



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 02:14 AM EST

PDB ID : 1DR6
Title : CRYSTAL STRUCTURES OF ORGANOMERCURIAL-ACTIVATED
CHICKEN LIVER DIHYDROFOLATE REDUCTASE COMPLEXES
Authors : Mctigue, M.A.; Davies /II, J.F.; Kaufman, B.T.; Xuong, N.-H.; Kraut, J.
Deposited on : unknown
Resolution : 2.40 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

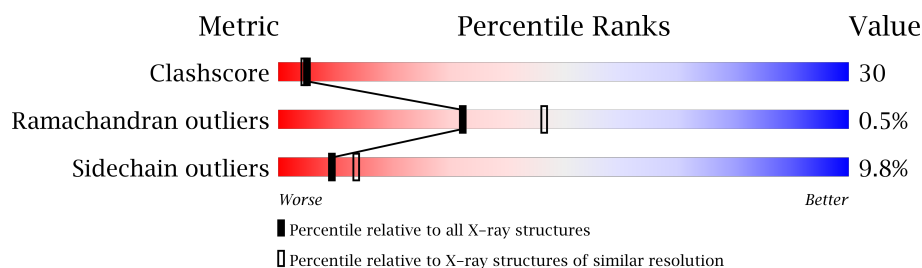
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	189	

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.

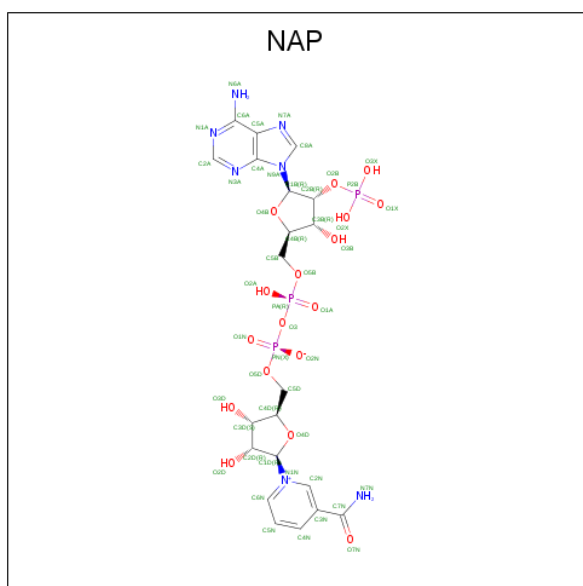
- Molecule 1 is a protein called DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	1	0
			1493	963	249	274	7			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

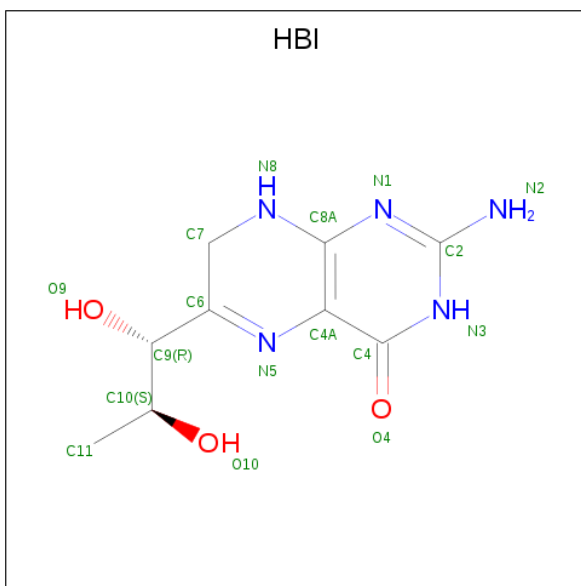
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $\text{C}_{21}\text{H}_{28}\text{N}_7\text{O}_{17}\text{P}_3$).



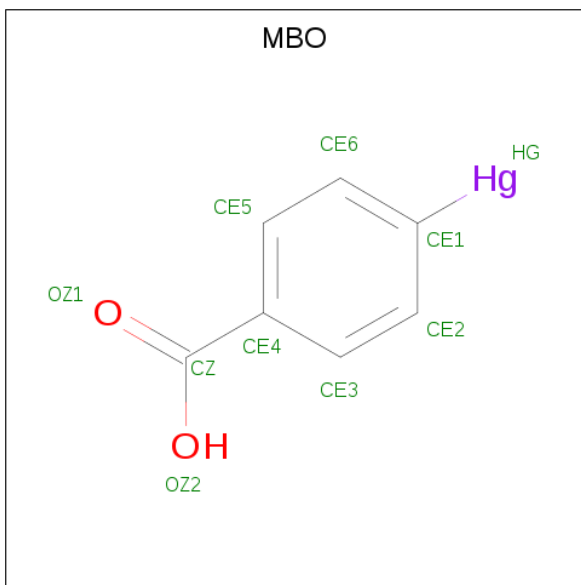
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is 7,8-DIHYDROBIOPTERIN (three-letter code: HBI) (formula: $C_9H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is MERCURIBENZOIC ACID (three-letter code: MBO) (formula: $C_7H_5HgO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Hg	O	0	1
			11	7	2	2		

- Molecule 6 is water.

