



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:59 pm BST

PDB ID : 1XJB  
Title : Crystal structure of human type 3 3alpha-hydroxysteroid dehydrogenase in complex with NADP(H), citrate and acetate molecules  
Authors : Couture, J.-F.; Pereira de Jesus-Tran, K.; Roy, A.-M.; Legrand, P.; Cantin, L.; Cote, P.-L.; Luu-The, V.; Labrie, F.; Breton, R.  
Deposited on : 2004-09-23  
Resolution : 1.90 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](mailto: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.

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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	:	2.11
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)	:	2.11

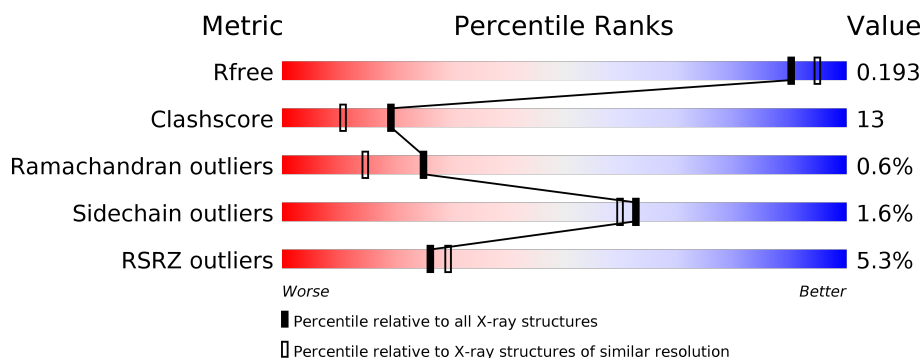
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	325	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>..</div> </div> </div>
1	B	325	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5865 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.

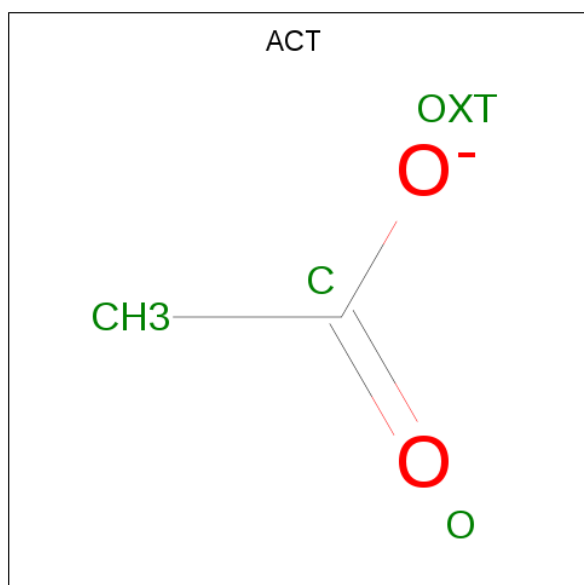
- Molecule 1 is a protein called Aldo-keto reductase family 1 member C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	3	0
			2628	1682	453	482	11			
1	B	322	Total	C	N	O	S	0	4	0
			2617	1673	453	479	12			

There are 6 discrepancies between the modelled and reference sequences:

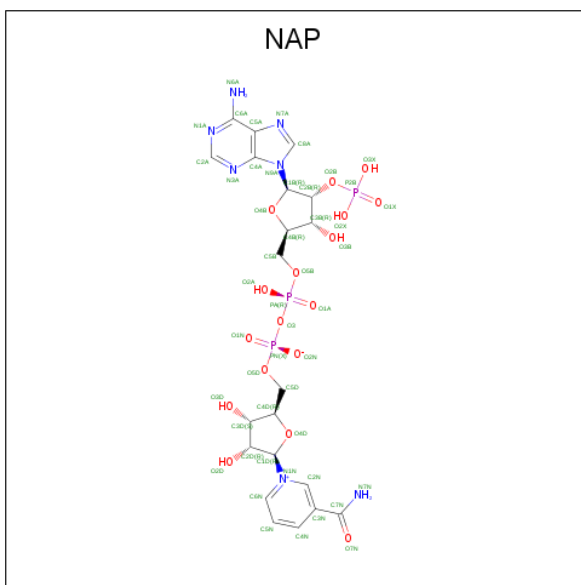
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	CLONING ARTIFACT	UNP P52895
A	0	VAL	-	CLONING ARTIFACT	UNP P52895
A	1	ASP	-	CLONING ARTIFACT	UNP P52895
B	-1	SER	-	CLONING ARTIFACT	UNP P52895
B	0	VAL	-	CLONING ARTIFACT	UNP P52895
B	1	ASP	-	CLONING ARTIFACT	UNP P52895

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



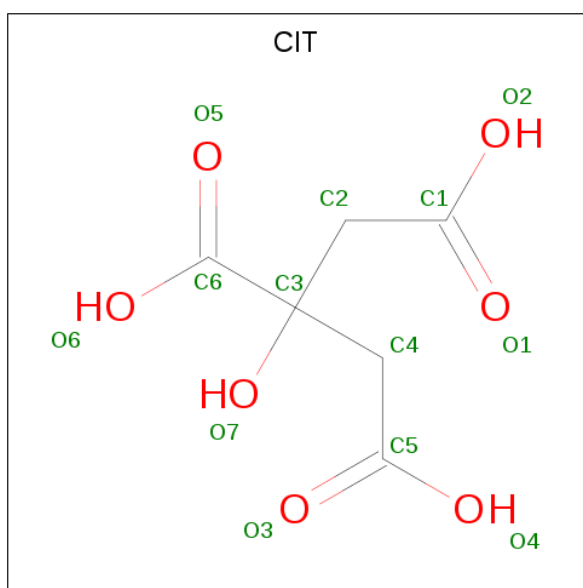
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

