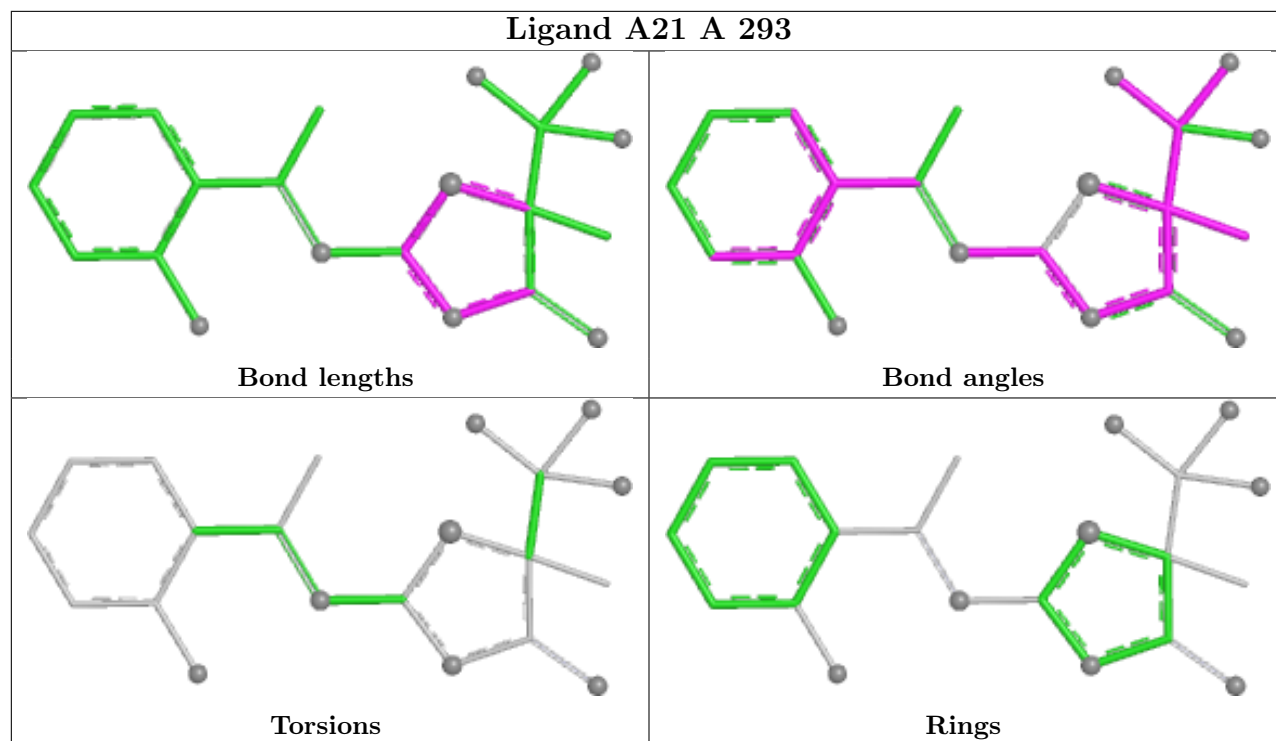
There are no ring outliers.

3 monomers are involved in 4 short contacts:

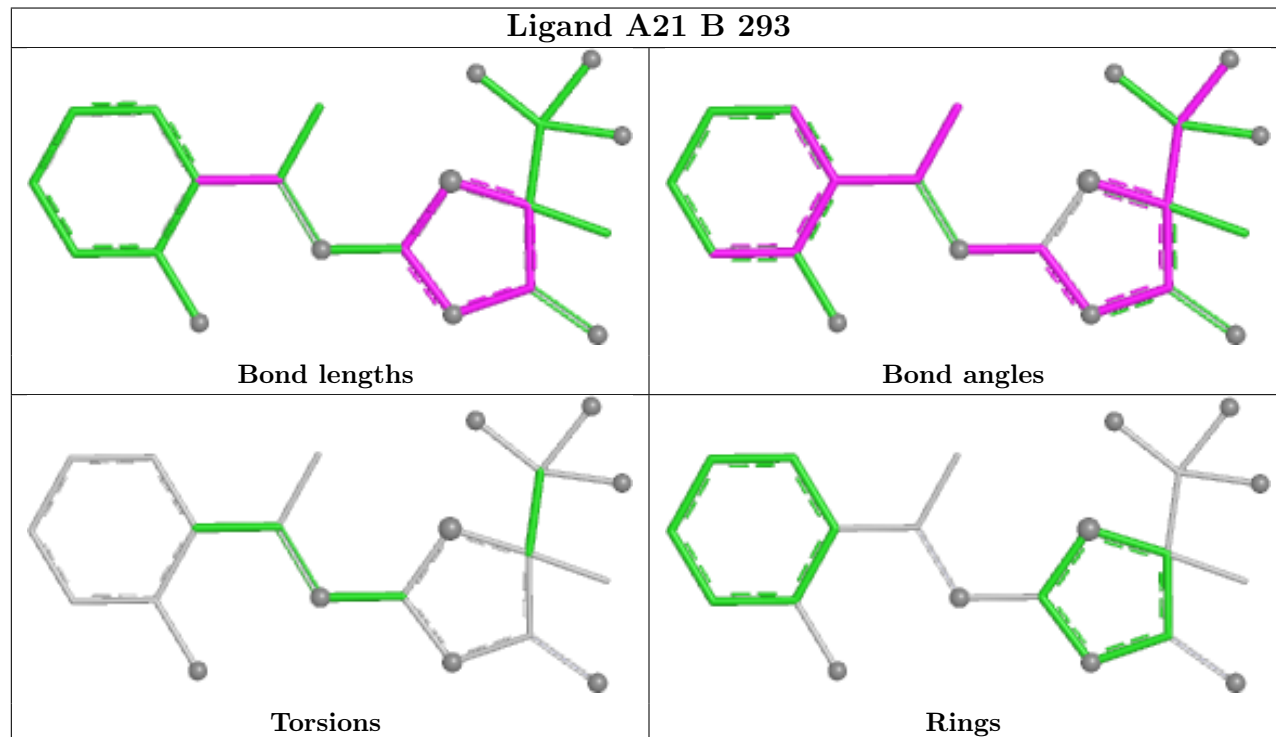
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	NAP	2	0
2	C	3	NAP	1	0
2	B	2	NAP	1	0