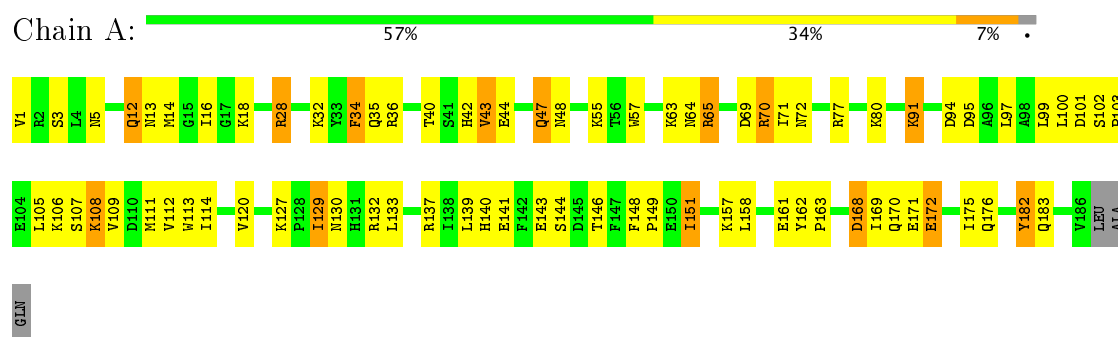
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	74	Total	O	0	0
			74	74		

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.

Note EDS was not executed.

• Molecule 1: DIHYDROFOLATE REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.72Å 48.74Å 63.87Å 90.00° 124.70° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.141 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1644	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MBO, HBI, 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	1.01	0/1533	1.61	12/2072 (0.6%)

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	3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	GLU	CA-CB-CG	9.07	133.36	113.40
1	A	65	ARG	CD-NE-CZ	7.92	134.69	123.60
1	A	168	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	97	LEU	CB-CA-C	6.57	122.68	110.20
1	A	182	TYR	N-CA-CB	6.54	122.37	110.60
1	A	70	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	64	ASN	CA-CB-CG	5.78	126.12	113.40
1	A	95	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	12	GLN	CB-CA-C	5.48	121.36	110.40
1	A	101	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	146	THR	CA-CB-CG2	5.08	119.51	112.40
1	A	44	GLU	CA-CB-CG	5.05	124.52	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ARG	Sidechain
1	A	28	ARG	Sidechain
1	A	77	ARG	Sidechain

