



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:42 PM UTC

PDB ID : 3CZR / pdb_00003czt
Title : Crystal Structure of Human 11-beta-Hydroxysteroid Dehydrogenase (HSD1)
in Complex with Arylsulfonylpiperazine Inhibitor
Authors : Wang, Z.; Sudom, A.; Walker, N.P.
Deposited on : 2008-04-29
Resolution : 2.35 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

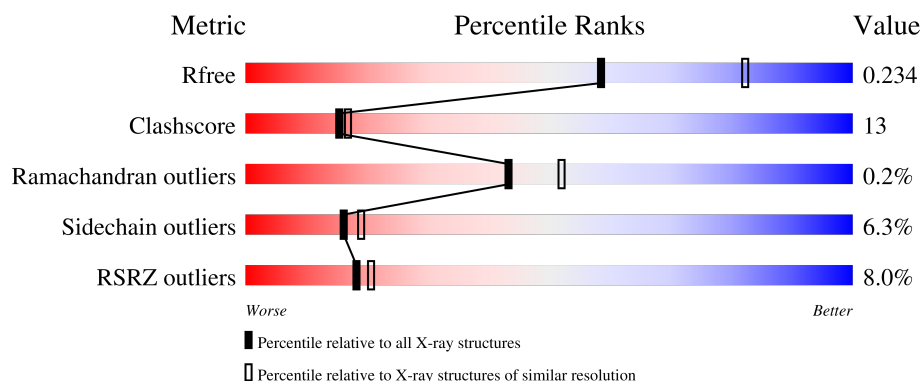
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	5% 67% 23% • 7%
1	B	286	10% 69% 21% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4390 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	265	Total	C	N	O	S	0	4	0
			2054	1308	348	383	15			
1	B	263	Total	C	N	O	S	0	1	0
			2023	1292	341	375	15			

There are 36 discrepancies between the modelled and reference sequences:

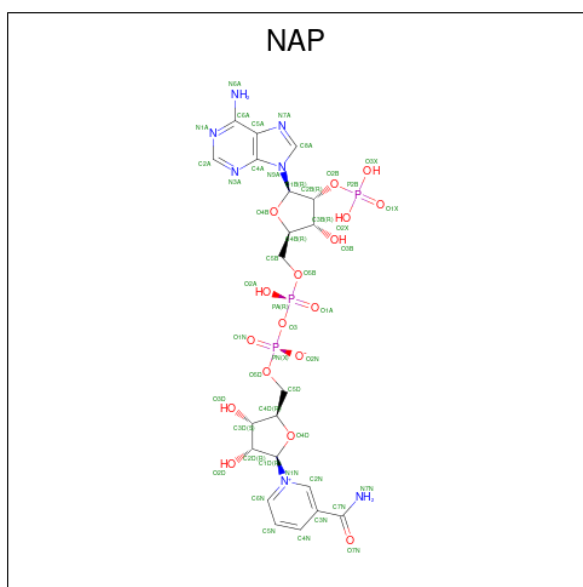
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP P28845
A	8	LYS	-	expression tag	UNP P28845
A	9	HIS	-	expression tag	UNP P28845
A	10	GLN	-	expression tag	UNP P28845
A	11	HIS	-	expression tag	UNP P28845
A	12	GLN	-	expression tag	UNP P28845
A	13	HIS	-	expression tag	UNP P28845
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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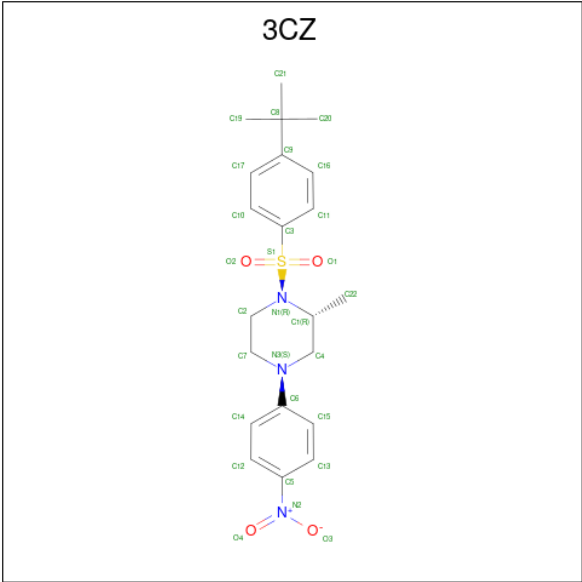
Chain	Residue	Modelled	Actual	Comment	Reference
B	14	GLN	-	expression tag	UNP P28845
B	15	HIS	-	expression tag	UNP P28845
B	16	GLN	-	expression tag	UNP P28845
B	17	HIS	-	expression tag	UNP P28845
B	18	GLN	-	expression tag	UNP P28845
B	19	HIS	-	expression tag	UNP P28845
B	20	GLN	-	expression tag	UNP P28845
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 (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



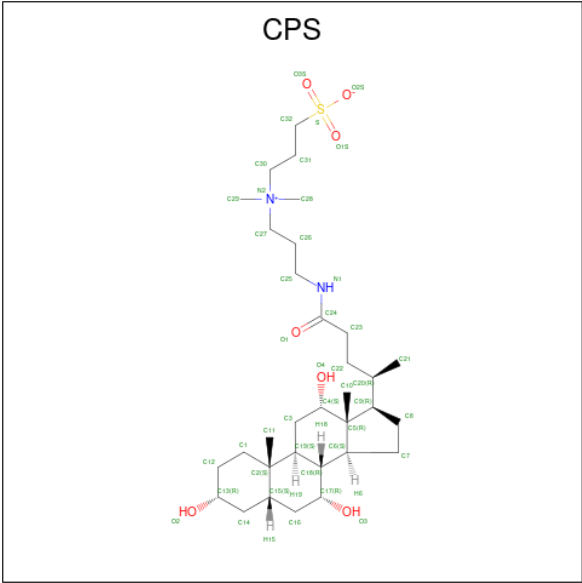
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is (2R)-1-[(4-tert-butylphenyl)sulfonyl]-2-methyl-4-(4-nitrophenyl)piperazine (CCD ID: 3CZ) (formula: $C_{21}H_{27}N_3O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			29	21	3	4	1		

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (CCD ID: CPS) (formula: C₃₂H₅₈N₂O₇S).

