



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:43 AM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

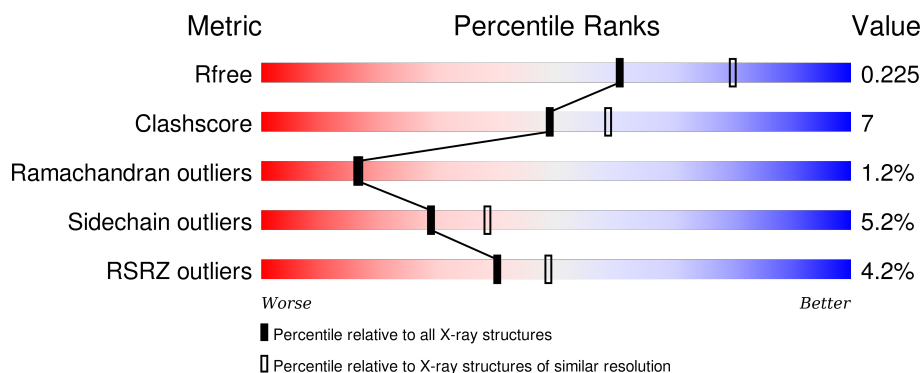
1 Overall quality at a glance

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>5%</div> <div>73%</div> <div>17%</div> <div>8%</div> </div>
1	B	286	<div> <div>2%</div> <div>75%</div> <div>15%</div> <div>7%</div> </div>

2 Entry composition

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:

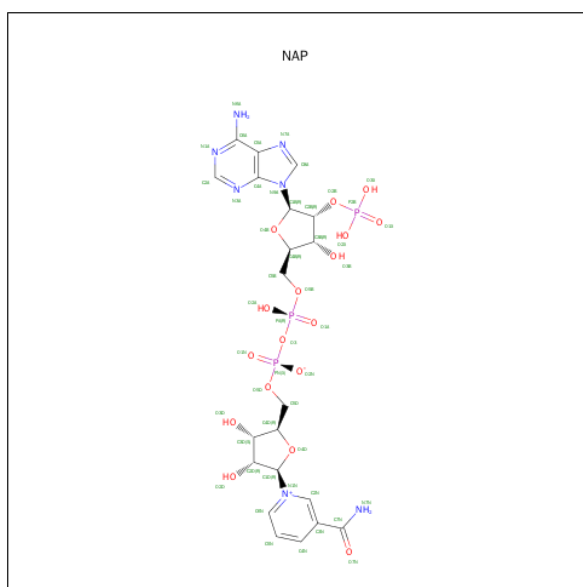
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	EXPRESSION TAG	UNP P28845
A	8	LYS	-	EXPRESSION TAG	UNP P28845
A	9	HIS	-	EXPRESSION TAG	UNP P28845
A	10	GLN	-	EXPRESSION TAG	UNP P28845
A	11	HIS	-	EXPRESSION TAG	UNP P28845
A	12	GLN	-	EXPRESSION TAG	UNP P28845
A	13	HIS	-	EXPRESSION TAG	UNP P28845
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	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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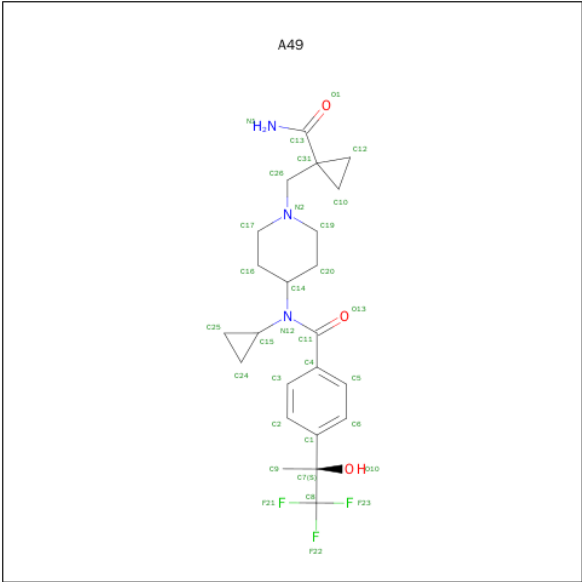
Chain	Residue	Modelled	Actual	Comment	Reference
B	14	GLN	-	EXPRESSION TAG	UNP P28845
B	15	HIS	-	EXPRESSION TAG	UNP P28845
B	16	GLN	-	EXPRESSION TAG	UNP P28845
B	17	HIS	-	EXPRESSION TAG	UNP P28845
B	18	GLN	-	EXPRESSION TAG	UNP P28845
B	19	HIS	-	EXPRESSION TAG	UNP P28845
B	20	GLN	-	EXPRESSION TAG	UNP P28845
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	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	
			48	21	7	17	3	0
2	B	1	Total	C	N	O	P	
			48	21	7	17	3	0