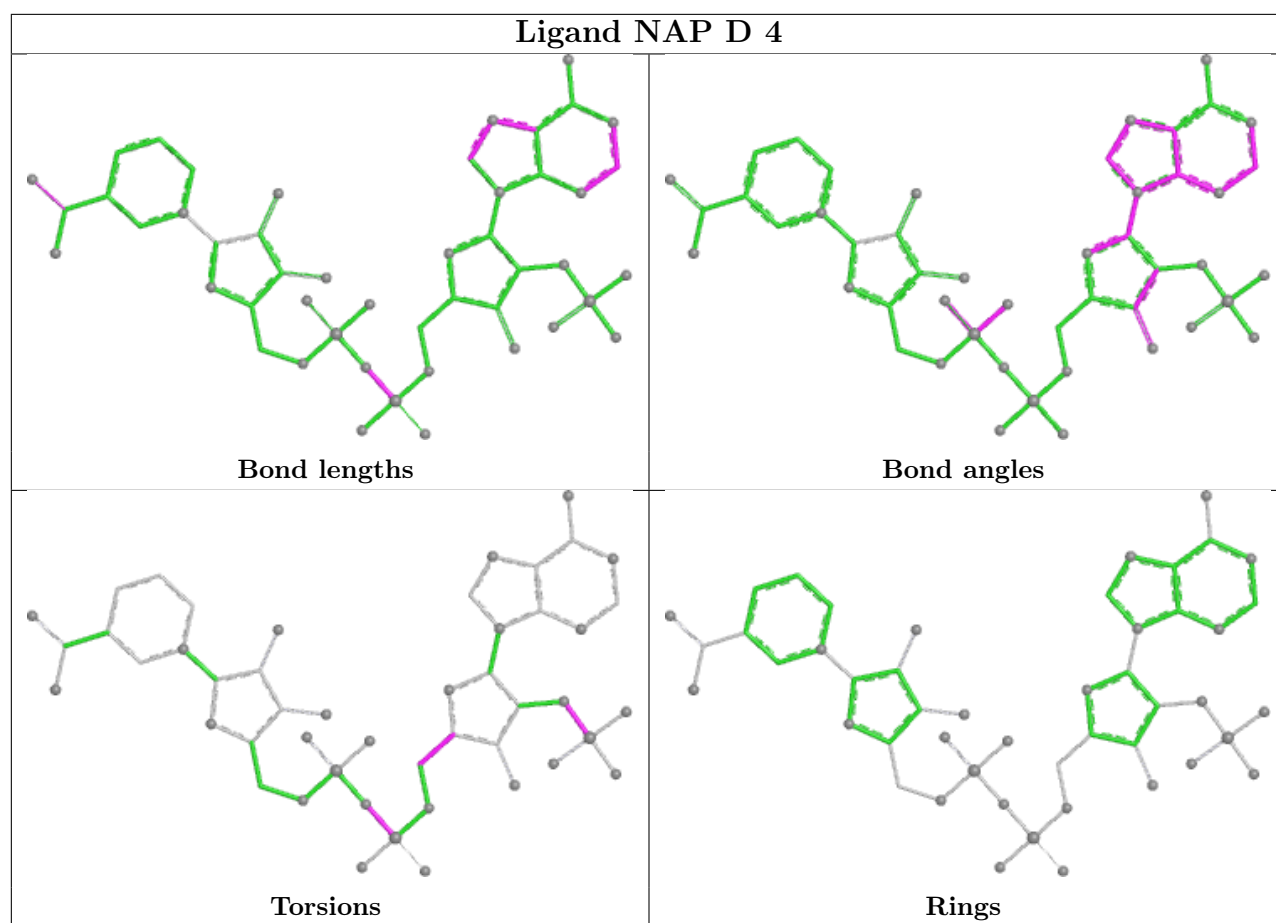
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