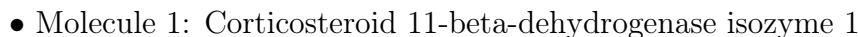


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			42	32	2	7	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total 81	O 81	0	0
5	B	65	Total 65	O 65	0	0

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.22Å 110.22Å 132.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.35 50.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.35) 99.8 (50.00-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.219 , 0.247 0.215 , 0.234	Depositor DCC
R_{free} test set	2423 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4390	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: NAP, 3CZ, CPS

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	0.75	0/2103	0.95	1/2839 (0.0%)
1	B	0.71	0/2061	0.97	0/2784
All	All	0.73	0/4164	0.96	1/5623 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	THR	N-CA-C	-5.34	106.53	112.57

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	2054	0	2094	55	0
1	B	2023	0	2072	61	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
3	A	29	0	27	1	0
4	B	42	0	58	3	0
5	A	81	0	0	1	0
5	B	65	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4390	0	4301	115	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 (115) 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:230:ILE:HG13	1:B:232:HIS:NE2	1.63	1.13
1:A:231:VAL:CG1	1:A:232:HIS:N	2.15	1.08
1:A:96:MET:HA	1:A:96:MET:HE3	1.31	1.08
1:A:231:VAL:HG13	1:A:232:HIS:H	1.21	1.03
1:A:231:VAL:CG1	1:A:232:HIS:H	1.72	1.02
1:B:230:ILE:CD1	1:B:232:HIS:CE1	2.45	0.99
1:A:231:VAL:HG12	1:A:232:HIS:N	1.76	0.96
1:B:224:MET:HE3	1:B:224:MET:HA	1.50	0.91
1:B:224:MET:HA	1:B:224:MET:CE	2.00	0.91
1:B:155:LEU:HB3	1:B:156:PRO:HD3	1.54	0.88
1:B:230:ILE:HD12	1:B:232:HIS:CE1	2.10	0.87
1:B:263:TRP:O	1:B:267:LEU:HD12	1.75	0.86
1:B:75:VAL:HG21	1:B:88:TYR:HB3	1.60	0.82
1:B:230:ILE:CD1	1:B:232:HIS:HE1	1.91	0.81
1:A:284:TYR:HE2	1:B:232:HIS:HD1	1.30	0.80
1:B:178:PRO:O	1:B:179:MET:HB2	1.81	0.80
1:A:122:THR:O	1:A:124:THR:HG22	1.82	0.79
1:B:103:VAL:HG11	1:B:154:ALA:HB2	1.65	0.77
1:A:279:LEU:O	1:A:283:SER:HB2	1.86	0.76
1:B:230:ILE:CG1	1:B:232:HIS:NE2	2.46	0.75
1:A:284:TYR:HE2	1:B:232:HIS:ND1	1.87	0.72
1:A:96:MET:HA	1:A:96:MET:CE	2.15	0.72
1:B:230:ILE:HD11	1:B:232:HIS:CE1	2.25	0.71
1:A:140:MET:HE3	1:A:140:MET:HA	1.74	0.69
1:A:191:ASP:O	1:A:195:SER:HB2	1.94	0.67
1:B:230:ILE:HD11	1:B:232:HIS:HE1	1.58	0.67
1:B:101:GLN:HA	1:B:101:GLN:HE21	1.60	0.67
1:B:200:GLU:OE1	5:B:411:HOH:O	2.14	0.66
1:A:224:MET:HA	1:A:224:MET:HE2	1.78	0.65
1:A:96:MET:HE1	1:A:146:SER:HA	1.79	0.65
1:B:155:LEU:HB3	1:B:156:PRO:CD	2.26	0.64
1:A:231:VAL:HG13	1:A:232:HIS:N	1.95	0.64
1:A:216:GLY:O	1:A:218:ILE:HG12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LEU:HD21	1:B:179:MET:HE1	1.84	0.60
1:B:97:THR:O	1:B:101:GLN:HG2	2.03	0.59
1:A:175:VAL:HG23	1:A:177:TYR:CE1	2.38	0.58
1:B:230:ILE:CG1	1:B:232:HIS:CE1	2.87	0.57
1:A:134[B]:HIS:NE2	1:A:138:LYS:NZ	2.53	0.56
1:B:224:MET:HE3	1:B:227:VAL:CG2	2.36	0.56
1:B:224:MET:CE	1:B:224:MET:CA	2.78	0.56
1:B:128:LEU:CD2	1:B:179:MET:HE1	2.36	0.56
1:B:224:MET:CE	1:B:227:VAL:CG2	2.85	0.55
1:B:230:ILE:HG13	1:B:232:HIS:CE1	2.38	0.55
1:A:215:LEU:HD11	1:A:245:ILE:HD11	1.89	0.55
1:B:224:MET:HE3	1:B:224:MET:CA	2.33	0.55
1:B:60:HIS:CD2	1:B:84:ALA:HB3	2.41	0.55
1:A:139:SER:O	1:A:143:ASN:HB2	2.07	0.54
1:B:36:LYS:O	1:B:113:LEU:HD12	2.07	0.54
1:B:178:PRO:O	1:B:179:MET:CB	2.49	0.54
1:A:96:MET:CE	1:A:146:SER:HA	2.37	0.54
1:A:155:LEU:HB3	1:A:156:PRO:HD3	1.89	0.54
1:B:42:ALA:HB3	1:B:63:VAL:HB	1.89	0.54
1:B:139:SER:O	1:B:143:ASN:HB2	2.08	0.53
1:A:140:MET:HE3	1:A:144:PHE:HB3	1.91	0.53
1:B:105:GLN:O	1:B:109:LEU:HD13	2.08	0.53
1:A:227:VAL:O	1:A:228:SER:C	2.52	0.53
1:B:127:ASN:ND2	5:B:386:HOH:O	2.42	0.52
1:A:221:GLU:O	1:A:225:LYS:HD3	2.09	0.52
1:A:212:LEU:O	1:A:255:GLU:HA	2.10	0.52
1:B:75:VAL:CG2	1:B:88:TYR:HB3	2.36	0.51
1:B:224:MET:HA	1:B:224:MET:HE2	1.87	0.51
1:A:119:ASN:HD22	1:A:168:VAL:HG21	1.75	0.51
1:B:36:LYS:HG2	1:B:110:MET:HB3	1.92	0.51
1:B:146:SER:O	1:B:150:LEU:HD12	2.10	0.51
1:A:223:ALA:O	1:A:227:VAL:HG22	2.11	0.51
1:A:178:PRO:O	1:A:179:MET:HB2	2.12	0.50
1:A:27:PHE:CD2	1:A:247:LYS:HD3	2.47	0.49
1:B:46:ILE:HG22	1:B:50:MET:HE2	1.94	0.49
1:A:133:ILE:HD13	1:B:149:VAL:HG22	1.94	0.49
1:B:75:VAL:HG13	1:B:86:ALA:HB1	1.94	0.49
1:A:191:ASP:O	1:A:195:SER:CB	2.60	0.48
4:B:1:CPS:H262	4:B:1:CPS:H30A	1.41	0.48
1:A:62:VAL:CG2	1:A:110:MET:HE2	2.44	0.47
1:B:37:VAL:HG13	1:B:115:MET:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:VAL:HG23	1:B:71:LEU:HD22	1.97	0.47
1:A:71:LEU:O	1:A:75:VAL:HG23	2.15	0.47
1:A:161:SER:O	1:A:162:ASN:HB2	2.14	0.46
1:B:103:VAL:HG11	1:B:154:ALA:CB	2.41	0.46
1:B:243:LEU:HG	1:B:247:LYS:HE3	1.97	0.46
1:A:54:LEU:HA	1:A:57:MET:HE3	1.97	0.46
1:B:220:THR:O	1:B:224:MET:HG2	2.17	0.45
1:A:266:LEU:O	1:A:269:ARG:HG2	2.16	0.45
1:A:45:GLY:O	1:A:49:GLU:HG2	2.17	0.44
1:B:103:VAL:CG1	1:B:154:ALA:HB2	2.42	0.44
1:B:64:THR:O	1:B:65:ALA:HB2	2.17	0.44
1:A:46:ILE:HG22	1:A:50:MET:HE2	1.98	0.44
1:B:236:ALA:HB2	1:B:260:SER:HB3	2.00	0.44
1:B:205:ARG:NH1	1:B:205:ARG:HG3	2.33	0.44
1:A:284:TYR:O	1:A:285:ASN:HB3	2.17	0.44
1:A:126:LEU:HD11	1:A:227:VAL:HG12	1.99	0.43
1:B:71:LEU:O	1:B:75:VAL:HG23	2.18	0.43
1:A:158:LEU:HD22	1:A:164:SER:H	1.82	0.43
1:A:128:LEU:HD23	1:B:200:GLU:HB3	2.00	0.43
1:B:270:ASN:HD21	1:B:272:SER:HB2	1.82	0.43
1:A:54:LEU:HA	1:A:57:MET:CE	2.49	0.42
1:B:212:LEU:O	1:B:255:GLU:HA	2.19	0.42
1:B:180:VAL:O	1:B:184:SER:HB2	2.19	0.42
1:A:96:MET:HE2	1:A:149:VAL:HG21	2.01	0.42
1:A:53:HIS:O	1:A:57:MET:HG3	2.19	0.42
3:A:293:3CZ:H15	3:A:293:3CZ:H7A	1.87	0.42
1:A:49:GLU:HB3	5:A:347:HOH:O	2.19	0.42
1:A:185:ALA:HB2	1:B:193:PHE:HB2	2.02	0.42
1:B:205:ARG:HG3	1:B:205:ARG:HH11	1.84	0.42
1:A:96:MET:HE1	1:A:146:SER:CB	2.50	0.41
1:A:40:THR:CB	1:A:120:HIS:HD1	2.31	0.41
1:A:133:ILE:H	1:A:133:ILE:HG13	1.64	0.41
1:A:96:MET:HE1	1:A:146:SER:HB2	2.03	0.41
1:A:61:VAL:O	1:A:86:ALA:HA	2.21	0.41
1:A:132:ASP:O	1:A:136:VAL:HG23	2.20	0.41
1:A:285:ASN:ND2	1:A:285:ASN:C	2.78	0.40
1:B:92:THR:OG1	1:B:94:GLU:OE2	2.35	0.40
4:B:1:CPS:O2S	4:B:1:CPS:C30	2.69	0.40
4:B:1:CPS:O2S	4:B:1:CPS:H30	2.18	0.40
1:B:101:GLN:HA	1:B:101:GLN:NE2	2.33	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	265/286 (93%)	247 (93%)	18 (7%)	0	100	100
1	B	262/286 (92%)	244 (93%)	17 (6%)	1 (0%)	30	34
All	All	527/572 (92%)	491 (93%)	35 (7%)	1 (0%)	43	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	65	ALA

