



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2014 – 10:15 AM EDT

PDB ID : 4B7F
Title : Structure of a liganded bacterial catalase
Authors : Gumiero, A.; Walsh, M.
Deposited on : 2012-08-20
Resolution : 1.76 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

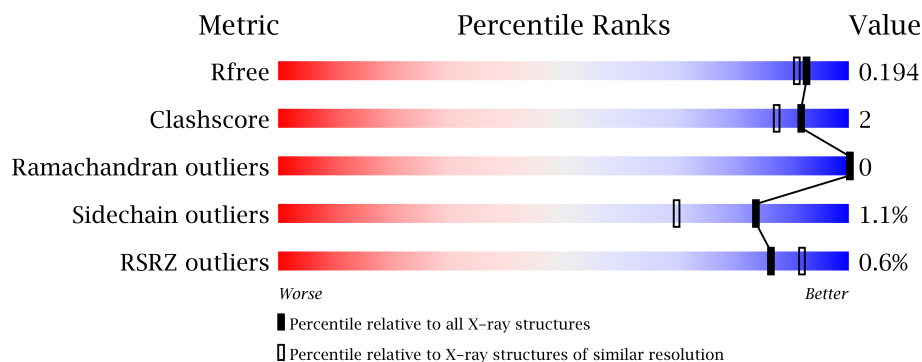
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 1.76 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}	66092	1134 (1.76-1.76)
Clashscore	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	515	
1	B	515	
1	C	515	
1	D	515	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NDP	A	1518	-	X
3	NDP	B	1517	-	X
3	NDP	C	1517	-	X
3	NDP	D	1518	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	NO	C	1519	-	X
4	NO	D	1520	-	X
5	EDO	B	1522	-	X
7	BTB	D	1517	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18258 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CATALASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	9	0
			4197	2638	736	814	9			
1	B	514	Total	C	N	O	S	0	6	0
			4170	2619	736	806	9			
1	C	514	Total	C	N	O	S	0	8	0
			4187	2628	743	807	9			
1	D	514	Total	C	N	O	S	0	6	0
			4173	2623	738	803	9			

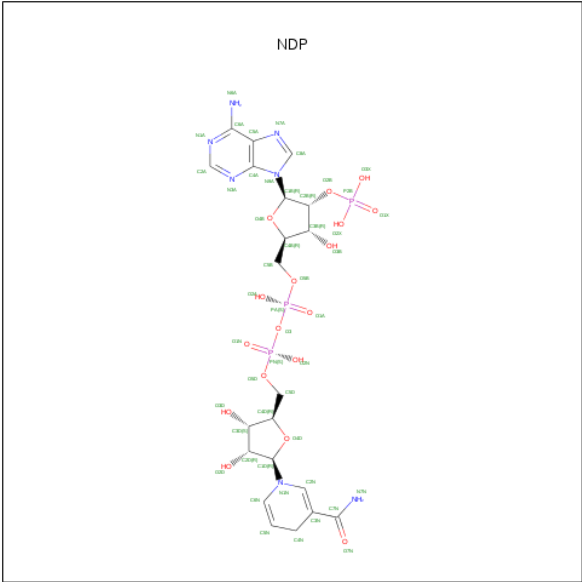
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ILE	LEU	CONFLICT	UNP Q6M8A6
B	327	ILE	LEU	CONFLICT	UNP Q6M8A6
C	327	ILE	LEU	CONFLICT	UNP Q6M8A6
D	327	ILE	LEU	CONFLICT	UNP Q6M8A6

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

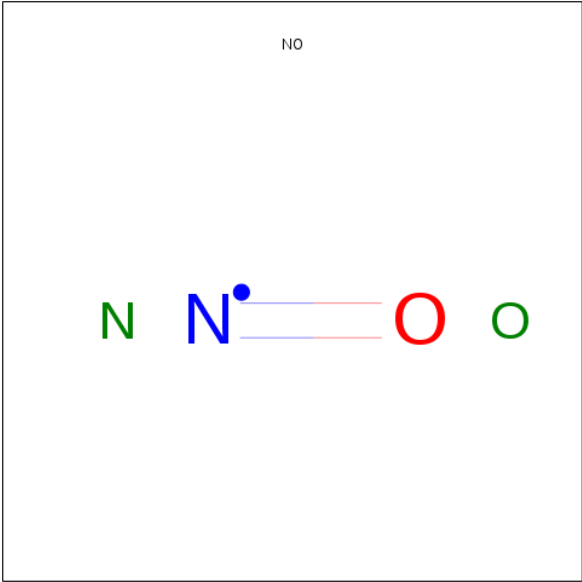
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