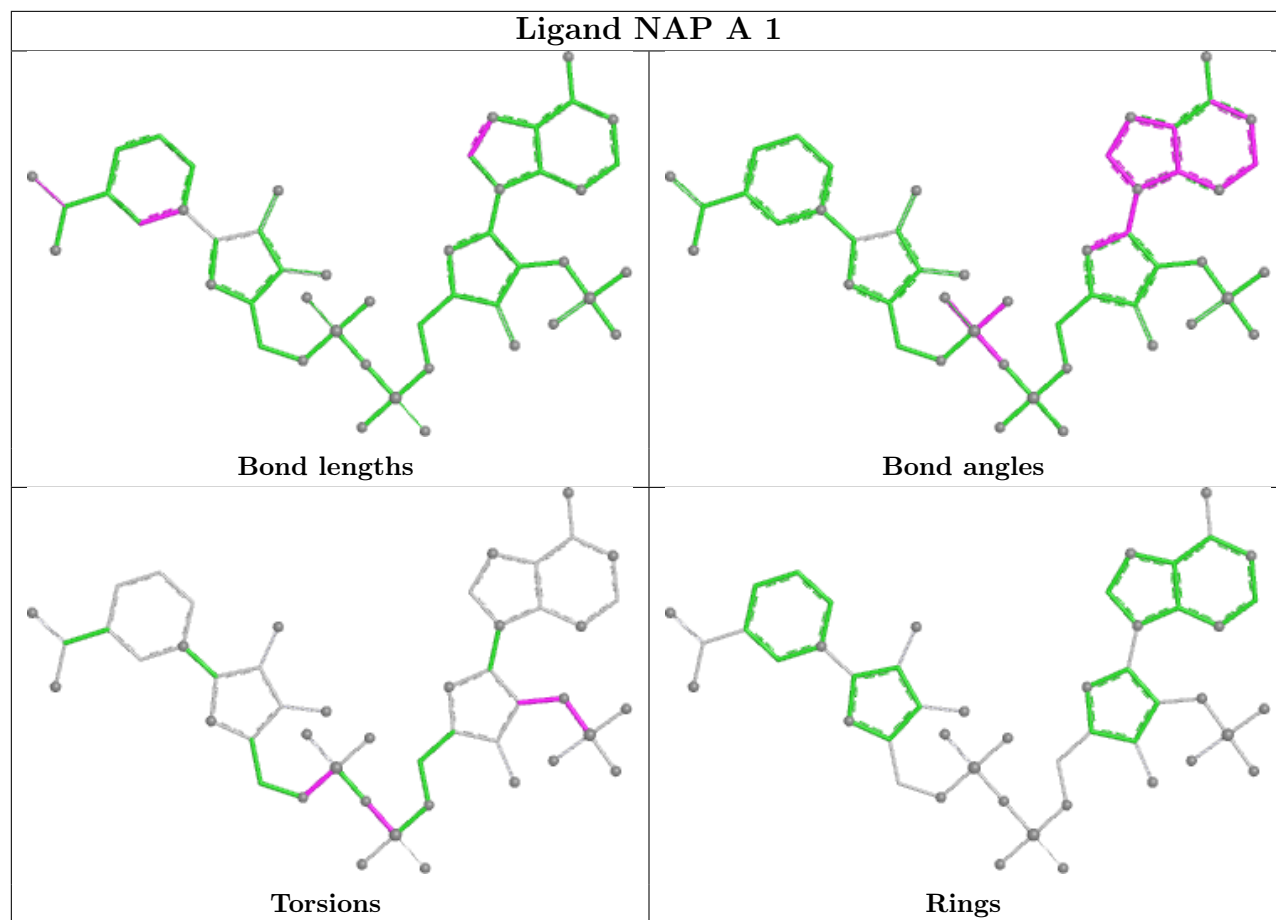
Ligand A21 A 293



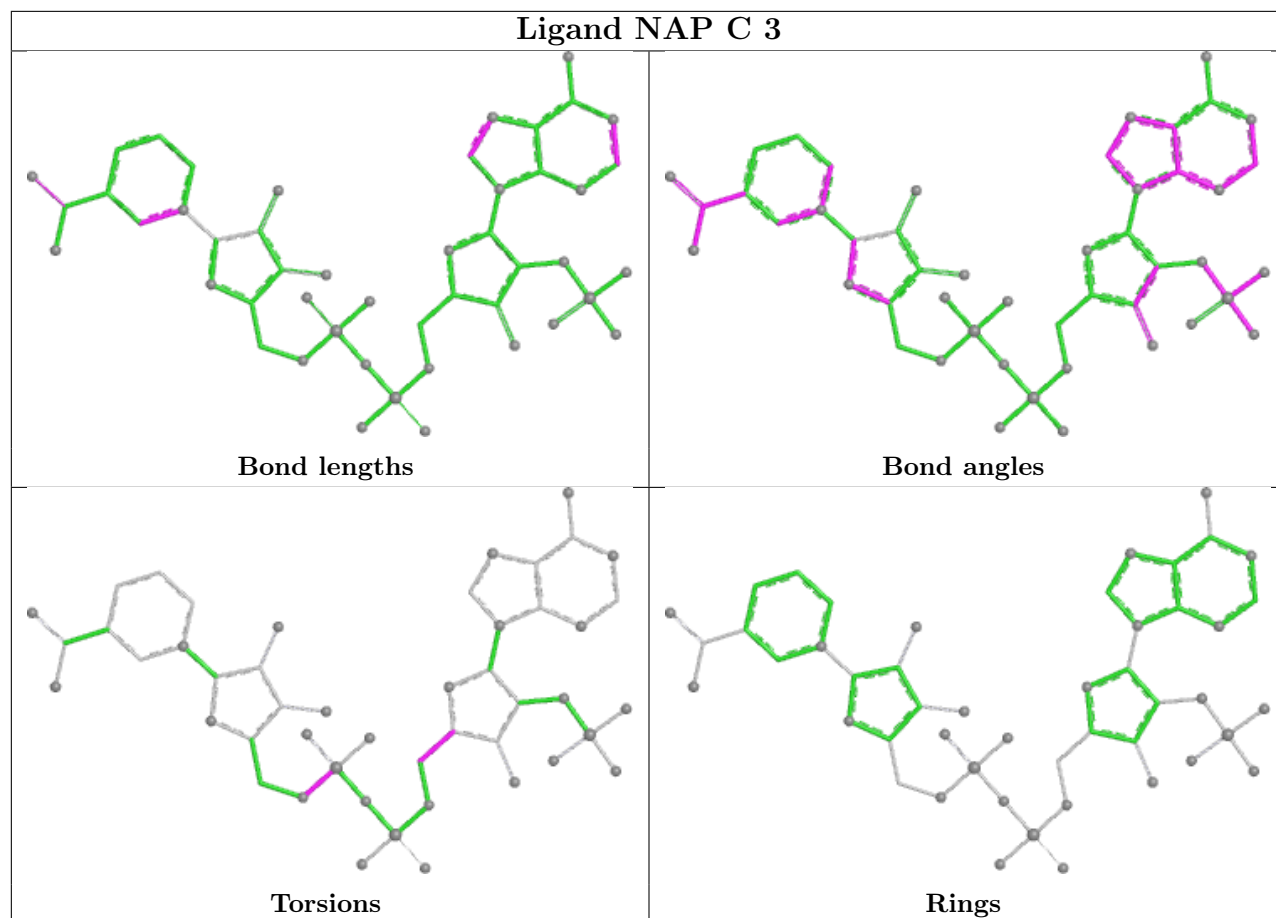
Ligand A21 B 293



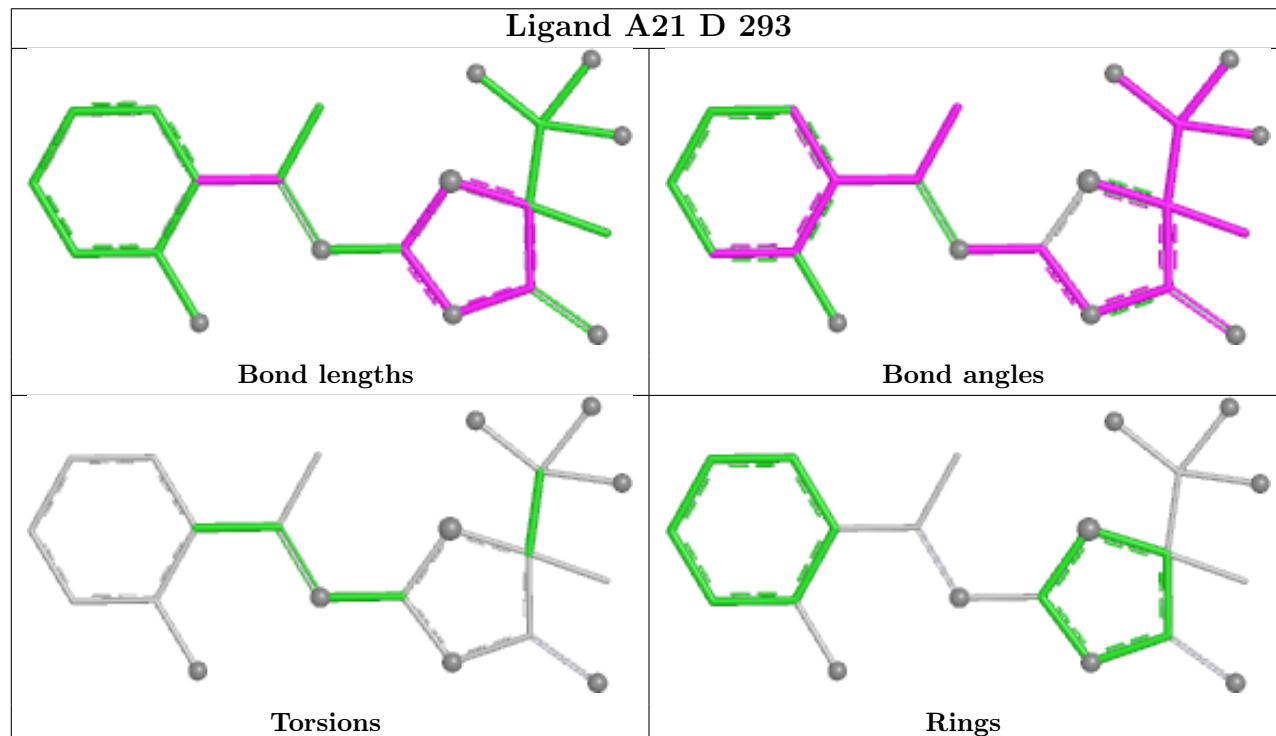




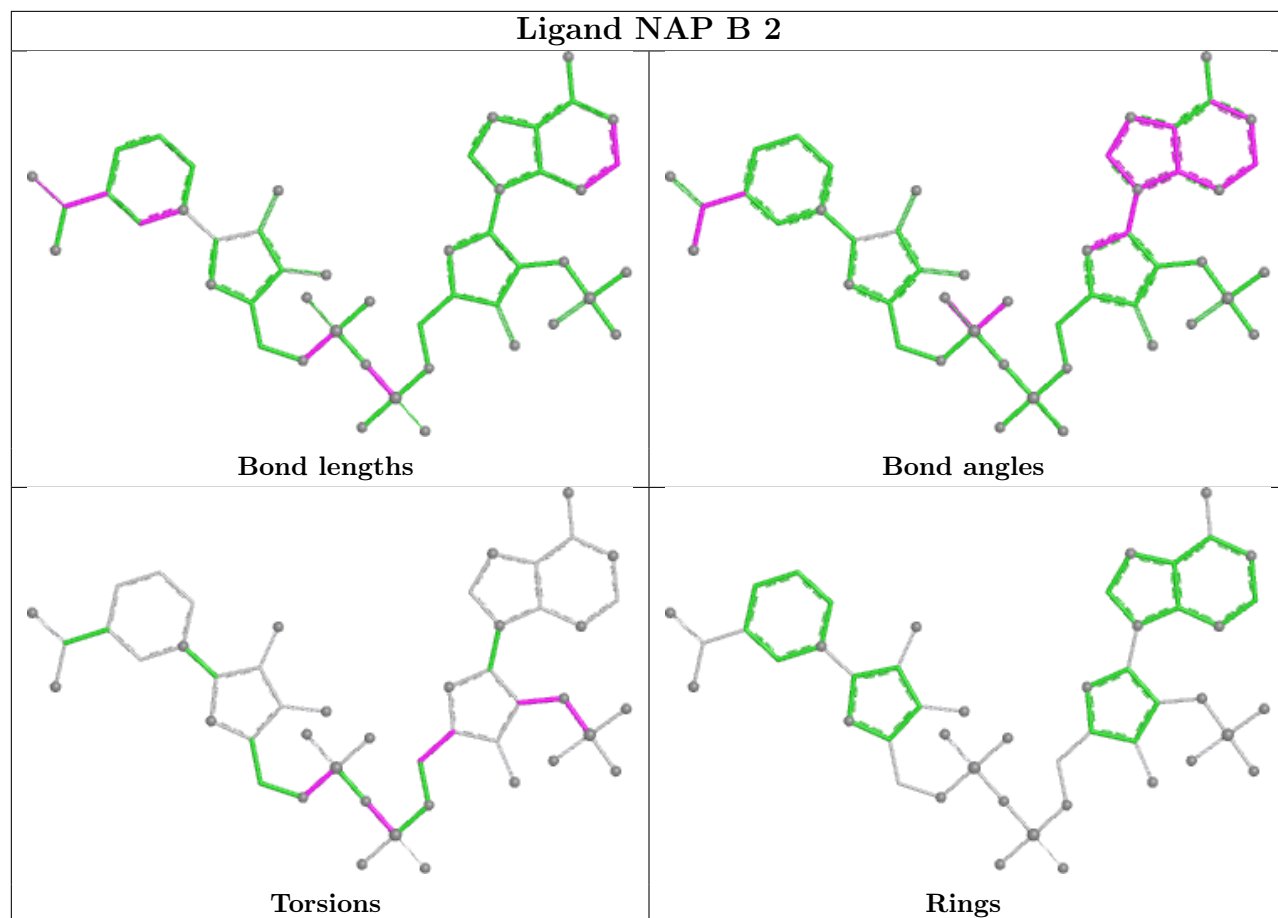
Ligand NAP C 3



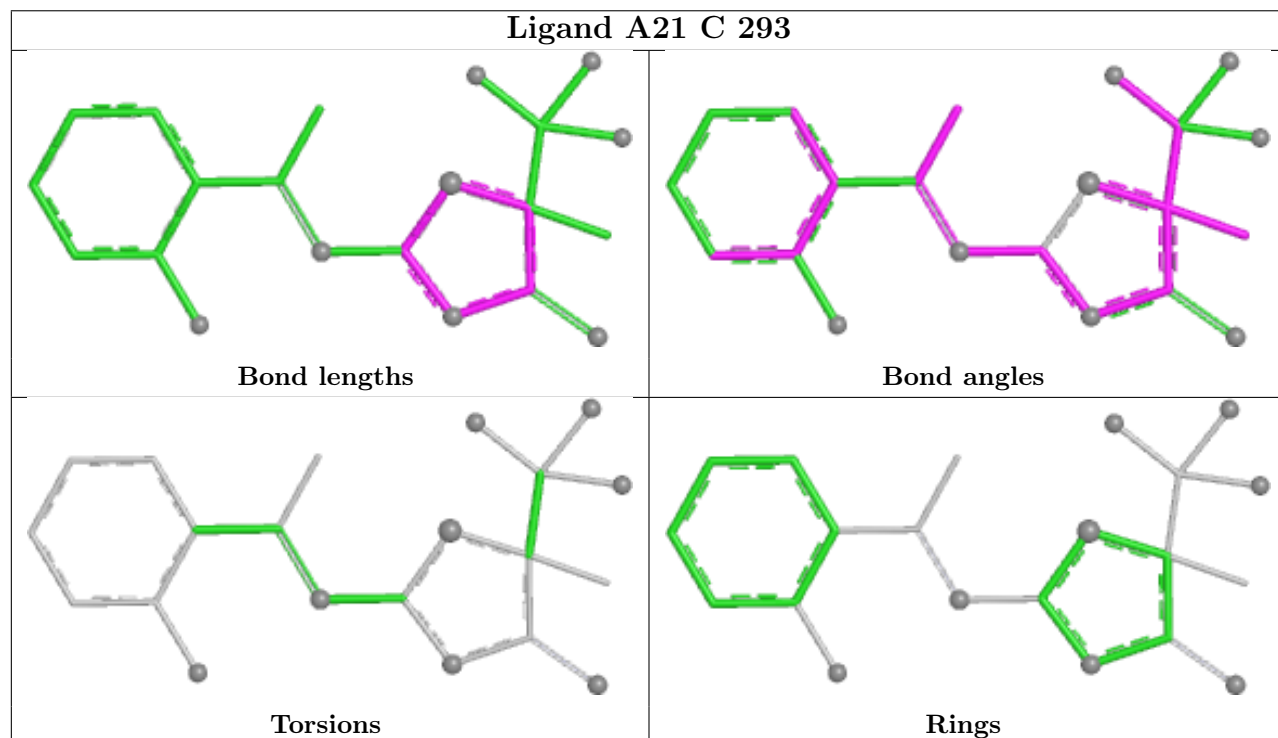
Ligand A21 D 293



Ligand NAP B 2



Ligand A21 C 293



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	263/286 (91%)	0.13	6 (2%) 61 61	24, 48, 76, 87	6 (2%)