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/243 (93%)	212 (94%)	14 (6%)	16	19
1	B	221/243 (91%)	207 (94%)	14 (6%)	16	19
All	All	447/486 (92%)	419 (94%)	28 (6%)	16	19

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	96	MET
1	A	109	LEU
1	A	117	ILE
1	A	124	THR

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Mol	Chain	Res	Type
1	A	133	ILE
1	A	179	MET
1	A	222	THR
1	A	231	VAL
1	A	247	LYS
1	A	266	LEU
1	A	269	ARG
1	A	281	SER
1	A	285	ASN
1	B	26	GLU
1	B	32	LEU
1	B	57	MET
1	B	70	THR
1	B	124	THR
1	B	126	LEU
1	B	127	ASN
1	B	150	LEU
1	B	170	SER
1	B	184	SER
1	B	224	MET
1	B	266	LEU
1	B	267	LEU
1	B	268	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	87	HIS
1	A	105	GLN
1	A	119	ASN
1	A	127	ASN
1	A	135	HIS
1	A	162	ASN
1	A	285	ASN
1	B	60	HIS
1	B	72	GLN
1	B	77	HIS
1	B	87	HIS
1	B	101	GLN
1	B	127	ASN
1	B	162	ASN

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Mol	Chain	Res	Type
1	B	270	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	2	-	50,52,52	1.70	5 (10%)	71,80,80	1.74	15 (21%)
4	CPS	B	1	-	45,45,45	1.44	1 (2%)	70,70,70	1.25	6 (8%)
3	3CZ	A	293	-	30,31,31	1.35	3 (10%)	43,47,47	1.18	4 (9%)
2	NAP	A	1	-	50,52,52	1.67	6 (12%)	71,80,80	1.65	11 (15%)

