Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 10:01 AM EDT

PDB ID	:	3FRJ
Title	:	Crystal Structure of 11b-Hydroxysteroid Dehydrogenase-1 (11b-HSD1) in Complex with Piperidyl Benzamide Inhibitor
Authors	:	Wang, Z.; Sudom, A.; Walker, N.P.
Deposited on	:	2009-01-08
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 following versions of software and data (see references ⓘ) were used in the production of this report:

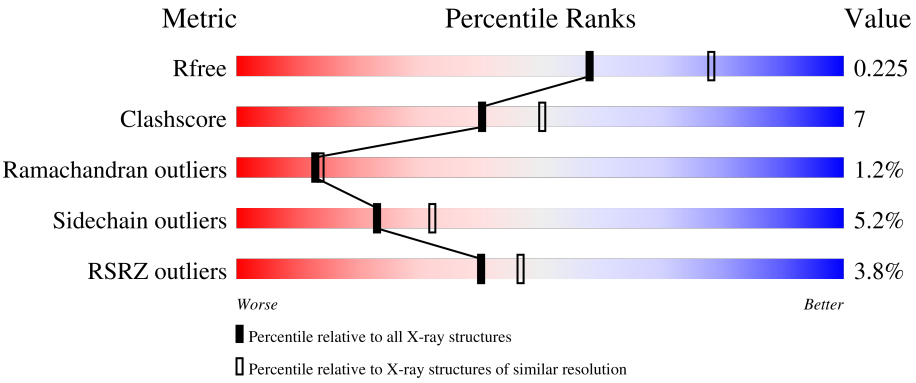
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	5% 73% 17% • 8%
1	B	286	2% 75% 15% • 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4351 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	262	Total	C	N	O	S	0	11	0
			2015	1285	340	375	15			
1	B	265	Total	C	N	O	S	0	12	0
			2043	1303	344	380	16			

There are 36 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
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

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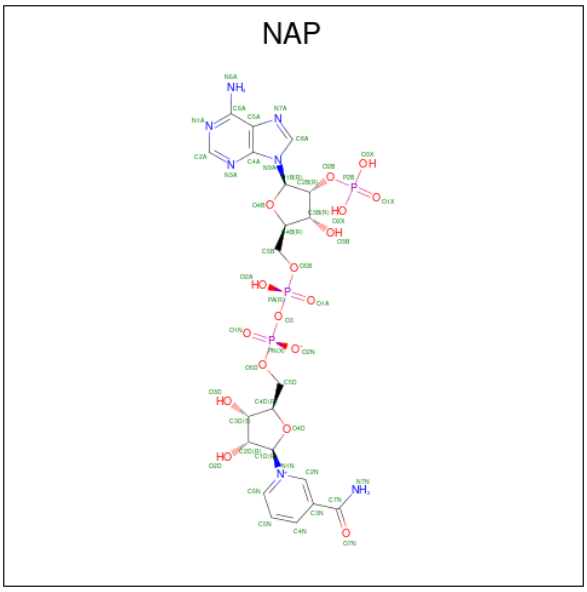
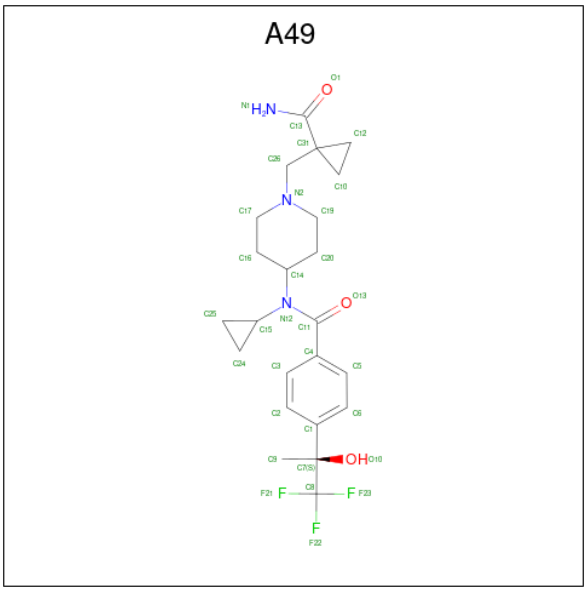
Chain	Residue	Modelled	Actual	Comment	Reference
B	14	GLN	-	expression tag	UNP P28845
B	15	HIS	-	expression tag	UNP P28845
B	16	GLN	-	expression tag	UNP P28845
B	17	HIS	-	expression tag	UNP P28845
B	18	GLN	-	expression tag	UNP P28845
B	19	HIS	-	expression tag	UNP P28845
B	20	GLN	-	expression tag	UNP P28845
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

- 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		

- Molecule 3 is N-{1-[(1-carbamoylcyclopropyl)methyl]piperidin-4-yl}-N-cyclopropyl-4-[(1S)-2,2,2-trifluoro-1-hydroxy-1-methylethyl]benzamide (three-letter code: A49) (formula: $C_{23}H_{30}F_3N_3O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C F N O 32 23 3 3 3	0	0

- Molecule 4 is water.