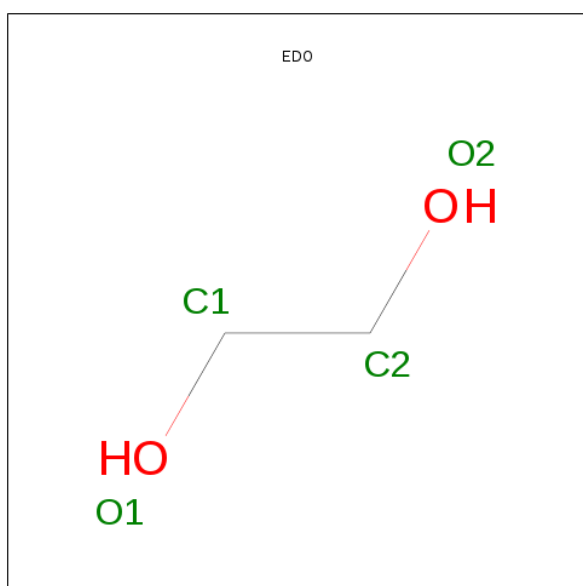
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is NITRIC OXIDE (three-letter code: NO) (formula: NO).



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

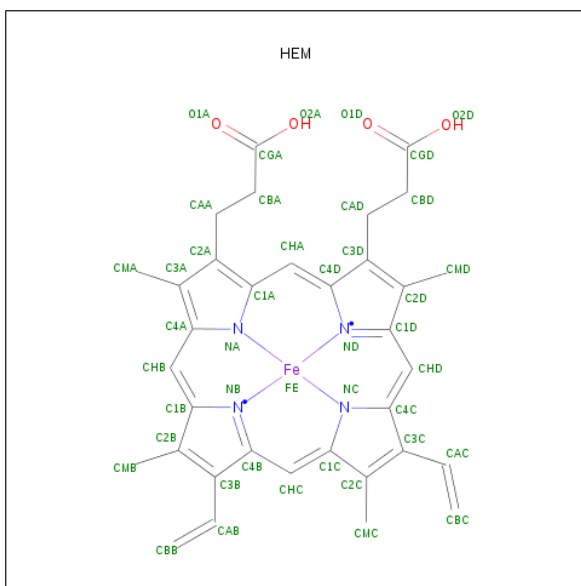
- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

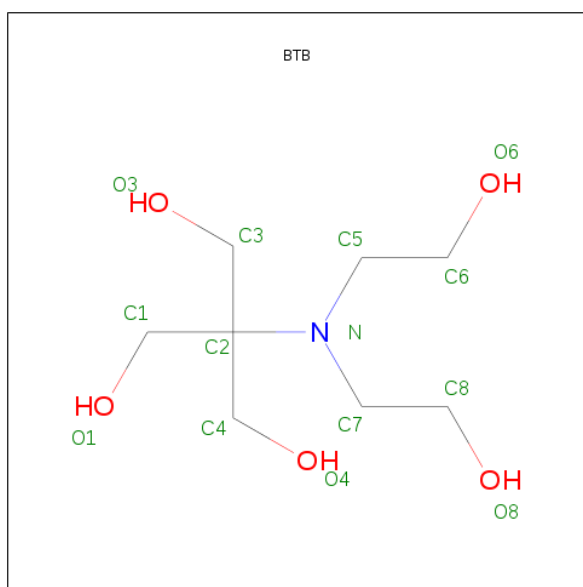
- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 7 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	378	Total	O	0	0
			378	378		
8	B	276	Total	O	0	0
			276	276		
8	C	265	Total	O	0	0
			265	265		
8	D	196	Total	O	0	0
			196	196		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: CATALASE