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	2	-	-	3/35/67/67	0/5/5/5
4	CPS	B	1	-	-	14/25/90/90	0/4/4/4
3	3CZ	A	293	-	-	0/24/39/39	0/3/3/3
2	NAP	A	1	-	-	6/35/67/67	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAP	O7N-C7N	8.70	1.40	1.24
2	B	2	NAP	O7N-C7N	8.64	1.40	1.24
4	B	1	CPS	C32-S	-7.97	1.66	1.77
3	A	293	3CZ	O2-S1	3.74	1.47	1.43
3	A	293	3CZ	C3-S1	3.27	1.80	1.76
2	B	2	NAP	PA-O3	3.19	1.62	1.59
2	B	2	NAP	C8A-N7A	3.01	1.37	1.31
2	B	2	NAP	C2N-N1N	2.93	1.38	1.35
2	A	1	NAP	C2A-N1A	2.84	1.39	1.33
2	A	1	NAP	C8A-N7A	2.81	1.37	1.31
3	A	293	3CZ	O1-S1	2.79	1.46	1.43
2	B	2	NAP	C2A-N1A	2.77	1.38	1.33
2	A	1	NAP	C2N-N1N	2.75	1.38	1.35
2	A	1	NAP	C2A-N3A	2.44	1.38	1.33
2	A	1	NAP	P2B-O2B	2.21	1.63	1.59

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAP	N3A-C2A-N1A	-6.58	118.62	128.58
2	A	1	NAP	N3A-C2A-N1A	-5.98	119.52	128.58
2	B	2	NAP	N9A-C8A-N7A	-4.31	107.82	113.94
2	A	1	NAP	N9A-C8A-N7A	-4.08	108.15	113.94
2	A	1	NAP	C3N-C7N-N7N	3.80	122.42	117.74
2	B	2	NAP	O2B-P2B-O1X	-3.70	96.16	109.33
4	B	1	CPS	C19-C18-C17	-3.52	107.42	111.86
2	B	2	NAP	C5A-N7A-C8A	3.45	108.88	103.45
2	A	1	NAP	C5A-C4A-N3A	-3.36	122.09	126.72
2	B	2	NAP	C5A-C4A-N3A	-3.32	122.14	126.72
2	A	1	NAP	C5A-N7A-C8A	3.32	108.67	103.45
2	A	1	NAP	O7N-C7N-C3N	-3.28	115.59	119.60
2	B	2	NAP	C2A-N3A-C4A	3.19	119.61	111.83
3	A	293	3CZ	O2-S1-O1	3.09	124.41	119.59
2	A	1	NAP	C2A-N3A-C4A	3.02	119.22	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAP	C2B-C1B-N9A	-2.93	108.93	113.75
2	B	2	NAP	C2N-C3N-C4N	2.89	121.62	118.26
4	B	1	CPS	C31-C32-S	-2.77	109.00	113.25
2	B	2	NAP	O4B-C1B-N9A	2.77	113.40	108.09
3	A	293	3CZ	O1S-S1-N1	-2.75	102.15	106.97
4	B	1	CPS	O1S-S-C32	2.71	110.82	106.73
2	A	1	NAP	C4D-O4D-C1D	-2.65	107.50	109.92
2	B	2	NAP	C4A-C5A-N7A	-2.59	107.62	110.58
4	B	1	CPS	C9-C5-C4	2.56	119.97	117.67
2	B	2	NAP	C4A-N9A-C8A	2.41	108.27	105.74
4	B	1	CPS	C19-C18-C6	2.35	113.04	109.75
2	B	2	NAP	C2A-N1A-C6A	2.35	122.59	118.73
2	A	1	NAP	C4A-C5A-N7A	-2.32	107.92	110.58
2	A	1	NAP	O2N-PN-O1N	2.32	123.23	112.44
2	B	2	NAP	C3N-C7N-N7N	2.24	120.50	117.74
2	B	2	NAP	O3X-P2B-O2B	2.22	114.50	105.85
3	A	293	3CZ	O4-N2-C5	-2.15	115.86	118.82
2	B	2	NAP	C5N-C4N-C3N	-2.08	118.32	120.36
3	A	293	3CZ	C13-C5-N2	-2.04	117.56	119.34
2	A	1	NAP	O4B-C1B-N9A	2.04	112.00	108.09
4	B	1	CPS	C3-C19-C2	2.02	115.75	113.70

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAP	C5D-O5D-PN-O3
2	A	1	NAP	C5D-O5D-PN-O1N
4	B	1	CPS	C23-C24-N1-C25
4	B	1	CPS	O1-C24-N1-C25
4	B	1	CPS	N2-C30-C31-C32
4	B	1	CPS	C31-C30-N2-C27
4	B	1	CPS	C31-C30-N2-C29
4	B	1	CPS	C31-C32-S-O3S
4	B	1	CPS	C31-C32-S-O1S
4	B	1	CPS	C26-C27-N2-C29
4	B	1	CPS	C31-C30-N2-C28
4	B	1	CPS	C31-C32-S-O2S
4	B	1	CPS	C26-C27-N2-C30
4	B	1	CPS	C26-C27-N2-C28
4	B	1	CPS	C30-C31-C32-S
4	B	1	CPS	N1-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
2	A	1	NAP	C5D-O5D-PN-O2N
2	A	1	NAP	C2B-O2B-P2B-O2X
2	A	1	NAP	C2B-O2B-P2B-O1X
2	B	2	NAP	C2B-O2B-P2B-O1X
2	B	2	NAP	PN-O3-PA-O2A
2	A	1	NAP	PN-O3-PA-O2A
2	B	2	NAP	O4B-C4B-C5B-O5B

