Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 02:14 AM EDT

PDB ID	:	3H6K
Title	:	Crystal Structure of Human 11-beta-hydroxysteroid-dehydrogenase Bound to an Ortho-chlro-sulfonyl-piperazine Inhibitor
Authors	:	Bard, J.; Svenson, K.
Deposited on	:	2009-04-23
Resolution	:	2.19 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 following versions of software and data (see references ⓘ) were used in the production of this report:

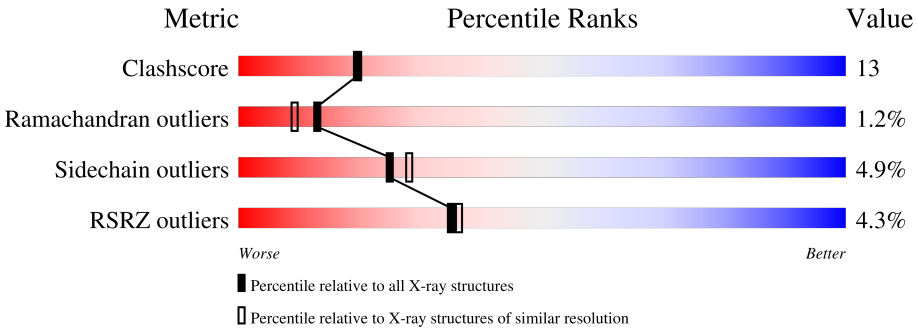
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.19 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))
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 <=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	3%, 63%, 25%, ·, 9%
1	B	286	4%, 62%, 26%, ·, 9%
1	C	286	5%, 70%, 19%, ·, 9%
1	D	286	4%, 60%, 26%, ·, 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8306 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	260	Total	C	N	O	S	0	0	0
			1957	1246	334	363	14			
1	B	261	Total	C	N	O	S	1	1	0
			1984	1265	335	370	14			
1	C	260	Total	C	N	O	S	1	0	0
			1966	1252	335	364	15			
1	D	256	Total	C	N	O	S	3	0	0
			1934	1232	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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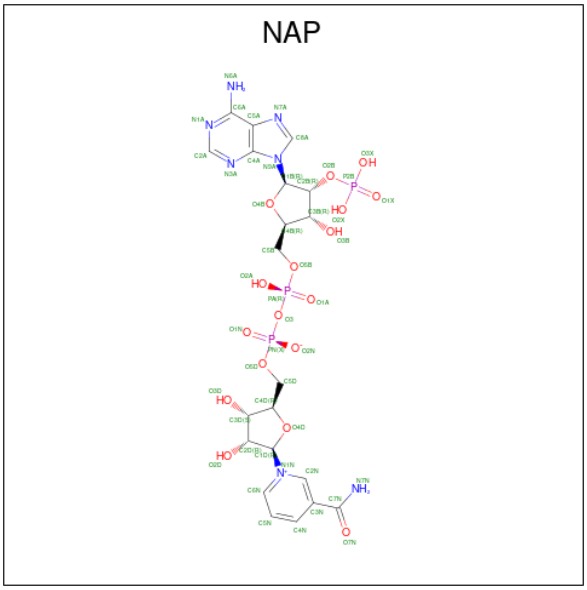
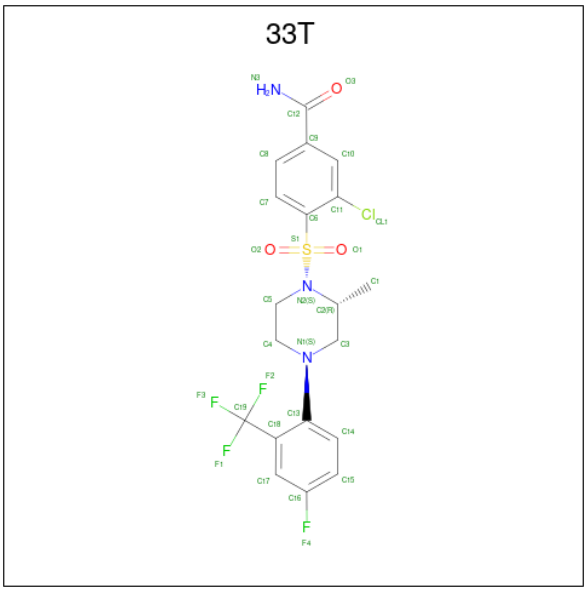
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	expression tag	UNP P28845
D	17	HIS	-	expression tag	UNP P28845
D	18	GLN	-	expression tag	UNP P28845
D	19	HIS	-	expression tag	UNP P28845
D	20	GLN	-	expression tag	UNP P28845
D	21	GLN	-	expression tag	UNP P28845
D	22	PRO	-	expression tag	UNP P28845
D	23	LEU	-	expression tag	UNP P28845
D	272	SER	CYS	engineered mutation	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: 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	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 3-chloro-4-({(2R)-4-[4-fluoro-2-(trifluoromethyl)phenyl]-2-methylpiperazin-1-yl}sulfonyl)benzamide (three-letter code: 33T) (formula: $C_{19}H_{18}ClF_4N_3O_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	0	0
			31	19	1	4	3	3	1		
3	B	1	Total	C	Cl	F	N	O	S	0	0
			31	19	1	4	3	3	1		
3	C	1	Total	C	Cl	F	N	O	S	0	0
			31	19	1	4	3	3	1		
3	D	1	Total	C	Cl	F	N	O	S	0	0
			31	19	1	4	3	3	1		

- Molecule 4 is water.

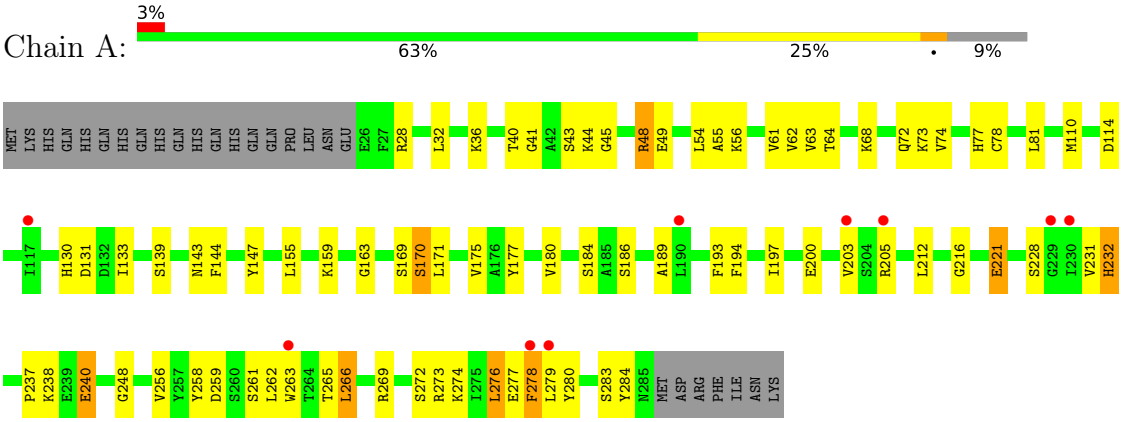
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	B	32	Total	O	0	0
			32	32		
4	C	54	Total	O	0	0
			54	54		
4	D	26	Total	O	0	0
			26	26		

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.

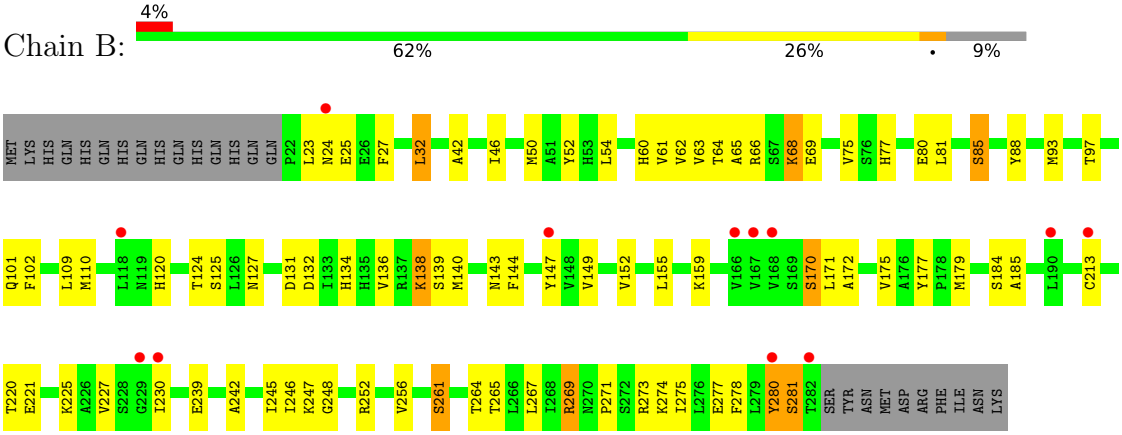
• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain A:



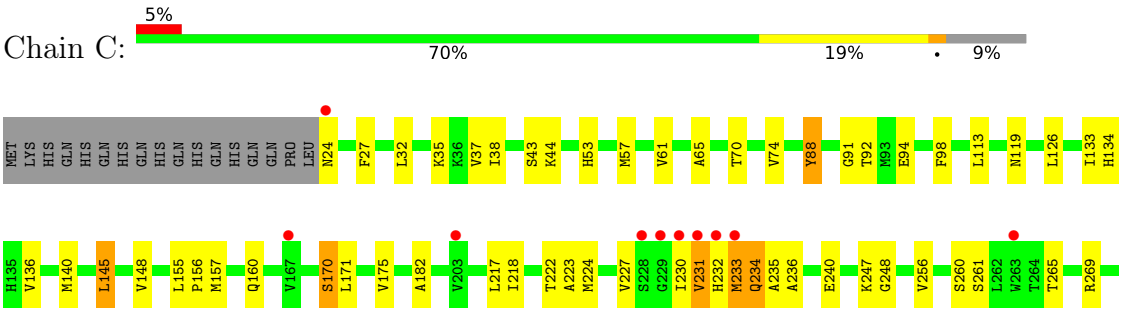
• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

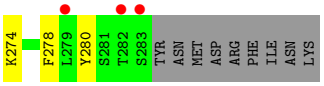
Chain B:



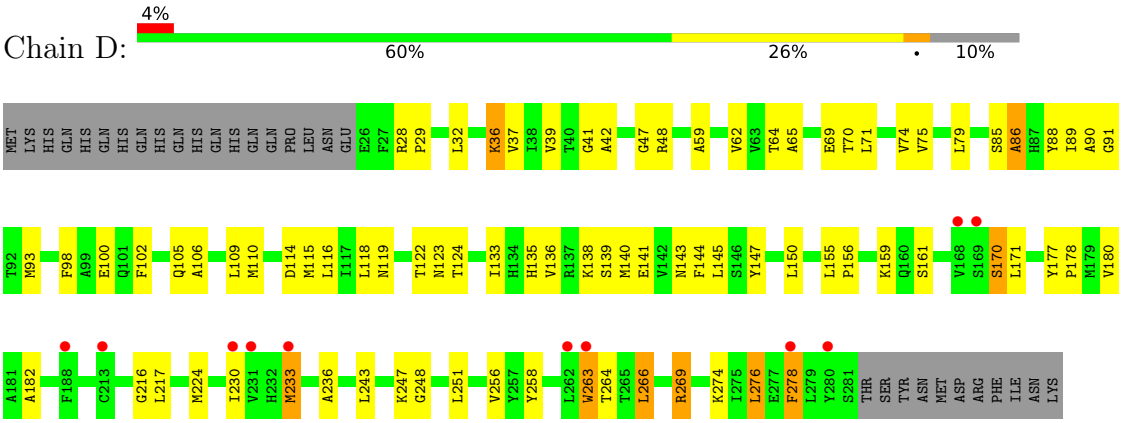
• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain C:





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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.20Å 152.01Å 74.54Å 90.00° 92.41° 90.00°	Depositor
Resolution (Å)	31.47 – 2.19 31.47 – 2.19	Depositor EDS
% Data completeness (in resolution range)	66.2 (31.47-2.19) 66.2 (31.47-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.190 , 0.275 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 53.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8306	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, 33T

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	0.32	0/1988	0.53	0/2685
1	B	0.32	0/2019	0.51	0/2726
1	C	0.33	0/1997	0.52	0/2697
1	D	0.30	0/1965	0.52	0/2652
All	All	0.32	0/7969	0.52	0/10760

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1957	0	1976	56	0
1	B	1984	0	2019	59	0
1	C	1966	0	2005	45	0
1	D	1934	0	1965	65	0
2	A	48	0	25	3	0
2	B	48	0	25	6	0
2	C	48	0	25	5	0
2	D	48	0	25	5	0
3	A	31	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	18	3	0
3	C	31	0	18	1	0
3	D	31	0	18	2	0
4	A	37	0	0	0	0
4	B	32	0	0	0	0
4	C	54	0	0	2	0
4	D	26	0	0	3	0
All	All	8306	0	8137	209	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 13.

