



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:47 PM EDT

PDB ID : 3HFG / pdb_00003hfg
Title : Crystal Structure of Human 11-beta-hydroxysteroid-dehydrogenase Bound to an Sulfonyl-piperazine Inhibitor
Authors : Bard, J.; Svenson, K.
Deposited on : 2009-05-11
Resolution : 2.30 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

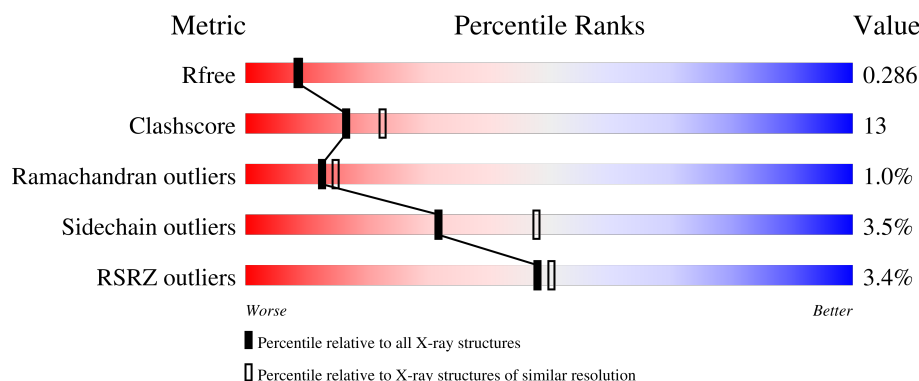
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	
1	B	286	
1	C	286	
1	D	286	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8217 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	258	Total	C	N	O	S	1	0	0
			1959	1248	331	365	15			
1	B	260	Total	C	N	O	S	3	0	0
			1977	1260	335	367	15			
1	C	254	Total	C	N	O	S	3	0	0
			1914	1217	327	356	14			
1	D	254	Total	C	N	O	S	0	0	0
			1905	1209	326	356	14			

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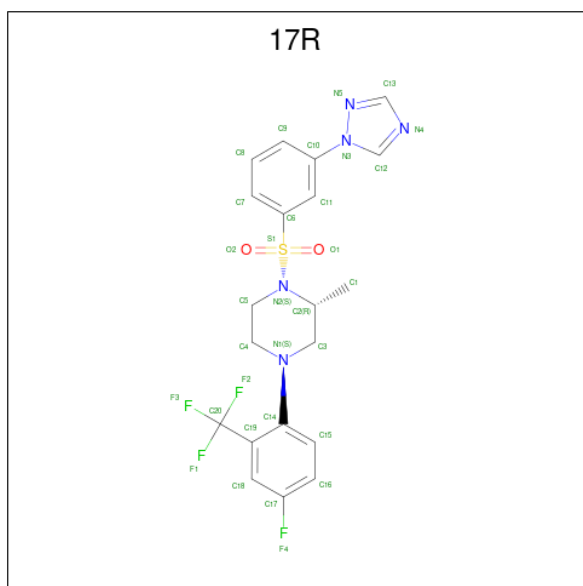
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	expression tag	UNP P28845
B	11	HIS	-	expression tag	UNP P28845
B	12	GLN	-	expression tag	UNP P28845
B	13	HIS	-	expression tag	UNP P28845
B	14	GLN	-	expression tag	UNP P28845
B	15	HIS	-	expression tag	UNP P28845
B	16	GLN	-	expression tag	UNP P28845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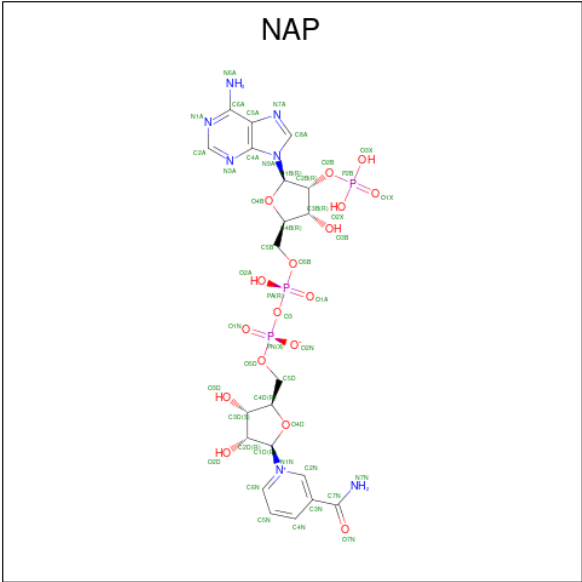
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	expression tag	UNP P28845
D	17	HIS	-	expression tag	UNP P28845
D	18	GLN	-	expression tag	UNP P28845
D	19	HIS	-	expression tag	UNP P28845
D	20	GLN	-	expression tag	UNP P28845
D	21	GLN	-	expression tag	UNP P28845
D	22	PRO	-	expression tag	UNP P28845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

- Molecule 2 is (2R)-4-[4-fluoro-2-(trifluoromethyl)phenyl]-2-methyl-1-{[3-(1H-1,2,4-triazol-1-yl)phenyl]sulfonyl}piperazine (CCD ID: 17R) (formula: C₂₀H₁₉F₄N₅O₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			32	20	4	5	2	1		
2	B	1	Total	C	F	N	O	S	0	0
			32	20	4	5	2	1		
2	C	1	Total	C	F	N	O	S	0	0
			32	20	4	5	2	1		
2	D	1	Total	C	F	N	O	S	0	0
			32	20	4	5	2	1		

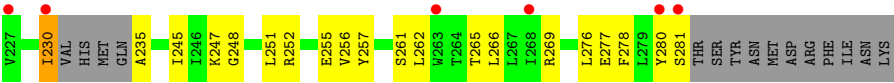
- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



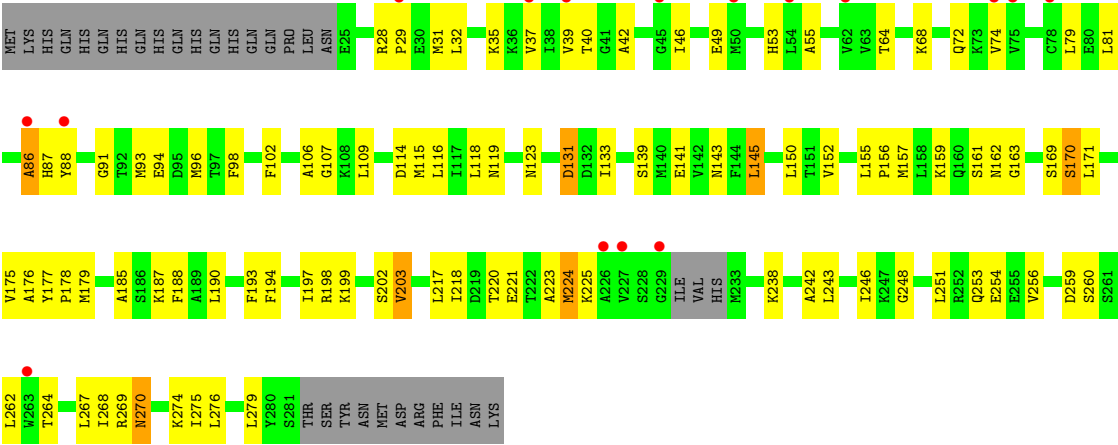
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	26	Total	O	0	0
			26	26		
4	C	52	Total	O	0	0
			52	52		
4	D	22	Total	O	0	0
			22	22		



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.44Å 152.67Å 74.20Å 90.00° 92.41° 90.00°	Depositor
Resolution (Å)	28.23 – 2.30 28.23 – 2.31	Depositor EDS
% Data completeness (in resolution range)	83.9 (28.23-2.30) 83.9 (28.23-2.31)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.31Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.4_6	Depositor
R, R_{free}	0.231 , 0.285 0.229 , 0.286	Depositor DCC
R_{free} test set	2330 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8217	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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: 17R, 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	0.36	0/1991	0.76	2/2689 (0.1%)
1	B	0.33	0/2009	0.71	0/2711
1	C	0.37	0/1943	0.78	0/2622
1	D	0.34	0/1934	0.78	4/2612 (0.2%)
All	All	0.35	0/7877	0.76	6/10634 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	270	ASN	CA-C-N	5.96	125.17	118.97
1	D	270	ASN	C-N-CA	5.96	125.17	118.97
1	D	106	ALA	N-CA-C	-5.52	106.59	113.55
1	A	270	ASN	CA-C-N	5.34	124.86	119.19
1	A	270	ASN	C-N-CA	5.34	124.86	119.19
1	D	94	GLU	N-CA-C	-5.28	105.53	111.28

