



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:06 PM UTC

PDB ID : 1DR6 / pdb_00001dr6
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 : 1992-03-14
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

<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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

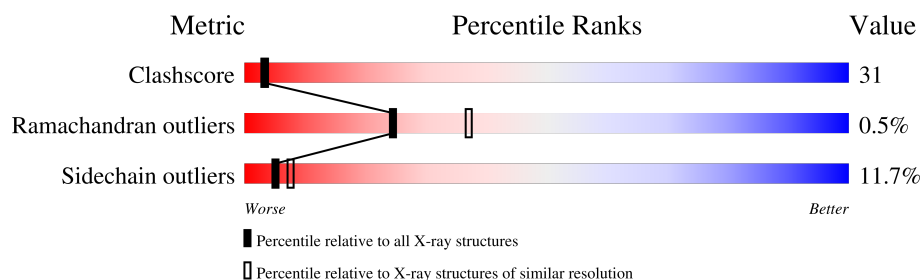
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	189	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 1644 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.

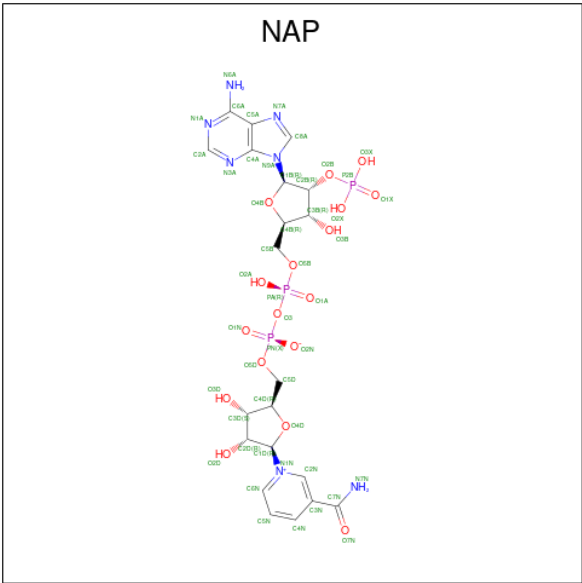
- Molecule 1 is a protein called DIHYDROFOLATE REDUCTASE.

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

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

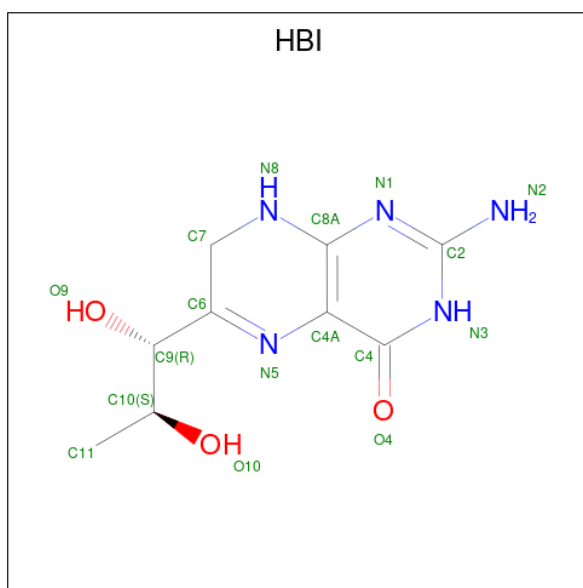
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



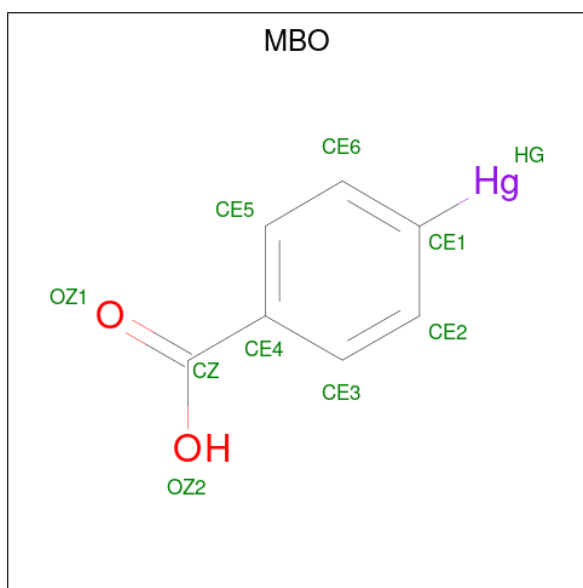
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0

- Molecule 4 is 7,8-DIHYDROBIOPTERIN (CCD ID: 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 (CCD ID: 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.