All (209) 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:269:ARG:NH2	1:B:274:LYS:HE2	1.80	0.96
1:D:170:SER:HB3	2:D:1:NAP:H5N	1.61	0.81
1:D:71:LEU:HD13	1:D:88:TYR:HB2	1.67	0.77
1:A:283:SER:N	1:A:284:TYR:HA	1.99	0.76
1:B:64:THR:HB	1:B:102:PHE:CE1	2.23	0.73
1:B:170:SER:OG	2:B:1:NAP:H6N	1.88	0.73
1:C:170:SER:HB3	2:C:1:NAP:H5N	1.71	0.73
1:A:221:GLU:CD	1:A:221:GLU:H	1.93	0.70
1:D:263:TRP:CD1	1:D:263:TRP:C	2.65	0.70
1:A:237:PRO:HG2	1:A:240:GLU:HB2	1.75	0.69
1:D:139:SER:O	1:D:143:ASN:HB2	1.93	0.68
1:A:170:SER:OG	2:A:1:NAP:H6N	1.97	0.64
1:C:170:SER:OG	2:C:1:NAP:H6N	1.97	0.64
1:B:271:PRO:O	1:B:275:ILE:HG13	1.99	0.63
1:A:283:SER:H	1:A:284:TYR:HA	1.62	0.63
1:C:92:THR:OG1	1:C:94:GLU:HG3	1.98	0.63
1:B:261:SER:HB3	1:B:264:THR:OG1	1.98	0.63
1:D:274:LYS:O	1:D:278:PHE:CD2	2.52	0.61
1:C:240:GLU:HB2	4:C:324:HOH:O	2.00	0.61
1:A:248:GLY:HA3	1:A:256:VAL:HG21	1.82	0.60
1:C:94:GLU:HB3	4:C:313:HOH:O	2.02	0.60
1:A:133:ILE:HD13	1:B:149:VAL:HG22	1.83	0.59
1:A:273:ARG:O	1:A:277:GLU:HG3	2.02	0.59
1:C:119:ASN:OD1	2:C:1:NAP:H4D	2.03	0.59
1:A:193:PHE:HB2	1:B:185:ALA:HB2	1.85	0.59
1:C:140:MET:HB3	1:D:140:MET:SD	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LEU:HD11	1:C:227:VAL:HG12	1.83	0.59
1:B:170:SER:HB3	2:B:1:NAP:H5N	1.84	0.58
1:D:170:SER:OG	2:D:1:NAP:H6N	2.03	0.58
1:C:223:ALA:O	1:C:227:VAL:HG22	2.03	0.58
1:A:130:HIS:O	1:A:131:ASP:HB2	2.04	0.57
1:B:132:ASP:O	1:B:136:VAL:HG23	2.05	0.56
1:B:273:ARG:O	1:B:277:GLU:HG3	2.05	0.56
1:D:39:VAL:HG12	1:D:42:ALA:HB2	1.88	0.56
1:C:27:PHE:CG	1:C:247:LYS:HG2	2.41	0.55
1:D:41:GLY:O	1:D:47:GLY:HA3	2.07	0.55
1:A:77:HIS:O	1:A:81:LEU:HG	2.06	0.55
1:A:48:ARG:HH22	1:A:73:LYS:HZ2	1.55	0.55
1:B:221:GLU:O	1:B:225:LYS:HG3	2.06	0.55
1:B:171:LEU:HD12	3:B:293:33T:C7	2.37	0.55
1:D:85:SER:O	1:D:86:ALA:HB2	2.06	0.55
1:A:131:ASP:OD1	1:B:152:VAL:HG13	2.07	0.54
1:B:46:ILE:O	1:B:50:MET:HG3	2.06	0.54
1:A:263:TRP:CE3	1:D:263:TRP:HH2	2.25	0.54
1:D:177:TYR:CD1	1:D:178:PRO:HD2	2.43	0.54
1:A:261:SER:O	1:A:265:THR:HG23	2.08	0.53
1:C:140:MET:HE2	1:D:140:MET:HG3	1.90	0.52
1:B:127:ASN:O	1:B:179:MET:HA	2.10	0.52
1:C:175:VAL:HG11	1:D:276:LEU:CD1	2.39	0.52
1:D:144:PHE:O	1:D:147:TYR:HB2	2.10	0.52
1:C:233:MET:O	1:C:234:GLN:CB	2.57	0.52
1:B:93:MET:HG2	2:B:1:NAP:H2A	1.92	0.52
1:D:119:ASN:OD1	2:D:1:NAP:H4D	2.10	0.52
1:D:36:LYS:HD3	1:D:36:LYS:N	2.25	0.52
1:D:89:ILE:HD13	1:D:105:GLN:HG3	1.91	0.52
1:A:62:VAL:HG23	1:A:110:MET:SD	2.49	0.52
1:D:48:ARG:HG3	1:D:74:VAL:HG21	1.92	0.51
1:C:230:ILE:O	1:C:231:VAL:O	2.28	0.51
1:A:56:LYS:HA	1:A:81:LEU:O	2.11	0.51
1:C:157:MET:O	1:C:160:GLN:HB2	2.11	0.51
1:B:23:LEU:HD13	1:B:252:ARG:HD3	1.92	0.51
1:D:32:LEU:O	1:D:59:ALA:HB2	2.11	0.51
1:D:180:VAL:O	1:D:180:VAL:HG23	2.09	0.51
3:A:293:33T:H10	1:B:280[A]:TYR:HE2	1.76	0.50
1:C:43:SER:HB3	1:C:65:ALA:HB3	1.92	0.50
1:D:116:LEU:HD11	1:D:118:LEU:HD21	1.92	0.50
1:A:279:LEU:HD23	1:A:280:TYR:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ILE:HG13	1:C:113:LEU:CD1	2.41	0.50
1:A:216:GLY:HA3	1:A:259:ASP:OD2	2.12	0.50
1:B:62:VAL:N	1:B:110:MET:HE3	2.26	0.50
2:B:1:NAP:H4N	3:B:293:33T:O2	2.12	0.49
1:B:60:HIS:O	1:B:110:MET:HE1	2.11	0.49
1:B:62:VAL:HG23	1:B:110:MET:HE3	1.94	0.49
1:D:170:SER:HB3	2:D:1:NAP:C5N	2.38	0.49
1:C:38:ILE:HG13	1:C:113:LEU:HD11	1.94	0.49
1:D:217:LEU:HD11	1:D:224:MET:CE	2.42	0.49
1:C:236:ALA:HB2	1:C:260:SER:HB3	1.94	0.49
1:D:135:HIS:CD2	4:D:308:HOH:O	2.65	0.49
1:B:52:TYR:CE1	1:B:77:HIS:HB3	2.47	0.49
1:B:97:THR:O	1:B:101:GLN:HG3	2.13	0.49
1:B:109:LEU:N	1:B:109:LEU:HD23	2.28	0.48
1:A:262:LEU:O	1:A:262:LEU:HD12	2.13	0.48
1:A:171:LEU:O	1:A:175:VAL:HG22	2.13	0.48
1:A:276:LEU:HD13	1:B:267:LEU:HD13	1.96	0.48
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.95	0.48
1:A:186:SER:O	1:A:189:ALA:HB3	2.14	0.48
1:A:269:ARG:NH2	1:A:274:LYS:HE3	2.29	0.48
1:D:122:THR:OG1	1:D:138:LYS:HE3	2.14	0.48
1:D:79:LEU:HD21	1:D:86:ALA:HB3	1.95	0.48
1:A:36:LYS:HB3	1:A:110:MET:HE3	1.95	0.48
1:B:75:VAL:HG21	1:B:88:TYR:HB3	1.94	0.48
1:B:124:THR:HG22	1:B:125:SER:N	2.29	0.48
1:D:71:LEU:O	1:D:75:VAL:HG23	2.14	0.48
1:D:156:PRO:HB2	4:D:318:HOH:O	2.13	0.48
1:A:32:LEU:HD23	1:A:54:LEU:CD2	2.44	0.48
1:D:243:LEU:HG	1:D:247:LYS:HE3	1.96	0.48
1:B:275:ILE:HG12	1:D:266:LEU:HD23	1.95	0.47
1:C:269:ARG:CZ	1:C:274:LYS:NZ	2.77	0.47
1:C:53:HIS:O	1:C:57:MET:HG3	2.15	0.47
1:C:217:LEU:O	1:C:218:ILE:HD13	2.14	0.47
1:D:278:PHE:CD2	1:D:278:PHE:N	2.83	0.47
1:A:55:ALA:HB1	1:A:78:CYS:O	2.14	0.47
1:C:280:TYR:CB	3:D:293:33T:N3	2.78	0.47
1:C:222:THR:HG21	2:C:1:NAP:O2A	2.14	0.47
1:B:68:LYS:HG2	1:B:69:GLU:N	2.29	0.47
1:B:139:SER:O	1:B:143:ASN:HB2	2.14	0.46
1:C:232:HIS:O	1:C:233:MET:HB2	2.15	0.46