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	1959	0	1993	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1977	0	2014	45	0
1	C	1914	0	1941	61	0
1	D	1905	0	1917	72	0
2	A	32	0	19	1	0
2	B	32	0	19	3	0
2	C	32	0	19	3	0
2	D	32	0	19	1	0
3	A	48	0	25	3	0
3	B	48	0	25	4	0
3	C	48	0	25	3	0
3	D	48	0	25	6	0
4	A	42	0	0	1	0
4	B	26	0	0	1	0
4	C	52	0	0	2	0
4	D	22	0	0	0	0
All	All	8217	0	8041	208	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 (208) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:MET:HE2	1:B:140:MET:HE2	1.54	0.88
1:D:39:VAL:HG12	1:D:42:ALA:HB2	1.61	0.83
1:A:233:MET:HG3	1:A:234:GLN:N	2.00	0.75
1:A:233:MET:HG3	1:A:234:GLN:H	1.52	0.74
1:A:133:ILE:HD13	1:B:149:VAL:HG22	1.71	0.72
1:C:171:LEU:HD12	2:C:1:17R:H7	1.72	0.72
1:D:223:ALA:HB2	3:D:293:NAP:H72N	1.55	0.71
1:C:39:VAL:HG12	1:C:42:ALA:HB2	1.74	0.69
1:B:64:THR:HB	1:B:102:PHE:CE1	2.29	0.68
1:B:91:GLY:HA3	1:B:98:PHE:CZ	2.29	0.67
1:D:46:ILE:HD11	1:D:218:ILE:HG13	1.75	0.66
1:C:60:HIS:C	1:C:110:MET:HE2	2.21	0.66
1:A:93:MET:HG2	3:A:293:NAP:H2A	1.77	0.66
1:C:62:VAL:HG23	1:C:110:MET:HE3	1.77	0.65
1:D:40:THR:HA	1:D:64:THR:HG22	1.78	0.65
1:D:64:THR:HB	1:D:102:PHE:CE1	2.32	0.65
1:D:141:GLU:HA	1:D:145:LEU:HB2	1.79	0.65
2:A:1:17R:C11	2:A:1:17R:H1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:LEU:HD21	1:D:86:ALA:HB3	1.79	0.64
1:C:134:HIS:HB2	4:C:324:HOH:O	1.99	0.63
1:C:180:VAL:HG23	1:C:180:VAL:O	1.99	0.63
1:D:91:GLY:HA3	1:D:98:PHE:CZ	2.35	0.62
1:D:139:SER:O	1:D:143:ASN:HB2	2.00	0.62
1:C:217:LEU:HD13	2:C:1:17R:H1B	1.83	0.61
1:C:261:SER:O	1:C:265:THR:HG23	2.01	0.61
1:B:39:VAL:HG12	1:B:42:ALA:HB2	1.82	0.61
2:B:1:17R:H1	2:B:1:17R:C11	2.33	0.59
1:C:193:PHE:HB2	1:D:185:ALA:HB2	1.85	0.58
1:D:118:LEU:HD22	1:D:150:LEU:HD12	1.84	0.58
1:D:72:GLN:HG2	1:D:88:TYR:CE2	2.40	0.57
1:A:194:PHE:HA	1:A:197:ILE:HG12	1.86	0.57
1:A:199:LYS:HE3	1:A:277:GLU:HB3	1.86	0.56
1:D:68:LYS:O	1:D:72:GLN:HG3	2.04	0.56
1:C:194:PHE:CD2	1:C:197:ILE:HD11	2.40	0.56
1:D:171:LEU:HD21	1:D:268:ILE:HD11	1.88	0.56
1:A:215:LEU:HD11	1:A:245:ILE:HD11	1.87	0.55
1:D:32:LEU:HA	1:D:35:LYS:HG3	1.87	0.55
1:C:137:ARG:O	1:C:141:GLU:HG2	2.07	0.55
1:A:233:MET:CG	1:A:234:GLN:N	2.70	0.55
1:D:55:ALA:HB1	1:D:81:LEU:HB2	1.89	0.55
1:C:280:TYR:O	1:C:281:SER:C	2.50	0.55
1:A:233:MET:CG	1:A:234:GLN:H	2.17	0.54
1:D:223:ALA:HB2	3:D:293:NAP:N7N	2.22	0.54
1:C:92:THR:OG1	1:C:94:GLU:HG3	2.07	0.54
1:A:185:ALA:HB2	1:B:193:PHE:HB2	1.89	0.54
1:A:48:ARG:NH2	1:A:73:LYS:HE3	2.23	0.54
1:B:40:THR:O	1:B:119:ASN:HB3	2.07	0.53
1:C:28:ARG:O	1:C:31:MET:HG3	2.08	0.53
1:C:93:MET:HG2	3:C:293:NAP:H2A	1.90	0.53
1:B:269:ARG:HH11	1:B:274:LYS:HE2	1.73	0.53
1:A:278:PHE:C	1:A:278:PHE:CD2	2.86	0.53
1:D:270:ASN:O	1:D:274:LYS:HG3	2.09	0.53
1:C:139:SER:O	1:C:143:ASN:HB2	2.10	0.52
1:C:230:ILE:C	1:C:230:ILE:HD13	2.34	0.52
1:D:187:LYS:HD2	1:D:190:LEU:HD12	1.90	0.52
1:D:107:GLY:HA3	1:D:157:MET:SD	2.50	0.52
1:D:40:THR:HA	1:D:64:THR:CG2	2.40	0.52
1:D:131:ASP:C	1:D:131:ASP:OD1	2.53	0.52
1:D:242:ALA:O	1:D:246:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:THR:HB	1:C:102:PHE:CE1	2.44	0.52
1:A:227:VAL:HG23	1:A:228:SER:N	2.25	0.51
1:B:261:SER:HG	1:B:263:TRP:CD1	2.27	0.51
1:C:43:SER:HB3	1:C:65:ALA:HB3	1.92	0.51
1:A:32:LEU:HA	1:A:35:LYS:HG3	1.92	0.51
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.93	0.51
1:C:251:LEU:C	1:C:252:ARG:HG3	2.35	0.51
1:D:248:GLY:HA3	1:D:256:VAL:HG21	1.91	0.51
1:A:155:LEU:HB3	1:A:156:PRO:HD3	1.92	0.50
1:B:66:ARG:HB2	3:B:293:NAP:O2X	2.11	0.50
1:D:102:PHE:CD2	1:D:102:PHE:C	2.89	0.50
1:C:26:GLU:O	1:C:31:MET:HE1	2.11	0.50
1:B:233:MET:HE1	2:B:1:17R:C8	2.42	0.50
1:D:49:GLU:HG3	1:D:238:LYS:HG3	1.93	0.50
1:D:194:PHE:HA	1:D:197:ILE:HG12	1.94	0.50
1:B:170:SER:OG	3:B:293:NAP:H6N	2.11	0.49
1:D:161:SER:O	1:D:162:ASN:C	2.55	0.49
1:A:280:TYR:CD2	1:B:233:MET:HE3	2.46	0.49
1:C:26:GLU:HG2	1:C:27:PHE:H	1.77	0.49
1:B:23:LEU:HD13	1:B:252:ARG:HD3	1.94	0.49
1:C:32:LEU:HD22	1:C:54:LEU:CD2	2.42	0.49
1:C:88:TYR:CD1	1:C:88:TYR:C	2.90	0.49
1:C:119:ASN:OD1	3:C:293:NAP:H4D	2.12	0.49
1:C:257:TYR:CE1	1:C:269:ARG:HG2	2.48	0.49
1:B:93:MET:HG2	3:B:293:NAP:H2A	1.95	0.49
1:B:114:ASP:O	1:B:163:GLY:HA3	2.14	0.48
1:D:40:THR:HG22	1:D:64:THR:HG21	1.95	0.48
1:A:279:LEU:HD11	1:B:263:TRP:CH2	2.47	0.48
1:D:224:MET:HA	1:D:224:MET:HE2	1.94	0.48
1:C:215:LEU:HD11	1:C:245:ILE:HD11	1.96	0.48
1:C:188:PHE:O	1:D:188:PHE:HB3	2.13	0.48
1:D:276:LEU:HA	1:D:279:LEU:HD12	1.96	0.48
1:C:194:PHE:HD2	1:C:197:ILE:HD11	1.79	0.47
1:D:264:THR:HA	1:D:267:LEU:HD12	1.96	0.47
1:D:175:VAL:CG2	1:D:177:TYR:CE1	2.97	0.47
1:B:46:ILE:HG13	1:B:220:THR:HG21	1.97	0.47
1:A:136:VAL:HG22	1:A:182:ALA:HB2	1.96	0.47
1:B:50:MET:O	1:B:54:LEU:HG	2.15	0.47
1:D:170:SER:HB3	3:D:293:NAP:H5N	1.96	0.47
1:A:46:ILE:HG22	1:A:50:MET:HE2	1.97	0.47
1:D:251:LEU:HB2	1:D:253:GLN:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:VAL:HG13	1:D:115:MET:HB3	1.97	0.46
1:D:178:PRO:O	1:D:179:MET:HB2	2.16	0.46
1:C:53:HIS:O	1:C:57:MET:HG3	2.15	0.46
1:C:63:VAL:HG23	1:C:71:LEU:HD22	1.97	0.46
1:C:171:LEU:CD1	2:C:1:17R:H7	2.44	0.46
1:C:178:PRO:O	1:C:179:MET:HB2	2.15	0.46
1:A:114:ASP:OD1	1:A:161:SER:HB2	2.16	0.46
1:B:134:HIS:HB2	4:B:308:HOH:O	2.16	0.46
1:C:27:PHE:CG	1:C:247:LYS:HG2	2.50	0.46
1:D:198:ARG:NH2	1:D:254:GLU:O	2.49	0.46
1:A:132:ASP:OD1	1:A:132:ASP:N	2.42	0.46
1:B:35:LYS:HA	1:B:35:LYS:HD3	1.75	0.45
1:B:114:ASP:OD1	1:B:161:SER:HB2	2.15	0.45
1:B:233:MET:HE1	2:B:1:17R:H8	1.98	0.45
1:D:177:TYR:CD2	2:D:1:17R:N5	2.84	0.45
1:D:169:SER:O	3:D:293:NAP:H6N	2.17	0.45
1:A:262:LEU:O	1:A:266:LEU:HD13	2.15	0.45
1:B:96:MET:HE3	1:B:141:GLU:OE2	2.17	0.45
1:B:105:GLN:O	1:B:109:LEU:HG	2.17	0.45
1:B:236:ALA:HB1	1:B:258:TYR:HE1	1.81	0.45
1:C:199:LYS:O	1:C:203:VAL:HG12	2.17	0.45
1:C:148:VAL:HG12	1:D:133:ILE:CD1	2.47	0.45
1:D:88:TYR:CD1	1:D:88:TYR:C	2.94	0.45
1:C:169:SER:O	3:C:293:NAP:H6N	2.17	0.45
1:B:244:GLU:HG3	1:B:258:TYR:CD2	2.51	0.45
1:C:178:PRO:O	1:C:179:MET:CB	2.64	0.45
1:A:223:ALA:HB2	3:A:293:NAP:H72N	1.82	0.44
1:B:170:SER:HB3	3:B:293:NAP:H5N	1.98	0.44
1:C:91:GLY:HA3	1:C:98:PHE:CZ	2.52	0.44
1:D:187:LYS:CD	1:D:190:LEU:HD12	2.48	0.44
1:C:43:SER:HB3	1:C:65:ALA:CB	2.48	0.44
1:B:62:VAL:HG11	1:B:106:ALA:HB2	2.00	0.44
1:D:28:ARG:NH1	1:D:31:MET:HE3	2.33	0.44
1:D:93:MET:HG2	3:D:293:NAP:H2A	1.98	0.44
1:A:156:PRO:HD2	4:A:317:HOH:O	2.17	0.44
1:C:269:ARG:HB2	4:C:340:HOH:O	2.16	0.44
1:C:140:MET:HE2	1:C:140:MET:HA	2.00	0.43
1:D:114:ASP:O	1:D:163:GLY:HA3	2.18	0.43
1:A:29:PRO:HB3	1:A:57:MET:HG2	2.00	0.43
1:B:201:TYR:CE2	1:B:210:ILE:HD11	2.53	0.43
1:C:196:SER:O	1:C:200:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HD12	1:A:276:LEU:HA	1.85	0.43
1:B:200:GLU:HA	1:B:203:VAL:HG22	2.00	0.43
1:A:137:ARG:NH2	1:B:96:MET:HG3	2.33	0.43
1:B:91:GLY:HA3	1:B:98:PHE:CE2	2.53	0.43
1:D:86:ALA:C	1:D:87:HIS:HD2	2.26	0.43
1:D:116:LEU:HD11	1:D:118:LEU:HD21	2.00	0.43
1:A:281:SER:C	1:A:283:SER:N	2.77	0.43
1:B:39:VAL:CG1	1:B:42:ALA:HB2	2.47	0.43
1:D:86:ALA:C	1:D:87:HIS:CD2	2.97	0.43
1:C:140:MET:HE2	1:C:186:SER:HB3	2.01	0.43
1:B:263:TRP:HE3	1:D:275:ILE:HD13	1.84	0.42
1:C:94:GLU:HG2	1:C:142:VAL:CG2	2.49	0.42
1:B:263:TRP:HB2	1:D:275:ILE:HG12	2.01	0.42
1:C:262:LEU:O	1:C:266:LEU:HG	2.20	0.42
1:C:278:PHE:C	1:C:280:TYR:H	2.25	0.42
1:D:53:HIS:CD2	1:D:243:LEU:HD13	2.54	0.42
1:D:217:LEU:O	1:D:218:ILE:HD13	2.19	0.42
1:C:212:LEU:O	1:C:255:GLU:HA	2.20	0.42
1:D:46:ILE:HG13	1:D:220:THR:HG21	2.01	0.42
1:A:28:ARG:HB2	1:A:30:GLU:OE2	2.19	0.42
1:A:236:ALA:HB1	1:A:237:PRO:HD2	2.01	0.42
1:A:237:PRO:HG2	1:A:240:GLU:HB2	2.01	0.42
1:C:185:ALA:HB2	1:D:193:PHE:HB2	2.01	0.42
1:A:170:SER:HB3	3:A:293:NAP:H5N	2.01	0.42
1:A:236:ALA:HB1	1:A:258:TYR:CE1	2.55	0.42
1:A:281:SER:O	1:A:282:THR:C	2.61	0.42
1:A:77:HIS:O	1:A:81:LEU:HG	2.20	0.42
1:B:36:LYS:HB3	1:B:110:MET:HE3	2.02	0.42
1:B:203:VAL:HG23	1:B:204:SER:N	2.34	0.42
1:C:194:PHE:HA	1:C:197:ILE:HG12	2.00	0.42
1:A:116:LEU:HG	1:A:118:LEU:HD21	2.02	0.42
1:A:281:SER:O	1:A:283:SER:N	2.53	0.42
1:D:269:ARG:NH1	1:D:274:LYS:NZ	2.67	0.42
1:B:46:ILE:HG13	1:B:220:THR:CG2	2.50	0.41
1:D:155:LEU:HB3	1:D:156:PRO:HD3	2.02	0.41
1:C:140:MET:HE3	1:C:140:MET:HB2	1.86	0.41
1:C:224:MET:HE2	1:C:235:ALA:HB3	2.02	0.41
1:A:257:TYR:CD2	1:A:268:ILE:HG21	2.55	0.41
1:A:263:TRP:N	1:A:263:TRP:CD1	2.89	0.41
1:C:168:VAL:O	1:C:187:LYS:NZ	2.53	0.41
1:D:119:ASN:OD1	3:D:293:NAP:H4D	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:PHE:CD2	1:A:197:ILE:HD11	2.55	0.41
1:D:116:LEU:HD11	1:D:118:LEU:CD2	2.51	0.41
1:D:199:LYS:O	1:D:203:VAL:HG13	2.21	0.41
1:B:221:GLU:O	1:B:225:LYS:HG3	2.20	0.41
1:C:64:THR:HB	1:C:102:PHE:CZ	2.55	0.41
1:C:133:ILE:O	1:C:133:ILE:HG13	2.19	0.41
1:B:242:ALA:O	1:B:246:ILE:HG13	2.21	0.41
1:D:259:ASP:CG	1:D:260:SER:N	2.79	0.41
1:A:279:LEU:HD11	1:B:263:TRP:CZ3	2.55	0.41
1:C:63:VAL:O	1:C:88:TYR:HA	2.21	0.41
1:D:87:HIS:ND1	1:D:109:LEU:HD23	2.36	0.41
1:D:171:LEU:HD23	1:D:171:LEU:HA	1.97	0.41
1:B:269:ARG:HH11	1:B:274:LYS:CE	2.34	0.41
1:D:155:LEU:HG	1:D:159:LYS:HE3	2.02	0.41
1:A:248:GLY:HA3	1:A:256:VAL:HG21	2.03	0.40
1:C:152:VAL:HG21	1:D:133:ILE:HD11	2.02	0.40
1:C:276:LEU:HD21	1:D:267:LEU:HB2	2.03	0.40
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.96	0.40
1:B:171:LEU:HD21	1:B:268:ILE:HD11	2.01	0.40
1:C:64:THR:O	1:C:65:ALA:HB2	2.21	0.40
1:A:155:LEU:HG	1:A:159:LYS:HE3	2.04	0.40
1:D:145:LEU:HD13	1:D:145:LEU:HA	1.78	0.40
1:D:221:GLU:OE2	1:D:225:LYS:HD2	2.21	0.40
1:D:93:MET:O	1:D:96:MET:CE	2.69	0.40
1:C:277:GLU:HG2	1:D:176:ALA:O	2.22	0.40
1:D:91:GLY:HA3	1:D:98:PHE:CE2	2.56	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	256/286 (90%)	240 (94%)	12 (5%)	4 (2%)	7	7
1	B	256/286 (90%)	236 (92%)	19 (7%)	1 (0%)	30	38
1	C	250/286 (87%)	234 (94%)	14 (6%)	2 (1%)	16	20
1	D	250/286 (87%)	227 (91%)	20 (8%)	3 (1%)	10	12
All	All	1012/1144 (88%)	937 (93%)	65 (6%)	10 (1%)	12	15