1	B	262/286 (91%)	0.20	5 (1%) 66 67	28, 47, 69, 84	3 (1%)
1	C	254/286 (88%)	0.12	7 (2%) 55 55	26, 46, 73, 84	3 (1%)
1	D	254/286 (88%)	0.75	18 (7%) 22 20	29, 62, 85, 89	1 (0%)
All	All	1033/1144 (90%)	0.30	36 (3%) 47 47	24, 50, 79, 89	13 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	281	SER	4.5
1	B	278	PHE	4.0
1	D	235	ALA	3.4
1	C	263	TRP	3.1
1	A	263	TRP	3.1
1	D	263	TRP	2.9
1	D	71	LEU	2.8
1	D	29	PRO	2.8
1	B	23	LEU	2.7
1	D	112	GLY	2.7
1	B	22	PRO	2.6
1	C	262	LEU	2.6
1	D	232	HIS	2.5
1	D	264	THR	2.4
1	C	278	PHE	2.4
1	D	223	ALA	2.4
1	A	287	ASP	2.4
1	C	236	ALA	2.4
1	D	39	VAL	2.4
1	D	261	SER	2.3
1	A	229	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	282	THR	2.3
1	A	235	ALA	2.3
1	D	236	ALA	2.3
1	C	281	SER	2.3
1	D	47	GLY	2.2
1	D	224	MET	2.2
1	D	52	TYR	2.2
1	C	233	MET	2.2
1	D	278	PHE	2.2
1	A	283	SER	2.1
1	C	265	THR	2.1
1	B	141	GLU	2.0
1	D	86	ALA	2.0
1	D	231	VAL	2.0
1	B	266	LEU	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](#)