1:D:263:TRP:CD1	1:D:264:THR:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:HD12	3:B:293:33T:C8	2.46	0.46
1:B:144:PHE:O	1:B:147:TYR:HB2	2.16	0.46
1:C:32:LEU:HA	1:C:35:LYS:HG3	1.96	0.46
1:D:145:LEU:HD12	1:D:145:LEU:HA	1.77	0.46
1:B:77:HIS:O	1:B:81:LEU:HG	2.15	0.46
1:A:169:SER:HB2	1:A:212:LEU:HD11	1.98	0.46
1:B:175:VAL:CG2	1:B:177:TYR:CE2	2.99	0.46
1:A:175:VAL:HG12	1:B:273:ARG:HG3	1.98	0.46
1:C:91:GLY:HA3	1:C:98:PHE:CZ	2.50	0.46
1:D:155:LEU:HG	1:D:159:LYS:HE3	1.98	0.46
1:C:148:VAL:HG12	1:D:133:ILE:CD1	2.46	0.45
1:A:49:GLU:HG3	1:A:238:LYS:HG3	1.98	0.45
1:A:240:GLU:HB3	1:A:258:TYR:OH	2.16	0.45
1:C:37:VAL:O	1:C:61:VAL:HA	2.16	0.45
1:D:217:LEU:HD23	1:D:233:MET:HB2	1.97	0.45
1:A:40:THR:HA	1:A:64:THR:HG22	1.98	0.45
1:A:248:GLY:HA3	1:A:256:VAL:CG2	2.46	0.45
1:C:136:VAL:HG22	1:C:182:ALA:HB2	1.99	0.45
1:B:248:GLY:HA3	1:B:256:VAL:HG21	1.97	0.45
1:B:23:LEU:O	1:B:25:GLU:N	2.49	0.45
1:A:48:ARG:HD3	1:A:74:VAL:HG22	1.99	0.45
1:D:155:LEU:HB3	1:D:156:PRO:HD3	1.99	0.45
1:C:233:MET:O	1:C:234:GLN:HB2	2.17	0.45
1:A:276:LEU:HD12	1:A:276:LEU:HA	1.81	0.45
1:B:242:ALA:O	1:B:246:ILE:HG13	2.16	0.45
1:D:135:HIS:HD2	4:D:308:HOH:O	2.00	0.45
1:A:114:ASP:O	1:A:163:GLY:HA3	2.18	0.44
1:C:261:SER:O	1:C:265:THR:HG23	2.18	0.44
1:D:171:LEU:HG	1:D:216:GLY:HA2	1.98	0.44
1:D:65:ALA:O	1:D:90:ALA:HA	2.17	0.44
1:D:91:GLY:HA3	1:D:98:PHE:CZ	2.52	0.44
1:A:144:PHE:O	1:A:147:TYR:HB2	2.18	0.44
1:A:170:SER:HB3	2:A:1:NAP:H5N	1.98	0.44
1:B:220:THR:HG21	2:B:1:NAP:O2N	2.18	0.44
1:C:145:LEU:HD23	1:D:140:MET:SD	2.58	0.44
1:D:64:THR:HB	1:D:102:PHE:CE1	2.53	0.44
1:A:263:TRP:CZ3	1:D:263:TRP:HH2	2.35	0.43
1:D:236:ALA:HB1	1:D:258:TYR:CE1	2.53	0.43
1:A:68:LYS:O	1:A:72:GLN:HG3	2.18	0.43
1:A:180:VAL:HG23	1:A:184:SER:OG	2.18	0.43
1:A:278:PHE:C	1:A:278:PHE:CD2	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:SER:O	1:A:143:ASN:HB2	2.17	0.43
1:A:194:PHE:HA	1:A:197:ILE:HG12	2.00	0.43
1:B:32:LEU:HD22	1:B:54:LEU:CD2	2.48	0.43
1:B:32:LEU:HD22	1:B:54:LEU:HD23	2.01	0.43
1:B:32:LEU:HD11	1:B:246:ILE:HG22	1.99	0.43
1:B:155:LEU:HG	1:B:159:LYS:HE3	1.99	0.43
1:D:136:VAL:HA	1:D:182:ALA:HB1	2.01	0.43
1:B:42:ALA:HB3	1:B:63:VAL:HB	2.01	0.43
1:D:62:VAL:HG23	1:D:110:MET:SD	2.59	0.43
1:D:105:GLN:O	1:D:109:LEU:HD13	2.18	0.43
1:A:43:SER:C	1:A:44:LYS:HG3	2.39	0.43
1:B:66:ARG:HB2	2:B:1:NAP:O2X	2.18	0.43
1:C:269:ARG:NH1	1:C:274:LYS:HZ3	2.16	0.43
1:C:278:PHE:CD2	1:C:278:PHE:C	2.91	0.43
1:D:28:ARG:HA	1:D:29:PRO:HD3	1.87	0.43
1:D:114:ASP:OD1	1:D:161:SER:HB2	2.19	0.43
1:A:48:ARG:NH2	1:A:73:LYS:HE3	2.34	0.42
1:A:175:VAL:HG23	1:A:177:TYR:CE1	2.54	0.42
1:B:239:GLU:CD	1:B:239:GLU:H	2.22	0.42
1:C:133:ILE:HG23	1:C:134:HIS:N	2.34	0.42
1:A:41:GLY:CA	2:A:1:NAP:H4B	2.49	0.42
1:B:54:LEU:HG	1:B:246:ILE:HD13	2.01	0.42
1:C:175:VAL:HG11	1:D:276:LEU:HD12	2.00	0.42
1:B:50:MET:HG2	1:B:242:ALA:HB1	2.00	0.42
1:D:88:TYR:O	1:D:89:ILE:HG12	2.19	0.42
1:A:130:HIS:O	1:A:131:ASP:CB	2.66	0.42
1:A:272:SER:HB3	1:B:267:LEU:HB3	2.02	0.42
1:C:88:TYR:CD1	1:C:88:TYR:C	2.93	0.42
1:C:171:LEU:HD12	3:C:293:33T:C7	2.50	0.42
1:D:278:PHE:N	1:D:278:PHE:HD2	2.18	0.42
1:B:27:PHE:CD2	1:B:247:LYS:HD3	2.55	0.42
1:B:60:HIS:ND1	1:B:85:SER:HB3	2.35	0.42
1:C:232:HIS:O	1:C:233:MET:CB	2.68	0.42
1:A:155:LEU:HG	1:A:159:LYS:HE3	2.02	0.41
1:A:231:VAL:O	1:A:232:HIS:CB	2.68	0.41
1:D:62:VAL:HG11	1:D:106:ALA:CB	2.50	0.41
1:C:70:THR:O	1:C:74:VAL:HG23	2.20	0.41
1:D:93:MET:HG2	2:D:1:NAP:H2A	2.02	0.41
1:B:120:HIS:CE1	1:B:147:TYR:CE1	3.09	0.41
1:B:213:CYS:SG	1:B:245:ILE:HG23	2.60	0.41
1:A:200:GLU:O	1:A:203:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:HIS:NE2	1:B:138:LYS:NZ	2.68	0.41
1:D:62:VAL:HG11	1:D:106:ALA:HB1	2.03	0.41
1:D:247:LYS:O	1:D:251:LEU:HG	2.21	0.41
1:C:170:SER:OG	2:C:1:NAP:C6N	2.66	0.41
1:D:269:ARG:NH1	1:D:274:LYS:HE2	2.36	0.41
1:C:224:MET:CE	1:C:235:ALA:HB3	2.50	0.41
1:D:177:TYR:CD2	3:D:293:33T:CL1	3.10	0.41
1:D:263:TRP:C	1:D:263:TRP:HD1	2.23	0.41
1:A:144:PHE:CD2	1:B:140:MET:HE3	2.56	0.41
1:A:262:LEU:HD12	1:A:266:LEU:HD13	2.03	0.41
1:B:172:ALA:HB1	1:B:184:SER:OG	2.20	0.41
1:B:227:VAL:O	1:B:227:VAL:CG1	2.70	0.40
1:C:155:LEU:N	1:C:156:PRO:CD	2.84	0.40
1:D:37:VAL:HG22	1:D:115:MET:HB3	2.04	0.40
1:A:61:VAL:HG12	1:A:63:VAL:HG13	2.03	0.40
1:B:275:ILE:CG1	1:D:266:LEU:HD23	2.50	0.40
1:D:118:LEU:HD22	1:D:150:LEU:HD13	2.03	0.40
1:D:248:GLY:HA3	1:D:256:VAL:HG21	2.02	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	258/286 (90%)	240 (93%)	15 (6%)	3 (1%)	13	9
1	B	260/286 (91%)	242 (93%)	15 (6%)	3 (1%)	13	9
1	C	258/286 (90%)	236 (92%)	19 (7%)	3 (1%)	13	9
1	D	254/286 (89%)	222 (87%)	29 (11%)	3 (1%)	13	9
All	All	1030/1144 (90%)	940 (91%)	78 (8%)	12 (1%)	13	9