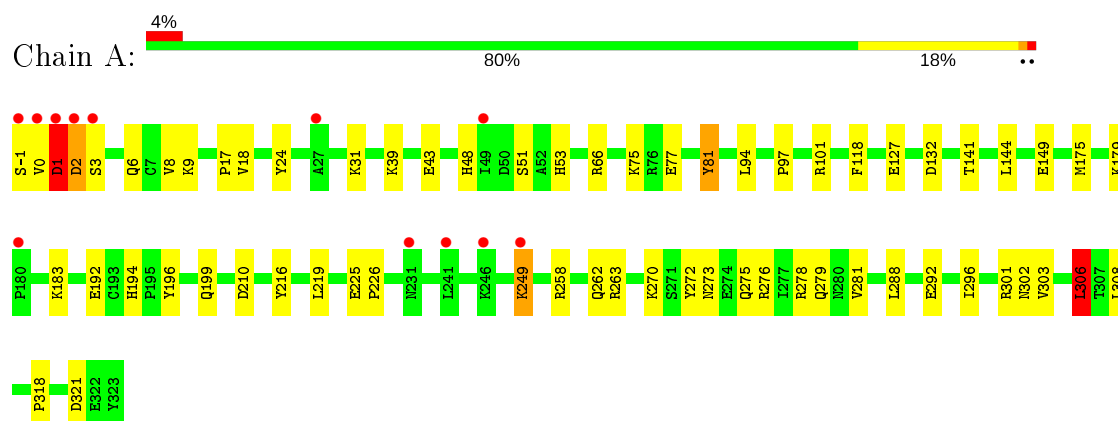
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	260	Total 260	O 260	0	0
8	B	217	Total 217	O 217	0	0

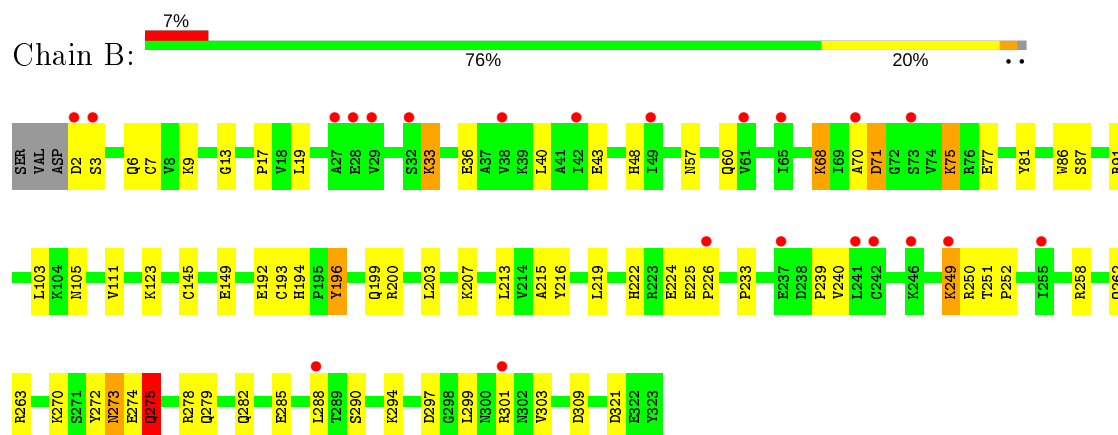
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Aldo-keto reductase family 1 member C2



- Molecule 1: Aldo-keto reductase family 1 member C2





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.12Å 143.12Å 204.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.17 – 1.90 19.17 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.17-1.90) 94.6 (19.17-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5, CNS	Depositor
R, $R_{free}$	0.174 , 0.199 0.179 , 0.193	Depositor DCC
$R_{free}$ test set	3025 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5865	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BME, CIT, EDO, NAP, SO4, ACT

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	1.17	4/2689 (0.1%)	0.94	5/3642 (0.1%)
1	B	1.30	11/2679 (0.4%)	1.04	9/3627 (0.2%)
All	All	1.24	15/5368 (0.3%)	0.99	14/7269 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	33	LYS	CD-CE	8.28	1.72	1.51
1	B	249	LYS	CG-CD	8.07	1.79	1.52
1	B	33	LYS	CE-NZ	7.00	1.66	1.49
1	B	249	LYS	CD-CE	6.23	1.66	1.51
1	B	68	LYS	CE-NZ	5.99	1.64	1.49
1	B	275	GLN	CG-CD	5.83	1.64	1.51
1	B	75	LYS	CE-NZ	5.80	1.63	1.49
1	B	81	TYR	CD2-CE2	5.70	1.47	1.39
1	A	183	LYS	CD-CE	5.65	1.65	1.51
1	A	81	TYR	CD2-CE2	5.60	1.47	1.39
1	B	81	TYR	CB-CG	5.52	1.59	1.51
1	B	216	TYR	CE2-CZ	5.33	1.45	1.38
1	A	318	PRO	CG-CD	5.16	1.67	1.50
1	B	196	TYR	CE1-CZ	5.13	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	TYR	CD2-CE2	5.08	1.47	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	A	210	ASP	CB-CG-OD2	7.92	125.42	118.30
1	B	250	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	B	263	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	B	297	ASP	CB-CG-OD1	6.71	124.34	118.30
1	B	309	ASP	CB-CG-OD2	6.53	124.17	118.30
1	B	71	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	321	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	249	LYS	CG-CD-CE	-5.85	94.36	111.90
1	B	91	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	306	LEU	CB-CG-CD2	5.51	120.38	111.00
1	A	132	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	1	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	321	ASP	CB-CG-OD2	5.28	123.05	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	GLU	Peptide
1	B	225	GLU	Mainchain,Peptide