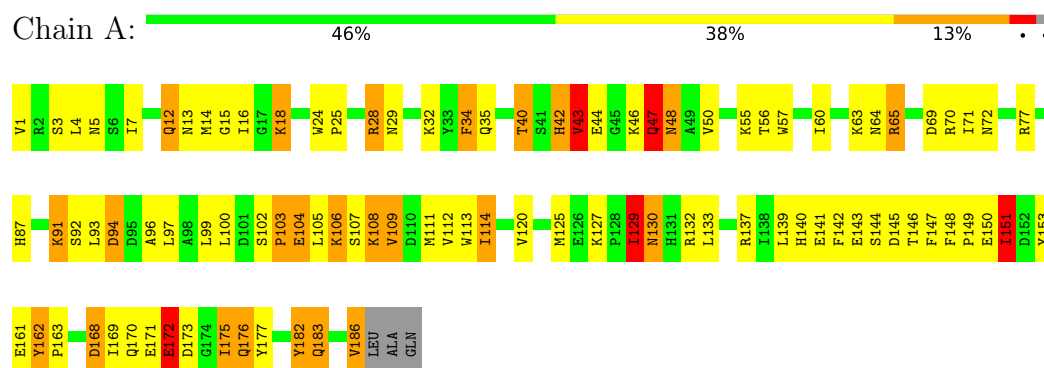
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	74	Total	O	0	0
			74	74		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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, HBI, NAP, MBO

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	1.34	5/1533 (0.3%)	2.02	55/2072 (2.7%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	THR	N-CA	6.81	1.54	1.45
1	A	48	ASN	N-CA	6.41	1.53	1.45
1	A	175	ILE	CA-CB	5.89	1.62	1.54
1	A	40	THR	CA-CB	5.82	1.60	1.53
1	A	114	ILE	C-N	-5.04	1.27	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ASN	CA-CB-CG	13.53	126.12	112.60
1	A	168	ASP	CA-CB-CG	9.83	122.43	112.60
1	A	172	GLU	CA-CB-CG	9.63	133.36	114.10
1	A	87	HIS	CA-CB-CG	-8.51	105.30	113.80
1	A	82	ALA	O-C-N	8.15	128.40	121.31
1	A	29	ASN	CA-CB-CG	-8.08	104.52	112.60
1	A	65	ARG	CD-NE-CZ	7.35	134.69	124.40
1	A	182	TYR	N-CA-CB	7.25	122.37	110.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	LEU	CB-CA-C	7.16	122.68	110.79
1	A	42	HIS	CA-CB-CG	-7.08	106.72	113.80
1	A	40	THR	N-CA-C	6.93	119.41	108.67
1	A	151	ILE	CB-CA-C	6.69	120.38	111.21
1	A	64	ASN	OD1-CG-ND2	-6.67	115.92	122.60
1	A	145	ASP	CB-CA-C	6.42	119.80	109.27
1	A	146	THR	CA-CB-OG1	-6.35	100.08	109.60
1	A	103	PRO	CA-C-N	6.31	129.59	120.38
1	A	103	PRO	C-N-CA	6.31	129.59	120.38
1	A	109	VAL	N-CA-C	6.14	117.14	108.36
1	A	94	ASP	CA-CB-CG	-6.07	106.53	112.60
1	A	142	PHE	CA-CB-CG	6.06	119.86	113.80
1	A	29	ASN	OD1-CG-ND2	6.05	128.65	122.60
1	A	24	TRP	O-C-N	5.94	126.55	121.20
1	A	47	GLN	CA-C-O	-5.86	114.59	121.44
1	A	129	ILE	CA-CB-CG2	5.81	120.38	110.50
1	A	12	GLN	CB-CA-C	5.80	121.36	110.63
1	A	56	THR	CA-CB-OG1	-5.70	101.05	109.60
1	A	186	VAL	CA-C-O	-5.59	111.29	120.80
1	A	4	LEU	N-CA-CB	-5.56	102.29	110.85
1	A	60	ILE	O-C-N	5.52	127.91	121.57
1	A	173	ASP	CA-C-O	-5.48	115.18	121.54
1	A	25	PRO	N-CA-C	-5.46	104.03	110.70
1	A	153	TYR	N-CA-CB	5.46	119.60	110.32
1	A	130	ASN	CB-CA-C	5.45	118.47	109.70
1	A	40	THR	CA-CB-OG1	-5.43	101.45	109.60
1	A	146	THR	N-CA-CB	-5.42	101.80	111.08
1	A	15	GLY	CA-C-N	5.39	131.68	121.97
1	A	15	GLY	C-N-CA	5.39	131.68	121.97
1	A	146	THR	CA-CB-CG2	5.30	119.51	110.50
1	A	50	VAL	O-C-N	5.26	128.94	123.26
1	A	44	GLU	CB-CG-CD	5.25	121.52	112.60
1	A	44	GLU	CA-CB-CG	5.21	124.52	114.10
1	A	92	SER	CA-C-O	-5.21	115.86	121.38
1	A	147	PHE	CA-CB-CG	-5.18	108.62	113.80
1	A	92	SER	O-C-N	5.13	128.65	123.26
1	A	176	GLN	CB-CG-CD	-5.13	103.87	112.60
1	A	43	VAL	N-CA-CB	-5.11	102.80	111.23
1	A	96	ALA	N-CA-C	-5.11	105.80	111.36
1	A	104	GLU	CB-CG-CD	5.09	121.26	112.60
1	A	183	GLN	CB-CG-CD	-5.09	103.94	112.60
1	A	46	LYS	N-CA-CB	5.08	119.42	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	LYS	N-CA-C	5.05	117.18	111.11
1	A	150	GLU	CA-C-N	-5.05	114.43	122.50
1	A	150	GLU	C-N-CA	-5.05	114.43	122.50
1	A	7	ILE	O-C-N	5.04	128.64	123.05
1	A	162	TYR	O-C-N	5.01	127.17	122.06