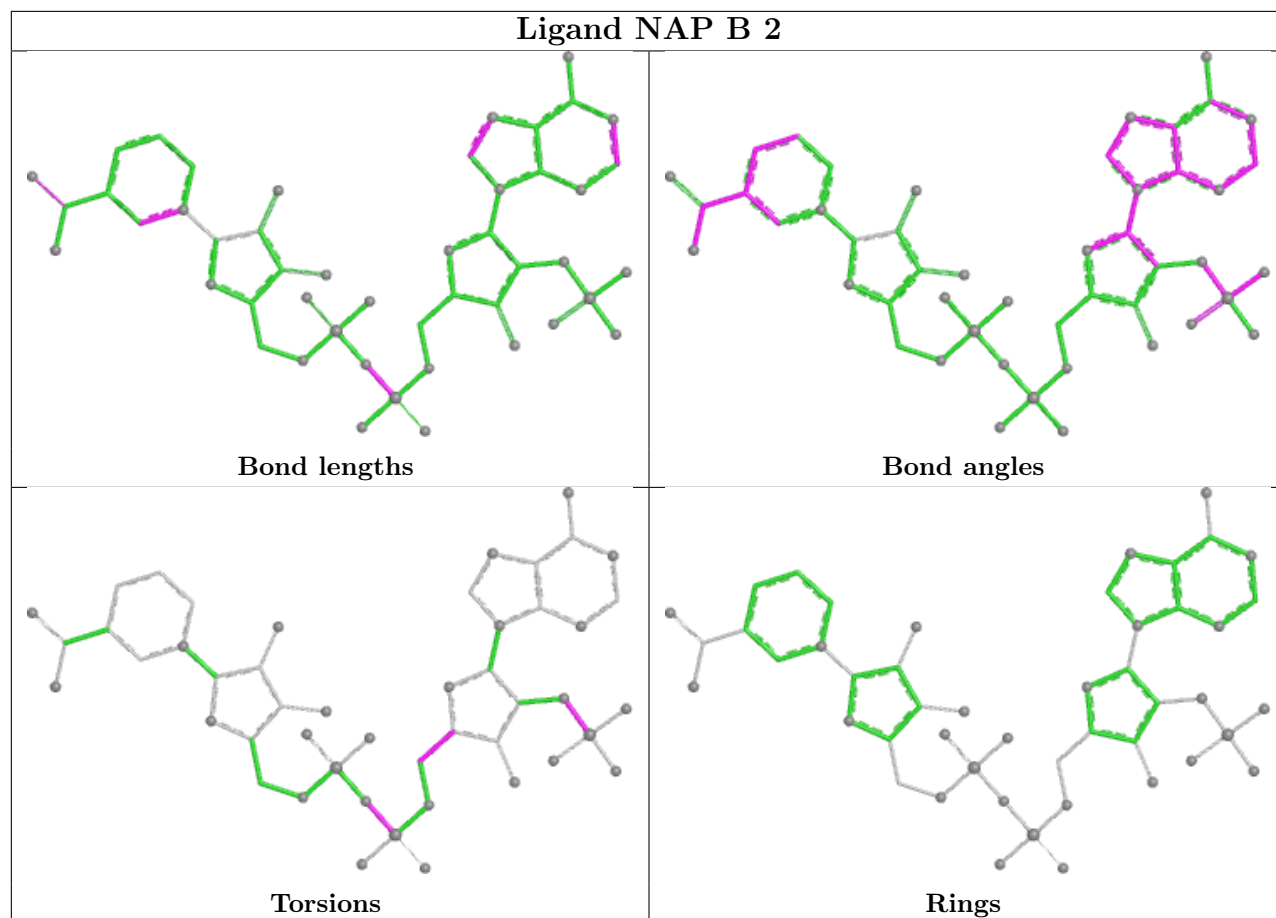
There are no ring outliers.

2 monomers are involved in 4 short contacts:

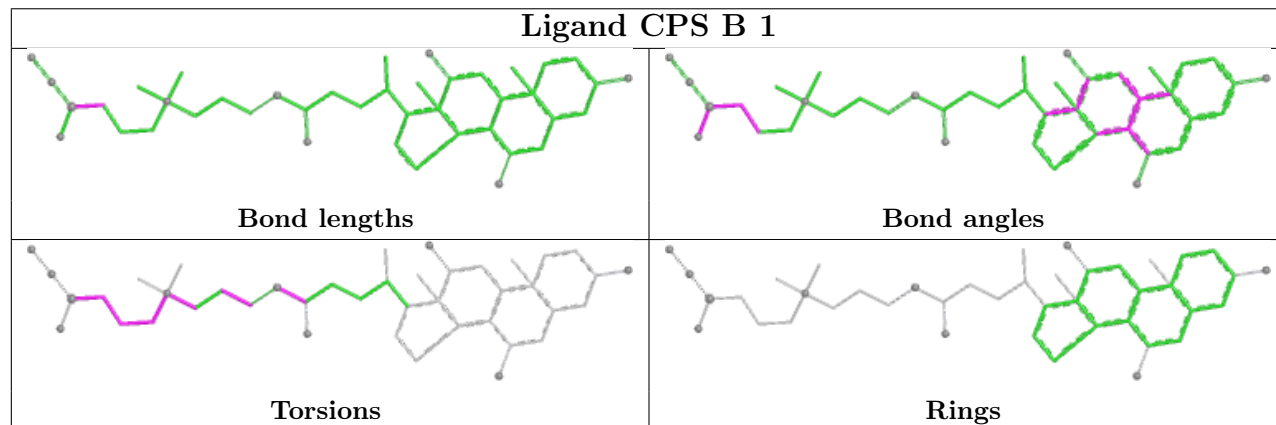
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	CPS	3	0
3	A	293	3CZ	1	0