## 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	2628	0	2638	56	0
1	B	2617	0	2614	86	0
2	A	8	0	6	0	0
2	B	4	0	3	0	0
3	A	48	0	25	6	0
3	B	48	0	25	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	6	1	0
4	B	4	0	6	1	0
5	A	13	0	5	0	0
6	A	4	0	6	0	0
7	B	10	0	0	0	0
8	A	260	0	0	9	0
8	B	217	0	0	11	0
All	All	5865	0	5334	138	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 (138) 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:249:LYS:CD	1:B:249:LYS:CG	1.79	1.55
1:B:301:ARG:HH21	1:B:303:VAL:HG11	1.17	1.04
1:B:301:ARG:NH2	1:B:303:VAL:HG11	1.78	0.98
1:A:258:ARG:HE	1:A:262:GLN:HE21	1.14	0.95
1:A:262:GLN:HE22	1:A:288:LEU:H	1.05	0.92
1:B:262:GLN:HE22	1:B:288:LEU:H	1.00	0.91
1:B:233:PRO:HG2	1:B:301:ARG:NH2	1.85	0.90
1:A:0:VAL:C	1:A:2:ASP:H	1.68	0.89
1:B:7[A]:CYS:SG	8:B:6219:HOH:O	2.29	0.89
1:B:233:PRO:HG2	1:B:301:ARG:CZ	2.03	0.88
1:A:219:LEU:HB2	3:A:1001:NAP:H52A	1.56	0.87
1:B:249:LYS:CG	1:B:249:LYS:CE	2.54	0.84
1:B:258:ARG:HE	1:B:262:GLN:HE21	1.23	0.84
1:A:301:ARG:HG3	1:A:303:VAL:HG23	1.62	0.81
1:B:219:LEU:HB2	3:B:5001:NAP:H52A	1.62	0.79
1:B:222:HIS:HD2	1:B:224:GLU:H	1.30	0.77
1:B:40:LEU:HB3	1:B:278[B]:ARG:HH12	1.50	0.76
1:B:36:GLU:HG3	8:B:6173:HOH:O	1.85	0.76
1:B:279:GLN:NE2	3:B:5001:NAP:H62A	1.83	0.75
1:B:249:LYS:CD	1:B:249:LYS:CB	2.66	0.74
1:B:273:ASN:HD22	1:B:274:GLU:N	1.86	0.74
1:B:43:GLU:HB2	1:B:278[B]:ARG:HH22	1.55	0.72
1:B:273:ASN:HD21	1:B:275:GLN:HE21	1.38	0.72
1:B:70:ALA:HB3	8:B:6176:HOH:O	1.90	0.71
1:A:0:VAL:C	1:A:2:ASP:N	2.42	0.71
1:A:279:GLN:NE2	3:A:1001:NAP:H62A	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ASN:C	1:B:273:ASN:HD22	1.93	0.71
1:A:273:ASN:HD22	1:A:276:ARG:H	1.36	0.69
1:B:262:GLN:NE2	1:B:288:LEU:H	1.84	0.67
1:A:306:LEU:HD13	1:A:308:LEU:HG	1.77	0.66
1:A:0:VAL:HB	8:A:5225:HOH:O	1.94	0.66
1:A:149:GLU:HG3	1:A:179:LYS:HE3	1.78	0.65
1:A:2:ASP:CG	1:A:3:SER:H	2.00	0.64
1:B:273:ASN:ND2	1:B:273:ASN:C	2.51	0.64
1:A:9:LYS:H	1:B:6:GLN:NE2	1.97	0.63
1:B:233:PRO:HG2	1:B:301:ARG:NH1	2.13	0.63
1:B:194:HIS:HD2	1:B:196:TYR:H	1.48	0.61
1:A:192:GLU:OE2	1:A:194:HIS:HE1	1.83	0.61
1:A:144:LEU:HB2	1:A:175:MET:HE1	1.82	0.60
1:A:301:ARG:HG3	1:A:303:VAL:CG2	2.31	0.60
1:B:2:ASP:O	1:B:3:SER:HB3	2.02	0.60
1:A:0:VAL:O	1:A:2:ASP:N	2.35	0.60
1:B:239:PRO:HG2	1:B:240:VAL:H	1.67	0.60
1:B:219:LEU:HB2	3:B:5001:NAP:C5B	2.31	0.60
1:B:262:GLN:HE22	1:B:288:LEU:N	1.84	0.59
1:A:262:GLN:NE2	1:A:288:LEU:H	1.89	0.59
1:B:233:PRO:HG2	1:B:301:ARG:HH22	1.68	0.59
1:A:17:PRO:HB2	1:A:48:HIS:HB2	1.85	0.59
1:B:145:CYS:O	1:B:149:GLU:HG3	2.03	0.59
1:A:-1:SER:HB3	1:B:13:GLY:HA3	1.84	0.58
1:B:303:VAL:CG1	8:B:6182:HOH:O	2.51	0.58
1:A:9:LYS:H	1:B:6:GLN:HE21	1.51	0.58
1:B:270:LYS:HE2	1:B:272:TYR:CD1	2.39	0.57
1:B:303:VAL:HG13	8:B:6182:HOH:O	2.02	0.57
1:B:222:HIS:CD2	1:B:224:GLU:H	2.19	0.57
1:B:273:ASN:ND2	1:B:275:GLN:H	2.04	0.56
1:B:290:SER:O	1:B:294:LYS:HG3	2.05	0.56
1:B:43:GLU:HG3	8:B:6172:HOH:O	2.04	0.56
1:A:194:HIS:HD2	1:A:196:TYR:H	1.53	0.56
1:A:2:ASP:OD2	1:A:3:SER:N	2.30	0.56
1:B:75:LYS:HG2	1:B:77:GLU:OE1	2.06	0.56
1:A:9:LYS:HE3	8:A:5153:HOH:O	2.05	0.55
1:B:43:GLU:HB2	1:B:278[B]:ARG:NH2	2.22	0.55
1:A:6:GLN:NE2	1:B:9:LYS:H	2.05	0.55
1:A:249:LYS:NZ	1:A:249:LYS:HA	2.21	0.54
1:B:203:LEU:HD11	1:B:207:LYS:HE3	1.88	0.54
1:A:262:GLN:HE22	1:A:288:LEU:N	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:HB3	1:B:278[B]:ARG:NH1	2.19	0.54
1:A:270:LYS:O	3:A:1001:NAP:H8A	2.07	0.54