Chain A: 



- Molecule 1: CATALASE

Chain B: 



- Molecule 1: CATALASE

Chain C: 



- Molecule 1: CATALASE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	151.51Å 151.51Å 156.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.58 – 1.76 100.58 – 1.76	Depositor EDS
% Data completeness (in resolution range)	93.0 (100.58-1.76) 93.0 (100.58-1.76)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.76Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8-1069)	Depositor
R, R_{free}	0.158 , 0.194 0.157 , 0.194	Depositor DCC
R_{free} test set	9382 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 28.4	EDS
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 186923 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18258	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NO, EDO, BTB, NDP, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.38	0/4334	0.55	1/5888 (0.0%)
1	B	0.38	1/4297 (0.0%)	0.55	0/5838
1	C	0.42	2/4317 (0.0%)	0.58	1/5863 (0.0%)
1	D	0.40	1/4301 (0.0%)	0.57	1/5843 (0.0%)
All	All	0.39	4/17249 (0.0%)	0.56	3/23432 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	419	ASN	C-N	-9.40	1.12	1.34
1	C	161	HIS	C-N	-6.57	1.19	1.34
1	B	161	HIS	C-N	-5.69	1.21	1.34
1	D	161	HIS	C-N	-5.53	1.21	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	161	HIS	O-C-N	-7.42	110.83	122.70
1	A	161	HIS	O-C-N	-5.81	113.40	122.70
1	D	161	HIS	O-C-N	-5.72	113.55	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4197	0	3937	10	0
1	B	4170	0	3912	18	0
1	C	4187	0	3939	15	0
1	D	4173	0	3919	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	48	0	26	1	0
3	B	48	0	26	0	0
3	C	48	0	26	1	0
3	D	48	0	26	0	0
4	A	2	0	0	4	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	4	0
5	A	4	0	6	0	0
5	B	12	0	18	0	0
5	C	4	0	6	0	0
5	D	8	0	12	0	0
6	A	43	0	30	4	0
6	B	43	0	30	1	0
6	C	43	0	30	0	0
6	D	43	0	30	4	0
7	D	14	0	19	0	0
8	A	378	0	0	0	0
8	B	276	0	0	2	0
8	C	265	0	0	2	0
8	D	196	0	0	1	0
All	All	18258	0	15992	60	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (60) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:216:GLN:HE22	1:D:431:VAL:H	1.09	0.98
1:B:216:GLN:HE22	1:B:431:VAL:H	1.12	0.91
1:A:69:ILE:H	1:A:356:GLN:HE22	1.21	0.89
1:D:401:ASN:HD22	1:D:403:TYR:H	1.20	0.87
1:C:401:ASN:HD22	1:C:403:TYR:H	1.25	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:401:ASN:HD22	1:B:403:TYR:H	1.22	0.84
1:A:401:ASN:HD22	1:A:403:TYR:H	1.24	0.83
1:B:235:GLN:HE22	1:B:271:ILE:H	1.28	0.81
1:C:235:GLN:HE22	1:C:271:ILE:H	1.34	0.75
1:D:3:GLU:HB3	1:D:4:LYS:HB3	1.71	0.72
1:D:3:GLU:HG3	1:D:315:ARG:HH12	1.58	0.68
1:D:11:VAL:HG22	1:D:318:ARG:HG2	1.80	0.64