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	ILE
1	C	65	ALA
1	A	65	ALA
1	A	282	THR
1	B	65	ALA
1	D	86	ALA
1	A	228	SER
1	C	68	LYS
1	D	262	LEU
1	D	29	PRO

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	211/243 (87%)	205 (97%)	6 (3%)	38	56
1	B	213/243 (88%)	205 (96%)	8 (4%)	29	44
1	C	203/243 (84%)	197 (97%)	6 (3%)	36	53
1	D	201/243 (83%)	192 (96%)	9 (4%)	24	37
All	All	828/972 (85%)	799 (96%)	29 (4%)	32	48

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	THR

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Mol	Chain	Res	Type
1	A	145	LEU
1	A	170	SER
1	A	239	GLU
1	A	276	LEU
1	A	279	LEU
1	B	76	SER
1	B	97	THR
1	B	145	LEU
1	B	170	SER
1	B	184	SER
1	B	234	GLN
1	B	239	GLU
1	B	274	LYS
1	C	30	GLU
1	C	140	MET
1	C	145	LEU
1	C	170	SER
1	C	203	VAL
1	C	230	ILE
1	D	74	VAL
1	D	123	ASN
1	D	131	ASP
1	D	145	LEU
1	D	152	VAL
1	D	170	SER
1	D	202	SER
1	D	203	VAL
1	D	224	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	C	72	GLN
1	C	77	HIS
1	C	134	HIS
1	C	162	ASN
1	C	207	ASN
1	D	33	GLN
1	D	53	HIS
1	D	253	GLN

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	NAP	D	293	-	50,52,52	1.21	4 (8%)	71,80,80	1.70	12 (16%)
2	17R	B	1	-	34,35,35	1.27	2 (5%)	50,53,53	1.14	7 (14%)
3	NAP	B	293	-	50,52,52	1.12	4 (8%)	71,80,80	1.65	12 (16%)
2	17R	D	1	-	34,35,35	1.24	2 (5%)	50,53,53	1.35	3 (6%)
2	17R	A	1	-	34,35,35	1.15	2 (5%)	50,53,53	1.12	4 (8%)
2	17R	C	1	-	34,35,35	1.23	2 (5%)	50,53,53	1.24	6 (12%)
3	NAP	A	293	-	50,52,52	1.16	4 (8%)	71,80,80	1.65	12 (16%)
3	NAP	C	293	-	50,52,52	1.08	3 (6%)	71,80,80	1.64	14 (19%)

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	NAP	D	293	-	-	2/35/67/67	0/5/5/5
2	17R	B	1	-	-	9/26/39/39	0/4/4/4
3	NAP	B	293	-	-	5/35/67/67	0/5/5/5
2	17R	D	1	-	-	9/26/39/39	0/4/4/4
2	17R	A	1	-	-	11/26/39/39	0/4/4/4
2	17R	C	1	-	-	11/26/39/39	0/4/4/4
3	NAP	A	293	-	-	3/35/67/67	0/5/5/5
3	NAP	C	293	-	-	6/35/67/67	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	17R	S1-N2	5.21	1.71	1.63
2	D	1	17R	S1-N2	4.78	1.70	1.63
2	C	1	17R	S1-N2	4.27	1.69	1.63
2	A	1	17R	S1-N2	4.03	1.69	1.63
3	D	293	NAP	O4D-C1D	3.34	1.45	1.40
3	A	293	NAP	O4D-C1D	3.17	1.45	1.40
3	C	293	NAP	O4D-C1D	3.10	1.45	1.40
3	D	293	NAP	C2N-N1N	-3.07	1.31	1.35
3	A	293	NAP	PN-O3	2.94	1.62	1.59
3	B	293	NAP	O4D-C1D	2.77	1.44	1.40
3	C	293	NAP	C2N-N1N	-2.71	1.32	1.35
3	D	293	NAP	PA-O3	2.57	1.62	1.59
3	A	293	NAP	PA-O3	2.51	1.62	1.59
3	D	293	NAP	PN-O3	2.50	1.62	1.59
2	D	1	17R	C12-N3	2.48	1.38	1.34
2	A	1	17R	C12-N3	2.47	1.38	1.34
3	B	293	NAP	PN-O3	2.47	1.62	1.59
3	B	293	NAP	C2N-N1N	-2.47	1.32	1.35
2	B	1	17R	C12-N3	2.44	1.38	1.34
3	B	293	NAP	PA-O3	2.34	1.62	1.59
2	C	1	17R	C12-N3	2.28	1.37	1.34
3	A	293	NAP	C2N-N1N	-2.22	1.32	1.35
3	C	293	NAP	PN-O3	2.20	1.61	1.59