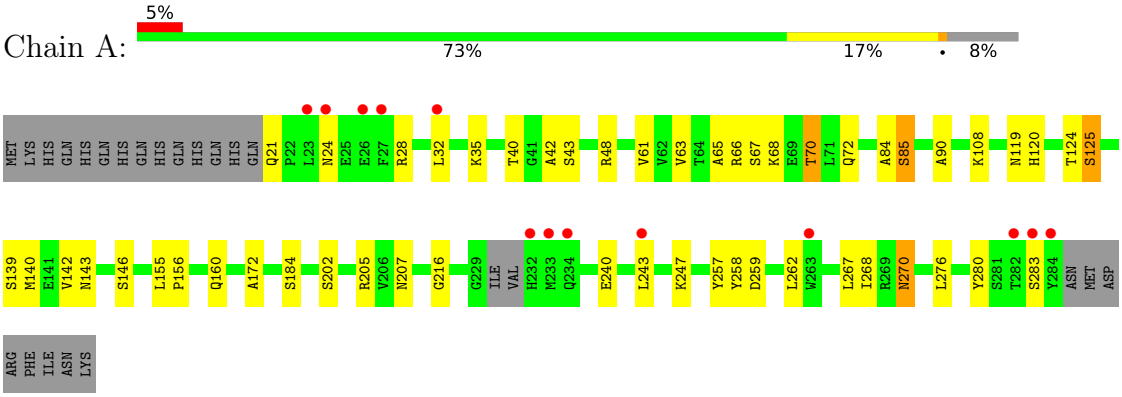
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	84	Total O 84 84	0	0
4	B	81	Total O 81 81	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

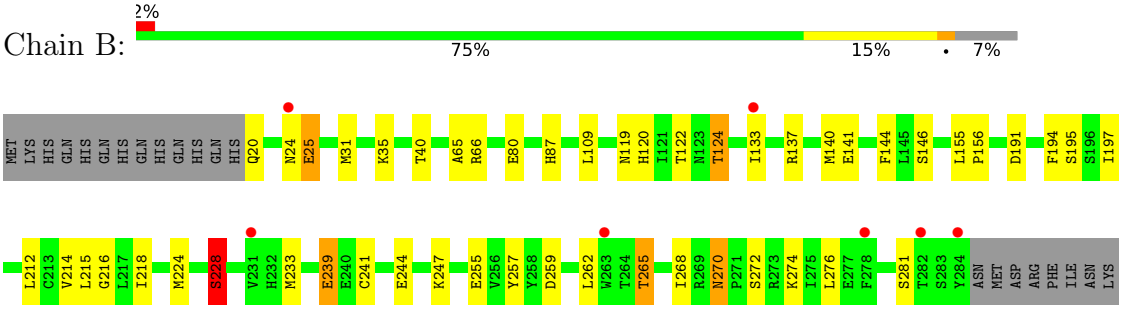
• Molecule 1: Corticosteroid 11-beta-Dehydrogenase, Isozyme 1

Chain A:



• Molecule 1: Corticosteroid 11-beta-Dehydrogenase, Isozyme 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	104.92Å 104.92Å 134.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.34 – 2.30 75.34 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (75.34-2.30) 99.8 (75.34-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	5.19 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.231 0.189 , 0.225	Depositor DCC
R_{free} test set	1935 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4351	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 3.76% 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: A49, 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	1.08	1/2059 (0.0%)	0.92	1/2779 (0.0%)
1	B	1.18	3/2098 (0.1%)	0.93	1/2833 (0.0%)
All	All	1.14	4/4157 (0.1%)	0.93	2/5612 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	137[A]	ARG	CB-CG	5.31	1.66	1.52
1	B	214	VAL	CB-CG1	5.16	1.63	1.52
1	A	142	VAL	CB-CG2	5.09	1.63	1.52
1	B	141	GLU	CG-CD	5.02	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	239	GLU	CA-CB-CG	5.09	124.60	113.40

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	2015	0	2039	32	0
1	B	2043	0	2076	31	0
2	A	48	0	25	1	0
2	B	48	0	25	2	0
3	B	32	0	30	0	0
4	A	84	0	0	4	0
4	B	81	0	0	2	0
All	All	4351	0	4195	61	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 7.