1:A:219:LEU:HB2	3:A:1001:NAP:C5B	2.35	0.54
1:B:19:LEU:HB3	4:B:1003:EDO:H22	1.90	0.54
1:B:192:GLU:OE2	1:B:194:HIS:HE1	1.91	0.53
1:A:144:LEU:HB2	1:A:175:MET:CE	2.38	0.53
1:A:6:GLN:HE21	1:B:9:LYS:H	1.55	0.53
1:A:306:LEU:HD11	1:A:308:LEU:HD21	1.92	0.51
1:B:301:ARG:CZ	1:B:303:VAL:HG11	2.39	0.51
1:B:222:HIS:CD2	1:B:224:GLU:HB3	2.46	0.50
1:B:3:SER:N	8:B:6150:HOH:O	2.42	0.50
1:A:0:VAL:HG21	8:B:6139:HOH:O	2.11	0.50
3:A:1001:NAP:H51N	8:A:5017:HOH:O	2.11	0.50
1:B:251:THR:OG1	1:B:279:GLN:NE2	2.44	0.50
1:B:279:GLN:O	1:B:282:GLN:HB2	2.11	0.50
1:A:75:LYS:HB3	1:A:77:GLU:OE2	2.12	0.50
1:B:301:ARG:HB2	1:B:303:VAL:HG12	1.92	0.50
1:B:270:LYS:HD3	1:B:270:LYS:C	2.34	0.48
1:A:1:ASP:O	1:A:2:ASP:O	2.32	0.48
1:A:127:GLU:CD	1:A:127:GLU:H	2.16	0.48
1:B:40:LEU:HD13	1:B:274:GLU:HA	1.96	0.48
1:A:39:LYS:O	1:A:43:GLU:HG3	2.15	0.47
1:B:233:PRO:CG	1:B:301:ARG:NH2	2.68	0.47
1:B:282:GLN:O	1:B:285[B]:GLU:HB2	2.16	0.46
1:A:43:GLU:HG2	8:A:5230:HOH:O	2.15	0.46
1:B:219:LEU:CB	3:B:5001:NAP:H52A	2.40	0.46
1:B:270:LYS:O	3:B:5001:NAP:H8A	2.15	0.45
1:A:270:LYS:HE2	1:A:272:TYR:CD1	2.51	0.45
1:B:70:ALA:N	8:B:6176:HOH:O	2.50	0.45
1:B:40:LEU:CB	1:B:278[B]:ARG:HH12	2.24	0.45
1:A:66:ARG:HD3	8:A:5197:HOH:O	2.15	0.45
1:A:53:HIS:HE1	8:A:5066:HOH:O	1.99	0.45
1:B:105:ASN:HD22	1:B:105:ASN:HA	1.65	0.45
1:B:200:ARG:C	1:B:200:ARG:HD2	2.38	0.44
1:B:123:LYS:NZ	8:B:6160:HOH:O	2.50	0.44
1:A:273:ASN:HD21	1:A:275:GLN:HB3	1.83	0.44
1:A:31:LYS:NZ	8:A:5172:HOH:O	2.50	0.44
1:A:118:PHE:CE1	1:A:308:LEU:HD12	2.53	0.44
1:B:270:LYS:HE2	1:B:272:TYR:CE1	2.53	0.44
1:B:273:ASN:ND2	1:B:275:GLN:N	2.66	0.44
1:B:299:LEU:O	1:B:301:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:CYS:HB3	1:B:215:ALA:CB	2.48	0.43
1:B:273:ASN:HD21	1:B:275:GLN:NE2	2.11	0.43
1:B:68:LYS:HE2	1:B:68:LYS:HA	2.01	0.43
1:A:94:LEU:C	1:A:97:PRO:HD2	2.38	0.43
1:B:282:GLN:O	1:B:285[A]:GLU:HB2	2.19	0.43
1:A:141:THR:HB	4:A:5003:EDO:H22	2.01	0.43
1:B:17:PRO:HB2	1:B:48[B]:HIS:HB2	2.01	0.43
1:B:273:ASN:HD21	1:B:275:GLN:H	1.66	0.43
1:B:33:LYS:HB3	1:B:272:TYR:HD2	1.83	0.43
1:B:252:PRO:HD2	8:B:6098:HOH:O	2.19	0.42
1:B:17:PRO:HB2	1:B:48[A]:HIS:HB2	2.01	0.42
1:A:51:SER:HB3	1:A:81:TYR:OH	2.20	0.42
1:A:219:LEU:HD12	3:A:1001:NAP:H51A	2.01	0.42
1:B:57:ASN:HA	1:B:60:GLN:NE2	2.35	0.42
1:B:233:PRO:CD	1:B:301:ARG:HH22	2.32	0.42
1:A:194:HIS:CD2	1:A:196:TYR:HB2	2.54	0.42
1:B:233:PRO:CG	1:B:301:ARG:HH22	2.30	0.42
1:B:103:LEU:HD21	1:B:111:VAL:HG13	2.01	0.42
1:A:66:ARG:CD	8:A:5197:HOH:O	2.67	0.42
1:B:213:LEU:HD23	1:B:213:LEU:C	2.41	0.41
1:A:101[A]:ARG:NH1	8:A:5090:HOH:O	2.53	0.41
1:A:8:VAL:HG13	1:A:18:VAL:CG1	2.51	0.41
1:B:86:TRP:CG	1:B:87:SER:N	2.89	0.41
1:B:43:GLU:CB	1:B:278[B]:ARG:NH2	2.84	0.41
1:A:2:ASP:CG	1:A:3:SER:N	2.70	0.41
1:A:292:GLU:O	1:A:296:ILE:HG13	2.20	0.41
1:A:302:ASN:O	1:A:302:ASN:CG	2.59	0.41
1:B:194:HIS:HD2	1:B:196:TYR:N	2.14	0.41
1:B:275:GLN:NE2	1:B:275:GLN:H	2.19	0.40
1:A:278:ARG:O	1:A:281[A]:VAL:HG22	2.22	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	326/325 (100%)	316 (97%)	7 (2%)	3 (1%)	17	7
1	B	324/325 (100%)	311 (96%)	12 (4%)	1 (0%)	41	31
All	All	650/650 (100%)	627 (96%)	19 (3%)	4 (1%)	25	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	1	ASP
1	B	226	PRO
1	A	226	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	290/287 (101%)	285 (98%)	5 (2%)	60	57
1	B	288/287 (100%)	284 (99%)	4 (1%)	67	65
All	All	578/574 (101%)	569 (98%)	9 (2%)	62	60