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	74	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	78	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 31.

All (78) 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:28:ARG:NE	1:A:32:LYS:HZ1	1.59	0.99
1:A:40:THR:O	1:A:111:MET:HE1	1.71	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:NE	1:A:32:LYS:NZ	2.15	0.89
1:A:48:ASN:HD21	1:A:111:MET:HE3	1.39	0.88
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
4:A:198:HBI:O10	6:A:756:HOH:O	2.03	0.77
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:HE	1:A:32:LYS:HZ1	0.77	0.73
1:A:42:HIS:C	1:A:43:VAL:HG23	2.12	0.72
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
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:71:ILE:HD11	1:A:108:LYS:HZ3	1.67	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:42:HIS:C	1:A:43:VAL:CG2	2.77	0.58
1:A:48:ASN:ND2	1:A:111:MET:HE3	2.15	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:139:LEU:C	1:A:140:HIS:CG	2.85	0.55
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: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:28:ARG:NE	1:A:32:LYS:HZ2	2.02	0.52
1:A:125:MET:HE2	1:A:149:PRO:HG2	1.92	0.50
1:A:158:LEU:HB2	1:A:182:TYR:CE2	2.47	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:5:ASN:O	1:A:113:TRP:HA	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:HG23	1:A:120:VAL:HG12	1.96	0.47
1:A:34:PHE:CD1	1:A:34:PHE:C	2.93	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:139:LEU:C	1:A:140:HIS:CD2	2.95	0.45
1:A:100:LEU:HD13	1:A:112:VAL:CG2	2.47	0.45
1:A:172:GLU:OE1	1:A:177:TYR:OH	2.29	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: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
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: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:100:LEU:HD23	1:A:100:LEU:HA	1.88	0.40
1:A:108:LYS:HZ3	1:A:108:LYS:HG2	1.78	0.40
1:A:63:LYS:HA	1:A:63:LYS:HD3	1.75	0.40
1:A:175:ILE:HA	1:A:175:ILE:HD13	1.88	0.40
1:A:93:LEU:O	1:A:94:ASP:C	2.64	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	185/189 (98%)	178 (96%)	6 (3%)	1 (0%)	24	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	VAL

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	164/168 (98%)	145 (88%)	19 (12%)	5 8

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	34	PHE
1	A	47	GLN
1	A	55	LYS
1	A	80	LYS
1	A	91	LYS
1	A	104	GLU
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	161	GLU
1	A	168	ASP
1	A	169	ILE
1	A	172	GLU
1	A	186	VAL

Sometimes 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 [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](#)