1:C:247:LYS:NZ	1:C:251:GLU:OE2	2.25	0.62
4:A:1519:NO:N	6:A:3000:HEM:NC	2.49	0.61
1:B:115[A]:GLN:O	8:B:2070:HOH:O	2.16	0.60
4:D:1520:NO:N	6:D:3003:HEM:ND	2.50	0.59
4:D:1520:NO:N	6:D:3003:HEM:NA	2.49	0.59
1:D:115[A]:GLN:NE2	8:D:2019:HOH:O	2.37	0.58
1:B:115[B]:GLN:OE1	8:B:2030:HOH:O	2.17	0.57
4:A:1519:NO:N	6:A:3000:HEM:NB	2.54	0.56
1:C:368:LEU:HD23	1:D:388[B]:TYR:CD1	2.44	0.53
1:B:235:GLN:NE2	1:B:271:ILE:H	2.04	0.53
1:C:367:ASP:HB2	1:D:388[B]:TYR:OH	2.10	0.52
1:D:216:GLN:NE2	1:D:431:VAL:H	1.93	0.52
4:A:1519:NO:N	6:A:3000:HEM:NA	2.59	0.51
1:C:515:LYS:N	1:C:516:ALA:HB2	2.26	0.51
1:C:235:GLN:NE2	1:C:271:ILE:H	2.07	0.50
4:A:1519:NO:N	6:A:3000:HEM:ND	2.59	0.50
1:A:388[A]:TYR:HB2	1:B:388:TYR:CZ	2.48	0.48
1:B:216:GLN:HE22	1:B:431:VAL:N	1.95	0.48
4:D:1520:NO:N	6:D:3003:HEM:NC	2.60	0.48
1:C:18:LYS:HZ1	1:D:404:ASP:HB2	1.78	0.48
1:A:198:ARG:O	1:A:201:PRO:HD3	2.14	0.47
1:B:71:HIS:CE1	1:B:111:VAL:HG22	2.49	0.47
1:A:388[B]:TYR:HB2	1:B:388:TYR:CZ	2.49	0.47
1:B:6:ALA:HB3	1:B:80:GLU:HG2	1.98	0.46
1:B:147:THR:HG23	1:B:190:GLN:HE21	1.81	0.45
1:C:347:GLN:HA	1:D:49:ASN:HD21	1.81	0.45
1:B:401:ASN:ND2	1:B:403:TYR:H	2.02	0.45
1:C:345:MET:O	1:C:349:ARG:HG3	2.17	0.45
4:D:1520:NO:N	6:D:3003:HEM:NB	2.64	0.45
1:D:3:GLU:N	1:D:314:ASN:O	2.51	0.44
1:C:460:LEU:HD13	3:C:1517:NDP:H1D	1.98	0.44
1:A:46:ASN:HD21	1:C:344:ARG:HG2	1.84	0.43
1:D:346:LEU:O	1:D:350:ILE:HG12	2.18	0.43
1:A:13:ARG:HB2	1:A:369:PRO:HB3	2.00	0.43
1:A:346:LEU:O	1:A:350:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:193:TYR:CD2	3:A:1518:NDP:H2A	2.54	0.42
1:B:461:TYR:O	1:B:470:LYS:HE2	2.19	0.42
1:D:147:THR:HG23	1:D:190:GLN:HE21	1.85	0.41
1:D:182:THR:HB	1:D:491:ARG:HG2	2.03	0.41
1:B:420:HIS:HE1	8:C:2240:HOH:O	2.02	0.41
1:C:332:GLY:HA2	1:C:350:ILE:HD12	2.03	0.41
1:C:388:TYR:CE1	1:D:388[B]:TYR:CD1	3.08	0.41
1:A:176:MET:HG3	1:D:398:TYR:CE1	2.56	0.41
1:B:346:LEU:O	1:B:350:ILE:HG12	2.21	0.40
1:B:128:ALA:HB2	6:B:3001:HEM:HMD3	2.03	0.40
1:C:25[A]:ARG:HD3	8:C:2014:HOH:O	2.20	0.40
1:D:69:ILE:HA	1:D:70:PRO:HA	1.89	0.40
1:B:173:ASP:O	1:B:177:GLN:HG3	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	522/515 (101%)	502 (96%)	20 (4%)	0	100	100
1	B	518/515 (101%)	494 (95%)	24 (5%)	0	100	100
1	C	520/515 (101%)	501 (96%)	19 (4%)	0	100	100
1	D	518/515 (101%)	496 (96%)	22 (4%)	0	100	100
All	All	2078/2060 (101%)	1993 (96%)	85 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	444/436 (102%)	439 (99%)	5 (1%)	84	70
1	B	440/436 (101%)	436 (99%)	4 (1%)	87	75
1	C	442/436 (101%)	437 (99%)	5 (1%)	84	70
1	D	440/436 (101%)	435 (99%)	5 (1%)	84	70
All	All	1766/1744 (101%)	1747 (99%)	19 (1%)	84	70