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

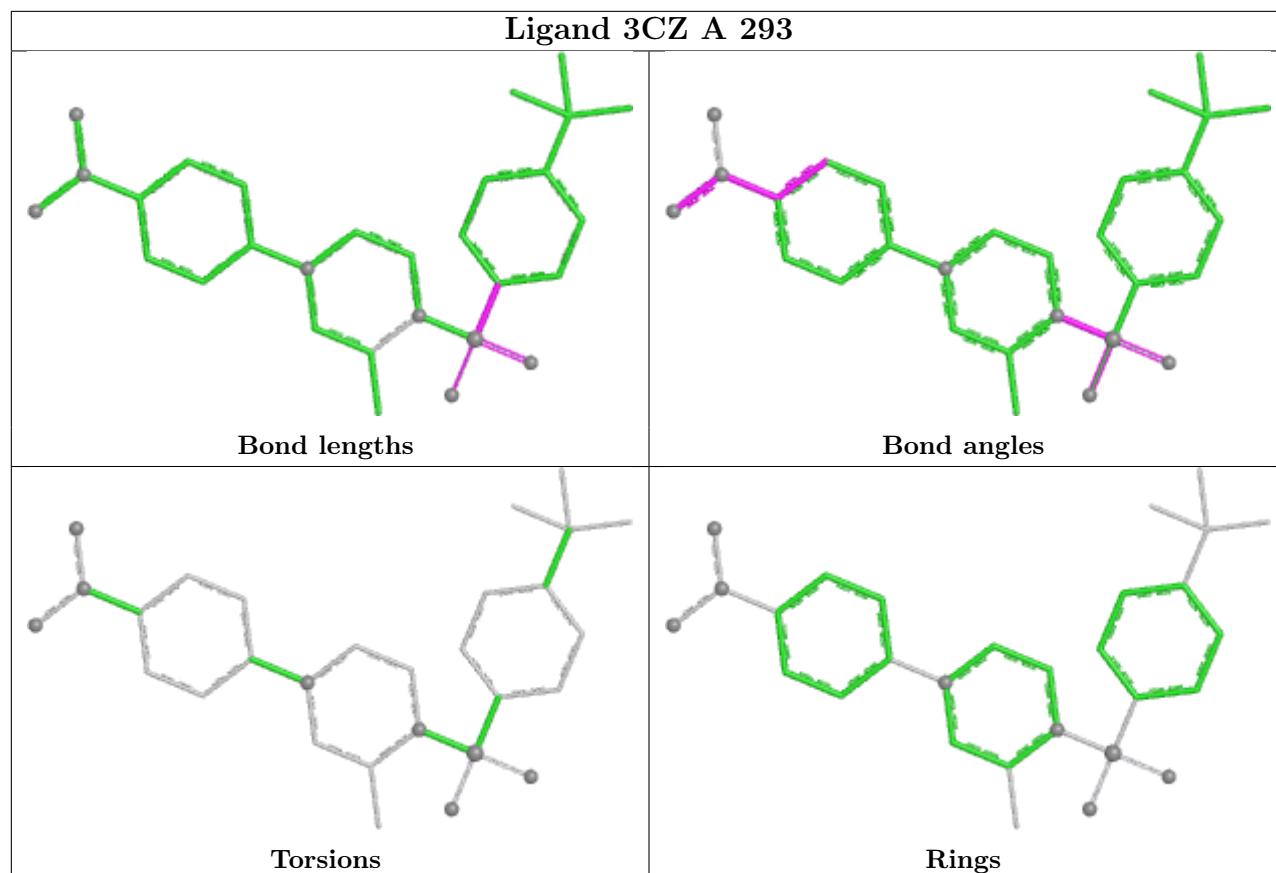
Ligand NAP B 2



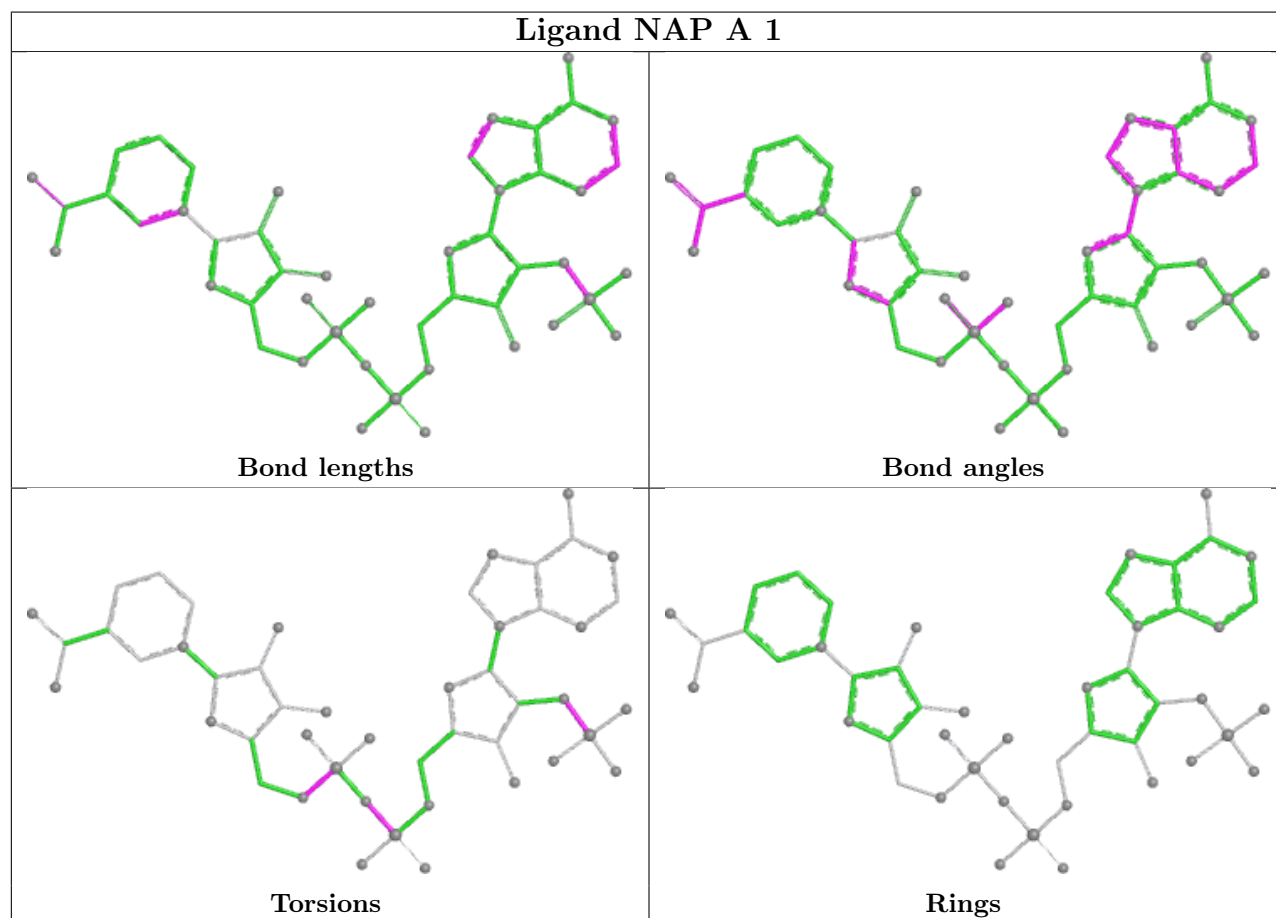
Ligand CPS B 1



Ligand 3CZ A 293



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, 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	265/286 (92%)	0.39	14 (5%)	32 37	31, 55, 79, 95	4 (1%)
1	B	263/286 (91%)	0.84	28 (10%)	11 13	32, 64, 95, 107	1 (0%)
All	All	528/572 (92%)	0.61	42 (7%)	18 21	31, 60, 92, 107	5 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280[A]	TYR	6.8
1	B	233	MET	5.0
1	A	231	VAL	4.7
1	B	231	VAL	4.7
1	B	23	LEU	3.9
1	A	232	HIS	3.7
1	B	112	GLY	3.7
1	A	229	GLY	3.5
1	B	79	LEU	3.4
1	B	84	ALA	3.4