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	$\# Z > 2$
4	HBI	A	198	-	15,18,18	4.19	5 (33%)	14,26,26	1.82	4 (28%)
5	MBO	A	201[B]	1	7,10,10	2.36	1 (14%)	11,13,13	2.38	5 (45%)
5	MBO	A	201[A]	1	7,10,10	2.36	1 (14%)	11,13,13	2.38	5 (45%)
3	NAP	A	191	2	50,52,52	3.51	18 (36%)	71,80,80	2.29	18 (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
4	HBI	A	198	-	-	0/4/17/17	0/2/2/2
5	MBO	A	201[B]	1	-	0/4/4/4	0/1/1/1
5	MBO	A	201[A]	1	-	0/4/4/4	0/1/1/1
3	NAP	A	191	2	-	2/35/67/67	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	191	NAP	O4B-C4B	-14.29	1.13	1.45
3	A	191	NAP	C4N-C3N	10.42	1.55	1.39
4	A	198	HBI	C7-C6	-10.21	1.38	1.49
4	A	198	HBI	C7-N8	-10.07	1.30	1.45
3	A	191	NAP	C5N-C4N	8.28	1.53	1.38
3	A	191	NAP	O4D-C1D	5.83	1.48	1.40
5	A	201[A]	MBO	OZ1-CZ	5.74	1.39	1.22
5	A	201[B]	MBO	OZ1-CZ	5.74	1.39	1.22
3	A	191	NAP	C5A-C6A	5.36	1.55	1.41
4	A	198	HBI	C6-N5	5.33	1.37	1.28
3	A	191	NAP	PA-O3	-4.39	1.54	1.59
3	A	191	NAP	C2N-N1N	4.34	1.39	1.35
3	A	191	NAP	C4A-N9A	-3.97	1.29	1.37
3	A	191	NAP	C5A-C4A	-3.66	1.32	1.39
3	A	191	NAP	C3N-C7N	-3.40	1.45	1.50
4	A	198	HBI	O4-C4	3.38	1.30	1.23
4	A	198	HBI	C2-N1	3.30	1.41	1.33
3	A	191	NAP	C6N-C5N	-3.27	1.31	1.38
3	A	191	NAP	C3B-C4B	3.15	1.61	1.53
3	A	191	NAP	O3B-C3B	3.11	1.50	1.43
3	A	191	NAP	C8A-N9A	-2.73	1.32	1.37
3	A	191	NAP	C5A-N7A	2.61	1.43	1.39
3	A	191	NAP	O3D-C3D	2.47	1.49	1.43
3	A	191	NAP	O4B-C1B	2.45	1.47	1.42
3	A	191	NAP	PN-O2N	-2.17	1.45	1.55

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	191	NAP	C5N-C4N-C3N	-11.56	109.00	120.36
3	A	191	NAP	C2N-C3N-C4N	4.79	123.83	118.26
3	A	191	NAP	O4B-C1B-C2B	-4.18	99.39	106.59
5	A	201[A]	MBO	OZ2-CZ-CE4	4.17	125.53	114.84
5	A	201[B]	MBO	OZ2-CZ-CE4	4.17	125.53	114.84
4	A	198	HBI	C6-C7-N8	4.14	127.13	114.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	201[A]	MBO	CE5-CE4-CZ	-4.05	112.36	120.37
5	A	201[B]	MBO	CE5-CE4-CZ	-4.05	112.36	120.37
3	A	191	NAP	C2B-C3B-C4B	-3.92	93.57	101.99
3	A	191	NAP	C2A-N1A-C6A	-3.71	112.64	118.73
3	A	191	NAP	C4A-N9A-C8A	3.68	109.61	105.74
3	A	191	NAP	N3A-C2A-N1A	3.67	134.13	128.58
5	A	201[A]	MBO	CE3-CE4-CZ	3.45	127.20	120.37
5	A	201[B]	MBO	CE3-CE4-CZ	3.45	127.20	120.37
3	A	191	NAP	O3B-C3B-C4B	-3.44	101.21	111.08
3	A	191	NAP	C4B-O4B-C1B	3.30	116.75	109.47
3	A	191	NAP	C6N-N1N-C1D	-2.86	114.12	119.73
4	A	198	HBI	N2-C2-N3	2.56	122.17	116.76
3	A	191	NAP	C6N-C5N-C4N	2.56	123.14	119.45
3	A	191	NAP	C2N-N1N-C1D	2.52	124.70	119.13
4	A	198	HBI	O4-C4-N3	2.50	124.82	120.11
3	A	191	NAP	O2D-C2D-C3D	-2.49	103.83	111.82
3	A	191	NAP	O3B-C3B-C2B	-2.33	104.68	111.19
3	A	191	NAP	C5N-C6N-N1N	2.33	123.56	120.38
4	A	198	HBI	C11-C10-C9	-2.29	106.14	111.57
3	A	191	NAP	O5B-C5B-C4B	2.26	116.68	108.99
5	A	201[A]	MBO	OZ1-CZ-CE4	-2.21	115.65	121.46
5	A	201[B]	MBO	OZ1-CZ-CE4	-2.21	115.65	121.46
3	A	191	NAP	C3N-C7N-N7N	2.21	120.47	117.74
5	A	201[A]	MBO	OZ2-CZ-OZ1	-2.19	118.64	123.35
5	A	201[B]	MBO	OZ2-CZ-OZ1	-2.19	118.64	123.35
3	A	191	NAP	C5A-C4A-N9A	2.10	108.09	105.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