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	1493	0	1497	72	0
2	A	1	0	0	0	0
3	A	48	0	25	4	0
4	A	17	0	13	3	0
5	A	11	0	0	0	0
6	A	74	0	0	2	0
All	All	1644	0	1535	76	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 30.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:HE	1:A:32:LYS:NZ	1.50	1.07
1:A:40:THR:O	1:A:111:MET:HE1	1.65	0.96
1:A:28:ARG:HE	1:A:32:LYS:HZ1	0.95	0.94
1:A:28:ARG:NE	1:A:32:LYS:NZ	2.15	0.93
1:A:40:THR:O	1:A:111:MET:CE	2.27	0.82
1:A:3:SER:HA	1:A:129:ILE:HD11	1.62	0.81
1:A:3:SER:CA	1:A:129:ILE:HD11	2.12	0.78
1:A:28:ARG:NE	1:A:32:LYS:HZ1	1.77	0.78
1:A:16:ILE:O	3:A:191:NAP:H2N	1.85	0.76
3:A:191:NAP:H4N	4:A:198:HBI:H71	1.67	0.76
1:A:28:ARG:NE	1:A:32:LYS:HZ2	1.82	0.75
4:A:198:HBI:O10	6:A:756:HOH:O	2.03	0.70
1:A:42:HIS:C	1:A:43:VAL:HG23	2.12	0.68
1:A:127:LYS:HB3	1:A:129:ILE:HG23	1.74	0.67
1:A:99:LEU:HG	1:A:105:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:191:NAP:C4N	4:A:198:HBI:H71	2.27	0.64
1:A:102:SER:HB2	1:A:103:PRO:HD2	1.81	0.63
1:A:71:ILE:HD12	1:A:109:VAL:HG22	1.83	0.61
1:A:139:LEU:O	1:A:140:HIS:CG	2.55	0.60
1:A:94:ASP:OD1	1:A:127:LYS:NZ	2.26	0.59
1:A:42:HIS:O	1:A:43:VAL:CG2	2.51	0.58
1:A:71:ILE:CD1	1:A:109:VAL:HG22	2.33	0.58
1:A:71:ILE:HD11	1:A:108:LYS:HZ3	1.68	0.58
1:A:47:GLN:HG2	1:A:69:ASP:O	2.04	0.57
1:A:42:HIS:O	1:A:43:VAL:HG23	2.05	0.57
1:A:18:LYS:HD3	1:A:143:GLU:HG3	1.87	0.57
1:A:99:LEU:HG	1:A:105:LEU:CD1	2.35	0.56
1:A:133:LEU:HD23	1:A:151:ILE:HD12	1.87	0.56
1:A:3:SER:HA	1:A:129:ILE:CD1	2.33	0.56
1:A:129:ILE:HG13	1:A:130:ASN:O	2.07	0.54
3:A:191:NAP:H8A	3:A:191:NAP:H52A	1.90	0.54
1:A:42:HIS:C	1:A:43:VAL:CG2	2.77	0.53
1:A:72:ASN:N	1:A:72:ASN:HD22	2.07	0.52
1:A:71:ILE:HD11	1:A:108:LYS:NZ	2.24	0.52
1:A:127:LYS:HB3	1:A:129:ILE:CG2	2.39	0.52
1:A:48:ASN:HD21	1:A:111:MET:HE3	1.74	0.50
1:A:158:LEU:HB2	1:A:182:TYR:CE2	2.47	0.50
1:A:139:LEU:C	1:A:140:HIS:CG	2.85	0.50
1:A:132:ARG:NH1	1:A:183:GLN:OE1	2.46	0.48
1:A:148:PHE:CD1	1:A:149:PRO:HD2	2.47	0.48
1:A:3:SER:N	1:A:129:ILE:HD11	2.29	0.48
1:A:114:ILE:HG23	1:A:120:VAL:HG12	1.96	0.47
1:A:5:ASN:O	1:A:113:TRP:HA	2.14	0.47
1:A:127:LYS:CB	1:A:129:ILE:HG23	2.45	0.46
1:A:35:GLN:NE2	1:A:70:ARG:HH12	2.14	0.45
1:A:57:TRP:CE2	1:A:65:ARG:HD3	2.51	0.45
1:A:100:LEU:HD13	1:A:112:VAL:CG2	2.47	0.45
1:A:140:HIS:CD2	1:A:175:ILE:HG23	2.53	0.44
1:A:100:LEU:HD13	1:A:112:VAL:HG21	1.99	0.44
1:A:170:GLN:O	1:A:176:GLN:HA	2.18	0.44
1:A:48:ASN:HD21	1:A:111:MET:CE	2.30	0.43
1:A:91:LYS:HD2	6:A:295:HOH:O	2.17	0.43
1:A:99:LEU:CG	1:A:105:LEU:HD12	2.47	0.43
1:A:13:ASN:O	1:A:14:MET:HB2	2.18	0.43
1:A:1:VAL:O	1:A:129:ILE:HD13	2.19	0.43
1:A:133:LEU:CD2	1:A:151:ILE:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLU:HA	1:A:175:ILE:O	2.19	0.42
1:A:162:TYR:HA	1:A:163:PRO:HD3	1.73	0.42
1:A:34:PHE:C	1:A:34:PHE:CD1	2.93	0.42
1:A:28:ARG:HH21	1:A:32:LYS:NZ	2.17	0.41
1:A:18:LYS:CD	1:A:143:GLU:HG3	2.51	0.41
1:A:161:GLU:HG2	1:A:162:TYR:N	2.29	0.41
1:A:129:ILE:HG13	1:A:130:ASN:N	2.35	0.41
1:A:139:LEU:C	1:A:140:HIS:CD2	2.95	0.41
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.88	0.40
1:A:175:ILE:HD13	1:A:175:ILE:HA	1.88	0.40
1:A:63:LYS:HD3	1:A:63:LYS:HA	1.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	185/189 (98%)	178 (96%)	6 (3%)	1 (0%)	32 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	VAL

5.3.2 Protein sidechains [i](#)

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	164/168 (98%)	148 (90%)	16 (10%)	9 14