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	A	216	TYR
1	A	249	LYS
1	A	263	ARG
1	A	306	LEU
1	B	71	ASP
1	B	199	GLN
1	B	273	ASN
1	B	275	GLN



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	53	HIS
1	A	105	ASN
1	A	167	ASN
1	A	178	ASN
1	A	194	HIS
1	A	199	GLN
1	A	231	ASN
1	A	262	GLN
1	A	273	ASN
1	A	279	GLN
1	A	287	GLN
1	B	6	GLN
1	B	53	HIS
1	B	56	ASN
1	B	60	GLN
1	B	105	ASN
1	B	167	ASN
1	B	178	ASN
1	B	194	HIS
1	B	199	GLN
1	B	222	HIS
1	B	262	GLN
1	B	273	ASN
1	B	275	GLN
1	B	279	GLN
1	B	287	GLN

### 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

11 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
4	EDO	B	1003	-	3,3,3	1.16	0	2,2,2	0.70	0
3	NAP	A	1001	-	45,52,52	1.87	9 (20%)	56,80,80	1.57	8 (14%)
7	SO4	B	5004	-	4,4,4	0.38	0	6,6,6	0.49	0
3	NAP	B	5001	-	45,52,52	1.80	9 (20%)	56,80,80	1.63	9 (16%)
6	BME	A	1005	-	3,3,3	0.83	0	1,2,2	1.01	0
2	ACT	B	6002	-	1,3,3	7.15	1 (100%)	0,3,3	0.00	-
5	CIT	A	1006	-	3,12,12	1.96	1 (33%)	3,17,17	2.19	1 (33%)
7	SO4	B	1004	-	4,4,4	1.03	0	6,6,6	0.72	0
2	ACT	A	5002	-	1,3,3	0.23	0	0,3,3	0.00	-
4	EDO	A	5003	-	3,3,3	0.44	0	2,2,2	0.61	0
2	ACT	A	1002	-	1,3,3	0.98	0	0,3,3	0.00	-

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
4	EDO	B	1003	-	-	1/1/1/1	-
3	NAP	A	1001	-	-	3/31/67/67	0/5/5/5
4	EDO	A	5003	-	-	1/1/1/1	-
6	BME	A	1005	-	-	1/1/1/1	-
5	CIT	A	1006	-	-	4/6/16/16	-
3	NAP	B	5001	-	-	8/31/67/67	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5001	NAP	O7N-C7N	7.23	1.38	1.24
2	B	6002	ACT	CH3-C	7.15	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	NAP	O7N-C7N	5.42	1.34	1.24
3	A	1001	NAP	C2N-N1N	4.43	1.40	1.35
3	A	1001	NAP	C2A-N3A	3.59	1.37	1.32
3	B	5001	NAP	O5B-C5B	-3.50	1.31	1.44
3	A	1001	NAP	C6N-N1N	3.41	1.43	1.35
3	B	5001	NAP	C2A-N3A	3.39	1.37	1.32
3	A	1001	NAP	O3D-C3D	3.23	1.50	1.43
3	A	1001	NAP	O5B-C5B	-3.19	1.32	1.44
5	A	1006	CIT	C2-C3	-2.65	1.51	1.54
3	A	1001	NAP	P2B-O2B	2.64	1.64	1.59
3	B	5001	NAP	C2N-N1N	2.61	1.38	1.35
3	B	5001	NAP	O4D-C1D	2.60	1.44	1.41
3	B	5001	NAP	C2N-C3N	2.57	1.43	1.39
3	A	1001	NAP	O4B-C4B	-2.41	1.39	1.45
3	A	1001	NAP	C2A-N1A	2.40	1.38	1.33
3	B	5001	NAP	PN-O1N	-2.37	1.42	1.50
3	B	5001	NAP	O4B-C4B	-2.36	1.39	1.45
3	B	5001	NAP	C3N-C7N	2.25	1.54	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5001	NAP	N3A-C2A-N1A	-5.77	119.66	128.68
3	B	5001	NAP	O4B-C4B-C5B	-5.70	90.63	109.37
3	A	1001	NAP	N3A-C2A-N1A	-5.12	120.67	128.68
3	A	1001	NAP	O4B-C4B-C5B	-4.92	93.19	109.37
3	A	1001	NAP	PN-O3-PA	4.37	147.84	132.83
3	A	1001	NAP	C2B-C3B-C4B	3.40	109.38	101.99
5	A	1006	CIT	C3-C2-C1	-3.33	109.65	114.98
3	B	5001	NAP	O2A-PA-O1A	3.01	127.12	112.24
3	B	5001	NAP	O2N-PN-O1N	2.71	125.66	112.24
3	A	1001	NAP	O5D-PN-O1N	-2.44	99.53	109.07
3	A	1001	NAP	O2A-PA-O1A	2.38	124.00	112.24
3	B	5001	NAP	C2N-C3N-C4N	2.29	120.85	118.26
3	B	5001	NAP	C3N-C2N-N1N	-2.25	118.23	120.43
3	B	5001	NAP	C2B-C3B-C4B	2.18	106.73	101.99
3	A	1001	NAP	O3X-P2B-O2X	2.16	115.87	107.64
3	B	5001	NAP	C2D-C3D-C4D	-2.08	98.59	102.64
3	B	5001	NAP	O2N-PN-O5D	-2.05	98.21	107.75
3	A	1001	NAP	C3N-C7N-N7N	2.03	120.18	117.75

There are no chirality outliers.