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	293	NAP	C5A-C4A-N3A	-5.81	118.72	126.72
3	A	293	NAP	C5A-C4A-N3A	-5.65	118.93	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	17R	C6-S1-N2	-5.59	97.60	107.36
3	B	293	NAP	C5A-C4A-N3A	-5.49	119.15	126.72
2	C	1	17R	C6-S1-N2	-5.39	97.96	107.36
3	C	293	NAP	C5A-C4A-N3A	-5.27	119.47	126.72
3	D	293	NAP	P2B-O2B-C2B	-5.17	109.63	123.43
3	D	293	NAP	N3A-C4A-N9A	4.67	135.12	127.17
3	A	293	NAP	N3A-C4A-N9A	4.61	135.01	127.17
3	B	293	NAP	N3A-C4A-N9A	4.44	134.71	127.17
3	C	293	NAP	N3A-C4A-N9A	4.30	134.48	127.17
2	D	1	17R	C2-C3-N1	4.21	117.08	110.86
3	B	293	NAP	C5A-N7A-C8A	4.13	109.93	103.45
3	A	293	NAP	N3A-C2A-N1A	-4.07	122.42	128.58
3	D	293	NAP	N3A-C2A-N1A	-4.06	122.44	128.58
3	B	293	NAP	N3A-C2A-N1A	-4.05	122.45	128.58
3	C	293	NAP	N3A-C2A-N1A	-4.03	122.49	128.58
3	B	293	NAP	P2B-O2B-C2B	-3.86	113.14	123.43
3	D	293	NAP	C5A-N7A-C8A	3.76	109.36	103.45
3	A	293	NAP	C2A-N3A-C4A	3.74	120.97	111.83
3	D	293	NAP	C2A-N3A-C4A	3.74	120.95	111.83
3	B	293	NAP	C2A-N3A-C4A	3.69	120.84	111.83
3	A	293	NAP	C5A-N7A-C8A	3.69	109.24	103.45
3	C	293	NAP	C5A-N7A-C8A	3.67	109.21	103.45
3	C	293	NAP	C2A-N3A-C4A	3.53	120.44	111.83
3	B	293	NAP	C4A-C5A-N7A	-3.33	106.77	110.58
2	A	1	17R	C20-C19-C14	-3.31	117.83	122.06
3	B	293	NAP	N9A-C8A-N7A	-3.13	109.50	113.94
3	C	293	NAP	P2B-O2B-C2B	-3.07	115.22	123.43
2	A	1	17R	C2-N2-S1	2.98	125.81	120.12
3	A	293	NAP	C4A-C5A-N7A	-2.93	107.23	110.58
3	A	293	NAP	C3N-C7N-N7N	2.93	121.35	117.74
3	A	293	NAP	P2B-O2B-C2B	-2.93	115.61	123.43
3	C	293	NAP	PN-O5D-C5D	-2.93	104.59	121.35
3	D	293	NAP	C4A-C5A-N7A	-2.92	107.24	110.58
3	C	293	NAP	C4A-C5A-N7A	-2.90	107.27	110.58
3	C	293	NAP	N9A-C8A-N7A	-2.85	109.89	113.94
3	B	293	NAP	PA-O5B-C5B	-2.82	105.18	121.35
3	B	293	NAP	PN-O5D-C5D	-2.73	105.72	121.35
3	A	293	NAP	N9A-C8A-N7A	-2.73	110.07	113.94
3	D	293	NAP	N9A-C8A-N7A	-2.61	110.23	113.94
3	C	293	NAP	C4D-O4D-C1D	-2.57	107.57	109.92
3	C	293	NAP	PA-O5B-C5B	-2.55	106.73	121.35
2	B	1	17R	C5-N2-C2	-2.52	112.73	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	293	NAP	PA-O5B-C5B	-2.51	106.95	121.35
2	B	1	17R	C2-C3-N1	2.44	114.47	110.86
3	D	293	NAP	PN-O5D-C5D	-2.43	107.42	121.35
2	B	1	17R	C7-C6-S1	-2.43	117.33	119.73
2	C	1	17R	C4-C5-N2	2.38	111.60	109.00
2	D	1	17R	C19-C18-C17	2.36	120.56	117.50
2	A	1	17R	C6-S1-N2	-2.34	103.27	107.36
2	A	1	17R	C18-C19-C20	2.34	122.28	116.60
2	B	1	17R	C20-C19-C14	-2.32	119.09	122.06
3	C	293	NAP	C5B-C4B-C3B	-2.27	107.03	115.21
3	C	293	NAP	O2B-C2B-C3B	-2.26	103.55	111.68
3	B	293	NAP	C3N-C7N-N7N	2.23	120.48	117.74
2	B	1	17R	C4-N1-C3	2.22	118.81	112.53
3	C	293	NAP	C3B-C2B-C1B	-2.20	98.59	102.81
2	C	1	17R	O1-S1-N2	2.19	110.80	106.97
2	C	1	17R	C5-N2-C2	2.18	118.95	116.06
3	A	293	NAP	PN-O5D-C5D	-2.16	108.97	121.35
3	D	293	NAP	O4B-C1B-N9A	2.12	112.16	108.09
3	B	293	NAP	O7N-C7N-N7N	-2.11	119.57	122.62
2	C	1	17R	C19-C18-C17	2.09	120.21	117.50
2	B	1	17R	C19-C18-C17	2.07	120.19	117.50
3	A	293	NAP	O2N-PN-O3	2.07	112.87	107.27
3	A	293	NAP	O7N-C7N-N7N	-2.06	119.64	122.62
2	C	1	17R	C18-C19-C20	2.02	121.49	116.60
3	D	293	NAP	C5N-C4N-C3N	-2.02	118.38	120.36
2	B	1	17R	C18-C19-C20	2.01	121.48	116.60

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	293	NAP	O4D-C4D-C5D-O5D
2	D	1	17R	C11-C6-S1-N2
2	D	1	17R	C5-N2-S1-O2
2	D	1	17R	C7-C6-S1-N2
3	C	293	NAP	C3D-C4D-C5D-O5D
2	C	1	17R	C11-C6-S1-N2
2	D	1	17R	C11-C6-S1-O1
3	B	293	NAP	O4B-C4B-C5B-O5B
2	D	1	17R	C7-C6-S1-O1
2	A	1	17R	C11-C6-S1-N2
2	C	1	17R	C11-C6-S1-O1

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Mol	Chain	Res	Type	Atoms
2	C	1	17R	C7-C6-S1-O1
2	A	1	17R	C11-C6-S1-O1
2	C	1	17R	C7-C6-S1-N2
2	A	1	17R	C7-C6-S1-O1
2	A	1	17R	C7-C6-S1-N2
2	C	1	17R	C5-N2-S1-O1
2	D	1	17R	C5-N2-S1-C6
2	A	1	17R	C15-C14-N1-C4
2	A	1	17R	C15-C14-N1-C3
2	C	1	17R	C15-C14-N1-C4
2	C	1	17R	C15-C14-N1-C3
2	B	1	17R	C15-C14-N1-C3
2	B	1	17R	C11-C6-S1-O1
3	C	293	NAP	C3B-C2B-O2B-P2B
2	B	1	17R	C7-C6-S1-O1
2	B	1	17R	C15-C14-N1-C4
2	C	1	17R	C5-N2-S1-O2
2	C	1	17R	C5-N2-S1-C6
2	D	1	17R	C5-N2-S1-O1
3	B	293	NAP	PN-O3-PA-O1A
2	A	1	17R	C5-N2-S1-O2
2	B	1	17R	C11-C6-S1-N2
2	A	1	17R	C5-N2-S1-O1
2	C	1	17R	C19-C14-N1-C4
2	B	1	17R	C7-C6-S1-N2
2	A	1	17R	C19-C14-N1-C3
2	B	1	17R	C19-C14-N1-C3
2	D	1	17R	C15-C14-N1-C4
2	A	1	17R	C19-C14-N1-C4
2	C	1	17R	C19-C14-N1-C3
3	A	293	NAP	C2B-O2B-P2B-O2X
2	D	1	17R	C15-C14-N1-C3
2	B	1	17R	C19-C14-N1-C4
3	C	293	NAP	O4B-C4B-C5B-O5B
3	D	293	NAP	O4B-C4B-C5B-O5B
2	A	1	17R	C5-N2-S1-C6
3	B	293	NAP	C2B-O2B-P2B-O3X
3	D	293	NAP	C2B-O2B-P2B-O2X
3	C	293	NAP	C2B-C1B-N9A-C8A
3	A	293	NAP	O4B-C4B-C5B-O5B
3	B	293	NAP	C3B-C4B-C5B-O5B
2	B	1	17R	C5-N2-S1-O2