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

Mol	Chain	Res	Type
1	A	4	LYS
1	A	133	THR
1	A	145	THR
1	A	155	LYS
1	A	360	ARG
1	B	133	THR
1	B	155	LYS
1	B	425	GLN
1	B	449	GLN
1	C	9	GLN
1	C	133	THR
1	C	145	THR
1	C	155	LYS
1	C	515	LYS
1	D	4	LYS
1	D	22	ASN
1	D	133	THR
1	D	155	LYS
1	D	401	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	49	ASN
1	A	61	ASN
1	A	97	GLN
1	A	300	GLN
1	A	316	ASN
1	A	356	GLN
1	A	401	ASN

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Mol	Chain	Res	Type
1	A	498	ASN
1	B	22	ASN
1	B	46	ASN
1	B	49	ASN
1	B	61	ASN
1	B	97	GLN
1	B	190	GLN
1	B	216	GLN
1	B	235	GLN
1	B	316	ASN
1	B	401	ASN
1	B	420	HIS
1	B	425	GLN
1	B	498	ASN
1	C	46	ASN
1	C	49	ASN
1	C	61	ASN
1	C	190	GLN
1	C	235	GLN
1	C	316	ASN
1	C	401	ASN
1	C	498	ASN
1	D	46	ASN
1	D	49	ASN
1	D	61	ASN
1	D	97	GLN
1	D	190	GLN
1	D	216	GLN
1	D	300	GLN
1	D	316	ASN
1	D	401	ASN
1	D	498	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	NDP	A	1518	-	52,52,52	1.39	5 (9%)	80,80,80	1.58	6 (7%)
4	NO	A	1519	6	0,1,1	0.00	-	0,0,0	0.00	-
5	EDO	A	1520	-	3,3,3	0.55	0	2,2,2	0.47	0
6	HEM	A	3000	1,4	42,50,50	3.45	12 (28%)	27,82,82	1.63	5 (18%)
3	NDP	B	1517	-	52,52,52	1.38	5 (9%)	80,80,80	1.61	9 (11%)
5	EDO	B	1519	-	3,3,3	0.55	0	2,2,2	0.45	0
4	NO	B	1520	6	0,1,1	0.00	-	0,0,0	0.00	-
5	EDO	B	1521	-	3,3,3	0.65	0	2,2,2	0.15	0
5	EDO	B	1522	-	3,3,3	0.50	0	2,2,2	0.42	0
6	HEM	B	3001	1,4	42,50,50	3.39	14 (33%)	27,82,82	1.70	6 (22%)
3	NDP	C	1517	-	52,52,52	1.41	5 (9%)	80,80,80	1.66	9 (11%)
5	EDO	C	1518	-	3,3,3	0.57	0	2,2,2	0.36	0
4	NO	C	1519	6	0,1,1	0.00	-	0,0,0	0.00	-
6	HEM	C	3002	1,4	42,50,50	3.44	13 (30%)	27,82,82	1.67	5 (18%)
7	BTB	D	1517	-	13,13,13	0.95	0	16,16,16	0.84	1 (6%)
3	NDP	D	1518	-	52,52,52	1.42	5 (9%)	80,80,80	1.67	8 (10%)
5	EDO	D	1519	-	3,3,3	0.62	0	2,2,2	0.40	0
4	NO	D	1520	6	0,1,1	0.00	-	0,0,0	0.00	-
5	EDO	D	1521	-	3,3,3	0.60	0	2,2,2	0.33	0
6	HEM	D	3003	1,4	42,50,50	3.50	12 (28%)	27,82,82	1.79	7 (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	NDP	A	1518	-	-	0/35/77/77	0/5/5/5
4	NO	A	1519	6	-	0/0/0/0	0/0/0/0
5	EDO	A	1520	-	-	0/1/1/1	0/0/0/0
6	HEM	A	3000	1,4	-	0/14/114/114	0/0/8/8
3	NDP	B	1517	-	-	0/35/77/77	0/5/5/5
5	EDO	B	1519	-	-	0/1/1/1	0/0/0/0
4	NO	B	1520	6	-	0/0/0/0	0/0/0/0
5	EDO	B	1521	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1522	-	-	0/1/1/1	0/0/0/0
6	HEM	B	3001	1,4	-	0/14/114/114	0/0/8/8
3	NDP	C	1517	-	-	0/35/77/77	0/5/5/5
5	EDO	C	1518	-	-	0/1/1/1	0/0/0/0
4	NO	C	1519	6	-	0/0/0/0	0/0/0/0
6	HEM	C	3002	1,4	-	0/14/114/114	0/0/8/8
7	BTB	D	1517	-	-	0/21/21/21	0/0/0/0
3	NDP	D	1518	-	-	0/35/77/77	0/5/5/5
5	EDO	D	1519	-	-	0/1/1/1	0/0/0/0
4	NO	D	1520	6	-	0/0/0/0	0/0/0/0
5	EDO	D	1521	-	-	0/1/1/1	0/0/0/0
6	HEM	D	3003	1,4	-	0/14/114/114	0/0/8/8