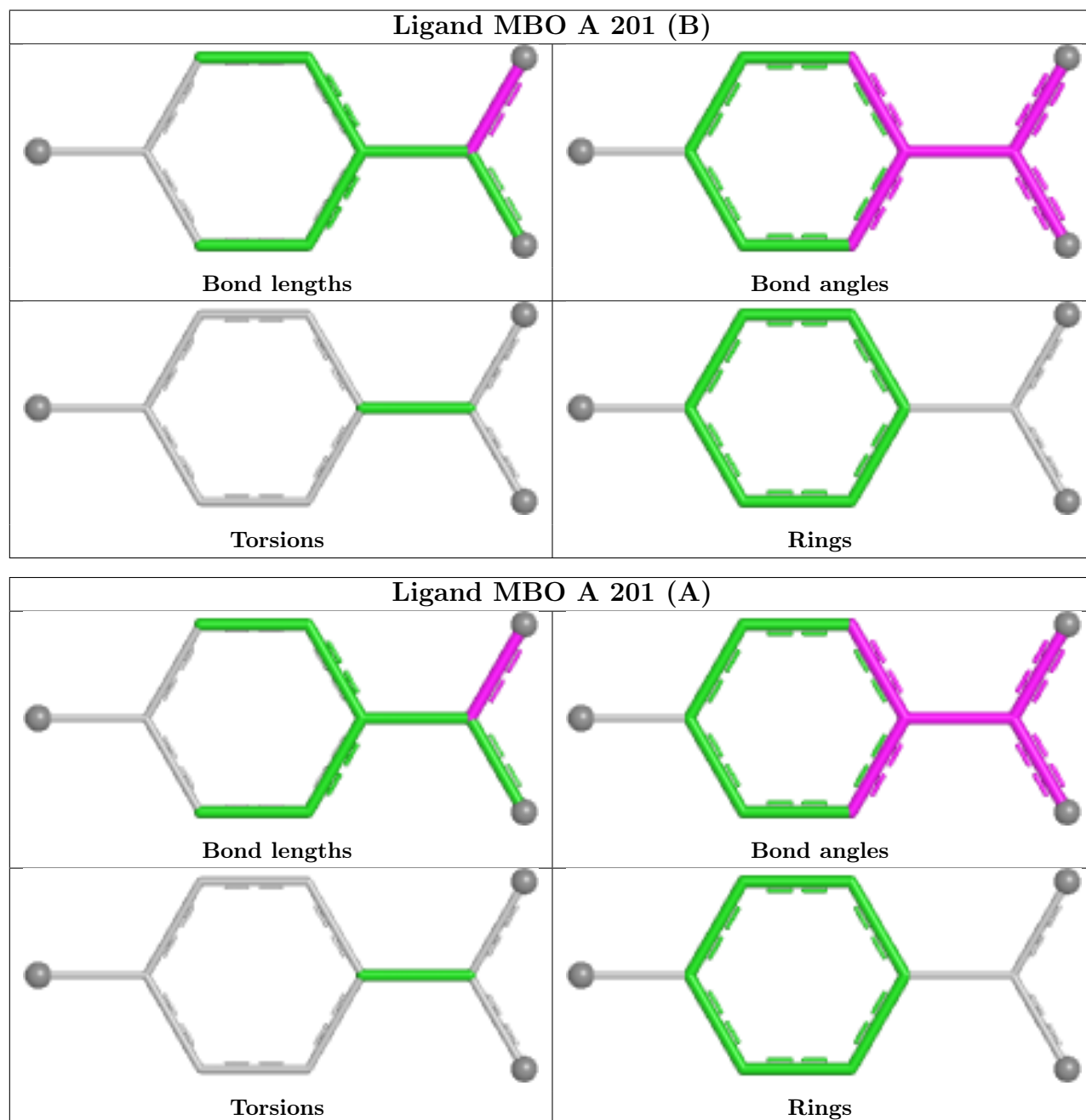
Mol	Chain	Res	Type	Atoms
3	A	191	NAP	O4D-C1D-N1N-C2N
3	A	191	NAP	C2B-O2B-P2B-O1X