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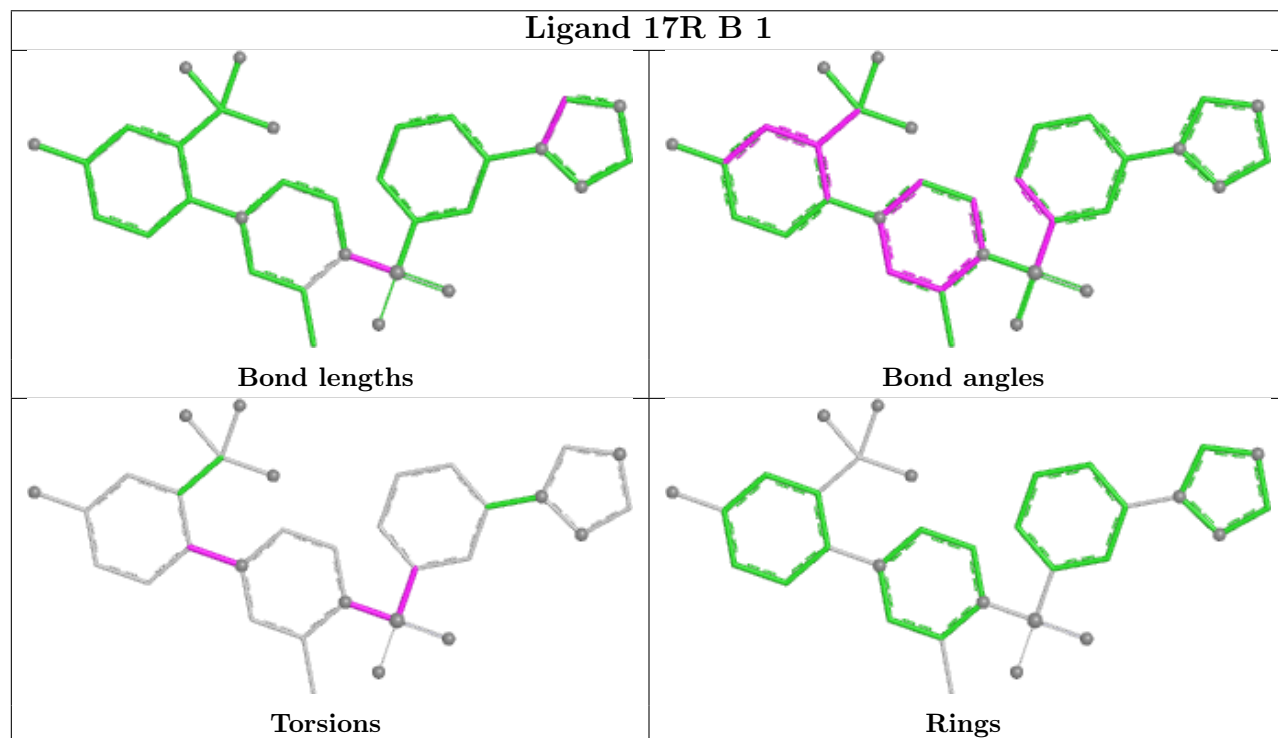
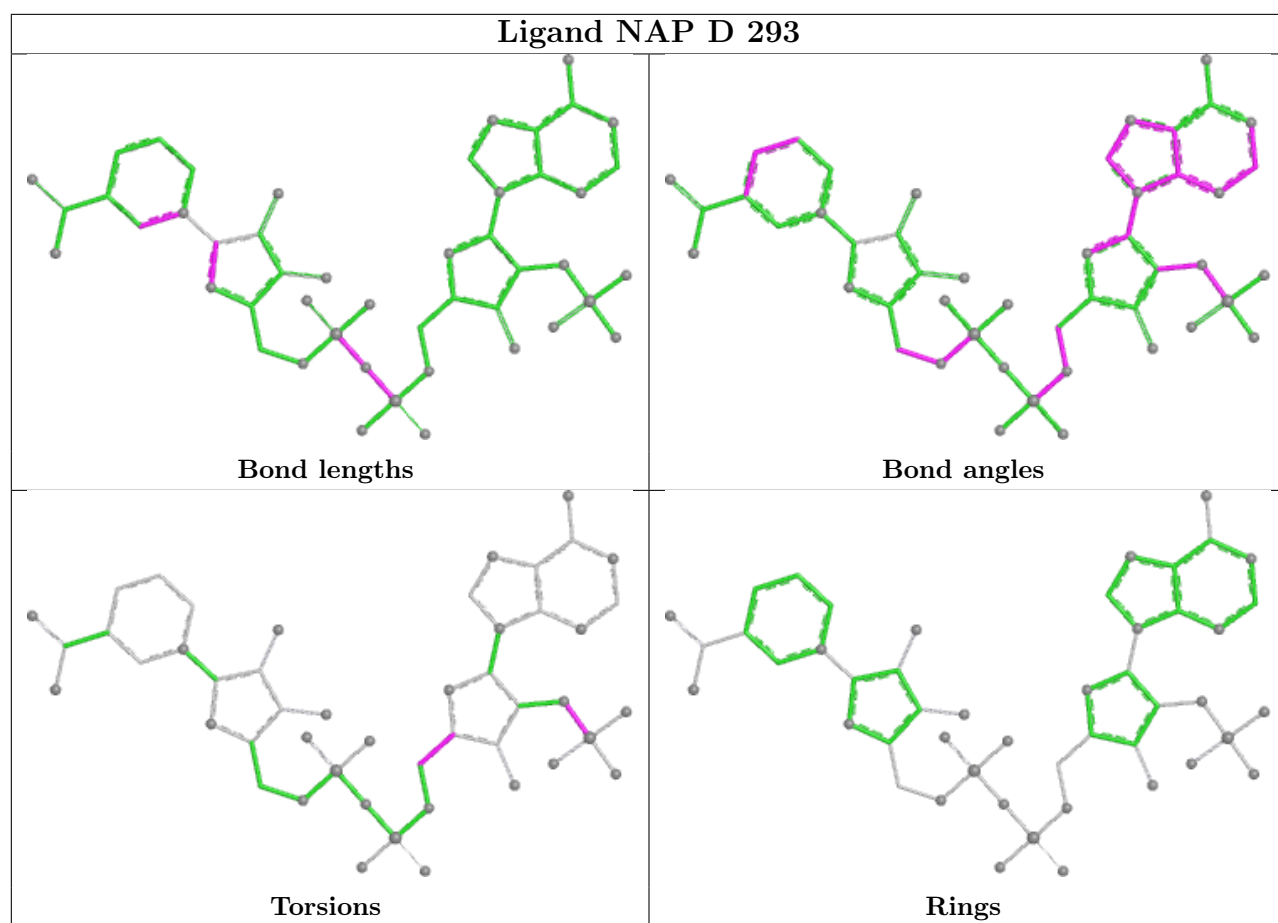
Mol	Chain	Res	Type	Atoms
3	A	293	NAP	PN-O3-PA-O2A
3	B	293	NAP	PN-O3-PA-O2A
3	C	293	NAP	PN-O3-PA-O2A

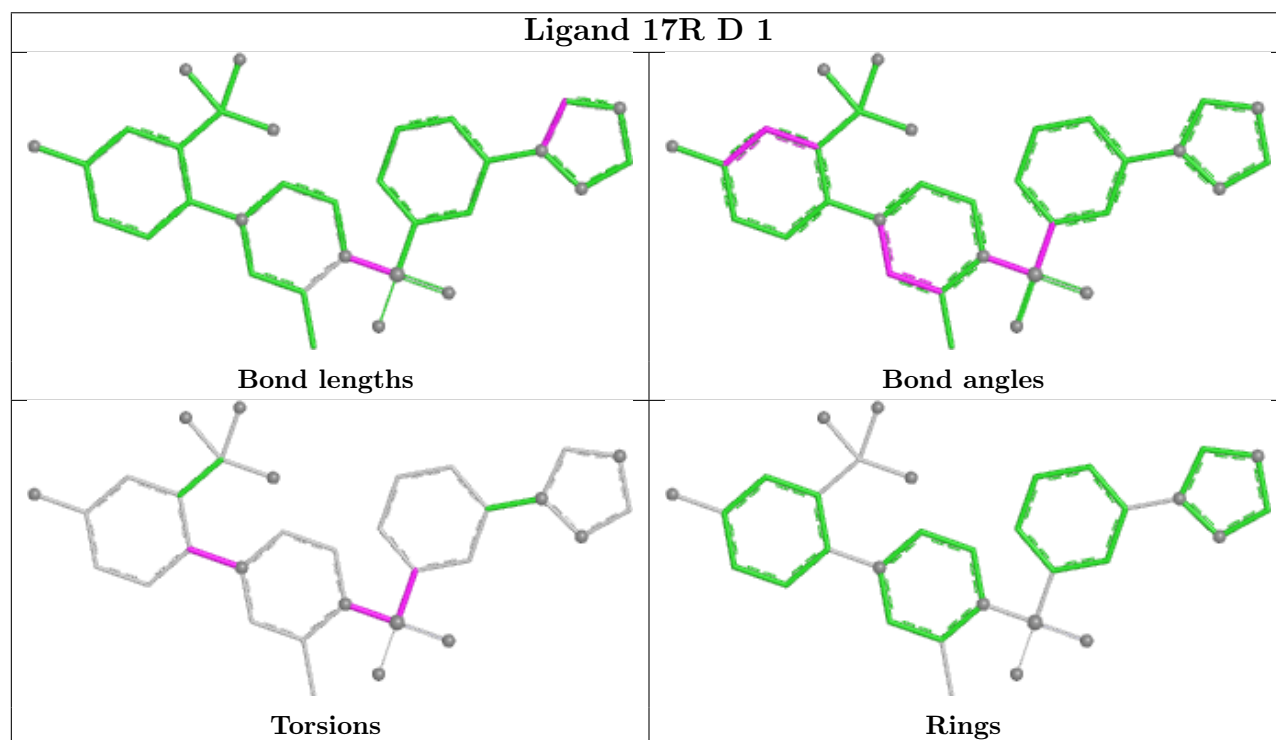
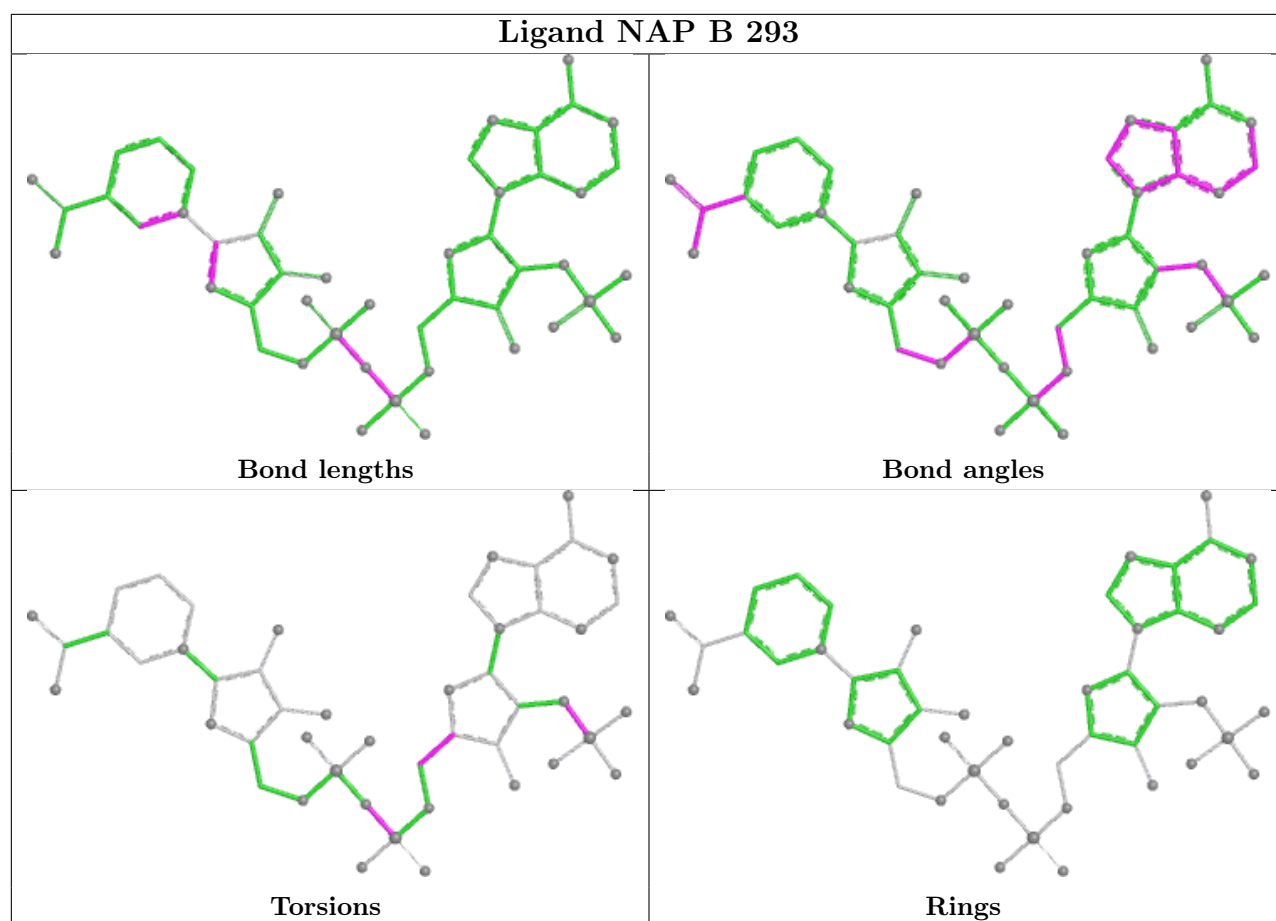
There are no ring outliers.