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	PHE
1	A	36	ARG
1	A	47	GLN
1	A	55	LYS
1	A	80	LYS
1	A	91	LYS
1	A	106	LYS
1	A	107	SER
1	A	108	LYS
1	A	129	ILE
1	A	144	SER
1	A	151	ILE
1	A	157	LYS
1	A	168	ASP
1	A	169	ILE
1	A	172	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	47	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

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAP	A	191	2	44,52,52	3.35	12 (27%)	51,80,80	2.55	15 (29%)
4	HBI	A	198	-	13,18,18	3.22	5 (38%)	10,26,26	6.15	6 (60%)
5	MBO	A	201[A]	1	4,10,10	0.60	0	8,13,13	2.90	2 (25%)
5	MBO	A	201[B]	1	4,10,10	0.60	0	8,13,13	2.90	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	A	191	2	-	0/27/67/67	0/5/5/5
4	HBI	A	198	-	-	0/4/17/17	0/2/2/2
5	MBO	A	201[A]	1	-	0/0/4/4	0/1/1/1
5	MBO	A	201[B]	1	-	0/0/4/4	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	191	NAP	O4B-C4B	-14.04	1.13	1.45
4	A	198	HBI	C7-N8	-7.49	1.30	1.45
3	A	191	NAP	C5A-C4A	-3.52	1.32	1.40
3	A	191	NAP	C3N-C7N	-3.21	1.45	1.50
3	A	191	NAP	C6N-C5N	-3.08	1.31	1.38
4	A	198	HBI	O4-C4	2.16	1.30	1.24
3	A	191	NAP	C6A-C5A	2.55	1.55	1.42
3	A	191	NAP	O3D-C3D	2.66	1.49	1.43
4	A	198	HBI	C4-N3	2.84	1.38	1.33
3	A	191	NAP	C3B-C4B	3.05	1.61	1.53
4	A	198	HBI	C2-N1	3.19	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	191	NAP	O3B-C3B	3.34	1.50	1.43
3	A	191	NAP	O4B-C1B	4.64	1.47	1.41
3	A	191	NAP	O4D-C1D	5.26	1.48	1.41
4	A	198	HBI	C6-N5	6.51	1.37	1.28
3	A	191	NAP	C5N-C4N	7.41	1.53	1.38
3	A	191	NAP	C4N-C3N	9.63	1.55	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	191	NAP	C5N-C4N-C3N	-9.65	109.00	120.35
4	A	198	HBI	C4A-C4-N3	-8.99	110.68	123.48
5	A	201[B]	MBO	CE5-CE4-CZ	-6.02	112.36	120.45
5	A	201[A]	MBO	CE5-CE4-CZ	-6.02	112.36	120.45
3	A	191	NAP	O4B-C1B-C2B	-4.12	99.39	106.59
3	A	191	NAP	C2B-C3B-C4B	-3.69	93.57	101.95
3	A	191	NAP	C2A-N1A-C6A	-3.50	112.64	118.77
3	A	191	NAP	O3B-C3B-C4B	-3.38	101.21	111.09
4	A	198	HBI	N3-C2-N1	-3.15	120.34	125.45
3	A	191	NAP	O2D-C2D-C3D	-2.50	103.83	111.83
3	A	191	NAP	O3B-C3B-C2B	-2.29	104.68	111.18
3	A	191	NAP	C5N-C6N-N1N	2.05	123.56	120.40
3	A	191	NAP	C5A-C6A-N6A	2.12	124.79	120.47
3	A	191	NAP	O5B-C5B-C4B	2.17	116.68	109.00
3	A	191	NAP	C3N-C7N-N7N	2.36	120.47	117.77
3	A	191	NAP	C6N-C5N-C4N	2.45	123.14	119.44
4	A	198	HBI	N2-C2-N3	3.08	122.17	117.24
4	A	198	HBI	C6-C7-N8	3.61	127.13	114.70
3	A	191	NAP	C2N-C3N-C4N	4.88	123.83	118.26
5	A	201[B]	MBO	CE3-CE4-CZ	5.02	127.20	120.45
5	A	201[A]	MBO	CE3-CE4-CZ	5.02	127.20	120.45
3	A	191	NAP	N3A-C2A-N1A	6.06	134.13	128.86
3	A	191	NAP	C4B-O4B-C1B	6.56	116.75	109.77
4	A	198	HBI	C4-N3-C2	7.28	126.53	116.06
4	A	198	HBI	C4-C4A-C8A	14.53	124.22	114.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	191	NAP	4	0
4	A	198	HBI	3	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 ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.