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3003	HEM	C3C-C2C	-13.62	1.34	1.45
6	A	3000	HEM	C3C-C2C	-13.21	1.35	1.45
6	C	3002	HEM	C3C-C2C	-13.02	1.35	1.45
6	B	3001	HEM	C3C-C2C	-12.43	1.35	1.45
6	C	3002	HEM	C3B-C2B	-10.83	1.35	1.45
6	D	3003	HEM	C3B-C2B	-10.67	1.35	1.45
6	A	3000	HEM	C3B-C2B	-10.61	1.35	1.45
6	B	3001	HEM	C3B-C2B	-10.38	1.35	1.45
3	D	1518	NDP	O7N-C7N	6.47	1.41	1.24
3	C	1517	NDP	O7N-C7N	6.41	1.40	1.24
3	B	1517	NDP	O7N-C7N	6.37	1.40	1.24
3	A	1518	NDP	O7N-C7N	6.35	1.40	1.24
6	A	3000	HEM	CMC-C2C	6.20	1.55	1.45
6	D	3003	HEM	CMC-C2C	6.10	1.55	1.45
6	D	3003	HEM	CMB-C2B	6.09	1.55	1.45
6	B	3001	HEM	CMB-C2B	6.08	1.55	1.45
6	C	3002	HEM	CMC-C2C	6.03	1.55	1.45
6	C	3002	HEM	CMB-C2B	6.01	1.55	1.45
6	B	3001	HEM	CMC-C2C	5.97	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3000	HEM	CMB-C2B	5.92	1.55	1.45
6	D	3003	HEM	CMD-C2D	5.61	1.54	1.45
6	B	3001	HEM	CMD-C2D	5.33	1.54	1.45
6	C	3002	HEM	CMD-C2D	5.16	1.53	1.45
6	A	3000	HEM	CMD-C2D	5.15	1.53	1.45
6	C	3002	HEM	C3B-CAB	4.67	1.55	1.40
6	C	3002	HEM	C3C-CAC	4.63	1.55	1.40
6	B	3001	HEM	C3B-CAB	4.62	1.55	1.40
6	A	3000	HEM	C3C-CAC	4.61	1.55	1.40
6	D	3003	HEM	C3B-CAB	4.59	1.55	1.40
6	B	3001	HEM	C3C-CAC	4.55	1.55	1.40
6	D	3003	HEM	C3C-CAC	4.53	1.55	1.40
6	A	3000	HEM	C3B-CAB	4.53	1.55	1.40
3	D	1518	NDP	C2A-N3A	3.80	1.38	1.32
3	C	1517	NDP	C2A-N3A	3.75	1.38	1.32
3	A	1518	NDP	C2A-N3A	3.70	1.38	1.32
3	B	1517	NDP	C2A-N3A	3.49	1.38	1.32
6	B	3001	HEM	C3D-C2D	3.46	1.52	1.43
6	A	3000	HEM	C3D-C2D	3.40	1.52	1.43
3	C	1517	NDP	C6N-C5N	3.35	1.40	1.33
3	B	1517	NDP	C6N-C5N	3.29	1.40	1.33
3	A	1518	NDP	C6N-C5N	3.29	1.40	1.33
3	D	1518	NDP	C6N-C5N	3.26	1.40	1.33
6	C	3002	HEM	C3D-C2D	3.22	1.51	1.43
6	D	3003	HEM	C3D-C2D	3.09	1.51	1.43
6	B	3001	HEM	C4D-ND	2.67	1.40	1.33
6	B	3001	HEM	FE-NC	2.64	2.06	1.95
6	B	3001	HEM	C1D-ND	2.63	1.40	1.33
6	C	3002	HEM	C1D-ND	2.62	1.40	1.33
3	B	1517	NDP	C2A-N1A	2.57	1.39	1.33
6	A	3000	HEM	C4D-ND	2.53	1.40	1.33
3	C	1517	NDP	C2A-N1A	2.50	1.38	1.33
6	D	3003	HEM	C4D-ND	2.47	1.39	1.33
3	D	1518	NDP	C2A-N1A	2.46	1.38	1.33
3	A	1518	NDP	C2A-N1A	2.46	1.38	1.33
6	A	3000	HEM	FE-ND	2.42	2.05	1.95
6	B	3001	HEM	FE-ND	2.38	2.05	1.95
3	D	1518	NDP	C2N-C3N	2.37	1.39	1.34
6	D	3003	HEM	C1D-ND	2.34	1.39	1.33
6	C	3002	HEM	C4D-ND	2.31	1.39	1.33
6	A	3000	HEM	C1D-ND	2.29	1.39	1.33
6	D	3003	HEM	FE-ND	2.27	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1518	NDP	C2N-C3N	2.23	1.39	1.34
3	B	1517	NDP	C2N-C3N	2.21	1.39	1.34
6	B	3001	HEM	FE-NB	2.15	2.03	1.95
6	C	3002	HEM	FE-NB	2.13	2.03	1.95
3	C	1517	NDP	C2N-C3N	2.09	1.39	1.34
6	A	3000	HEM	C1C-NC	2.07	1.39	1.33
6	C	3002	HEM	FE-ND	2.06	2.04	1.95
6	D	3003	HEM	C4C-NC	2.04	1.38	1.33
6	B	3001	HEM	CAA-C2A	2.01	1.55	1.52
6	C	3002	HEM	C4C-NC	2.00	1.38	1.33