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	ASN
1	C	231	VAL
1	C	233	MET
1	C	234	GLN
1	D	86	ALA
1	A	232	HIS
1	B	65	ALA
1	B	281	SER
1	A	45	GLY
1	D	69	GLU
1	A	228	SER
1	D	230	ILE

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	206/243 (85%)	197 (96%)	9 (4%)	28	33
1	B	213/243 (88%)	198 (93%)	15 (7%)	15	14
1	C	211/243 (87%)	206 (98%)	5 (2%)	49	59
1	D	206/243 (85%)	193 (94%)	13 (6%)	18	18
All	All	836/972 (86%)	794 (95%)	42 (5%)	25	27

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	48	ARG
1	A	170	SER
1	A	205	ARG
1	A	221	GLU
1	A	240	GLU
1	A	266	LEU
1	A	276	LEU
1	A	278	PHE
1	B	32	LEU

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Mol	Chain	Res	Type
1	B	61	VAL
1	B	68	LYS
1	B	80	GLU
1	B	85	SER
1	B	131	ASP
1	B	138	LYS
1	B	170	SER
1	B	230	ILE
1	B	261	SER
1	B	265	THR
1	B	269	ARG
1	B	278	PHE
1	B	280[A]	TYR
1	B	280[B]	TYR
1	C	24	ASN
1	C	44	LYS
1	C	88	TYR
1	C	145	LEU
1	C	170	SER
1	D	36	LYS
1	D	70	THR
1	D	100	GLU
1	D	123	ASN
1	D	124	THR
1	D	141	GLU
1	D	170	SER
1	D	233	MET
1	D	263	TRP
1	D	266	LEU
1	D	269	ARG
1	D	276	LEU
1	D	278	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
2	NAP	C	1	-	45,52,52	1.70	3 (6%)	56,80,80	1.20	3 (5%)
2	NAP	D	1	-	45,52,52	1.67	3 (6%)	56,80,80	1.19	3 (5%)
2	NAP	B	1	-	45,52,52	1.64	3 (6%)	56,80,80	1.14	3 (5%)
3	33T	C	293	-	32,33,33	1.64	3 (9%)	48,51,51	1.35	7 (14%)
2	NAP	A	1	-	45,52,52	1.66	3 (6%)	56,80,80	1.23	4 (7%)
3	33T	B	293	-	32,33,33	1.62	2 (6%)	48,51,51	1.10	6 (12%)
3	33T	D	293	-	32,33,33	1.53	3 (9%)	48,51,51	1.41	5 (10%)
3	33T	A	293	-	32,33,33	1.53	2 (6%)	48,51,51	1.12	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	C	1	-	-	6/31/67/67	0/5/5/5
2	NAP	D	1	-	-	6/31/67/67	0/5/5/5
2	NAP	B	1	-	-	5/31/67/67	0/5/5/5
3	33T	C	293	-	-	9/26/39/39	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	A	1	-	-	6/31/67/67	0/5/5/5
3	33T	B	293	-	-	9/26/39/39	0/3/3/3
3	33T	D	293	-	-	11/26/39/39	0/3/3/3
3	33T	A	293	-	-	11/26/39/39	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAP	O7N-C7N	9.07	1.41	1.24
2	A	1	NAP	O7N-C7N	8.85	1.41	1.24
2	B	1	NAP	O7N-C7N	8.80	1.41	1.24
2	D	1	NAP	O7N-C7N	8.61	1.40	1.24
3	B	293	33T	S1-N2	6.94	1.74	1.63
3	D	293	33T	S1-N2	6.35	1.73	1.63
3	C	293	33T	S1-N2	6.28	1.73	1.63
3	A	293	33T	S1-N2	6.25	1.72	1.63
2	D	1	NAP	C2A-N3A	3.97	1.38	1.32
2	A	1	NAP	C2A-N3A	3.69	1.38	1.32
2	B	1	NAP	C2A-N3A	3.61	1.37	1.32
2	C	1	NAP	C2A-N3A	3.59	1.37	1.32
3	C	293	33T	C12-N3	3.12	1.38	1.33
3	B	293	33T	C12-N3	2.87	1.38	1.33
3	A	293	33T	C12-N3	2.83	1.38	1.33
3	D	293	33T	C12-N3	2.76	1.38	1.33
2	D	1	NAP	C2A-N1A	2.61	1.38	1.33
2	B	1	NAP	C2A-N1A	2.58	1.38	1.33
2	A	1	NAP	C2A-N1A	2.16	1.37	1.33
2	C	1	NAP	C2A-N1A	2.16	1.37	1.33
3	C	293	33T	O1-S1	2.15	1.45	1.43
3	D	293	33T	O1-S1	2.03	1.45	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAP	N3A-C2A-N1A	-5.62	119.90	128.68
3	D	293	33T	C6-C11-CL1	5.58	125.58	121.49
2	B	1	NAP	N3A-C2A-N1A	-5.53	120.04	128.68
2	A	1	NAP	N3A-C2A-N1A	-5.51	120.06	128.68
2	C	1	NAP	N3A-C2A-N1A	-5.34	120.33	128.68
3	C	293	33T	C6-C11-CL1	3.66	124.17	121.49
2	C	1	NAP	O4D-C1D-C2D	-3.63	101.62	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	293	33T	C4-C5-N2	-3.34	106.17	108.96
3	A	293	33T	C6-C11-CL1	3.11	123.77	121.49
2	D	1	NAP	O4D-C1D-C2D	-3.09	102.42	106.93
3	C	293	33T	C10-C11-C6	-3.01	118.35	121.38
3	B	293	33T	C4-C5-N2	2.95	111.42	108.96
3	C	293	33T	C6-S1-N2	-2.84	99.44	106.56
2	A	1	NAP	O4D-C1D-C2D	-2.74	102.92	106.93
3	C	293	33T	C7-C6-C11	2.58	120.85	119.02
3	B	293	33T	C10-C11-C6	-2.55	118.80	121.38
2	B	1	NAP	O4D-C1D-C2D	-2.54	103.22	106.93
2	A	1	NAP	C6N-N1N-C2N	-2.52	119.68	121.97
3	D	293	33T	C6-S1-N2	-2.34	100.69	106.56
2	D	1	NAP	C2N-C3N-C4N	2.33	120.90	118.26
2	A	1	NAP	C2B-C3B-C4B	2.32	107.04	101.99
3	C	293	33T	C4-C5-N2	2.29	110.87	108.96
3	B	293	33T	C7-C6-C11	2.23	120.60	119.02
3	D	293	33T	C18-C17-C16	2.22	120.61	117.56
3	C	293	33T	C18-C17-C16	2.20	120.59	117.56
3	B	293	33T	C18-C17-C16	2.18	120.56	117.56
3	D	293	33T	C10-C11-CL1	-2.17	114.99	118.49
3	A	293	33T	C15-C16-C17	-2.16	120.48	123.29
2	B	1	NAP	C2B-C3B-C4B	2.10	106.56	101.99
3	B	293	33T	C6-C11-CL1	2.09	123.02	121.49
3	A	293	33T	C18-C17-C16	2.07	120.40	117.56
2	C	1	NAP	C2B-C3B-C4B	2.07	106.48	101.99
3	C	293	33T	C17-C18-C19	2.05	121.54	116.50
3	B	293	33T	C6-S1-N2	-2.01	101.53	106.56

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAP	C5B-O5B-PA-O3
2	B	1	NAP	C5B-O5B-PA-O2A
2	B	1	NAP	C5B-O5B-PA-O3
2	B	1	NAP	O4B-C4B-C5B-O5B
2	C	1	NAP	C5B-O5B-PA-O1A
2	C	1	NAP	C5B-O5B-PA-O2A
2	C	1	NAP	C5B-O5B-PA-O3
2	C	1	NAP	O4B-C4B-C5B-O5B
2	D	1	NAP	C5B-O5B-PA-O3
3	A	293	33T	O3-C12-C9-C8

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Mol	Chain	Res	Type	Atoms
3	A	293	33T	N3-C12-C9-C8
2	D	1	NAP	O4B-C4B-C5B-O5B
3	A	293	33T	N3-C12-C9-C10
3	A	293	33T	O3-C12-C9-C10
2	A	1	NAP	O4B-C4B-C5B-O5B
2	A	1	NAP	C3B-C4B-C5B-O5B
2	B	1	NAP	C3B-C4B-C5B-O5B
2	C	1	NAP	C3B-C4B-C5B-O5B
3	C	293	33T	C5-N2-S1-O2
3	A	293	33T	C5-N2-S1-O2
3	B	293	33T	C5-N2-S1-O2
3	B	293	33T	C5-N2-S1-C6
3	C	293	33T	C5-N2-S1-C6
3	B	293	33T	C14-C13-N1-C4
3	D	293	33T	C14-C13-N1-C3
3	B	293	33T	C14-C13-N1-C3
3	D	293	33T	C14-C13-N1-C4
3	A	293	33T	C5-N2-S1-C6
3	C	293	33T	C14-C13-N1-C3
3	D	293	33T	C5-N2-S1-O1
3	A	293	33T	C14-C13-N1-C3
3	A	293	33T	C14-C13-N1-C4
3	D	293	33T	C5-N2-S1-O2
3	D	293	33T	C18-C13-N1-C4
2	D	1	NAP	C3B-C4B-C5B-O5B
3	A	293	33T	C18-C13-N1-C3
3	B	293	33T	C18-C13-N1-C3
3	B	293	33T	C18-C13-N1-C4
3	C	293	33T	C18-C13-N1-C3
3	D	293	33T	C18-C13-N1-C3
2	A	1	NAP	C2B-O2B-P2B-O2X
2	A	1	NAP	C5B-O5B-PA-O1A
2	A	1	NAP	C5B-O5B-PA-O2A
2	B	1	NAP	C5B-O5B-PA-O1A
2	D	1	NAP	C5B-O5B-PA-O2A
3	B	293	33T	C11-C6-S1-N2
3	B	293	33T	C11-C6-S1-O1
3	C	293	33T	C14-C13-N1-C4
3	C	293	33T	C5-N2-S1-O1
3	D	293	33T	C5-N2-S1-C6
3	D	293	33T	O3-C12-C9-C8
3	D	293	33T	N3-C12-C9-C8

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Mol	Chain	Res	Type	Atoms
3	D	293	33T	O3-C12-C9-C10
3	A	293	33T	C18-C13-N1-C4
3	D	293	33T	N3-C12-C9-C10
3	A	293	33T	C5-N2-S1-O1
2	D	1	NAP	O4D-C4D-C5D-O5D
3	B	293	33T	C7-C6-S1-O1
2	C	1	NAP	O4D-C4D-C5D-O5D
3	C	293	33T	N3-C12-C9-C10
3	C	293	33T	O3-C12-C9-C10
2	D	1	NAP	C5B-O5B-PA-O1A
3	C	293	33T	N3-C12-C9-C8

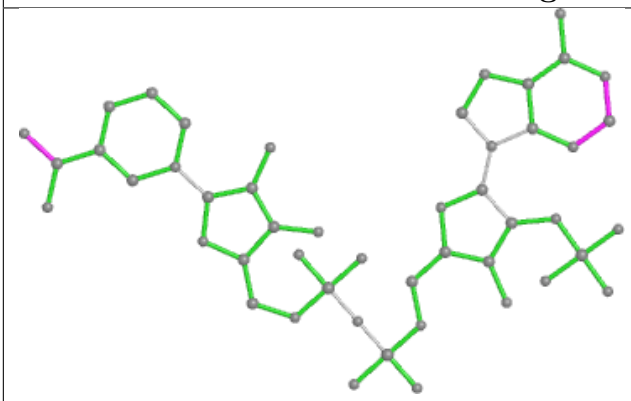
There are no ring outliers.

8 monomers are involved in 25 short contacts:

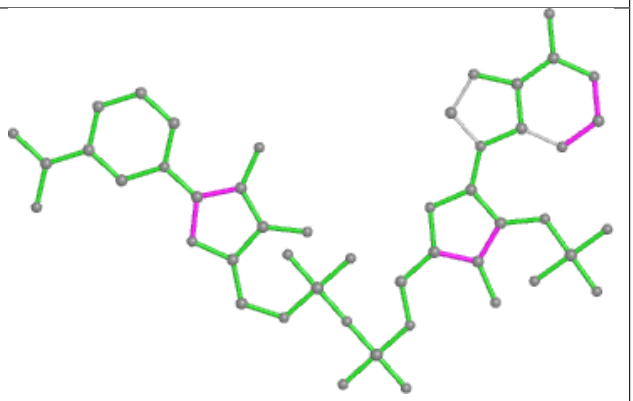
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAP	5	0
2	D	1	NAP	5	0
2	B	1	NAP	6	0
3	C	293	33T	1	0
2	A	1	NAP	3	0
3	B	293	33T	3	0
3	D	293	33T	2	0
3	A	293	33T	1	0

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 then 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.