- Molecule 3 is N-{1-[(1-CARBAMOYL-CYCLOPROPYL)-METHYL]PIPERIDIN-4-YL}-N-CYCLOPROPYL-4-[(1S)-2,2,2-TRIFLUORO-1-HYDROXY-1-METHYLETHYL]BENZAMIDE (three-letter code: A49) (formula: $C_{23}H_{30}F_3N_3O_3$).

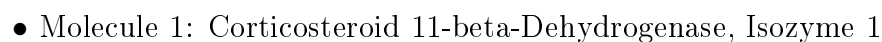


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			32	23	3	3	3		

- Molecule 4 is water.

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

- 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	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
$\langle I/\sigma(I) \rangle$ ¹	5.19 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.192 , 0.231 0.189 , 0.225	Depositor DCC
R_{free} test set	1935 reflections (5.28%)	DCC
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
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 38608 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, A49

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(°)	Ideal(°)
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 [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	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:C	1:A:270:ASN:HD22	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:HE2	1:B:224:MET:HA	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:257:TYR:CE2	1:A:268:ILE:HG22	2.51	0.46
1:A:84:ALA:O	1:A:85:SER:HB3	2.15	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:119:ASN:ND2	2:B:1:NAP:H4D	2.34	0.42
1:B:66:ARG:HB2	2:B:1:NAP:O2X	2.18	0.42
1:B:262:LEU:HA	1:B:265:THR:HG23	2.01	0.42
1:A:270:ASN:ND2	1:A:270:ASN:C	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:HD3	1:A:35:LYS:HA	1.81	0.41
1:B:215:LEU:HD13	1:B:241:CYS:SG	2.60	0.41
1:A:28:ARG:HD3	1:A:28:ARG:HH11	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:255:GLU:OE1	1:B:257:TYR:OH	2.22	0.41
1:B:35:LYS:HA	1:B:35:LYS:HD3	1.81	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%)	24	27
1	B	267/286 (93%)	248 (93%)	15 (6%)	4 (2%)	13	12
All	All	527/572 (92%)	494 (94%)	27 (5%)	6 (1%)	16	18

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%)	24	32
1	B	226/243 (93%)	216 (96%)	10 (4%)	35	46
All	All	447/486 (92%)	424 (95%)	23 (5%)	29	39

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

Some 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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	1	-	42,52,52	1.60	5 (11%)	54,80,80	2.73	14 (25%)
2	NAP	B	1	-	42,52,52	1.50	4 (9%)	54,80,80	2.73	13 (24%)
3	A49	B	2	-	33,35,35	1.34	4 (12%)	45,55,55	2.44	15 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	A	1	-	-	0/27/67/67	0/5/5/5
2	NAP	B	1	-	-	0/27/67/67	0/5/5/5
3	A49	B	2	-	-	0/36/58/58	0/2/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAP	PA-O2A	-2.35	1.44	1.54
2	A	1	NAP	PA-O2A	-2.35	1.44	1.54
3	B	2	A49	C14-N12	-2.11	1.45	1.48
2	A	1	NAP	C5A-C4A	-2.10	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAP	PN-O5D	2.02	1.68	1.59
3	B	2	A49	C17-N2	2.06	1.52	1.46
3	B	2	A49	C25-C15	2.37	1.54	1.48
2	A	1	NAP	O4B-C1B	2.59	1.44	1.41
2	B	1	NAP	C2A-N1A	2.76	1.39	1.33
2	B	1	NAP	C2A-N3A	3.46	1.38	1.32
3	B	2	A49	C11-N12	3.88	1.42	1.36
2	B	1	NAP	O7N-C7N	5.68	1.36	1.24
2	A	1	NAP	O7N-C7N	7.17	1.39	1.24