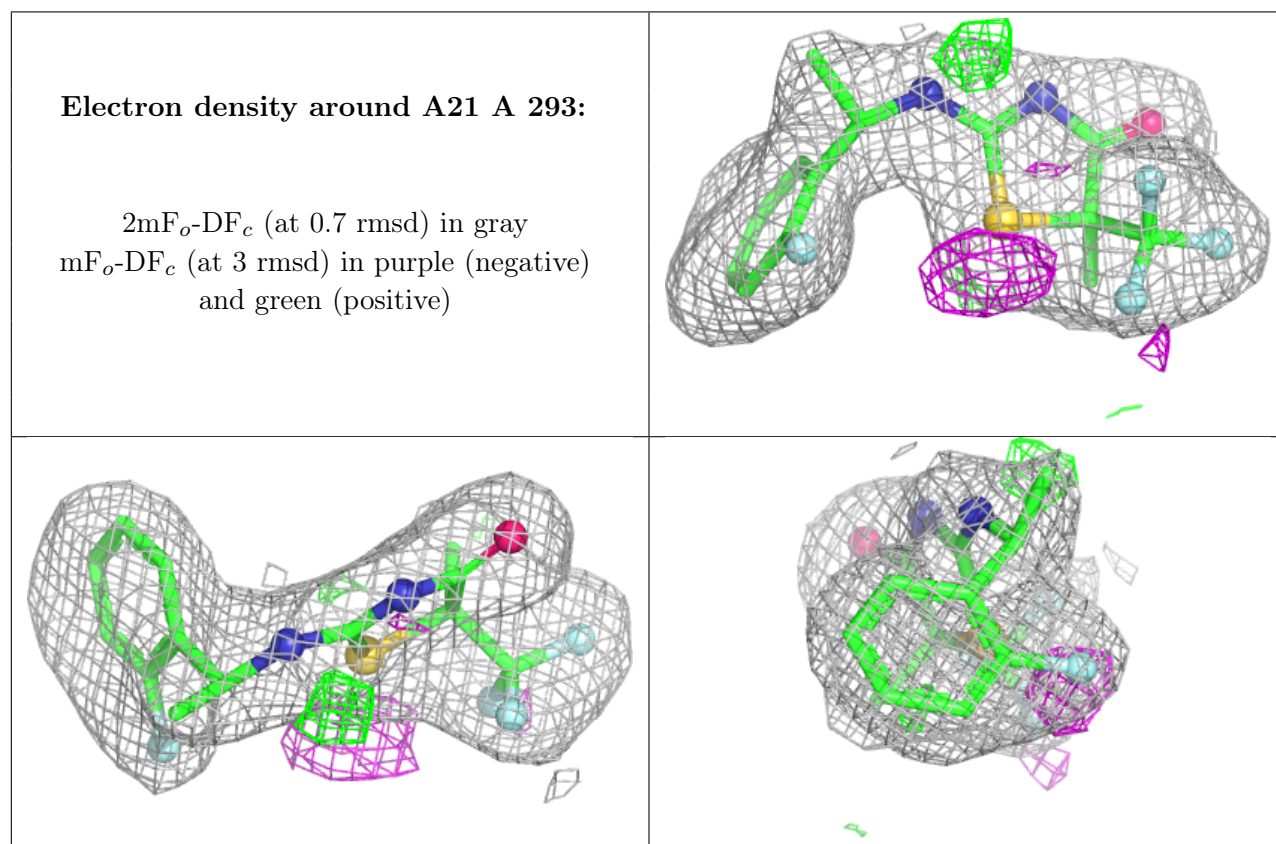
There are no oligosaccharides in this entry.

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.

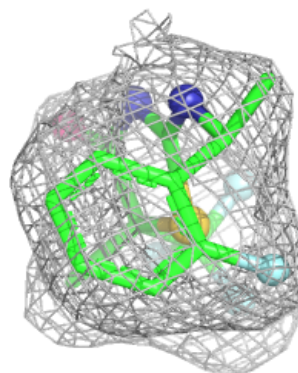
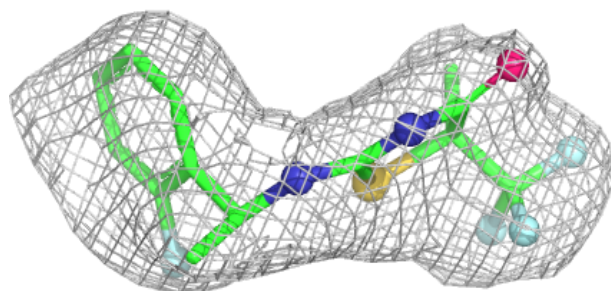
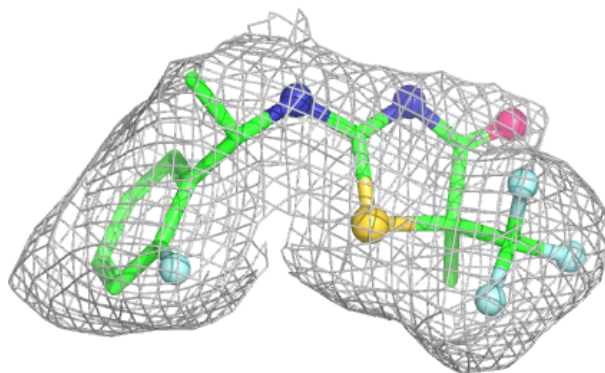
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A21	A	293	21/21	0.93	0.08	39,43,45,47	0
3	A21	D	293	21/21	0.94	0.09	51,54,58,61	0
2	NAP	D	4	48/48	0.95	0.08	47,52,57,60	0
3	A21	C	293	21/21	0.96	0.06	39,45,49,52	0
3	A21	B	293	21/21	0.96	0.07	42,46,50,52	0
2	NAP	C	3	48/48	0.97	0.07	31,38,41,44	0
2	NAP	A	1	48/48	0.97	0.06	31,36,41,45	0
2	NAP	B	2	48/48	0.97	0.06	30,33,43,46	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.