All (18) torsion outliers are listed below:

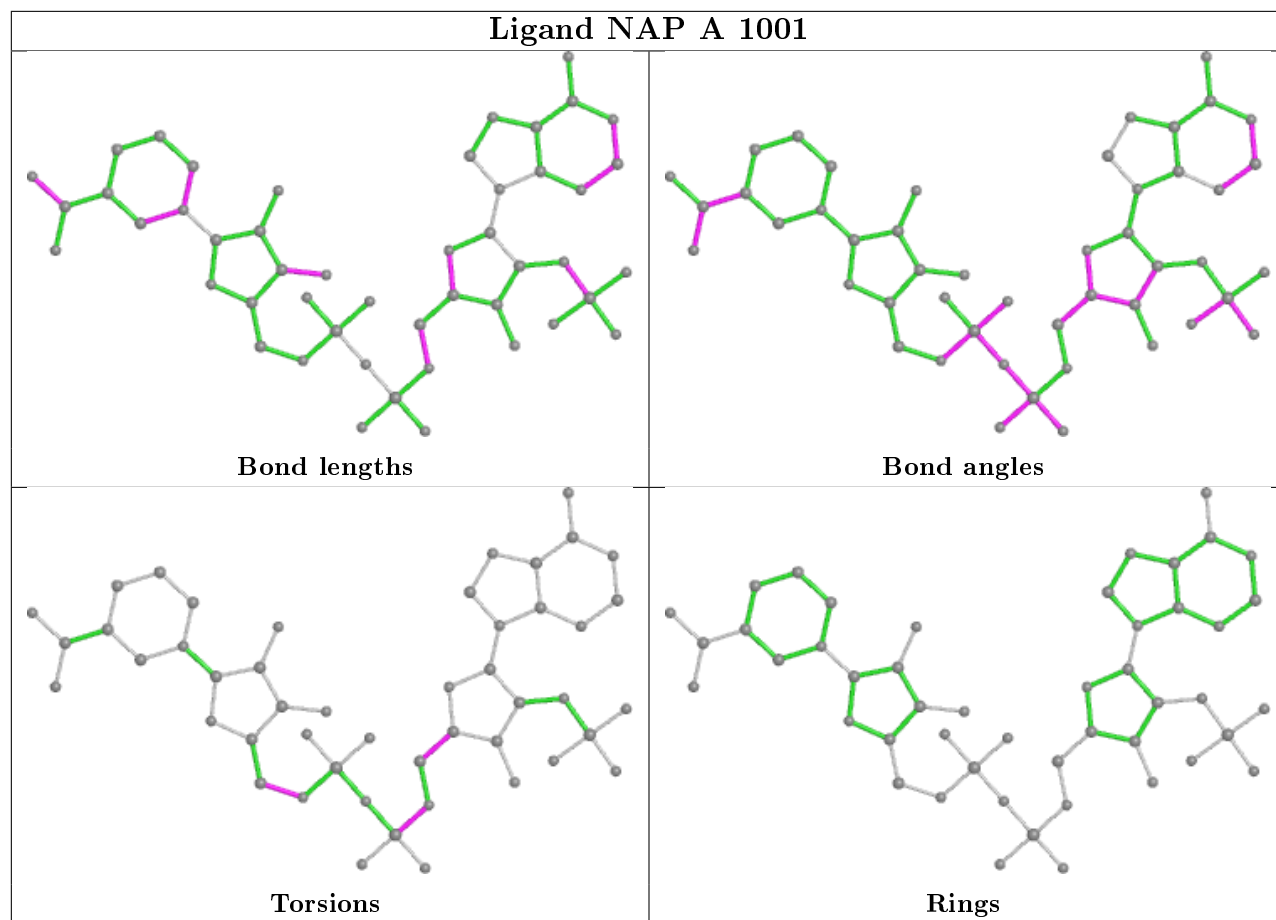
Mol	Chain	Res	Type	Atoms
3	B	5001	NAP	PA-O3-PN-O5D
6	A	1005	BME	O1-C1-C2-S2
5	A	1006	CIT	C1-C2-C3-C4
4	A	5003	EDO	O1-C1-C2-O2
3	B	5001	NAP	PN-O3-PA-O2A
5	A	1006	CIT	O7-C3-C4-C5
5	A	1006	CIT	C1-C2-C3-C6
5	A	1006	CIT	C6-C3-C4-C5
3	B	5001	NAP	C4D-C5D-O5D-PN
3	A	1001	NAP	C4D-C5D-O5D-PN
3	B	5001	NAP	PN-O3-PA-O1A
4	B	1003	EDO	O1-C1-C2-O2
3	B	5001	NAP	C5B-O5B-PA-O3
3	B	5001	NAP	C5D-O5D-PN-O3
3	A	1001	NAP	O4B-C4B-C5B-O5B
3	A	1001	NAP	C5B-O5B-PA-O1A
3	B	5001	NAP	C5B-O5B-PA-O1A
3	B	5001	NAP	O4B-C4B-C5B-O5B