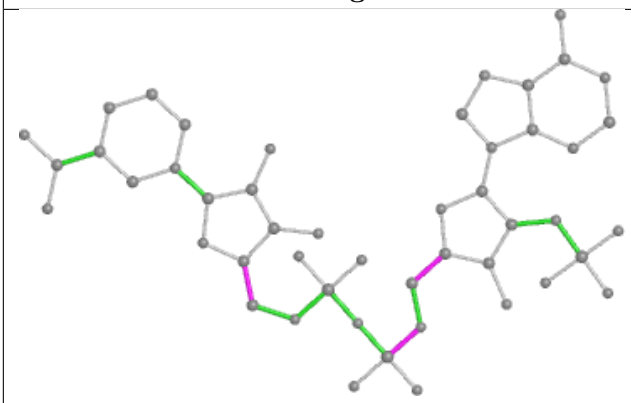
Ligand NAP C 1



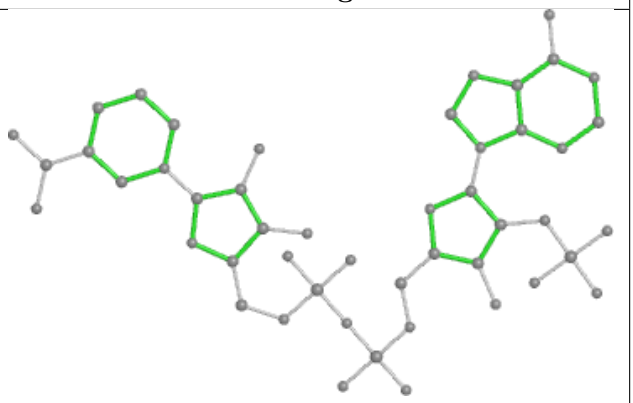
Bond lengths



Bond angles

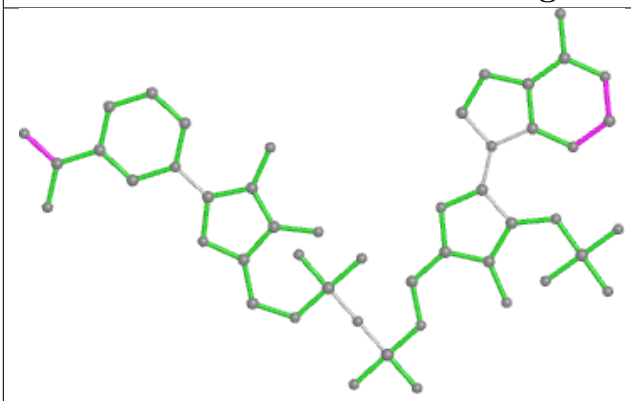


Torsions

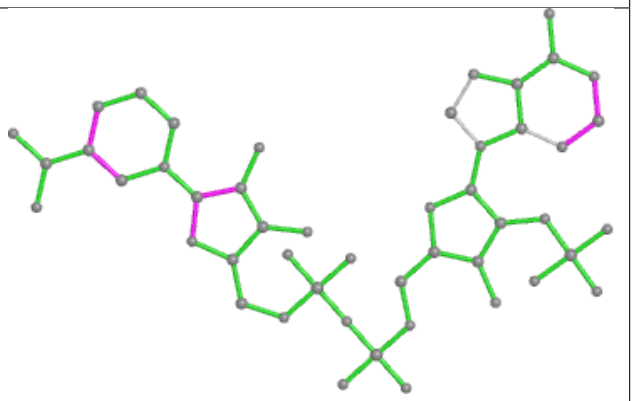


Rings

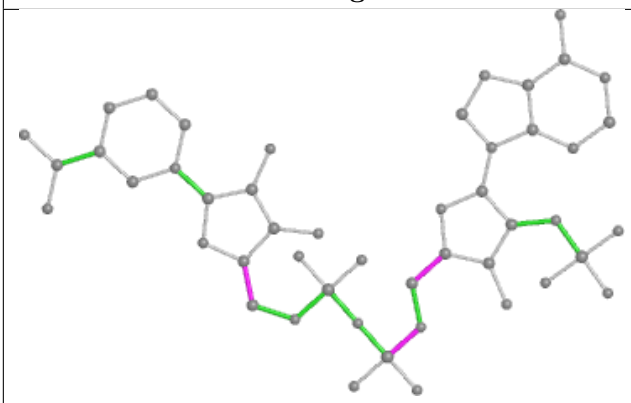
Ligand NAP D 1



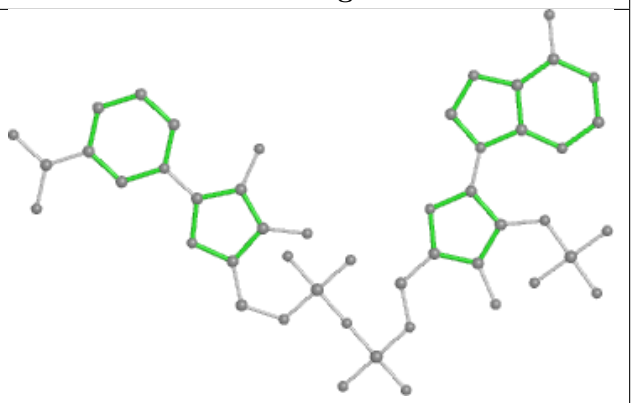
Bond lengths



Bond angles

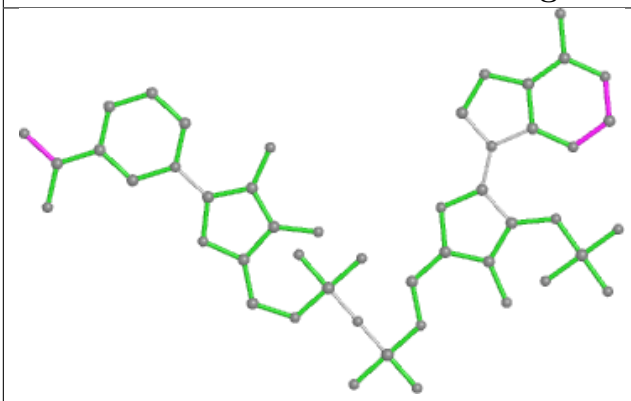


Torsions

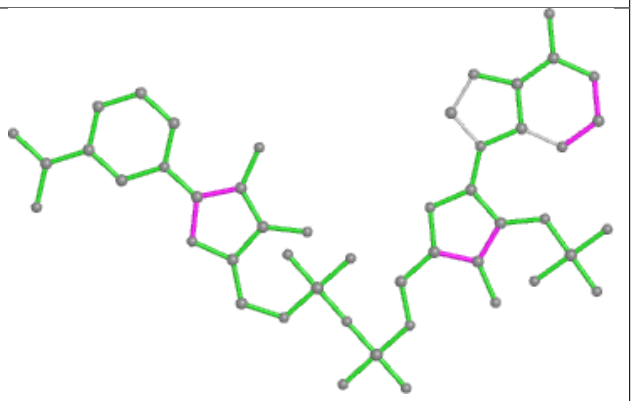


Rings

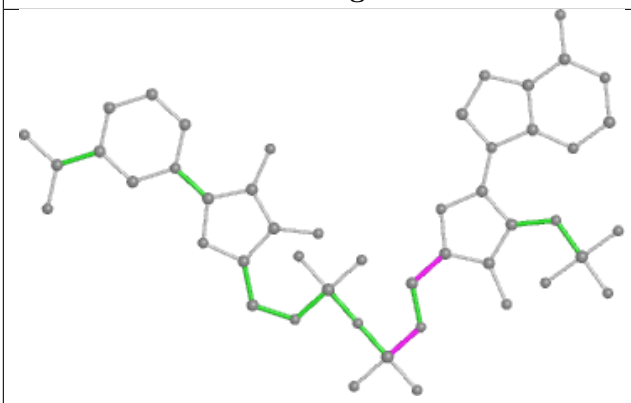
Ligand NAP B 1



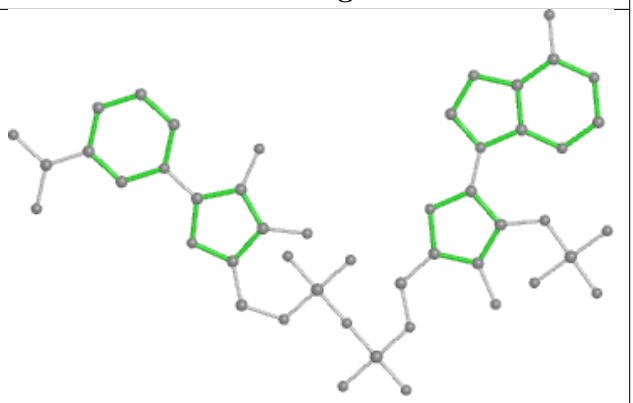
Bond lengths



Bond angles

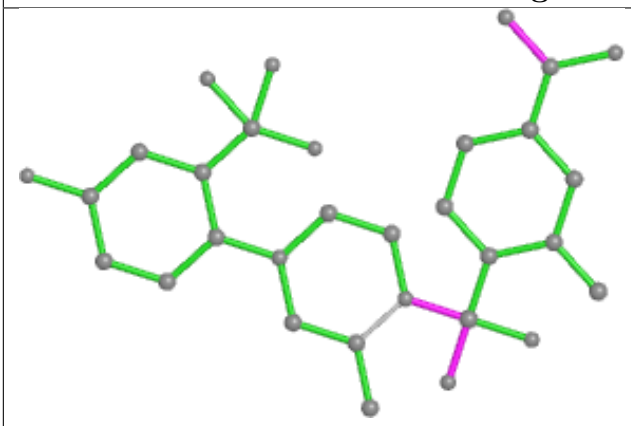


Torsions

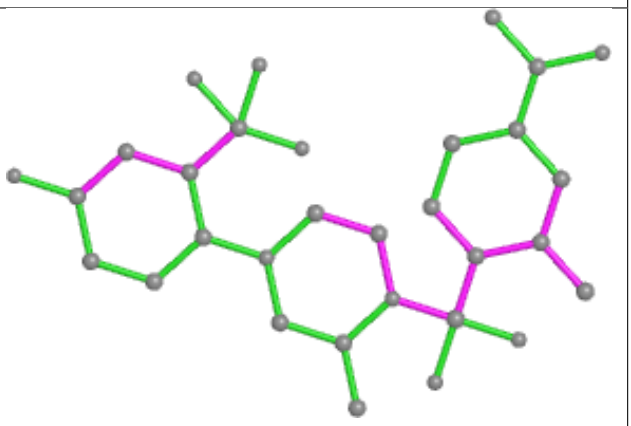


Rings

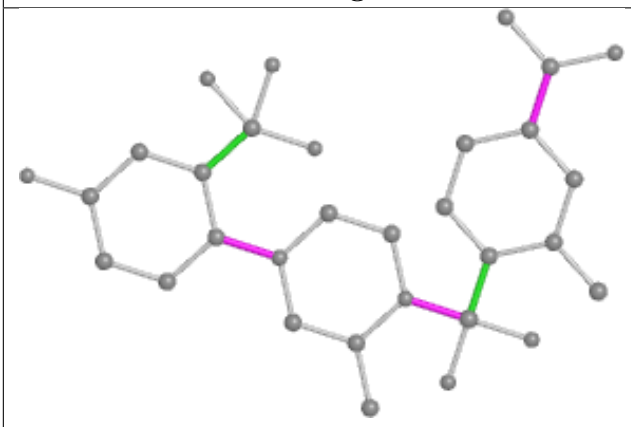
Ligand 33T C 293



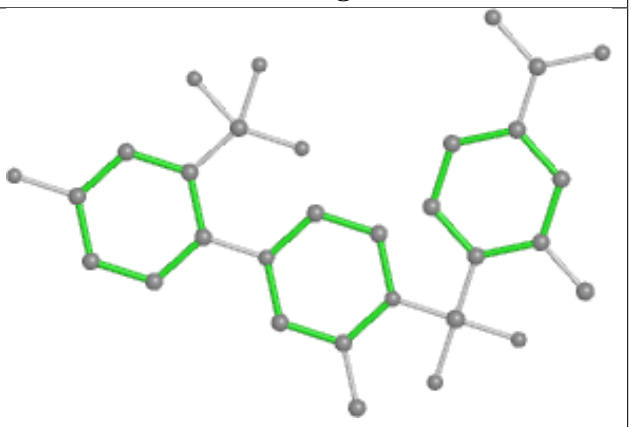
Bond lengths



Bond angles

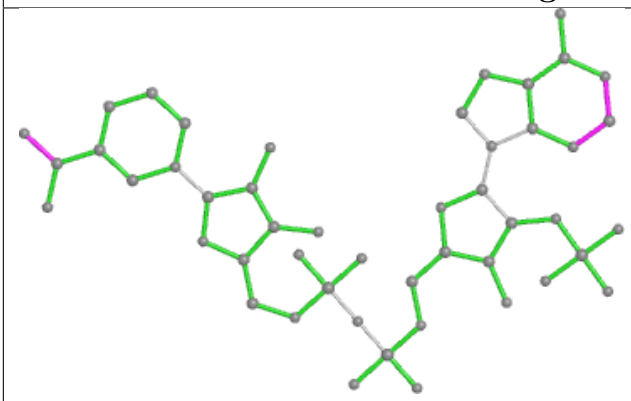


Torsions

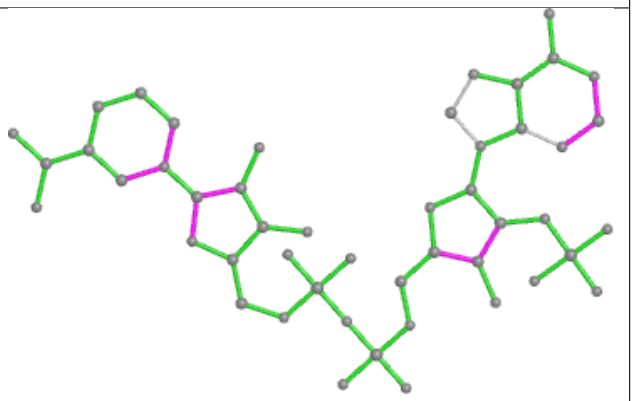


Rings

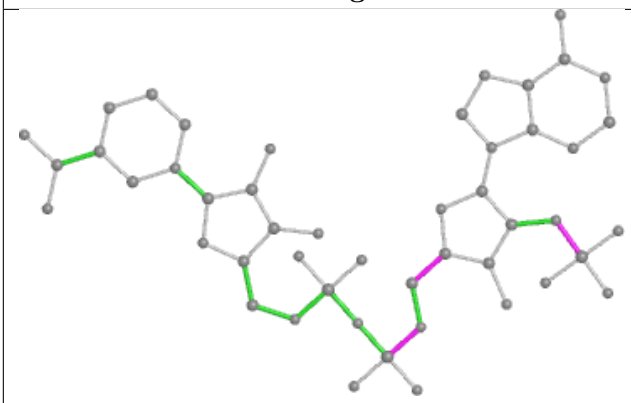
Ligand NAP A 1



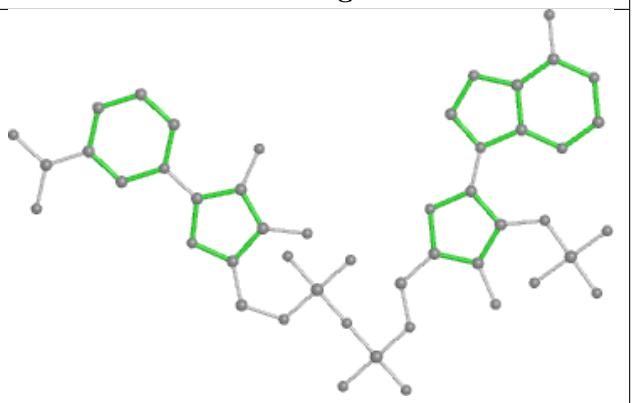
Bond lengths



Bond angles

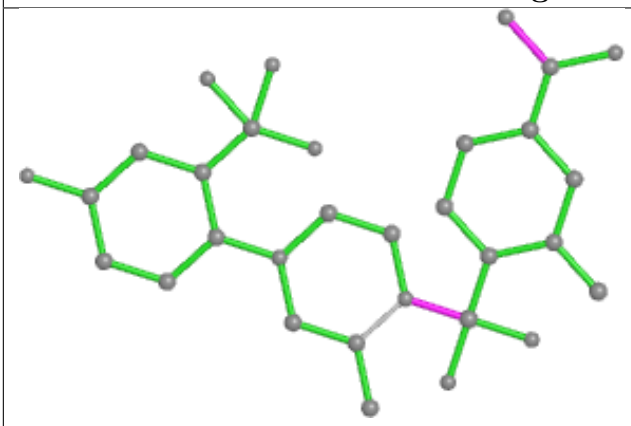


Torsions

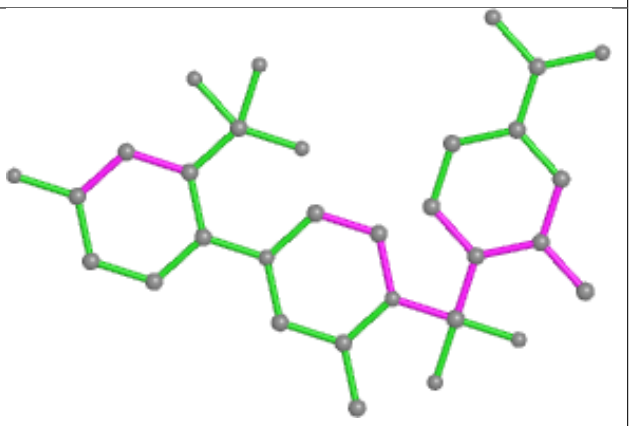


Rings

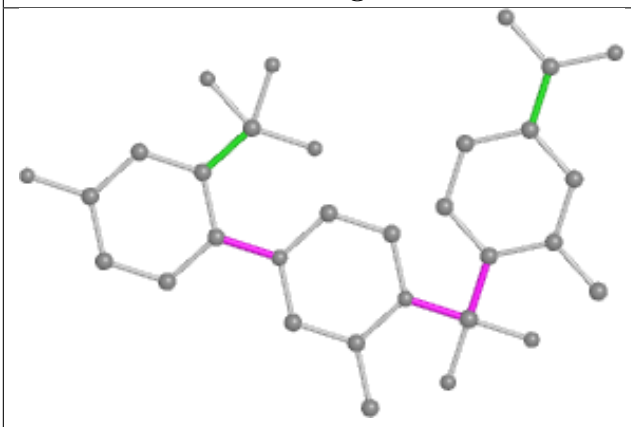
Ligand 33T B 293



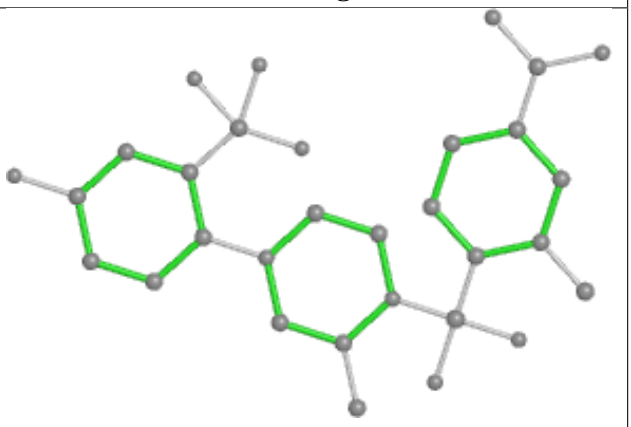
Bond lengths



Bond angles