All (61) 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:228:SER:HA	4:B:350:HOH:O	1.60	1.00
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.60	0.84
1:A:67[A]:SER:HB3	1:A:70:THR:HG23	1.63	0.79
1:A:120:HIS:HE1	1:A:146:SER:OG	1.65	0.77
1:A:140:MET:HG2	1:B:140[B]:MET:HG3	1.67	0.75
1:B:122:THR:O	1:B:124[A]:THR:HG22	1.86	0.75
1:B:87:HIS:HD2	4:B:295:HOH:O	1.75	0.69
1:A:125:SER:HA	4:A:318:HOH:O	1.92	0.69
1:B:122:THR:O	1:B:124[A]:THR:CG2	2.42	0.66
1:B:216:GLY:HA3	1:B:259:ASP:OD2	1.96	0.65
1:A:216:GLY:HA3	1:A:259:ASP:OD2	1.98	0.63
1:A:172:ALA:O	1:A:184[A]:SER:HB2	1.99	0.62
1:A:139:SER:O	1:A:143:ASN:HB2	1.99	0.62
1:B:270:ASN:C	1:B:270:ASN:HD22	2.04	0.61
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.85	0.59
1:A:270:ASN:HD22	1:A:270:ASN:C	2.06	0.59
1:A:119:ASN:ND2	2:A:1:NAP:H4D	2.21	0.56
1:A:257:TYR:CD2	1:A:268:ILE:HG21	2.41	0.56
1:B:191:ASP:O	1:B:195:SER:HB2	2.07	0.55
1:B:24:ASN:O	1:B:25:GLU:HB3	2.06	0.54
1:A:120:HIS:CE1	1:A:146:SER:OG	2.55	0.52
1:A:43:SER:O	1:A:48:ARG:NH1	2.43	0.50
1:B:224:MET:HA	1:B:224:MET:HE2	1.94	0.50
1:A:243:LEU:HG	1:A:247:LYS:HE3	1.95	0.49
1:B:212:LEU:O	1:B:255:GLU:HA	2.13	0.49
1:B:120:HIS:HE1	1:B:146:SER:OG	1.95	0.48
1:B:257:TYR:CD2	1:B:268:ILE:HG21	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ILE:HA	1:A:268:ILE:HD13	1.71	0.48
1:B:216:GLY:O	1:B:218:ILE:HG12	2.14	0.48
1:B:270:ASN:HD21	1:B:272:SER:HB2	1.79	0.48
1:B:244:GLU:OE1	1:B:247:LYS:NZ	2.39	0.47
1:A:268:ILE:HD12	1:A:268:ILE:HG23	1.60	0.47
1:A:61[A]:VAL:HG12	1:A:63:VAL:HG13	1.96	0.46
1:A:84:ALA:O	1:A:85:SER:HB3	2.15	0.46
1:A:257:TYR:CE2	1:A:268:ILE:HG22	2.51	0.46
4:A:356:HOH:O	1:B:133:ILE:HD13	2.17	0.45
1:A:32:LEU:O	1:A:35:LYS:HB2	2.16	0.45
1:B:270:ASN:C	1:B:270:ASN:ND2	2.70	0.45
1:A:68:LYS:HG3	1:A:90:ALA:CB	2.47	0.44
1:A:70:THR:HG21	4:A:366:HOH:O	2.18	0.44
1:B:194:PHE:HA	1:B:197:ILE:HG12	1.99	0.44
1:A:155:LEU:HB3	1:A:156:PRO:HD3	2.00	0.43
1:B:140[A]:MET:CE	1:B:144:PHE:CD2	3.01	0.43
1:B:66:ARG:HB2	2:B:1:NAP:O2X	2.18	0.42
1:B:119:ASN:ND2	2:B:1:NAP:H4D	2.34	0.42
1:B:262:LEU:HA	1:B:265:THR:HG23	2.01	0.42
1:A:270:ASN:C	1:A:270:ASN:ND2	2.72	0.42
1:B:155:LEU:HB3	1:B:156:PRO:HD3	2.01	0.42
1:A:267:LEU:O	1:B:272:SER:HB3	2.20	0.42
1:A:257:TYR:CD2	1:A:268:ILE:CG2	3.03	0.42
1:A:280:TYR:O	1:A:283:SER:OG	2.33	0.42
1:A:35:LYS:HA	1:A:35:LYS:HD3	1.81	0.41
1:B:215:LEU:HD13	1:B:241:CYS:SG	2.60	0.41
1:A:28:ARG:HH11	1:A:28:ARG:HD3	1.74	0.41
1:A:42:ALA:HB3	1:A:63:VAL:HB	2.01	0.41
1:A:207[A]:ASN:ND2	4:A:369:HOH:O	2.53	0.41
1:A:240:GLU:HB3	1:A:258:TYR:OH	2.20	0.41
1:B:35:LYS:HD3	1:B:35:LYS:HA	1.81	0.41
1:B:255:GLU:OE1	1:B:257:TYR:OH	2.22	0.41
1:B:274:LYS:HA	1:B:274:LYS:HD2	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/286 (91%)	246 (95%)	12 (5%)	2 (1%)	19	23
1	B	267/286 (93%)	248 (93%)	15 (6%)	4 (2%)	10	10
All	All	527/572 (92%)	494 (94%)	27 (5%)	6 (1%)	13	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	228	SER
1	B	25	GLU
1	B	31	MET
1	A	65	ALA
1	A	85	SER
1	B	65	ALA

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	221/243 (91%)	208 (94%)	13 (6%)	19	27
1	B	226/243 (93%)	216 (96%)	10 (4%)	28	39
All	All	447/486 (92%)	424 (95%)	23 (5%)	23	33

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	24	ASN
1	A	70	THR
1	A	72	GLN
1	A	108	LYS
1	A	124[A]	THR
1	A	125	SER
1	A	160	GLN
1	A	202	SER
1	A	205	ARG
1	A	262	LEU
1	A	270	ASN
1	A	276	LEU
1	B	20	GLN
1	B	109	LEU
1	B	124[A]	THR
1	B	228	SER
1	B	233	MET
1	B	239	GLU
1	B	265	THR
1	B	270	ASN
1	B	276	LEU
1	B	281	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	87	HIS
1	A	119	ASN
1	A	120	HIS
1	A	207[A]	ASN
1	A	270	ASN
1	B	119	ASN
1	B	120	HIS
1	B	207[A]	ASN
1	B	234	GLN
1	B	270	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	B	1	-	45,52,52	1.62	6 (13%)	56,80,80	2.08	17 (30%)
3	A49	B	2	-	33,35,35	1.35	4 (12%)	42,55,55	2.03	14 (33%)
2	NAP	A	1	-	45,52,52	1.79	6 (13%)	56,80,80	1.87	15 (26%)

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	B	1	-	-	6/31/67/67	0/5/5/5
3	A49	B	2	-	-	7/38/58/58	0/4/4/4
2	NAP	A	1	-	-	4/31/67/67	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAP	O7N-C7N	8.00	1.39	1.24
2	B	1	NAP	O7N-C7N	6.34	1.36	1.24
3	B	2	A49	C11-N12	3.90	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAP	C2A-N3A	3.86	1.38	1.32
2	A	1	NAP	P2B-O2B	3.39	1.65	1.59
2	A	1	NAP	C2D-C1D	-3.15	1.49	1.53
2	B	1	NAP	C2A-N1A	2.82	1.39	1.33
2	B	1	NAP	C2N-N1N	2.59	1.38	1.35
2	A	1	NAP	O4B-C1B	2.43	1.44	1.41
3	B	2	A49	C25-C15	2.39	1.54	1.48
3	B	2	A49	C14-N12	-2.25	1.45	1.48
2	B	1	NAP	PA-O2A	-2.22	1.44	1.55
2	A	1	NAP	PA-O2A	-2.21	1.44	1.55
2	A	1	NAP	PN-O5D	2.21	1.68	1.59
2	B	1	NAP	C3N-C7N	2.05	1.53	1.50
3	B	2	A49	C17-N2	2.04	1.52	1.46