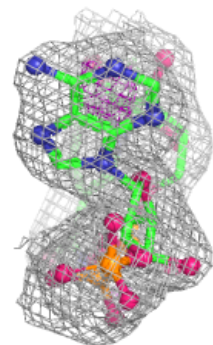
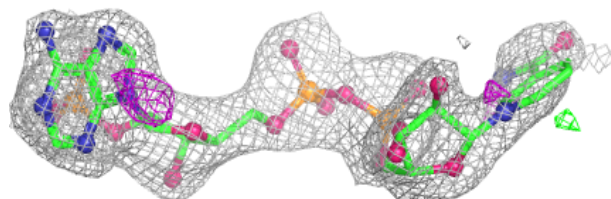
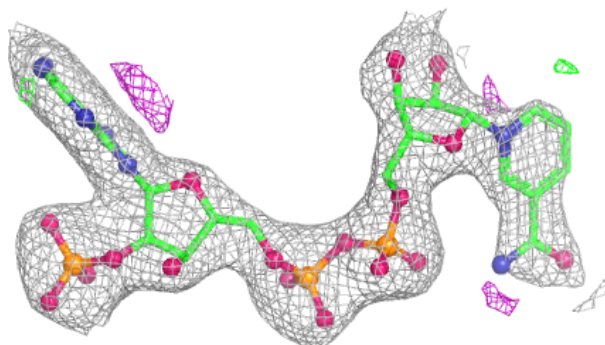


Electron density around A21 D 293:

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

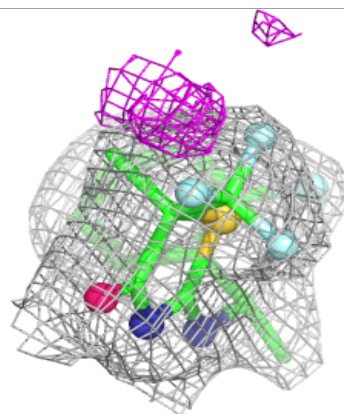
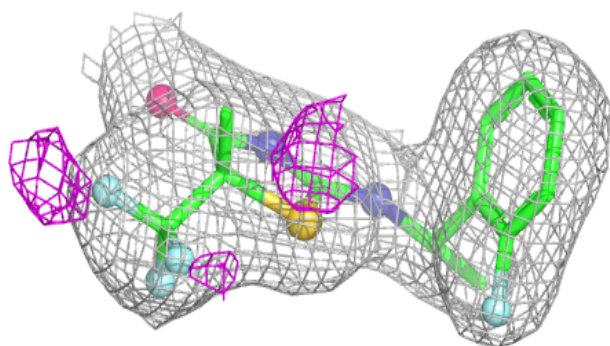
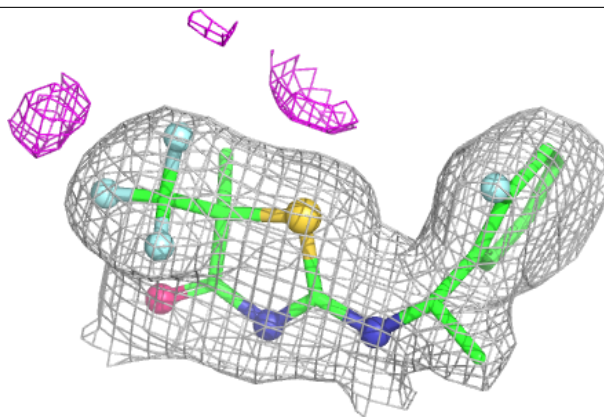
**Electron density around NAP D 4:**

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

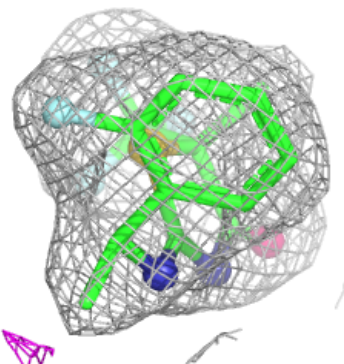
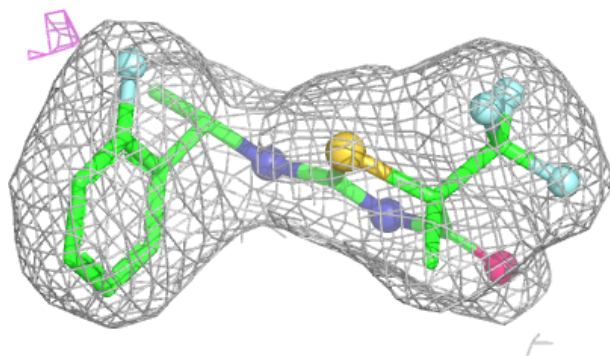
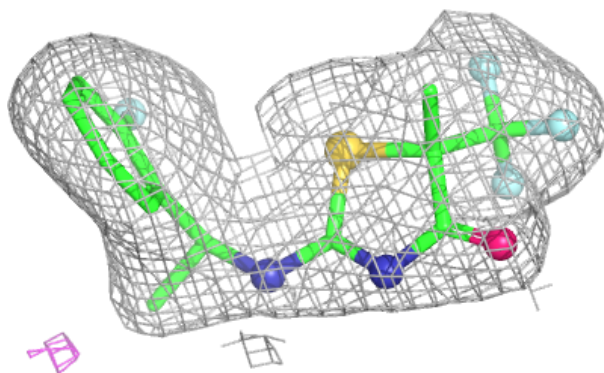


Electron density around A21 C 293:

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

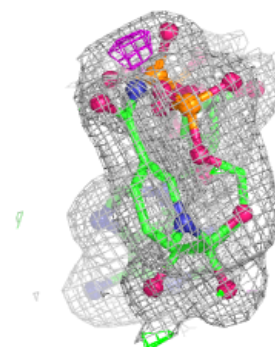
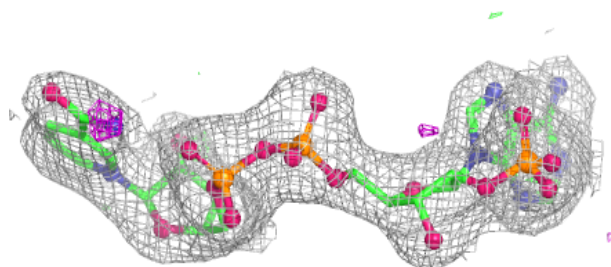
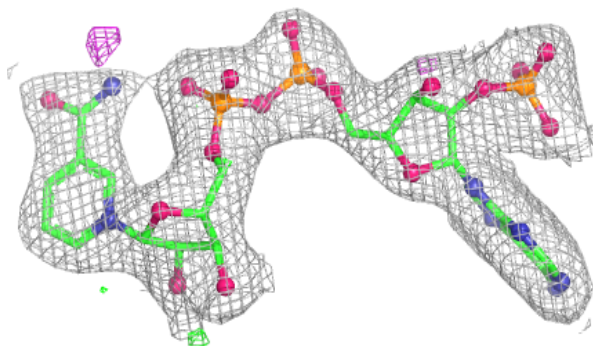
**Electron density around A21 B 293:**

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

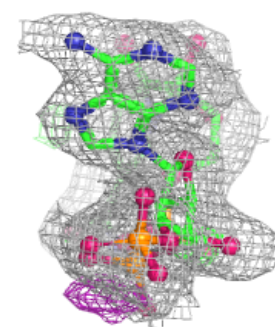
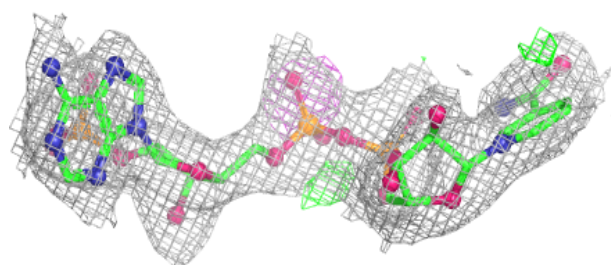
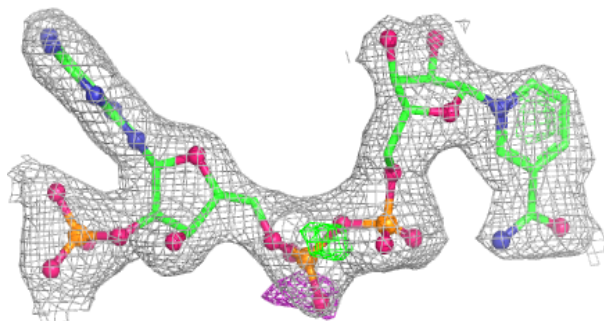


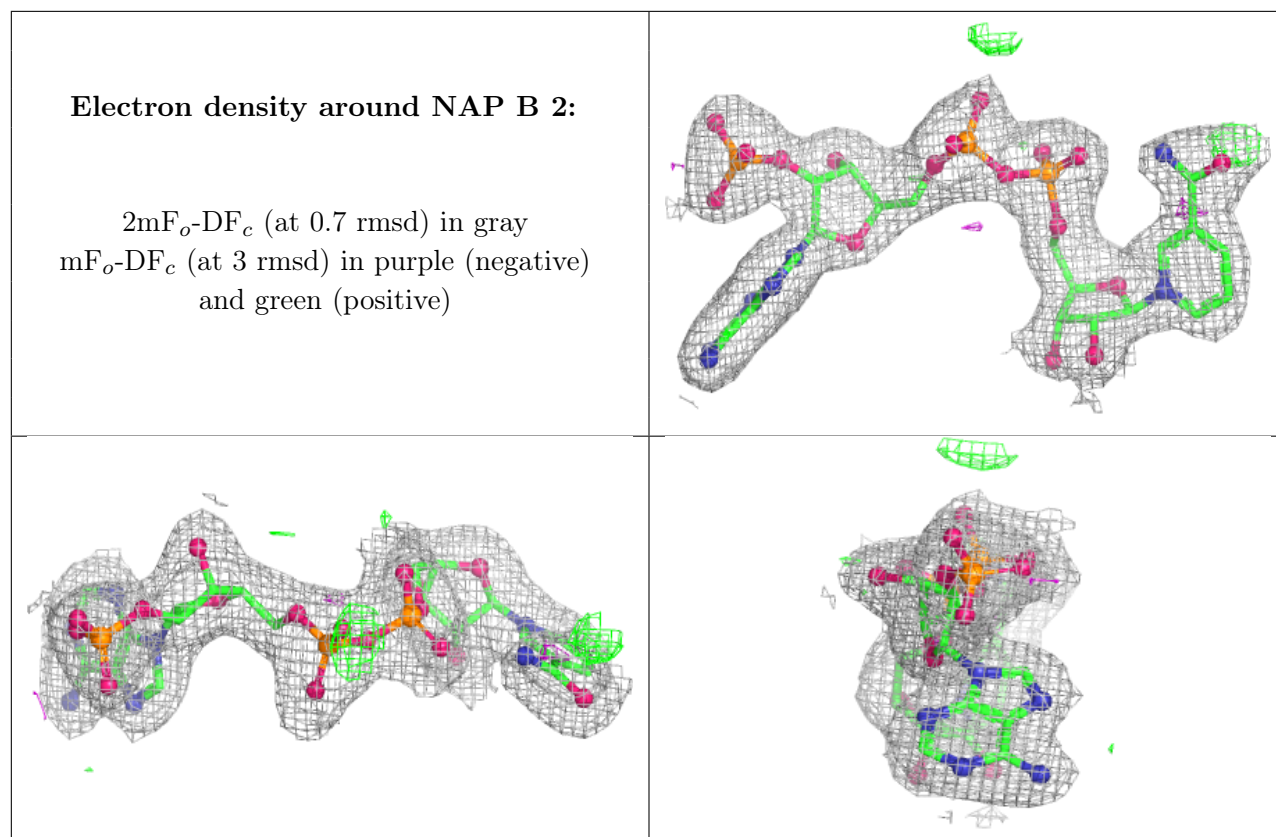
Electron density around NAP C 3:

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

**Electron density around NAP A 1:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.