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAP	N3A-C2A-N1A	-13.64	118.45	128.89
2	B	1	NAP	N3A-C2A-N1A	-12.62	119.23	128.89
3	B	2	A49	C25-C15-N12	-7.48	108.17	118.91
3	B	2	A49	C24-C15-N12	-6.25	109.93	118.91
3	B	2	A49	C20-C14-N12	-4.52	104.22	112.65
2	B	1	NAP	C1B-N9A-C4A	-4.38	120.33	126.94
3	B	2	A49	C6-C1-C7	-4.12	116.90	121.51
2	B	1	NAP	O7N-C7N-N7N	-4.11	116.81	122.59
3	B	2	A49	C12-C31-C26	-4.04	110.59	116.87
3	B	2	A49	C17-C16-C14	-4.01	104.71	110.80
2	A	1	NAP	O2B-P2B-O1X	-3.79	97.65	107.11
2	A	1	NAP	O5B-C5B-C4B	-3.22	97.23	109.12
2	B	1	NAP	C3B-C2B-C1B	-2.99	96.95	102.73
2	A	1	NAP	O4B-C1B-C2B	-2.97	101.23	106.60
3	B	2	A49	C19-N2-C26	-2.94	106.08	111.72
3	B	2	A49	C3-C2-C1	-2.93	117.38	121.26
3	B	2	A49	C16-C17-N2	-2.78	106.42	110.96
2	A	1	NAP	O3B-C3B-C2B	-2.69	103.38	111.16
2	B	1	NAP	O3X-P2B-O2X	-2.66	97.26	107.38
2	B	1	NAP	O3-PN-O5D	-2.63	95.96	102.94
2	B	1	NAP	O7N-C7N-C3N	-2.60	116.75	119.59
3	B	2	A49	C10-C12-C31	-2.58	59.01	60.53
2	A	1	NAP	C5N-C4N-C3N	-2.54	117.14	120.33
3	B	2	A49	C5-C4-C11	-2.07	115.05	120.31
2	A	1	NAP	C2N-C3N-C4N	2.03	120.55	118.29
2	B	1	NAP	O3X-P2B-O1X	2.13	117.43	110.58
3	B	2	A49	C4-C11-N12	2.14	122.27	118.43
2	B	1	NAP	C2B-C3B-C4B	2.19	107.04	101.85
2	B	1	NAP	O2A-PA-O1A	2.19	124.41	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1	NAP	C2A-N1A-C6A	2.26	122.80	118.77
3	B	2	A49	C16-C14-N12	2.30	116.93	112.65
2	A	1	NAP	O3X-P2B-O1X	2.83	119.70	110.58
3	B	2	A49	C6-C1-C2	2.87	122.25	117.94
2	A	1	NAP	C4B-O4B-C1B	2.88	112.88	109.72
3	B	2	A49	C10-C31-C13	3.06	118.13	115.24
2	A	1	NAP	O4B-C1B-N9A	3.22	114.83	108.10
2	A	1	NAP	C3N-C7N-N7N	3.45	121.59	117.82
2	A	1	NAP	C4D-O4D-C1D	3.45	113.51	109.72
2	B	1	NAP	C2A-N1A-C6A	3.75	125.46	118.77
2	B	1	NAP	O4D-C1D-N1N	6.41	115.17	108.13
2	B	1	NAP	C3N-C7N-N7N	7.79	126.34	117.82
2	A	1	NAP	O4D-C1D-N1N	8.62	117.60	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

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	262/286 (91%)	0.34	15 (5%) 27 36	30, 50, 77, 96	9 (3%)
1	B	265/286 (92%)	0.13	7 (2%) 59 68	29, 45, 69, 102	8 (3%)
All	All	527/572 (92%)	0.23	22 (4%) 40 49	29, 47, 74, 102	17 (3%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	SER	8.8
1	B	282	THR	6.2
1	A	232	HIS	5.2
1	B	278	PHE	4.1
1	A	24	ASN	4.0
1	A	282	THR	4.0
1	A	263	TRP	3.8
1	A	23	LEU	3.6
1	B	284[A]	TYR	3.4
1	A	284[A]	TYR	3.1
1	A	27	PHE	3.0
1	A	243	LEU	2.7
1	A	233	MET	2.5
1	B	263	TRP	2.5
1	B	24	ASN	2.5
1	B	231	VAL	2.4
1	B	133	ILE	2.2
1	A	32	LEU	2.2
1	A	234	GLN	2.1
1	A	26	GLU	2.0
1	A	126	LEU	2.0
1	A	30	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	NAP	B	1	48/48	0.99	0.14	0.45	30,37,42,47	0
2	NAP	A	1	48/48	0.99	0.12	-0.44	26,37,43,45	0
3	A49	B	2	32/32	0.96	0.11	-0.62	38,43,47,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.