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAP	C3N-C7N-N7N	7.16	126.34	117.75
2	A	1	NAP	N3A-C2A-N1A	-6.54	118.45	128.68
2	B	1	NAP	N3A-C2A-N1A	-6.04	119.23	128.68
3	B	2	A49	C20-C14-N12	-4.83	104.22	112.76
2	A	1	NAP	C6N-N1N-C2N	-4.45	117.91	121.97
3	B	2	A49	C6-C1-C7	-4.16	116.90	121.46
2	B	1	NAP	O7N-C7N-N7N	-4.06	116.81	122.58
3	B	2	A49	C12-C31-C26	-4.04	110.59	116.87
2	B	1	NAP	C2A-N1A-C6A	3.92	125.46	118.75
2	B	1	NAP	C1B-N9A-C4A	-3.59	120.33	126.64
2	A	1	NAP	O5B-C5B-C4B	-3.42	97.23	108.99
2	A	1	NAP	O4D-C1D-C2D	-3.34	102.04	106.93
3	B	2	A49	C19-N2-C26	-3.21	106.08	111.81
3	B	2	A49	C17-C16-C14	-3.21	104.71	110.81
2	A	1	NAP	C3N-C7N-N7N	3.20	121.59	117.75
2	B	1	NAP	C3B-C2B-C1B	-3.16	96.95	102.89
2	A	1	NAP	O4B-C1B-C2B	-3.09	101.23	106.59
3	B	2	A49	C10-C31-C13	3.06	118.13	115.24
2	A	1	NAP	O2B-P2B-O1X	-3.04	97.65	109.39
3	B	2	A49	C16-C17-N2	-3.02	106.42	111.11
3	B	2	A49	C6-C1-C2	2.87	122.25	117.97
3	B	2	A49	C3-C2-C1	-2.87	117.38	121.22
2	B	1	NAP	O4D-C1D-C2D	-2.76	102.89	106.93
2	A	1	NAP	O3B-C3B-C2B	-2.74	103.38	111.17
2	B	1	NAP	O3X-P2B-O2X	-2.71	97.26	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	NAP	C5N-C4N-C3N	-2.71	117.14	120.34
2	A	1	NAP	C3D-C2D-C1D	2.63	104.94	100.98
3	B	2	A49	C10-C12-C31	-2.53	59.01	60.69
2	B	1	NAP	O2A-PA-O1A	2.46	124.41	112.24
2	B	1	NAP	O7N-C7N-C3N	-2.41	116.75	119.63
2	A	1	NAP	C2A-N1A-C6A	2.37	122.80	118.75
3	B	2	A49	C16-C14-N12	2.36	116.93	112.76
2	B	1	NAP	C2B-C3B-C4B	2.32	107.04	101.99
2	A	1	NAP	O3X-P2B-O1X	2.30	119.70	110.68
2	B	1	NAP	C5A-C6A-N1A	-2.30	115.15	120.35
2	B	1	NAP	O2N-PN-O1N	2.23	123.26	112.24
3	B	2	A49	C4-C11-N12	2.20	122.27	118.47
2	B	1	NAP	O3X-P2B-O2B	2.20	115.85	105.99
2	B	1	NAP	C6N-N1N-C2N	-2.20	119.97	121.97
2	B	1	NAP	O2X-P2B-O2B	2.13	115.52	105.99
2	A	1	NAP	O2N-PN-O1N	2.12	122.72	112.24
2	A	1	NAP	O3X-P2B-O2B	2.11	115.43	105.99
2	B	1	NAP	C5B-C4B-C3B	-2.10	107.30	115.18
3	B	2	A49	C5-C4-C11	-2.07	115.05	120.29
3	B	2	A49	C12-C31-C10	2.06	60.92	58.63
2	A	1	NAP	C2N-C3N-C4N	2.02	120.55	118.26

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAP	C2B-O2B-P2B-O2X
2	A	1	NAP	C5D-O5D-PN-O1N
2	B	1	NAP	C2B-O2B-P2B-O2X
2	B	1	NAP	C5D-O5D-PN-O1N
3	B	2	A49	O1-C13-C31-C10
3	B	2	A49	O1-C13-C31-C12
3	B	2	A49	C4-C11-N12-C14
3	B	2	A49	C16-C14-N12-C15
3	B	2	A49	O13-C11-N12-C14
2	B	1	NAP	C5D-O5D-PN-O3
2	B	1	NAP	PN-O3-PA-O1A
2	A	1	NAP	C5D-O5D-PN-O3
2	B	1	NAP	O4B-C4B-C5B-O5B
2	B	1	NAP	PN-O3-PA-O2A
2	A	1	NAP	O4B-C4B-C5B-O5B
3	B	2	A49	C31-C26-N2-C17

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Mol	Chain	Res	Type	Atoms
3	B	2	A49	C31-C26-N2-C19

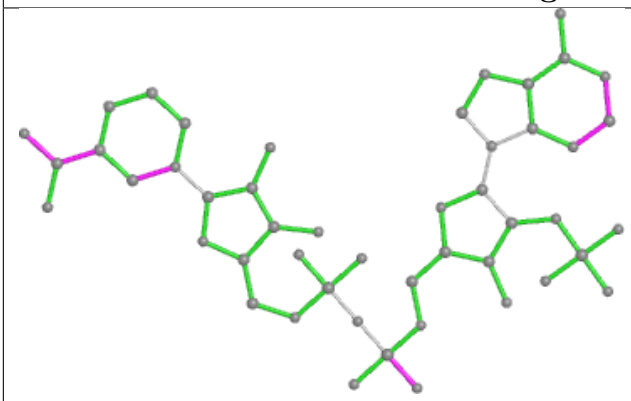
There are no ring outliers.