8 monomers are involved in 24 short contacts:

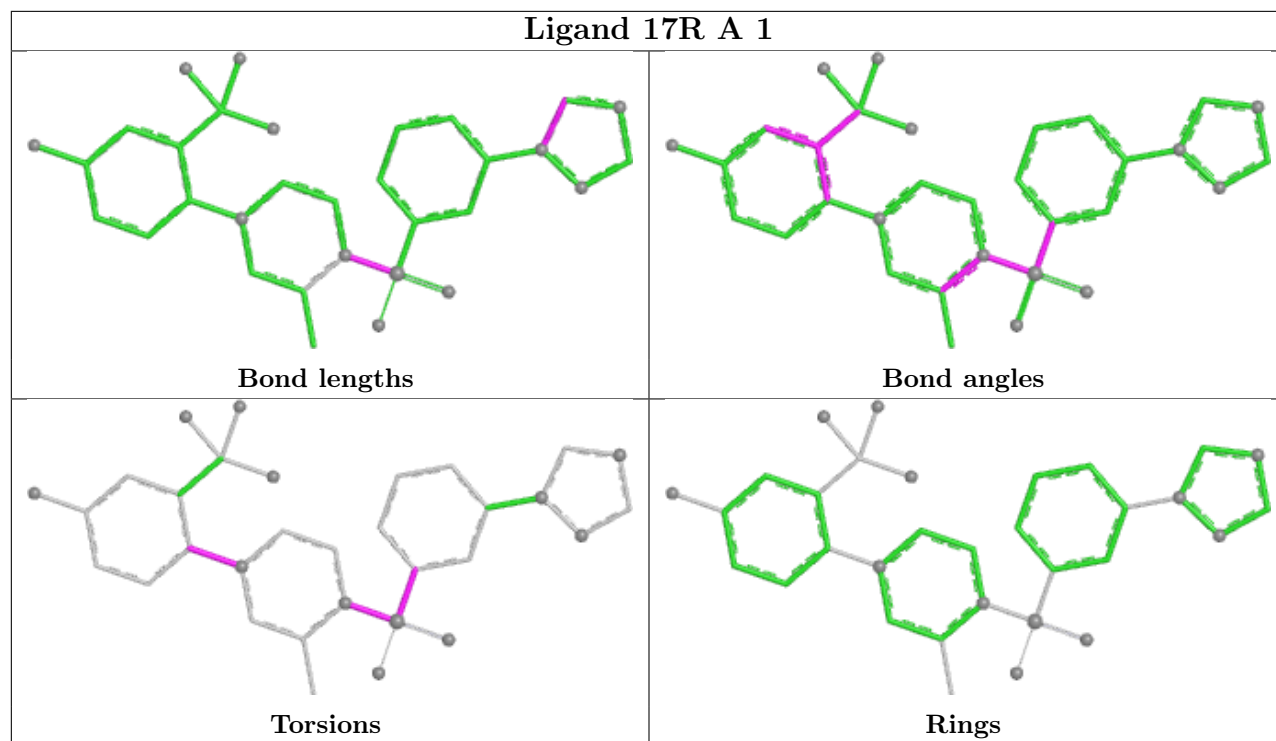
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	293	NAP	6	0
2	B	1	17R	3	0
3	B	293	NAP	4	0
2	D	1	17R	1	0
2	A	1	17R	1	0
2	C	1	17R	3	0
3	A	293	NAP	3	0
3	C	293	NAP	3	0

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.