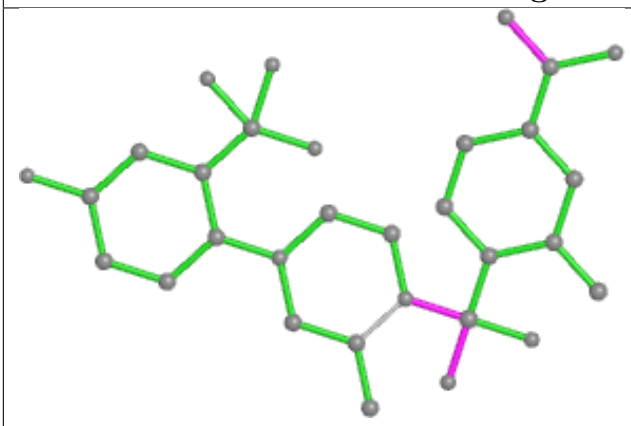


Torsions

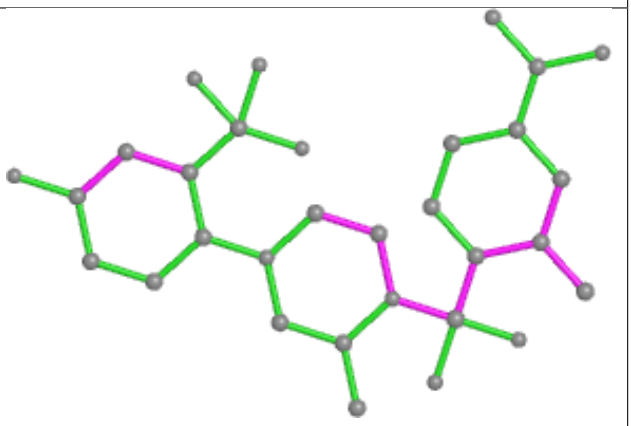


Rings

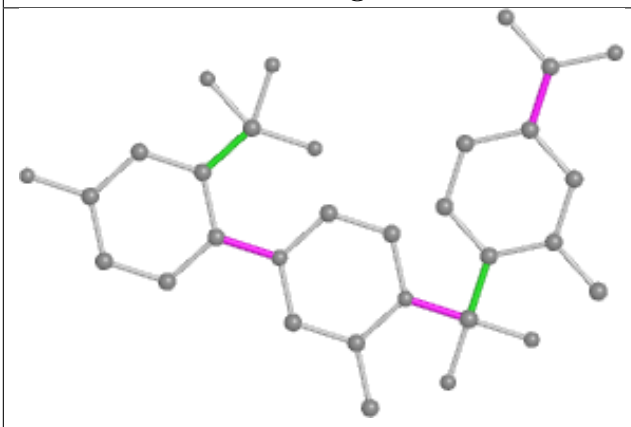
Ligand 33T D 293



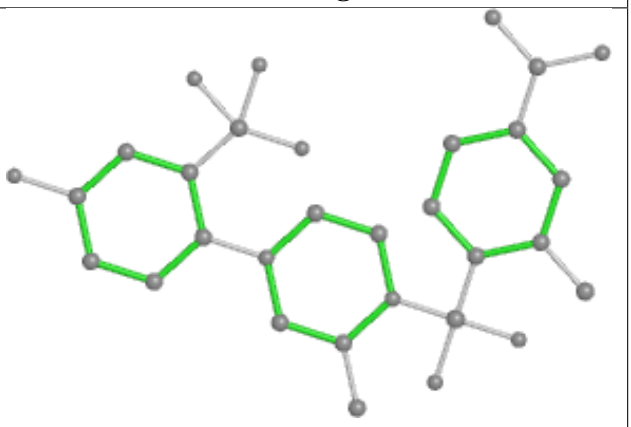
Bond lengths



Bond angles

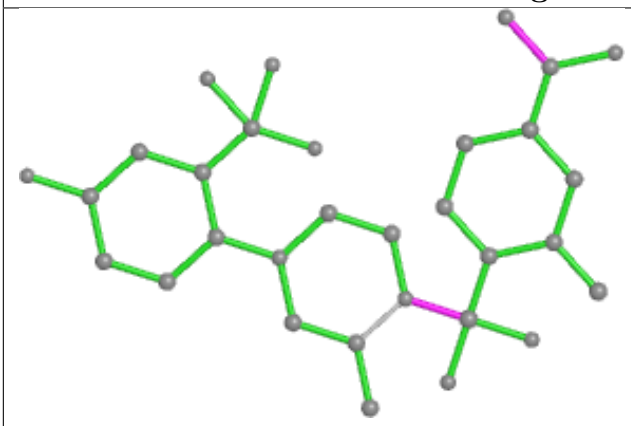


Torsions

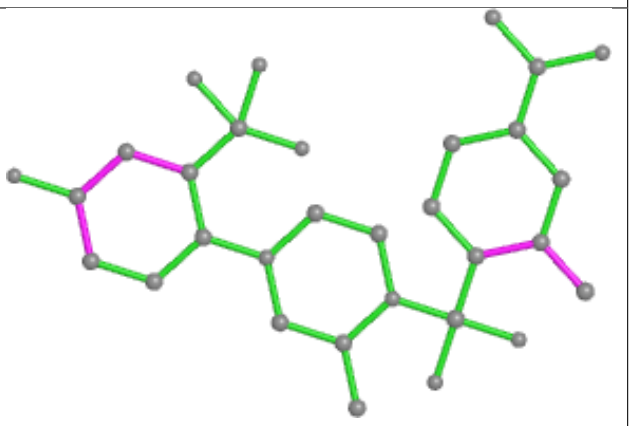


Rings

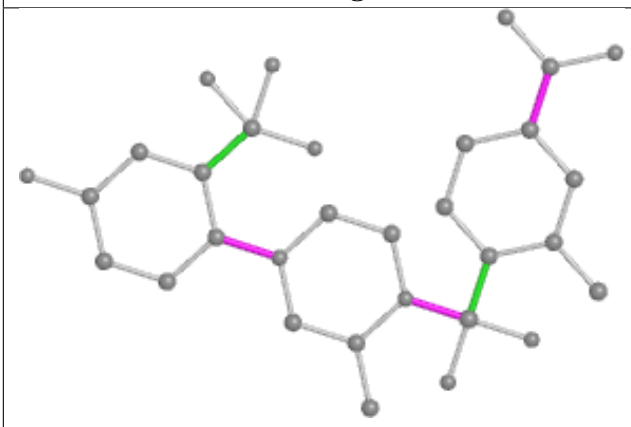
Ligand 33T A 293



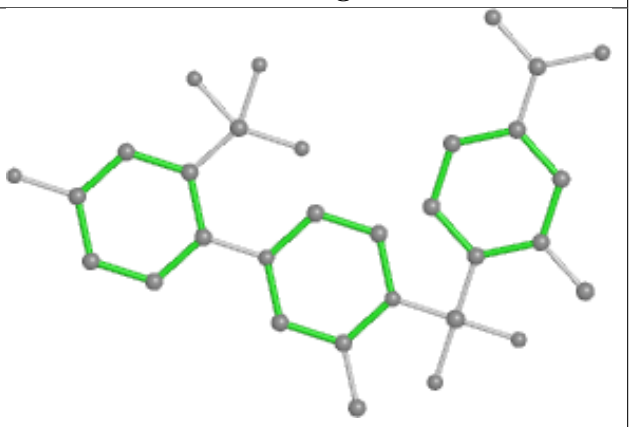
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	260/286 (90%)	-0.11	9 (3%)	44	44	21, 42, 88, 130	2 (0%)
1	B	261/286 (91%)	-0.01	12 (4%)	32	33	23, 44, 84, 116	3 (1%)
1	C	260/286 (90%)	-0.04	13 (5%)	28	30	20, 39, 85, 127	2 (0%)
1	D	256/286 (89%)	0.09	11 (4%)	35	36	20, 53, 91, 128	6 (2%)
All	All	1037/1144 (90%)	-0.02	45 (4%)	35	36	20, 45, 87, 130	13 (1%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	262	LEU	4.9
1	C	231	VAL	4.3
1	C	263	TRP	4.1
1	A	263	TRP	3.8
1	C	279	LEU	3.7
1	C	232	HIS	3.4
1	A	229	GLY	3.4
1	A	279	LEU	3.3
1	D	230	ILE	3.3
1	B	24	ASN	3.0
1	C	24	ASN	3.0
1	B	229	GLY	3.0
1	B	230	ILE	2.9
1	A	278	PHE	2.9
1	D	280	TYR	2.9
1	C	230	ILE	2.8
1	D	213	CYS	2.8
1	B	167	VAL	2.7
1	A	205	ARG	2.6
1	B	280[A]	TYR	2.6
1	D	231	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	190	LEU	2.6
1	C	283	SER	2.6
1	B	166	VAL	2.6
1	C	282	THR	2.5
1	B	118	LEU	2.4