2 monomers are involved in 3 short contacts:

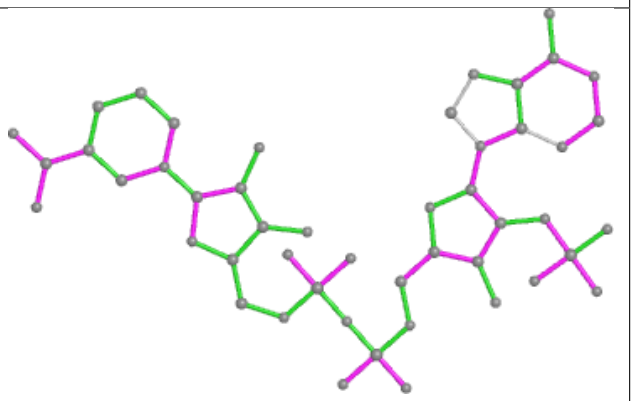
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAP	2	0
2	A	1	NAP	1	0

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

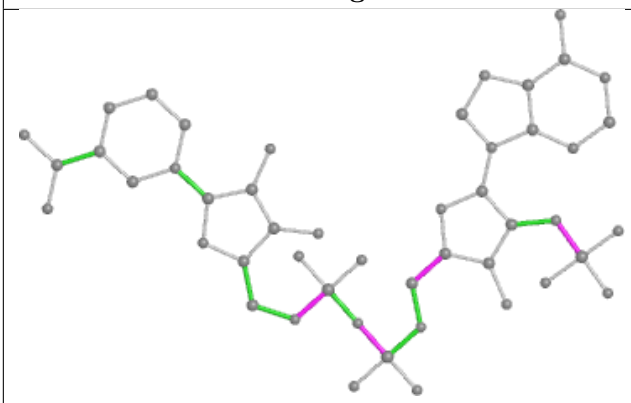
Ligand NAP B 1



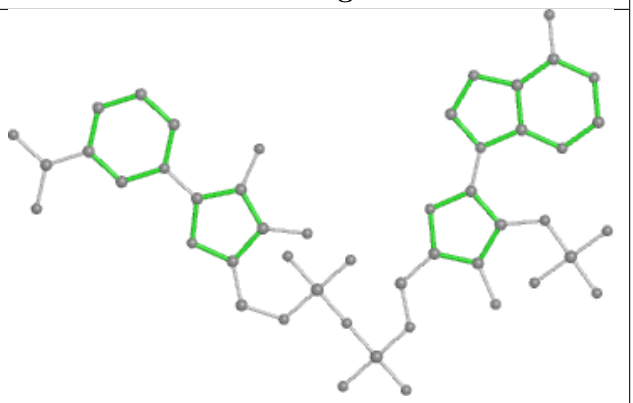
Bond lengths



Bond angles

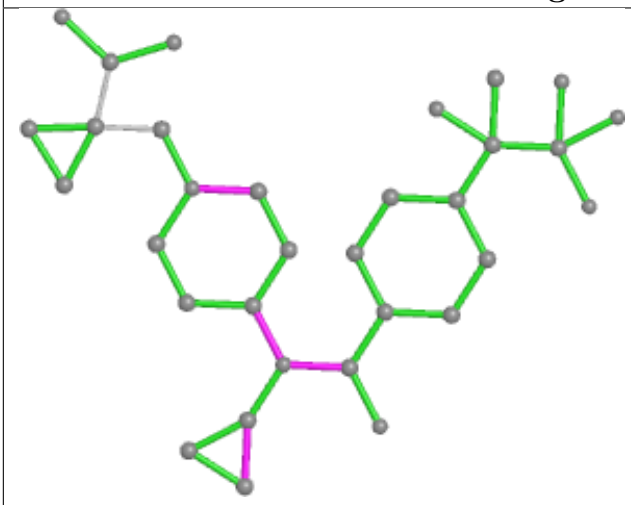


Torsions

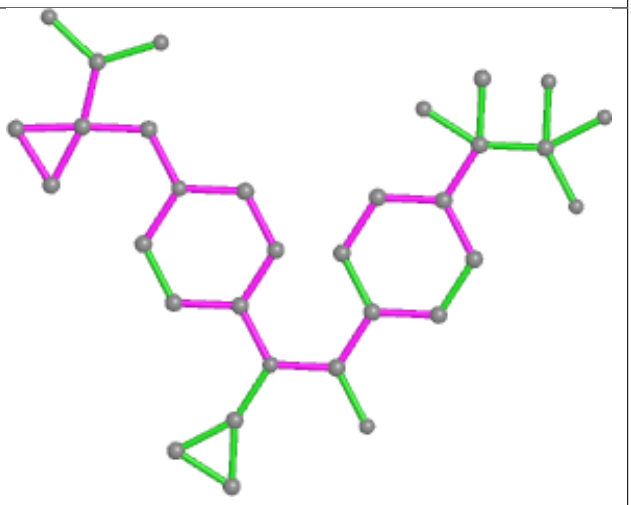


Rings

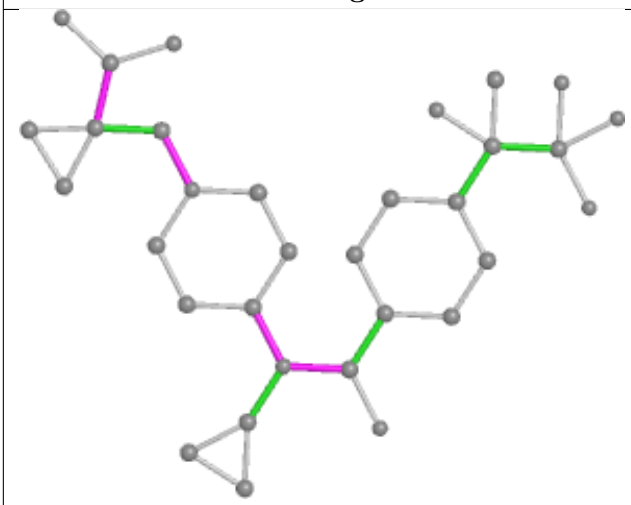
Ligand A49 B 2



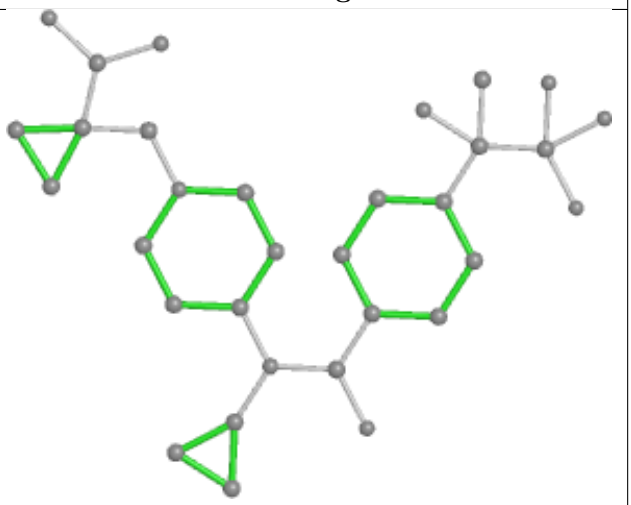
Bond lengths



Bond angles

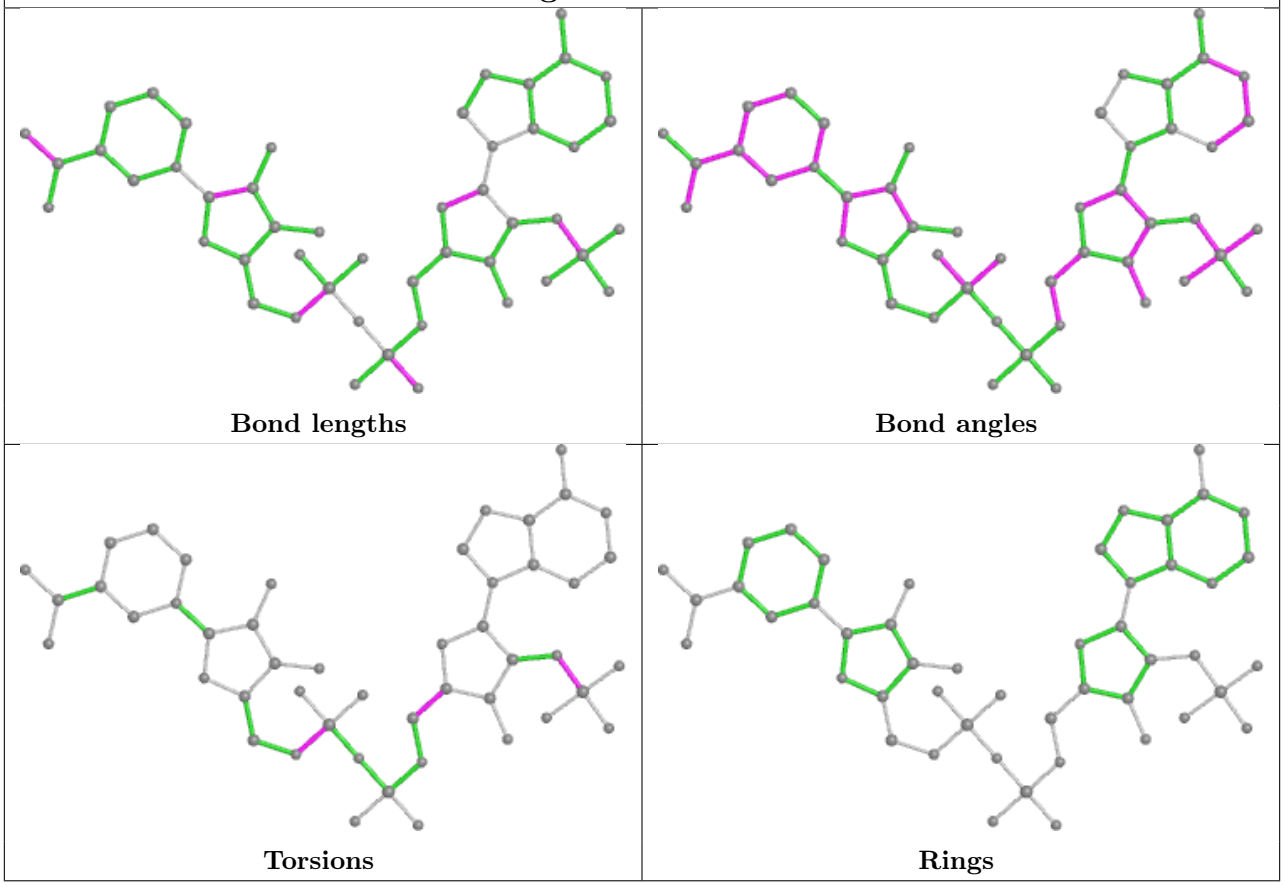


Torsions



Rings

Ligand NAP A 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, 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	262/286 (91%)	0.28	13 (4%) 28 35	30, 50, 77, 96	9 (3%)
1	B	265/286 (92%)	0.07	7 (2%) 56 63	29, 45, 69, 102	8 (3%)
All	All	527/572 (92%)	0.17	20 (3%) 40 47	29, 47, 74, 102	17 (3%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	SER	8.6
1	B	282	THR	6.0
1	A	232	HIS	5.0
1	A	24	ASN	3.9
1	B	278	PHE	3.9
1	A	282	THR	3.8
1	A	263	TRP	3.7
1	A	23	LEU	3.5
1	B	284[A]	TYR	3.3
1	A	284[A]	TYR	3.0
1	A	27	PHE	2.8
1	A	243	LEU	2.6
1	A	233	MET	2.4
1	B	263	TRP	2.4
1	B	24	ASN	2.4
1	B	231	VAL	2.2
1	A	32	LEU	2.1
1	A	234	GLN	2.0
1	B	133	ILE	2.0
1	A	26	GLU	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)