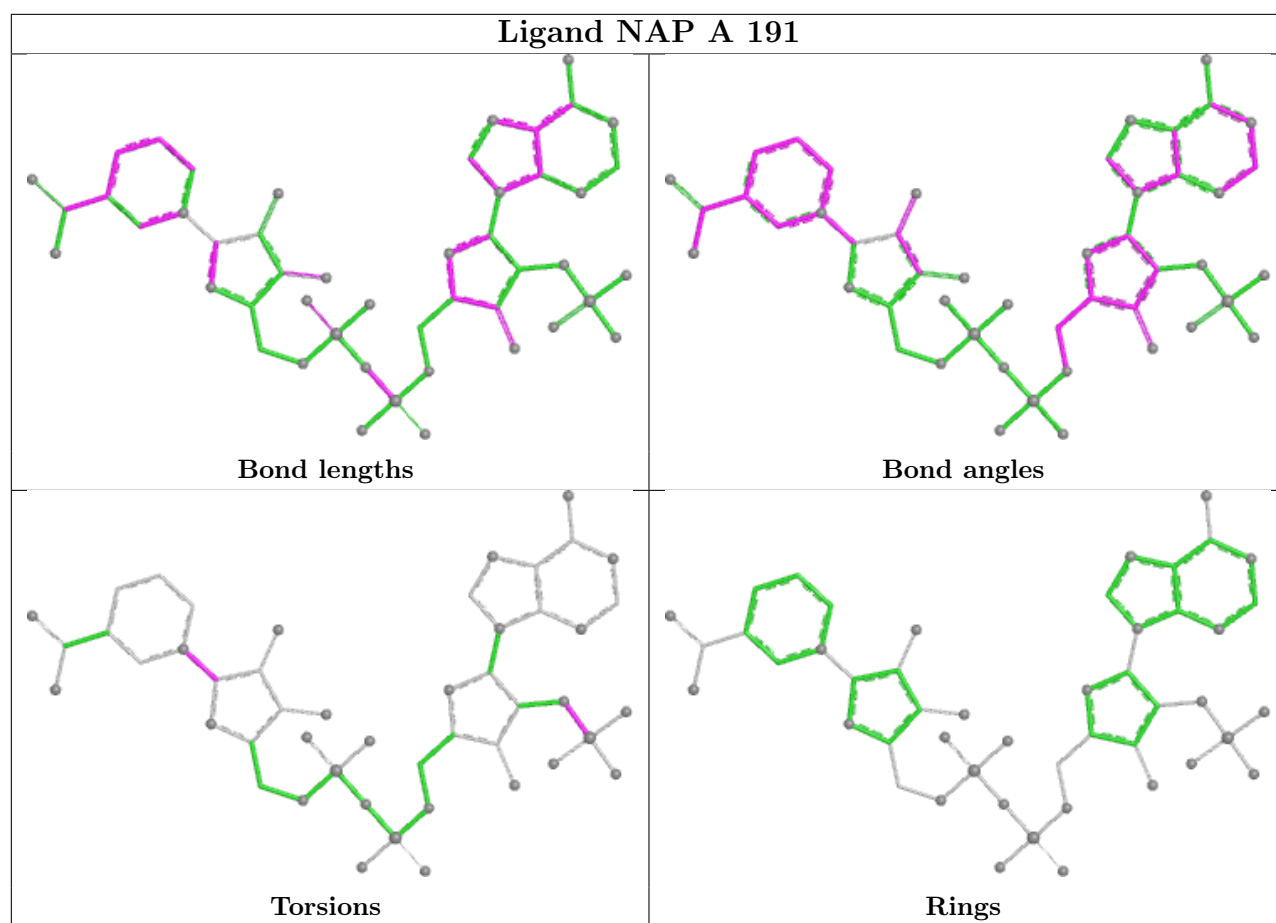
There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

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.