1	A	117	ILE	2.4
1	D	233	MET	2.4
1	B	282	THR	2.4
1	B	168	VAL	2.3
1	D	278	PHE	2.3
1	D	188	PHE	2.2
1	D	169	SER	2.2
1	C	167	VAL	2.2
1	A	190	LEU	2.1
1	D	168	VAL	2.1
1	A	230	ILE	2.1
1	A	203	VAL	2.1
1	B	213	CYS	2.1
1	C	228	SER	2.1
1	C	233	MET	2.1
1	B	147	TYR	2.1
1	D	263	TRP	2.1
1	C	203	VAL	2.0
1	C	229	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

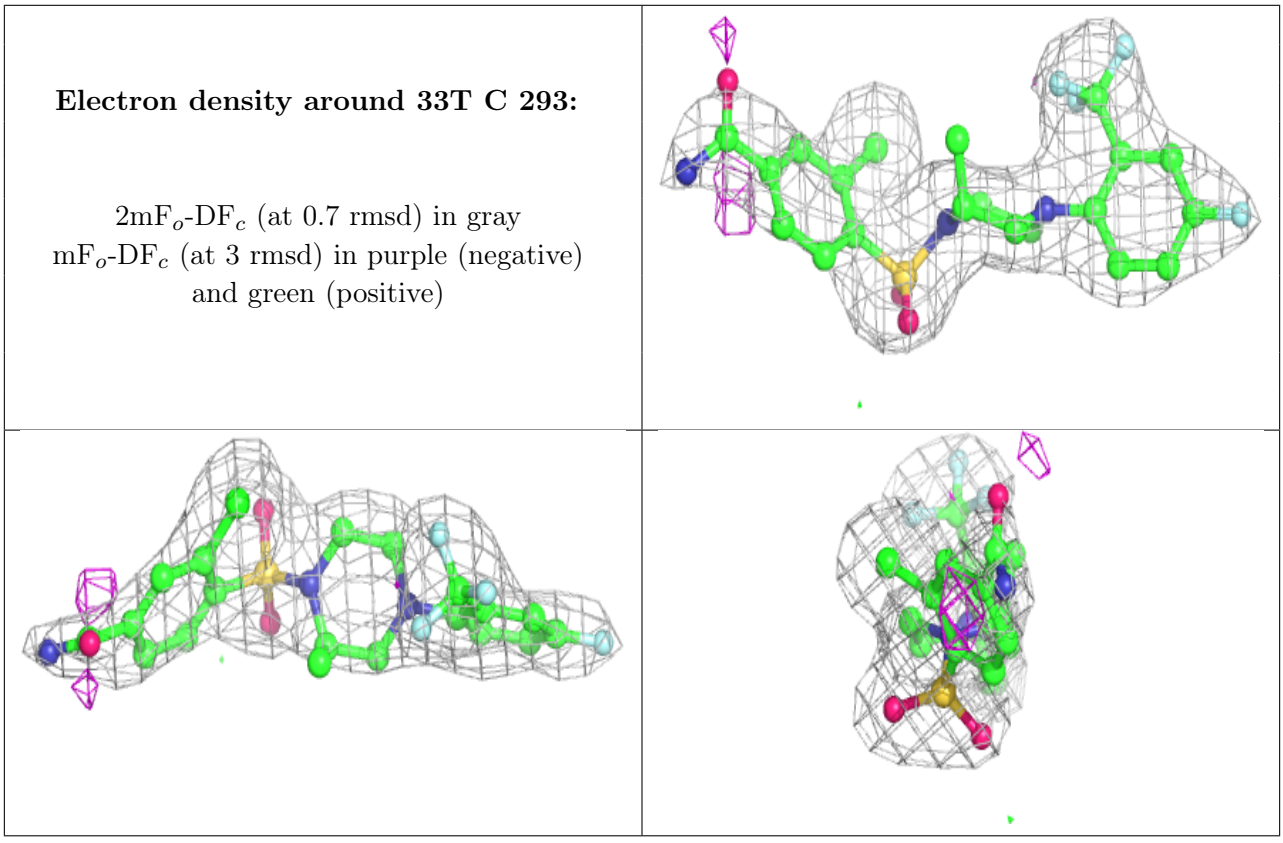
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	33T	C	293	31/31	0.96	0.12	31,63,100,129	0
2	NAP	D	1	48/48	0.97	0.10	24,47,70,77	0
3	33T	A	293	31/31	0.97	0.10	35,55,87,136	0
2	NAP	A	1	48/48	0.97	0.10	18,37,55,58	0
3	33T	D	293	31/31	0.97	0.12	33,64,125,128	0
3	33T	B	293	31/31	0.98	0.09	24,56,105,120	0
2	NAP	B	1	48/48	0.98	0.09	12,41,73,111	0
2	NAP	C	1	48/48	0.98	0.12	17,35,57,82	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.

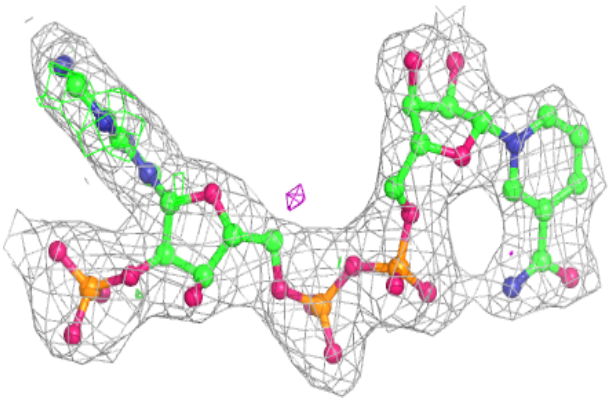
Electron density around 33T C 293:

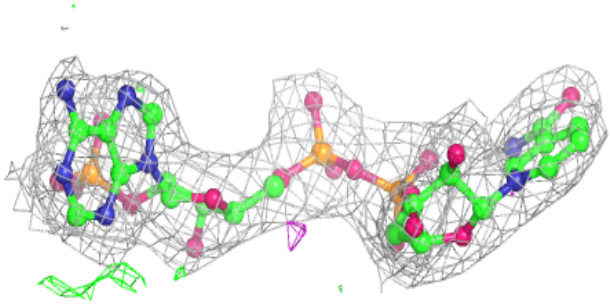
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

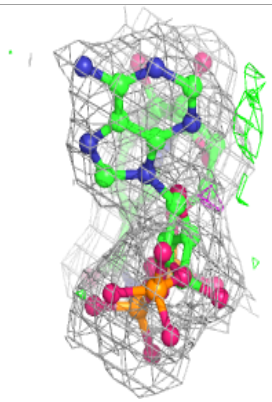


Electron density around NAP D 1:

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

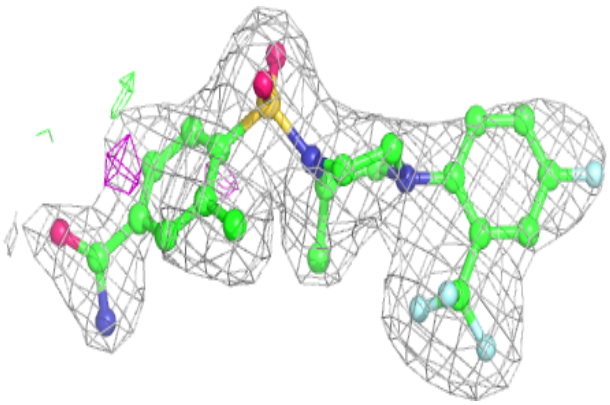


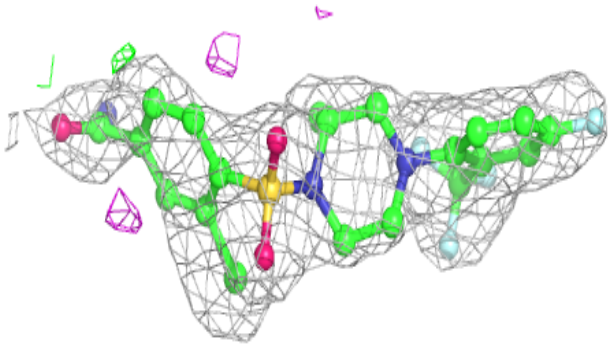


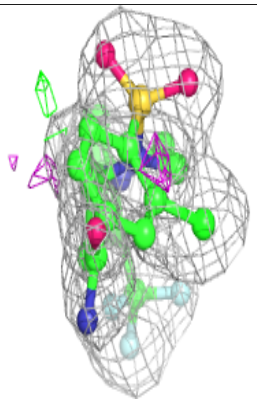


Electron density around 33T A 293:

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

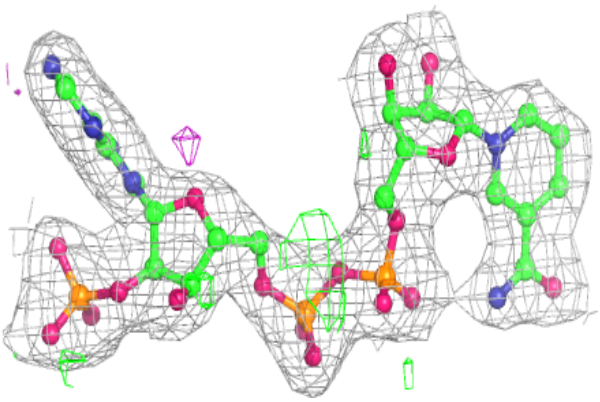


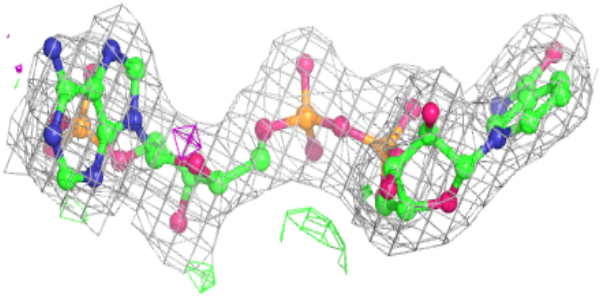


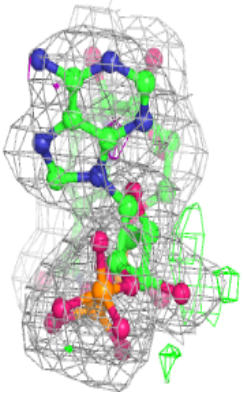


Electron density around NAP A 1:

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

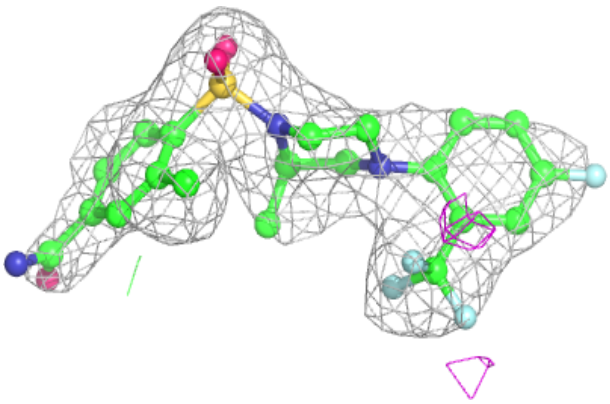


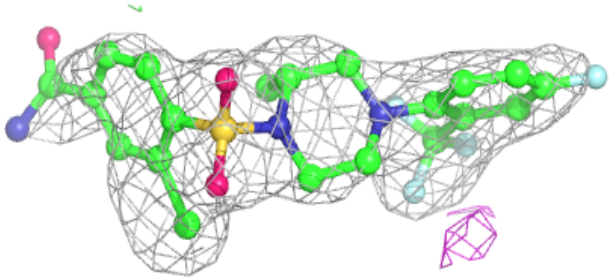


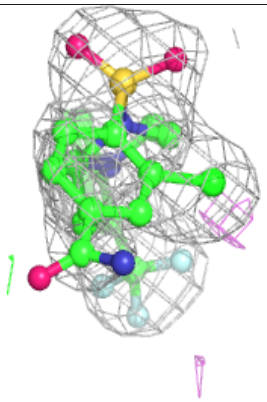


Electron density around 33T D 293:

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

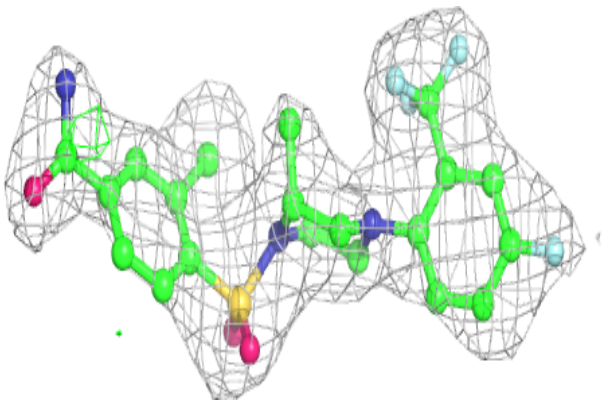


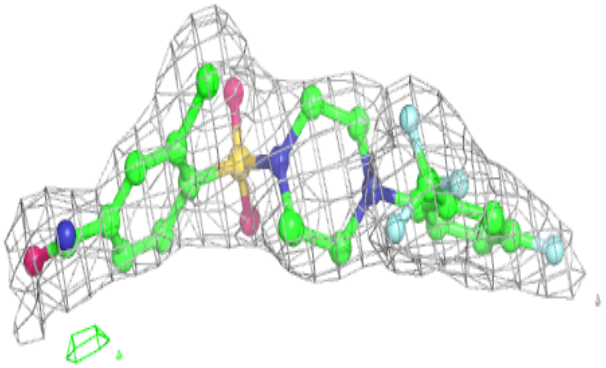


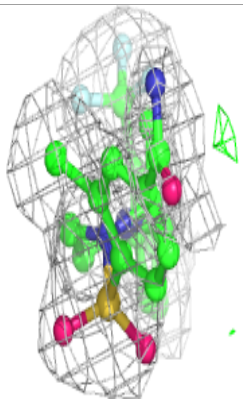


Electron density around 33T B 293:

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

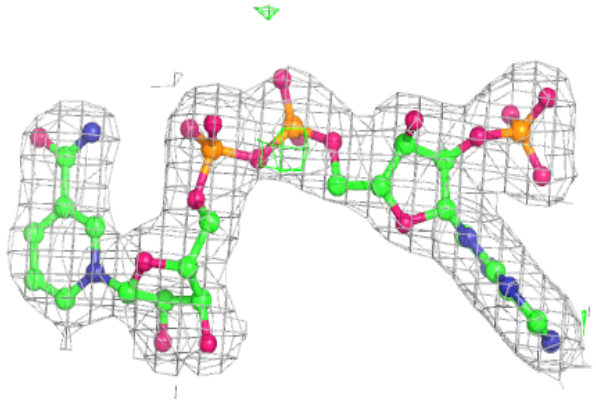


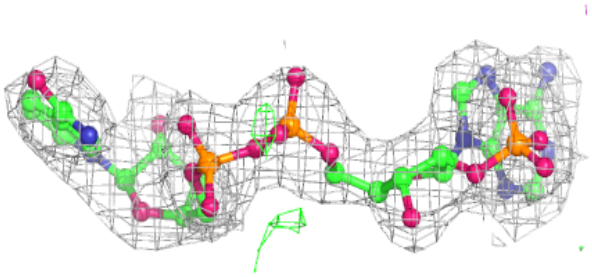


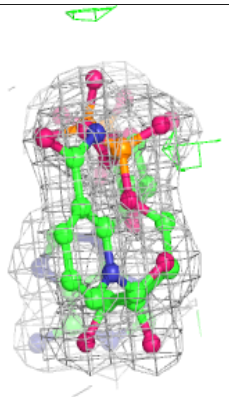


Electron density around NAP B 1:

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

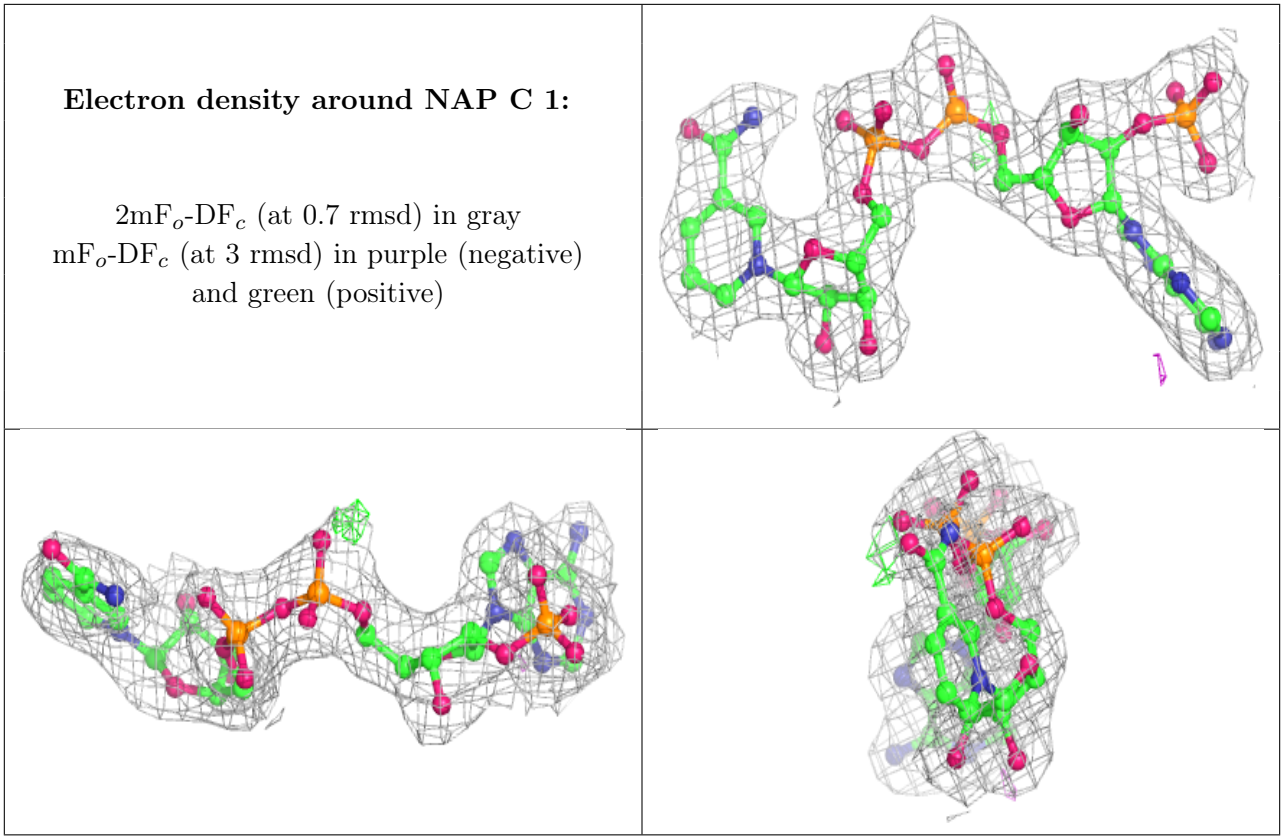






Electron density around NAP C 1:

$2mF_o$-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 (i)

There are no such residues in this entry.