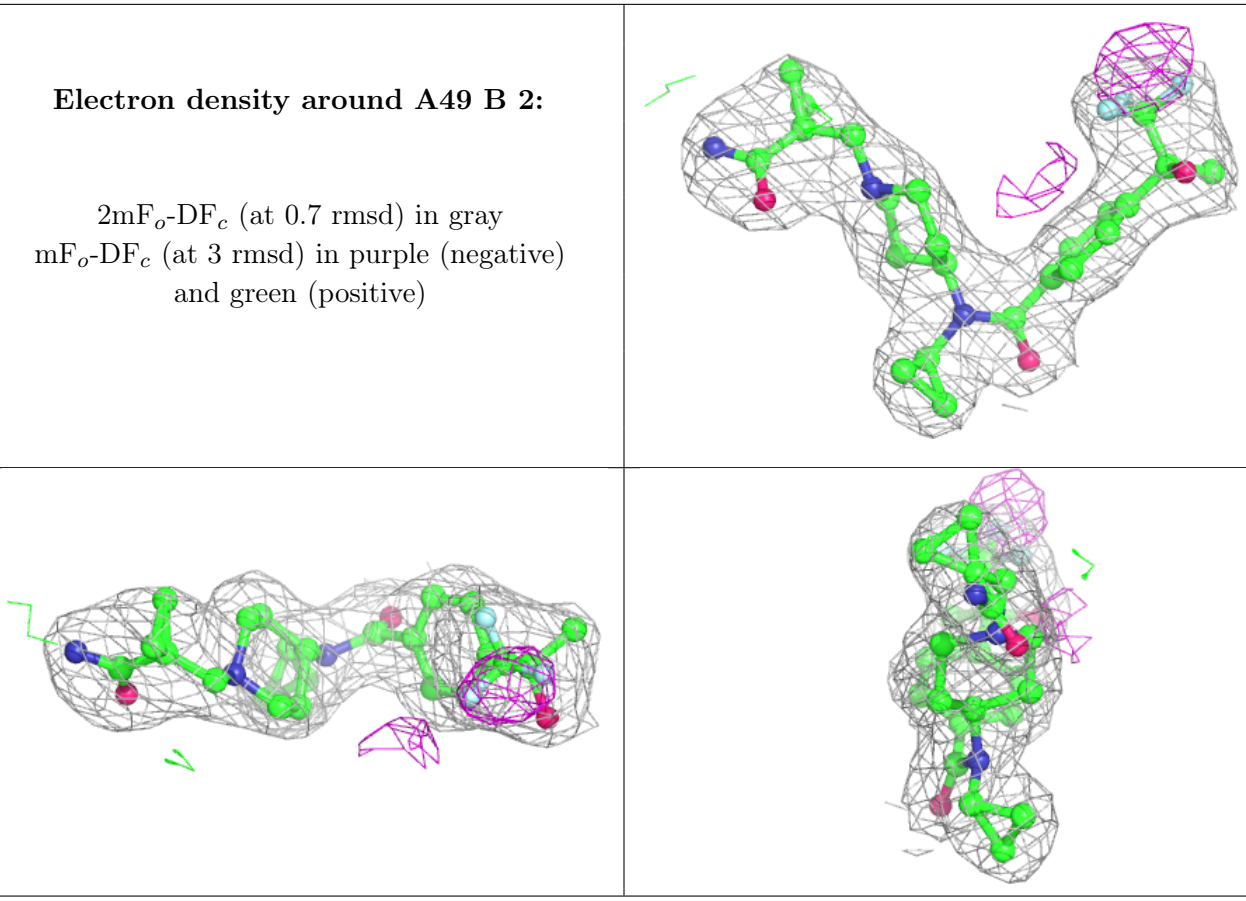
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	A49	B	2	32/32	0.96	0.11	38,43,47,52	0
2	NAP	B	1	48/48	0.99	0.14	30,37,42,47	0
2	NAP	A	1	48/48	0.99	0.12	26,37,43,45	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.