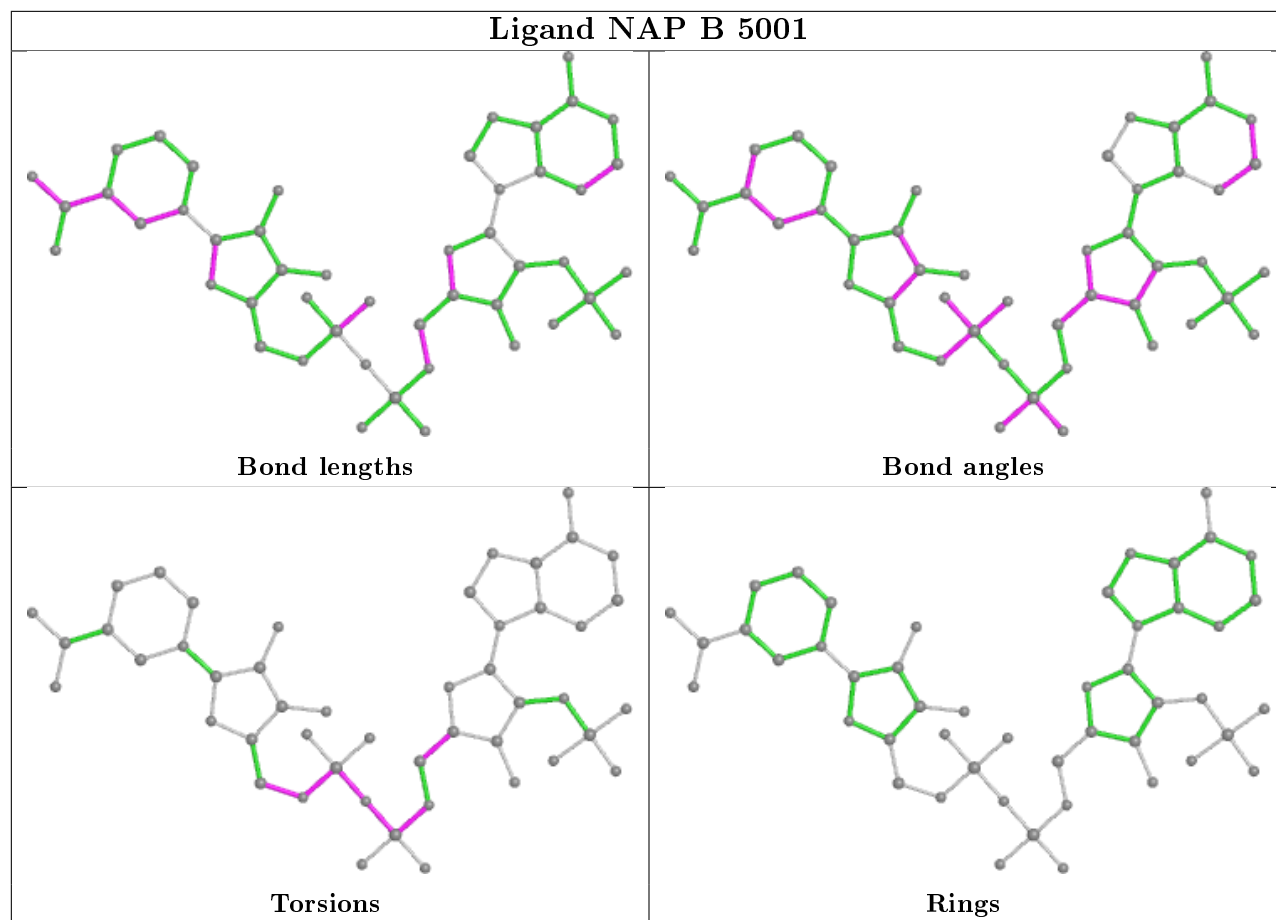
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1003	EDO	1	0
3	A	1001	NAP	6	0
3	B	5001	NAP	5	0
4	A	5003	EDO	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.





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	325/325 (100%)	0.19	12 (3%) 41 44	22, 30, 43, 79	15 (4%)
1	B	322/325 (99%)	0.30	22 (6%) 17 19	18, 30, 49, 59	11 (3%)
All	All	647/650 (99%)	0.24	34 (5%) 26 29	18, 30, 46, 79	26 (4%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	VAL	9.2
1	A	-1	SER	7.5
1	A	1	ASP	4.3
1	B	38	VAL	4.0
1	B	2	ASP	3.7
1	A	2	ASP	3.6
1	B	28	GLU	3.4
1	B	301	ARG	3.3
1	B	27	ALA	3.2
1	B	237	GLU	3.2
1	B	49	ILE	3.1
1	B	255	ILE	2.9
1	B	70	ALA	2.8
1	A	3	SER	2.8
1	A	231	ASN	2.6
1	B	73	SER	2.5
1	B	226	PRO	2.5
1	A	27	ALA	2.5
1	B	241	LEU	2.4
1	B	3	SER	2.4
1	B	65	ILE	2.4
1	B	32	SER	2.3
1	B	246	LYS	2.3
1	A	180	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	242	CYS	2.2
1	B	29	VAL	2.2
1	B	42	ILE	2.2
1	A	241	LEU	2.2
1	B	249	LYS	2.2
1	B	61	VAL	2.2
1	A	246	LYS	2.1
1	A	249	LYS	2.1
1	B	288	LEU	2.0
1	A	49[A]	ILE	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
5	CIT	A	1006	13/13	0.65	0.35	37,41,47,47	13
7	SO4	B	1004	5/5	0.86	0.37	38,38,41,42	5
2	ACT	B	6002	4/4	0.88	0.15	38,40,40,40	0
2	ACT	A	1002	4/4	0.89	0.13	28,29,31,35	0
4	EDO	A	5003	4/4	0.91	0.27	63,64,64,65	0
6	BME	A	1005	4/4	0.92	0.16	42,42,43,44	4
3	NAP	B	5001	48/48	0.93	0.16	24,36,48,49	0
3	NAP	A	1001	48/48	0.97	0.12	24,28,35,37	0
2	ACT	A	5002	4/4	0.97	0.07	32,32,34,35	0
7	SO4	B	5004	5/5	0.97	0.14	40,44,46,47	5
4	EDO	B	1003	4/4	0.97	0.08	28,30,34,37	0