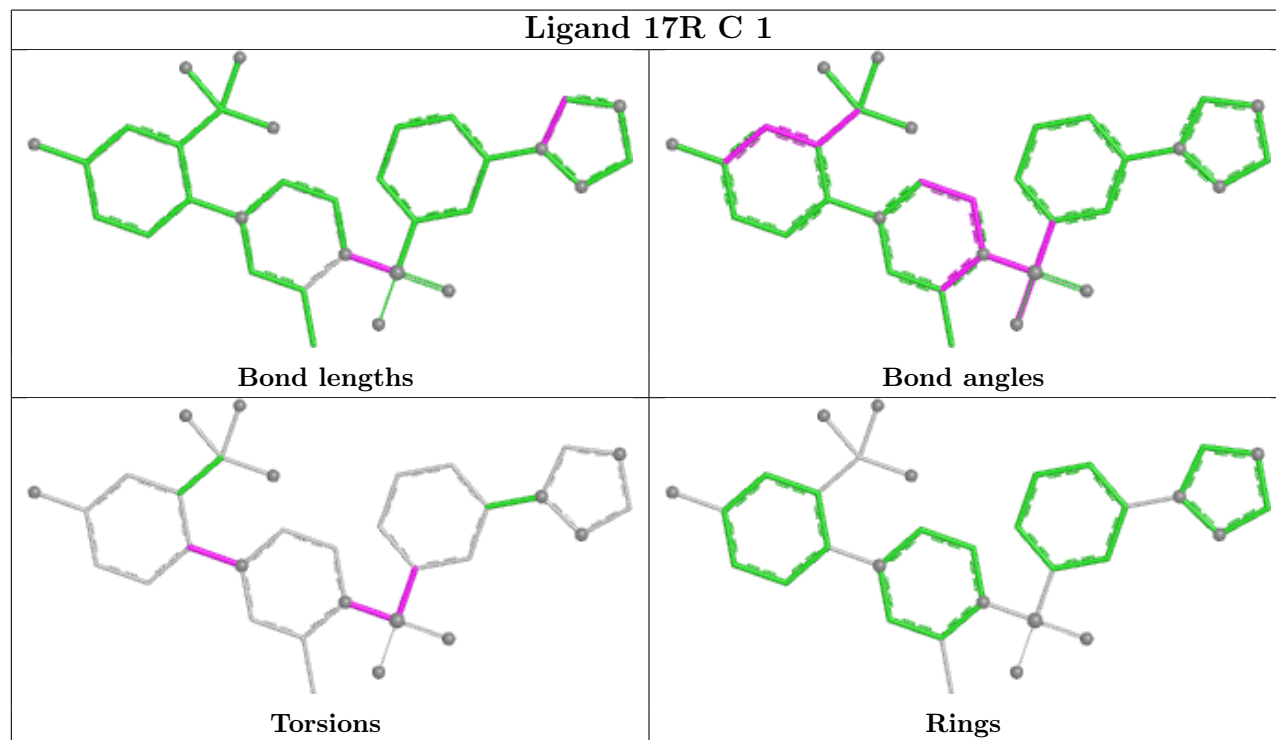


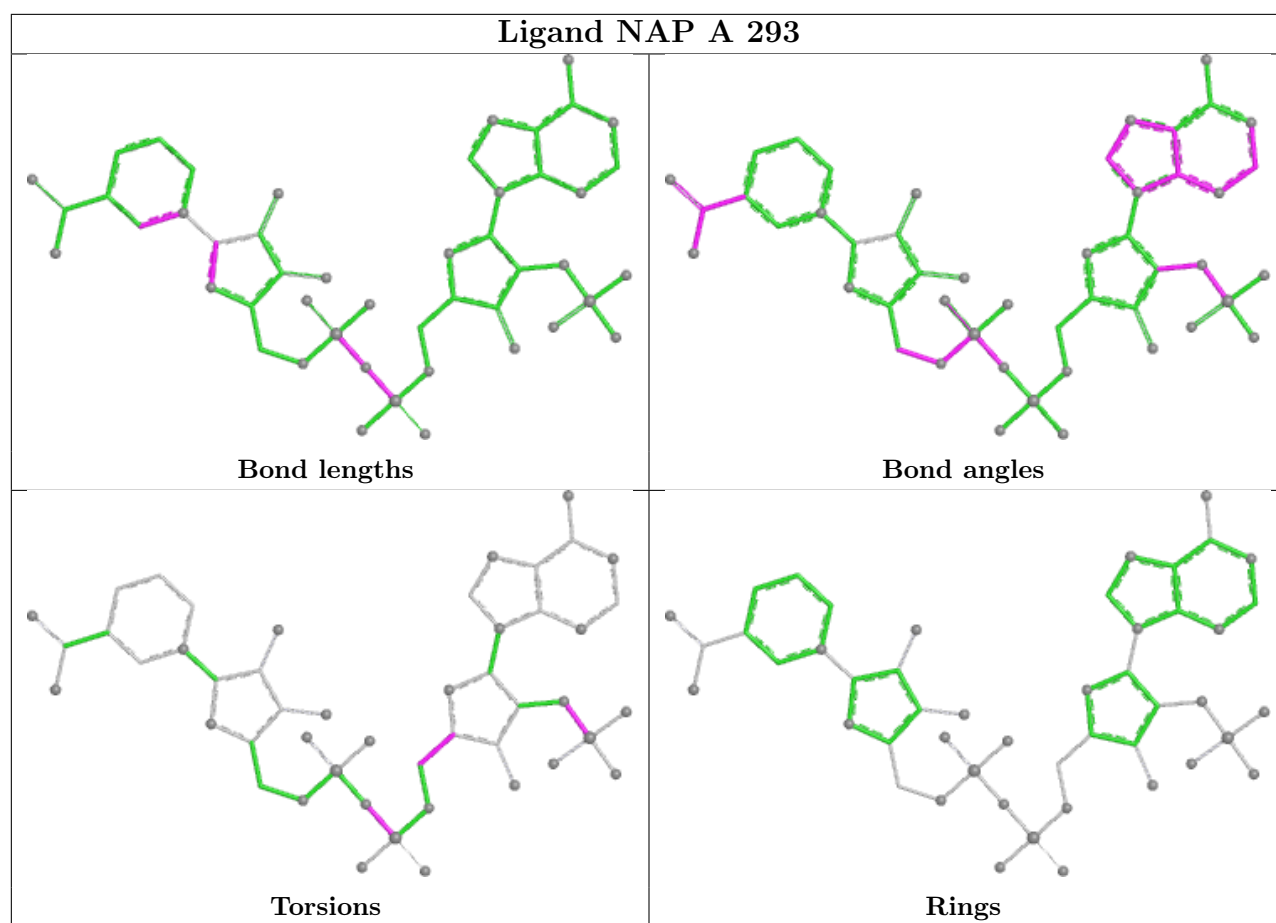


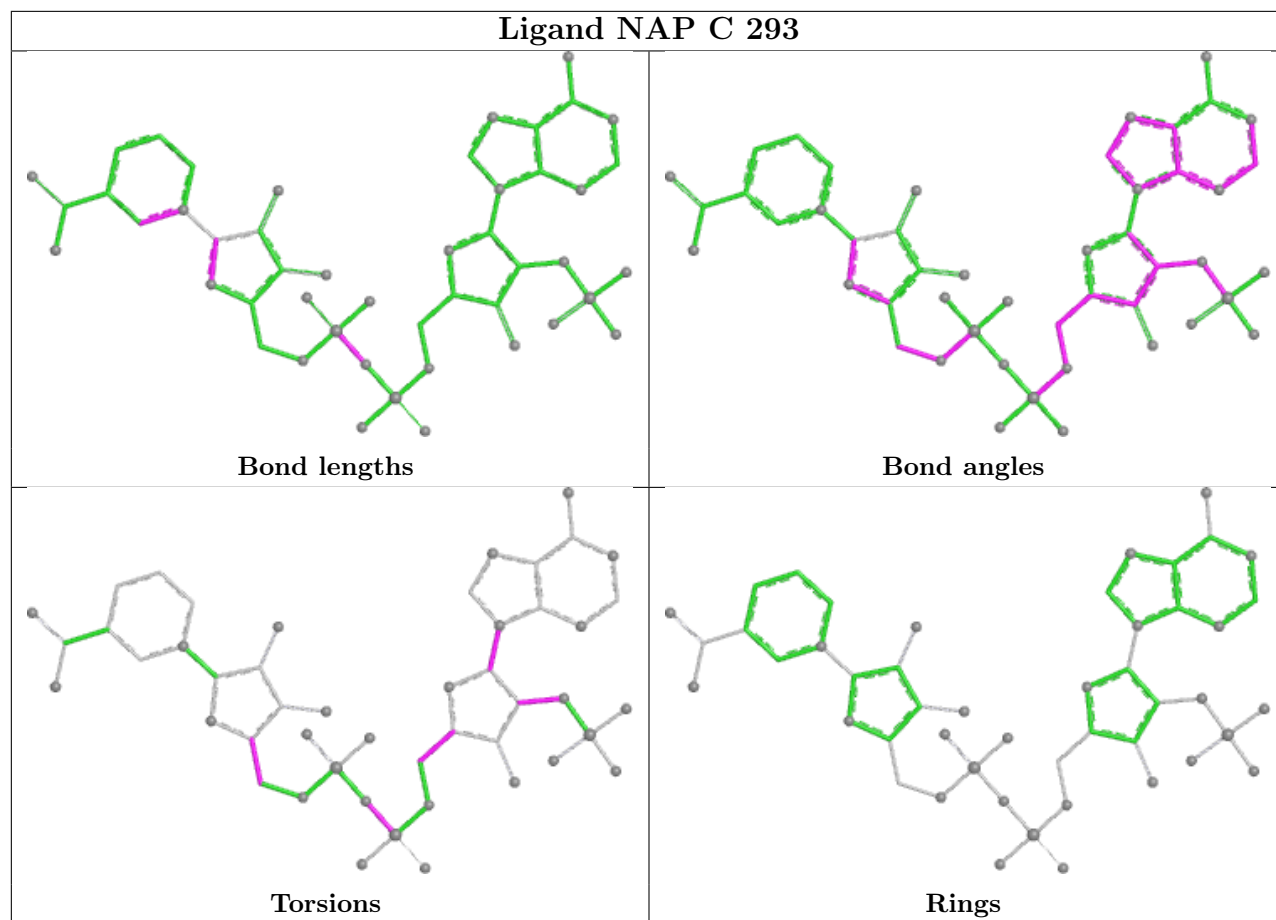
Ligand 17R A 1



Ligand 17R C 1







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	258/286 (90%)	0.30	7 (2%) 56 58	34, 50, 80, 98	2 (0%)
1	B	260/286 (90%)	0.36	2 (0%) 82 83	36, 54, 75, 97	4 (1%)
1	C	254/286 (88%)	0.39	10 (3%) 43 45	32, 49, 76, 90	2 (0%)
1	D	254/286 (88%)	0.79	16 (6%) 26 28	35, 62, 85, 94	4 (1%)
All	All	1026/1144 (89%)	0.46	35 (3%) 48 50	32, 53, 82, 98	12 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	230	ILE	3.5
1	D	75	VAL	3.3
1	D	29	PRO	3.2
1	A	227	VAL	3.1
1	A	263	TRP	3.0
1	C	281	SER	2.9
1	A	63	VAL	2.9
1	C	227	VAL	2.9
1	D	263	TRP	2.9
1	D	62	VAL	2.9
1	D	226	ALA	2.9
1	D	39	VAL	2.8
1	A	229	GLY	2.8
1	C	263	TRP	2.7
1	D	74	VAL	2.6
1	D	54	LEU	2.6
1	A	231	VAL	2.5
1	C	175	VAL	2.5
1	D	50	MET	2.5
1	D	78	CYS	2.5
1	D	45	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	227	VAL	2.4
1	C	268	ILE	2.4
1	B	81	LEU	2.4
1	D	88	TYR	2.3
1	C	280	TYR	2.2
1	A	228	SER	2.2
1	D	86	ALA	2.2
1	C	126	LEU	2.1
1	D	229	GLY	2.1
1	A	233	MET	2.1
1	C	130	HIS	2.1
1	D	37	VAL	2.1
1	B	83	ALA	2.0
1	C	172	ALA	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](#)

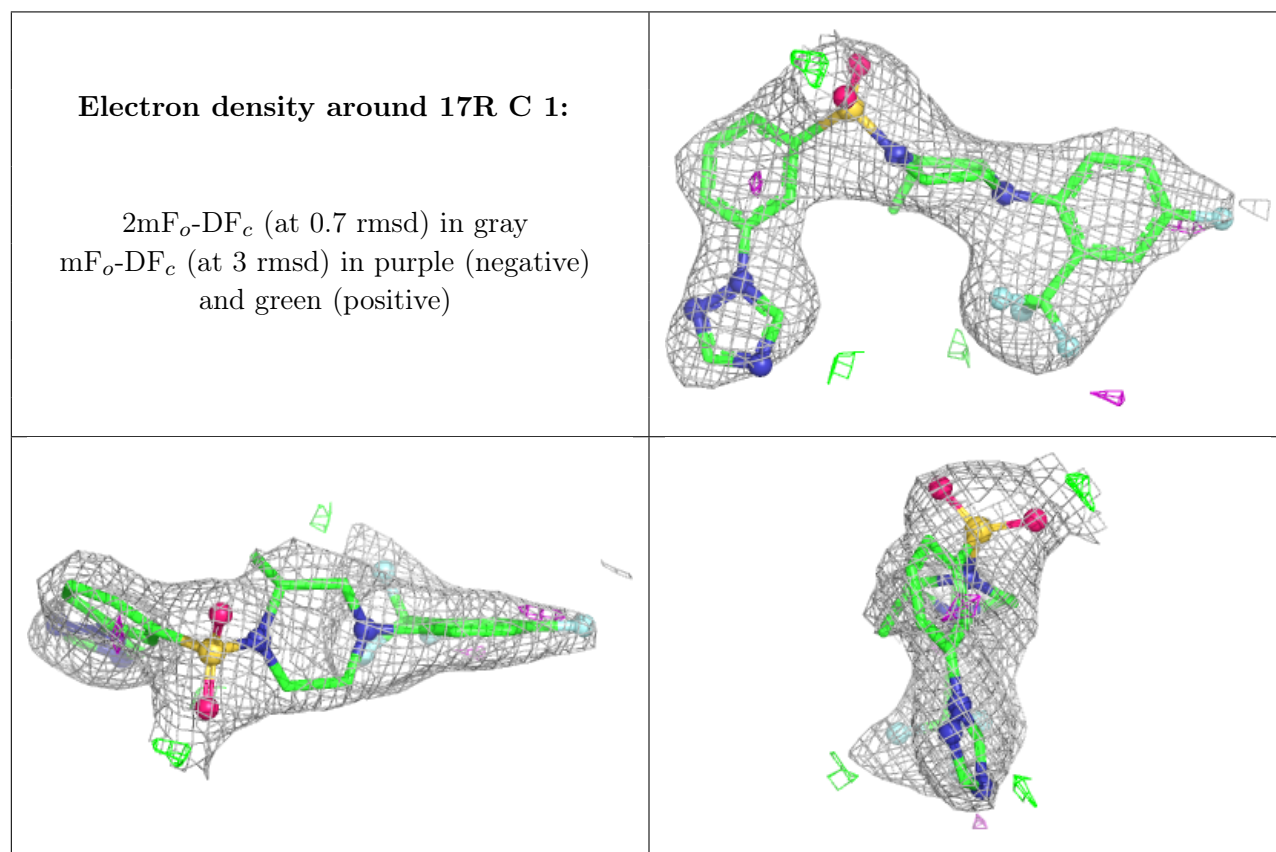
There are no oligosaccharides in this entry.

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.

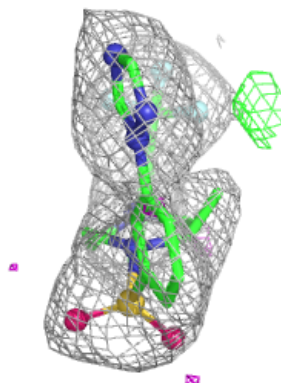
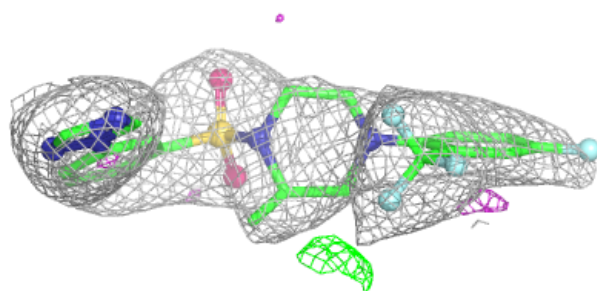
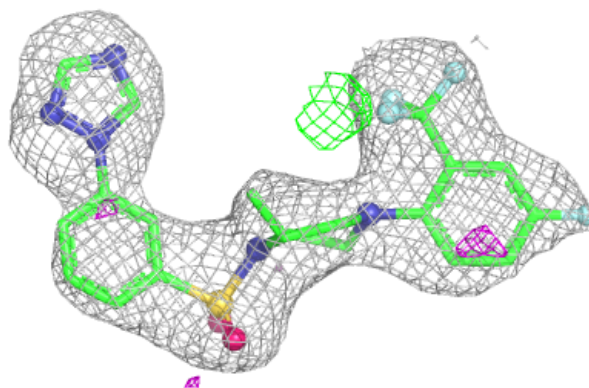
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	17R	C	1	32/32	0.91	0.11	38,58,71,73	0
2	17R	D	1	32/32	0.92	0.11	55,62,71,74	0
3	NAP	D	293	48/48	0.92	0.09	47,57,69,73	0
3	NAP	C	293	48/48	0.94	0.08	35,42,51,60	0
2	17R	A	1	32/32	0.94	0.11	42,51,61,66	0
3	NAP	B	293	48/48	0.95	0.07	37,47,56,61	0
2	17R	B	1	32/32	0.95	0.10	48,57,65,69	0
3	NAP	A	293	48/48	0.95	0.08	34,42,50,55	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.