1	B	22	PRO	3.4
1	A	134[A]	HIS	3.3
1	B	232	HIS	3.3
1	A	284	TYR	3.0
1	B	230	ILE	3.0
1	B	88	TYR	2.9
1	B	82	GLY	2.9
1	B	87	HIS	2.9
1	B	229	GLY	2.8
1	A	84	ALA	2.8
1	B	83	ALA	2.7
1	B	62	VAL	2.6
1	B	81	LEU	2.6
1	B	34	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	86	ALA	2.5
1	A	285	ASN	2.5
1	B	283	SER	2.4
1	B	59	ALA	2.4
1	B	206	VAL	2.4
1	A	79	LEU	2.4
1	A	83	ALA	2.3
1	B	89	ILE	2.3
1	A	69	GLU	2.3
1	B	39	VAL	2.3
1	B	58	GLY	2.2
1	B	37	VAL	2.2
1	B	236	ALA	2.2
1	A	233	MET	2.1
1	A	228	SER	2.1
1	A	75	VAL	2.1
1	A	126	LEU	2.0
1	B	21	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

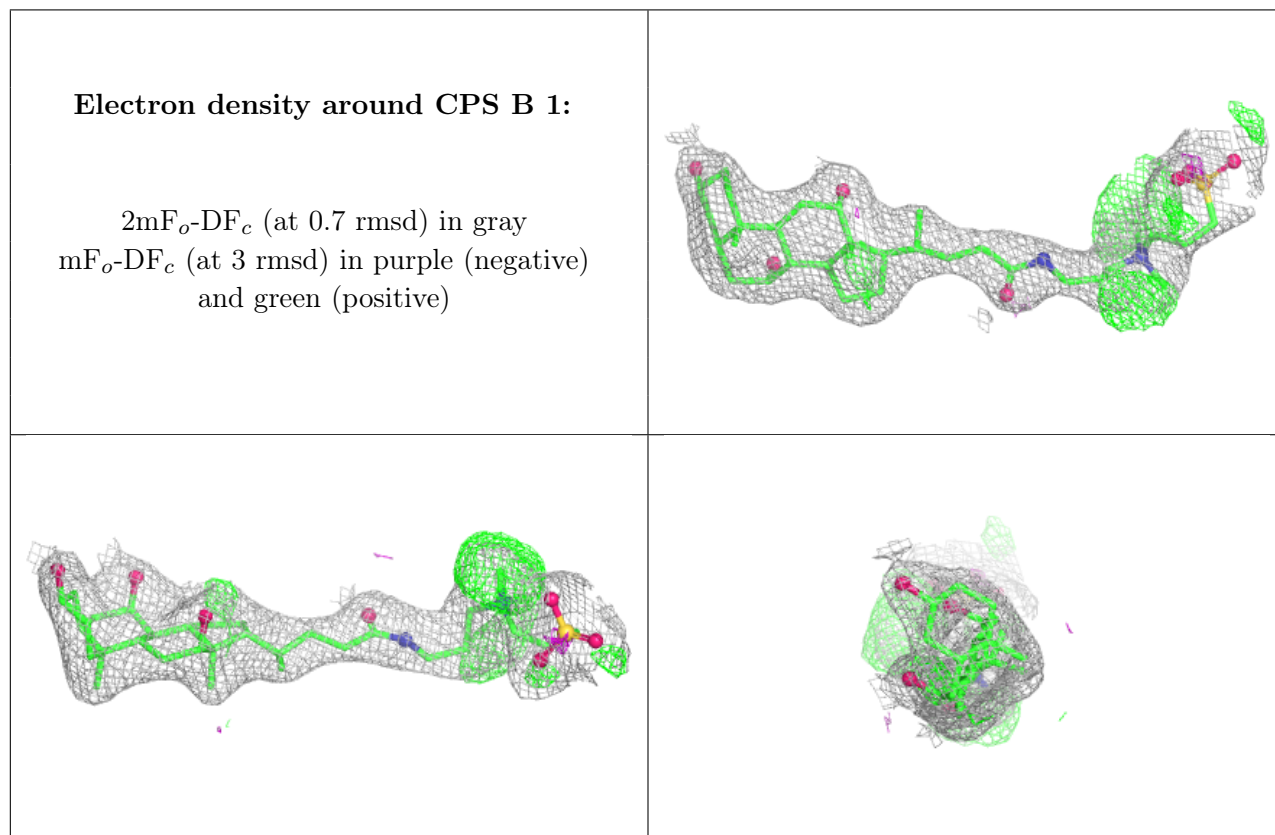
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