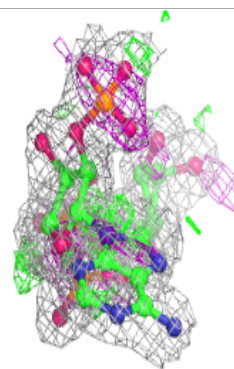
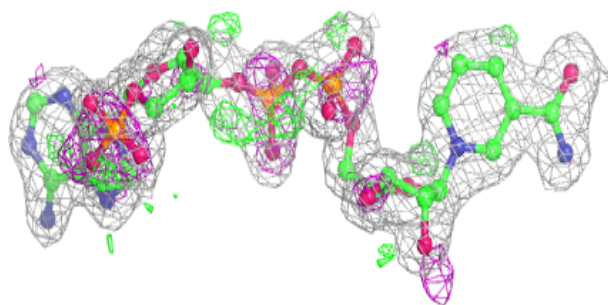
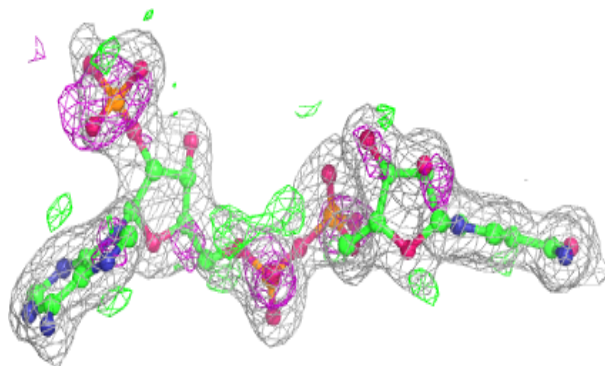
The following is a graphical depiction of the model fit to experimental electron density of all

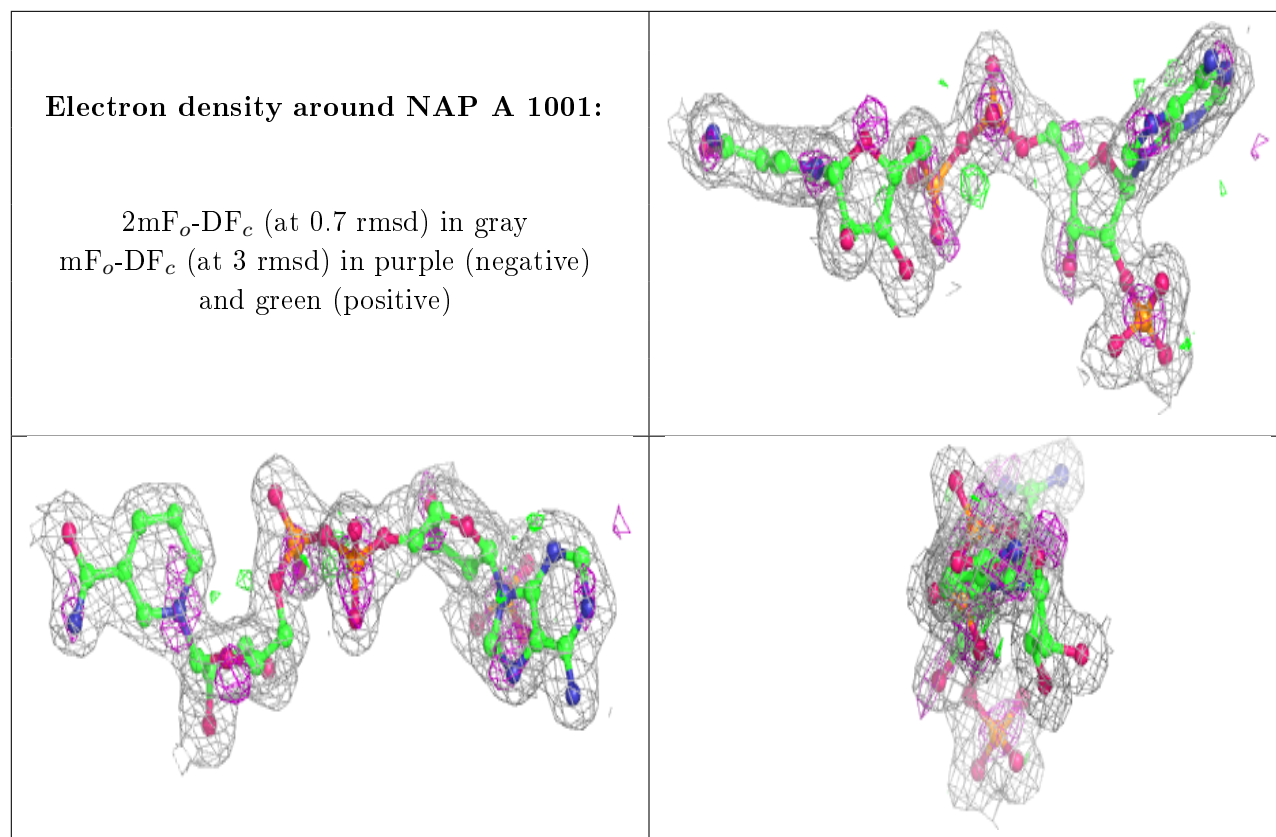


instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around NAP B 5001:**

$2mF_o-DF_c$  (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.