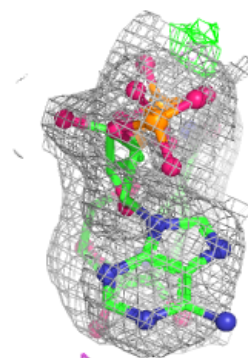
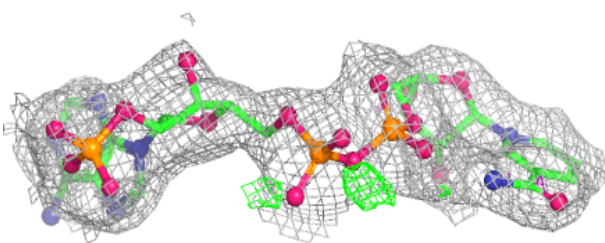
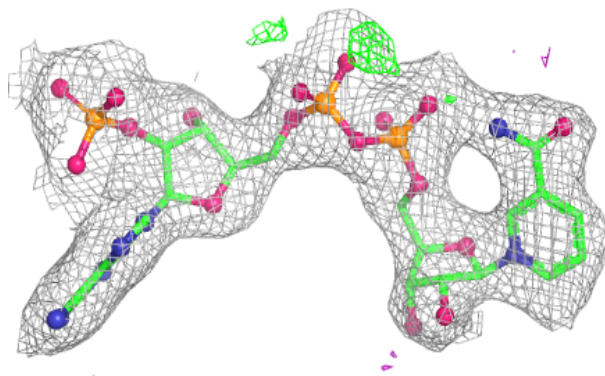


Electron density around 17R D 1:

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

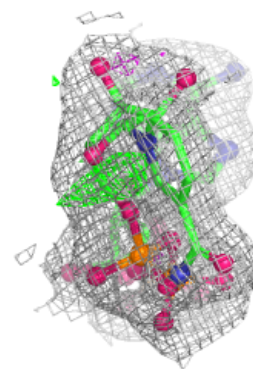
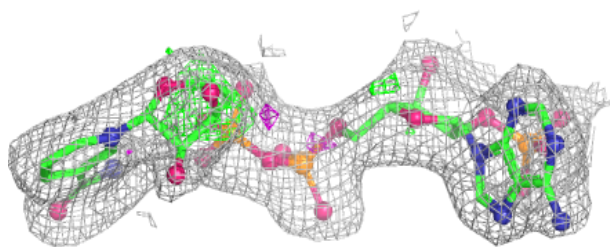
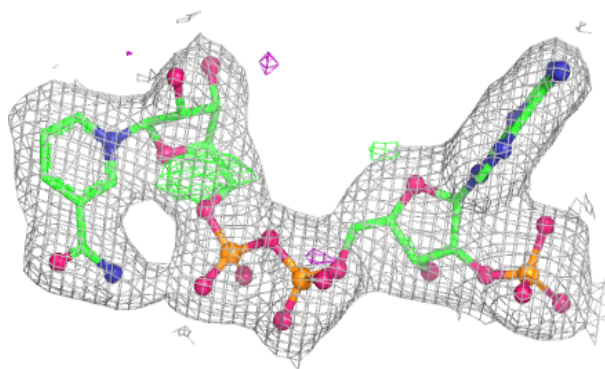
**Electron density around NAP D 293:**

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

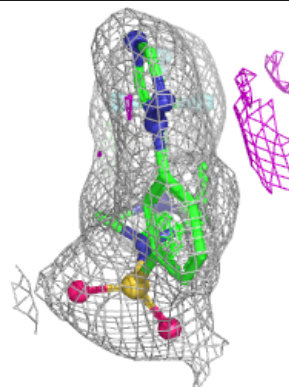
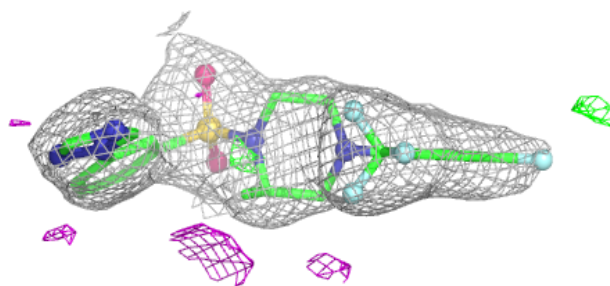
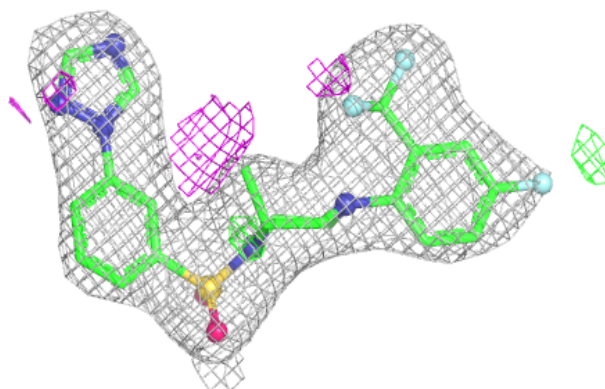


Electron density around NAP C 293:

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

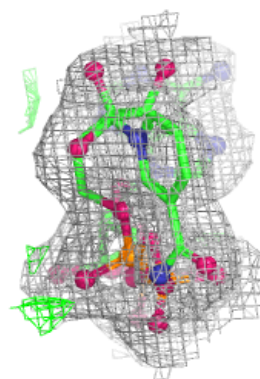
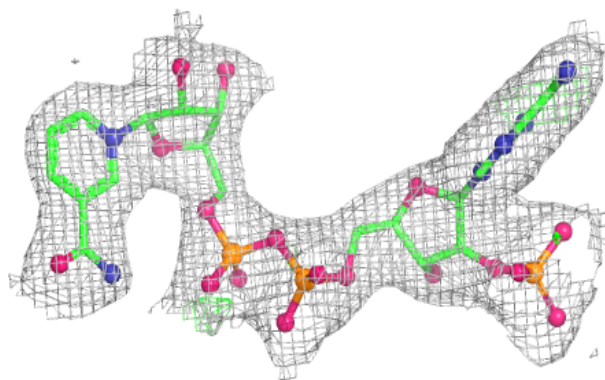
**Electron density around 17R A 1:**

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

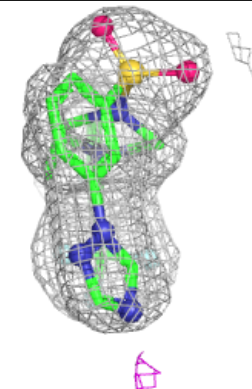
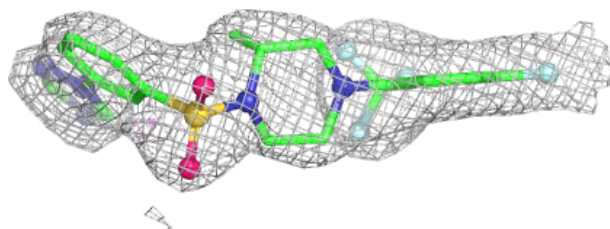
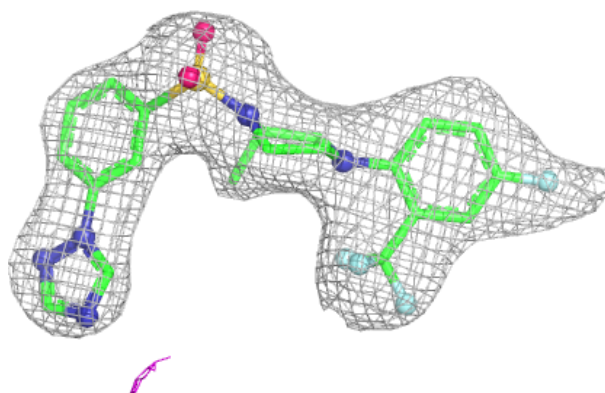


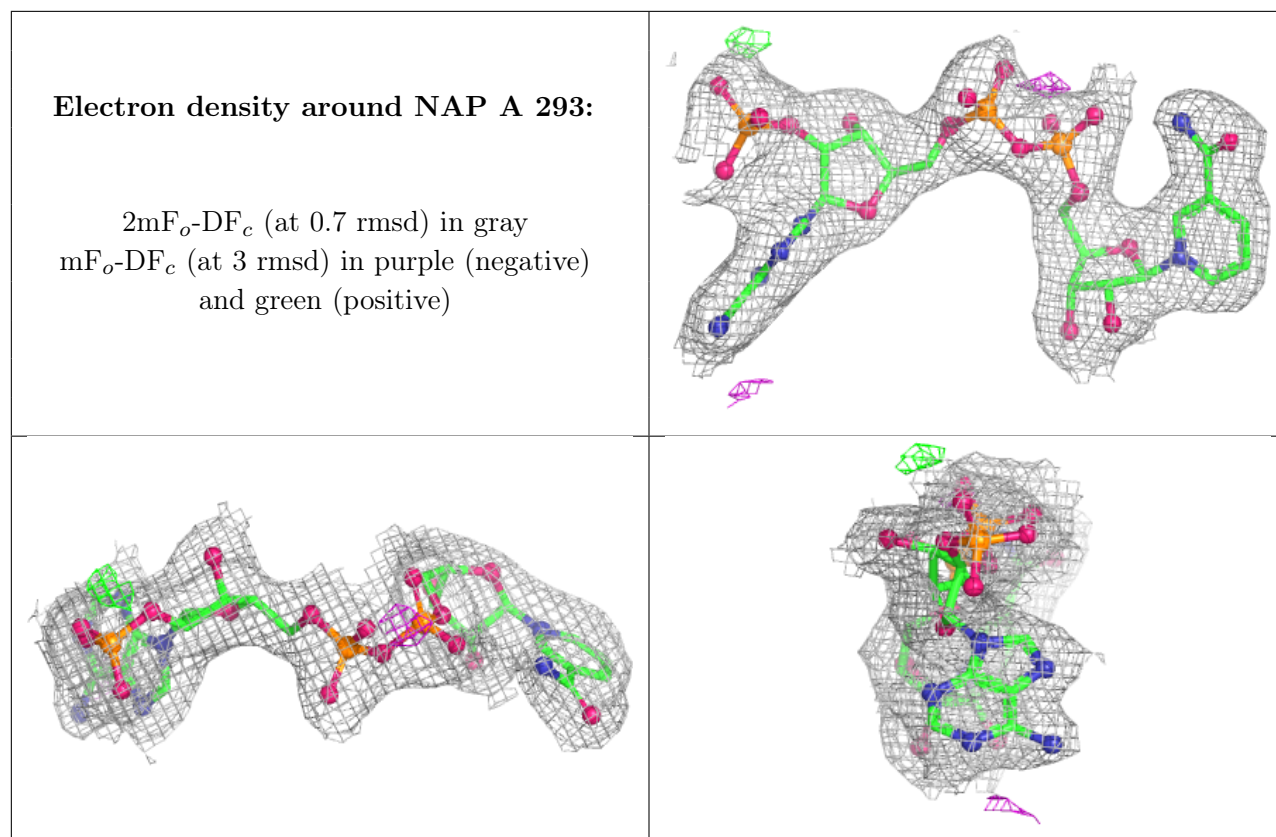
Electron density around NAP B 293:

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

**Electron density around 17R 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.