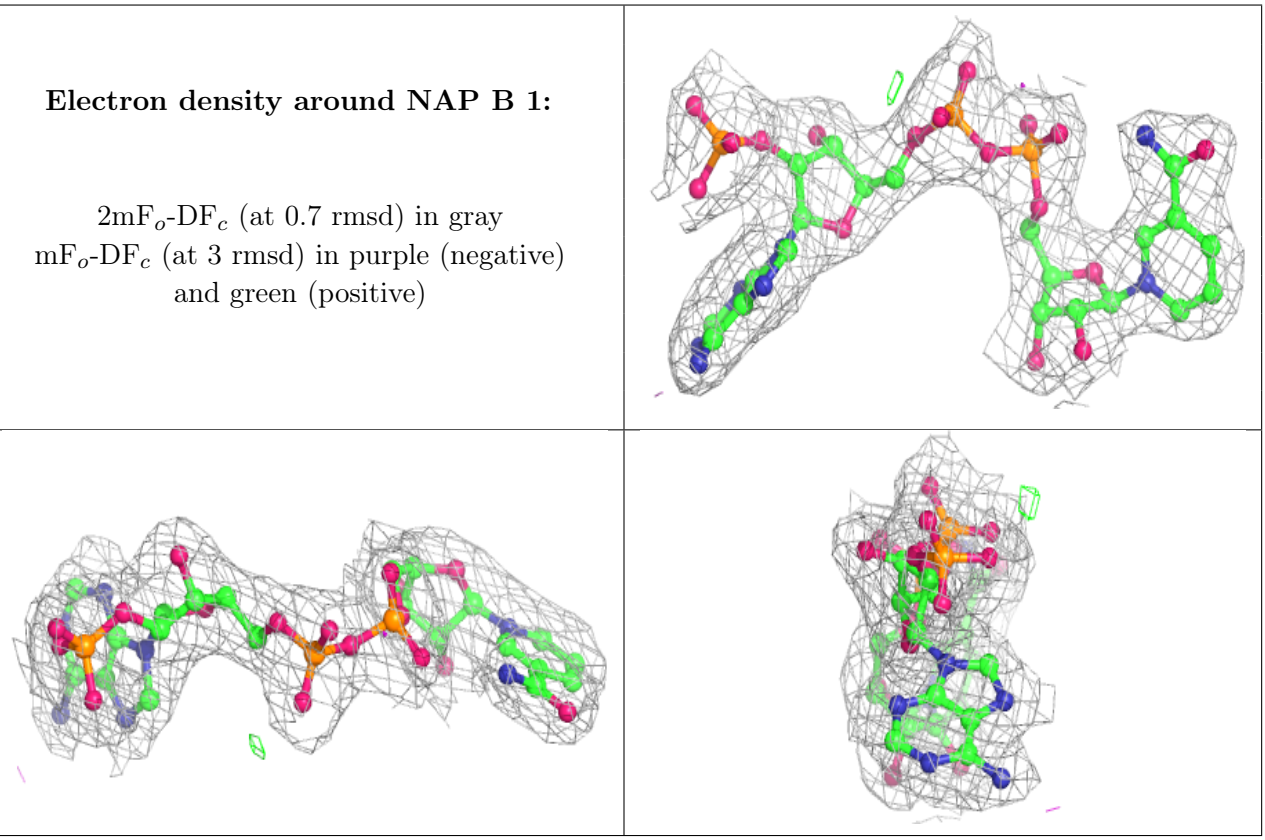
Electron density around A49 B 2:

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



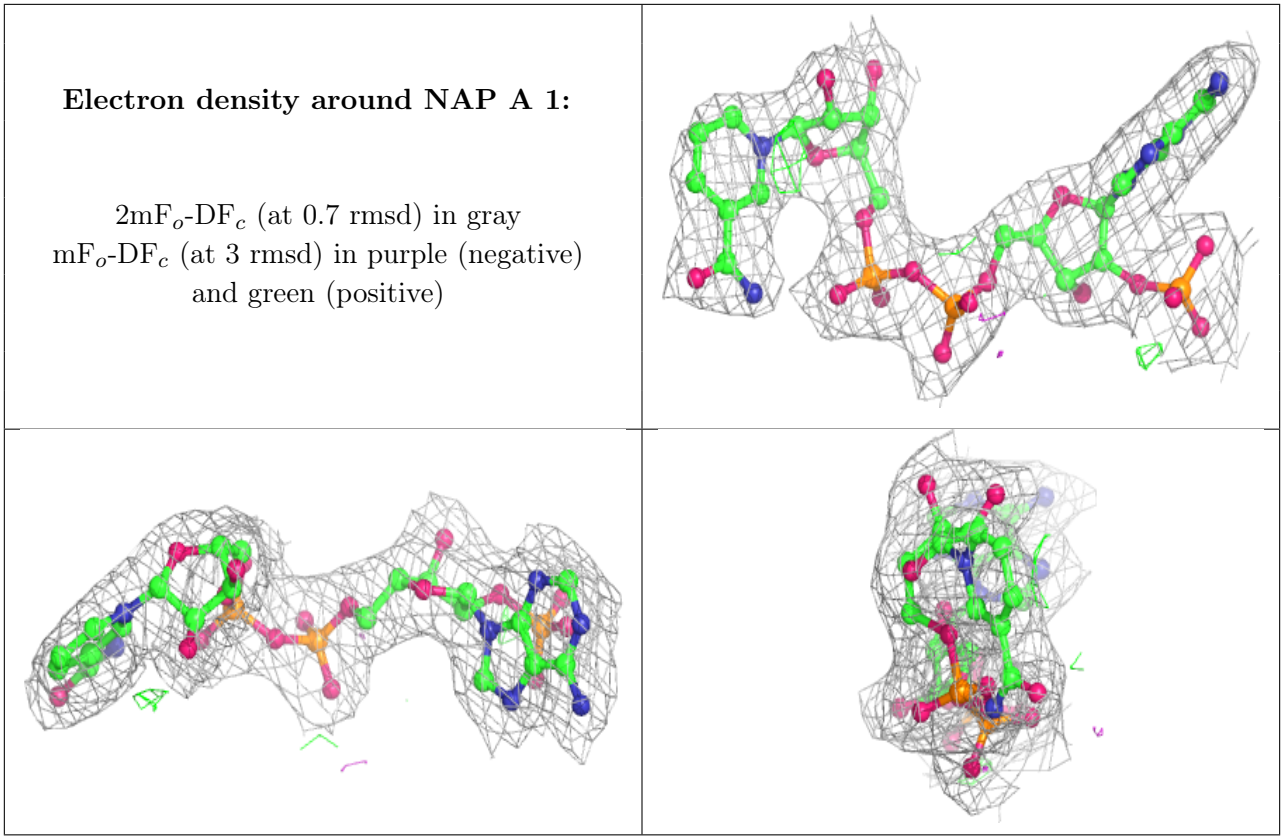
Electron density around NAP B 1:

$2mF_o$-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 A 1:

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



6.5 Other polymers (i)

There are no such residues in this entry.