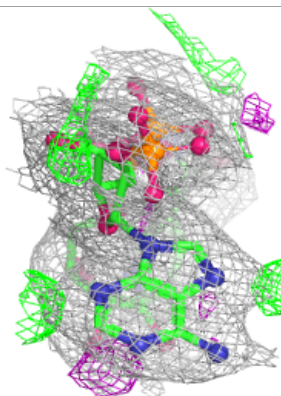
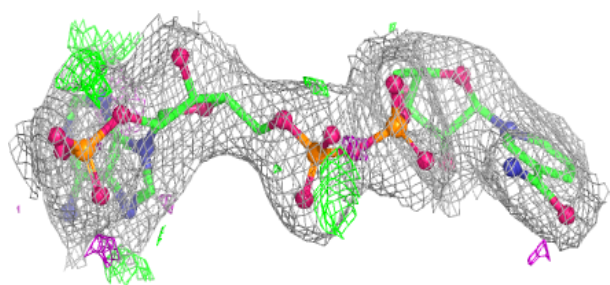
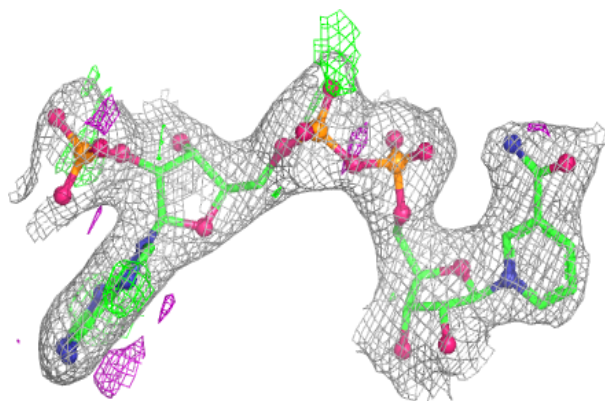
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CPS	B	1	42/42	0.87	0.15	48,53,97,98	0
2	NAP	A	1	48/48	0.95	0.09	38,46,60,63	0
3	3CZ	A	293	29/29	0.96	0.10	45,49,67,70	0
2	NAP	B	2	48/48	0.97	0.06	38,45,54,56	0

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.

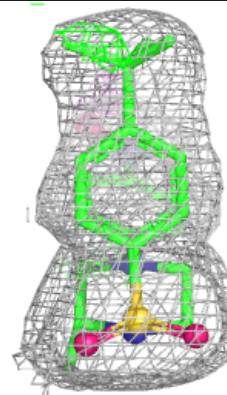
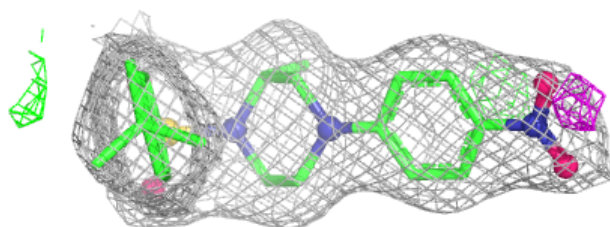
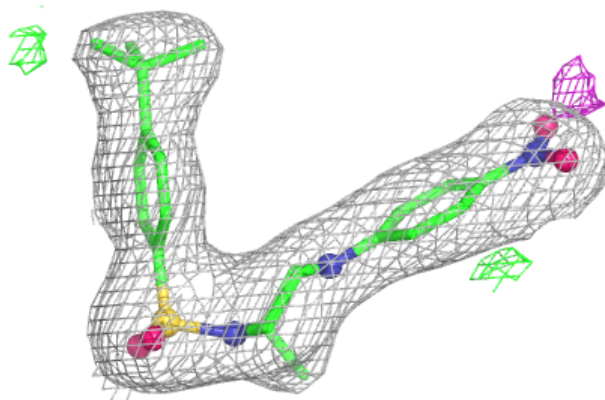


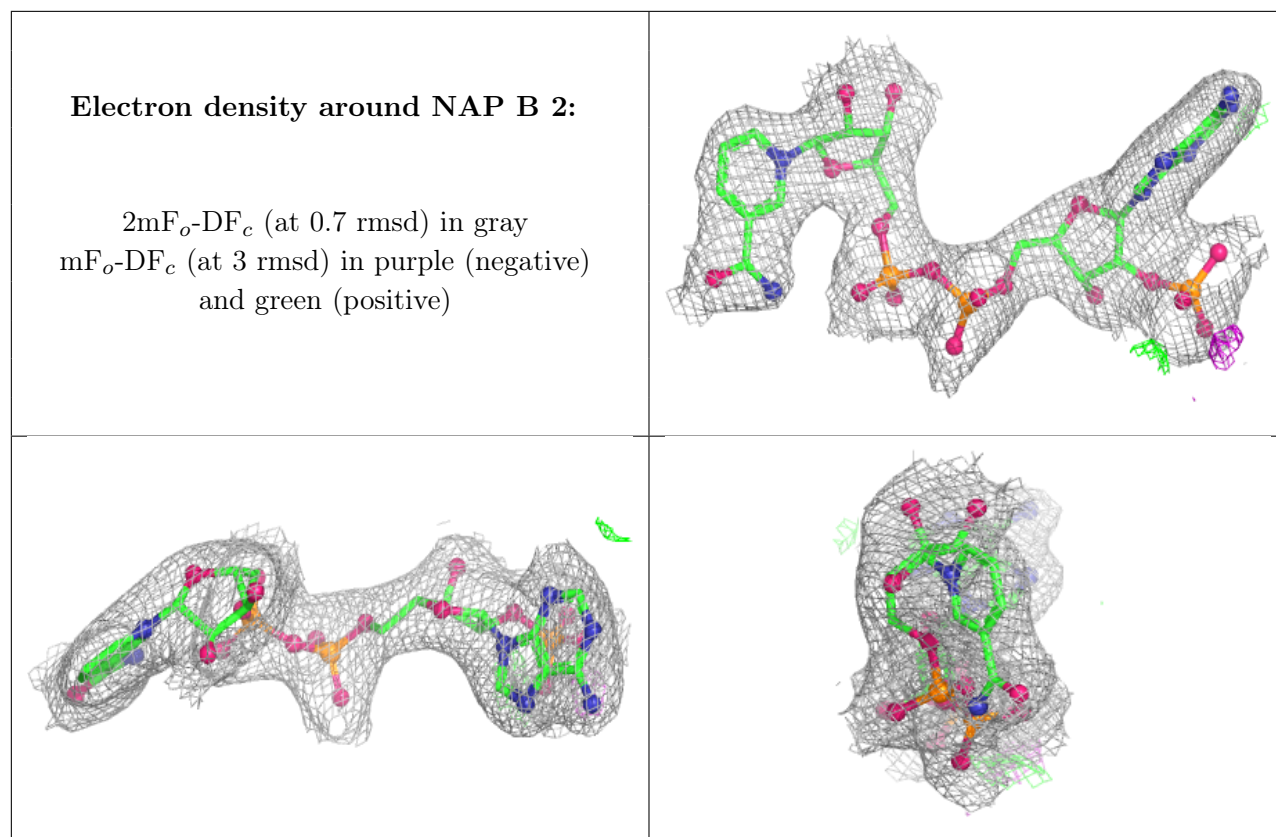
Electron density around NAP A 1:

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

**Electron density around 3CZ 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.