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1518	NDP	N3A-C2A-N1A	-10.08	120.02	128.89
3	B	1517	NDP	N3A-C2A-N1A	-9.59	120.45	128.89
3	C	1517	NDP	N3A-C2A-N1A	-9.58	120.46	128.89
3	A	1518	NDP	N3A-C2A-N1A	-9.23	120.77	128.89
3	C	1517	NDP	C5A-C4A-N3A	-5.28	120.83	125.98
3	D	1518	NDP	C5A-C4A-N3A	-5.23	120.88	125.98
3	A	1518	NDP	C5A-C4A-N3A	-4.98	121.12	125.98
6	A	3000	HEM	CAD-CBD-CGD	-4.87	104.34	113.53
6	D	3003	HEM	CAD-CBD-CGD	-4.79	104.51	113.53
3	B	1517	NDP	C5A-C4A-N3A	-4.70	121.40	125.98
6	B	3001	HEM	CAD-CBD-CGD	-4.55	104.96	113.53
3	D	1518	NDP	N3A-C4A-N9A	3.68	131.70	125.39
6	C	3002	HEM	CBD-CAD-C3D	-3.62	106.65	114.51
6	C	3002	HEM	CAD-CBD-CGD	-3.62	106.70	113.53
6	B	3001	HEM	CBD-CAD-C3D	-3.54	106.83	114.51
3	C	1517	NDP	N3A-C4A-N9A	3.52	131.43	125.39
6	D	3003	HEM	CMA-C3A-C4A	-3.43	123.19	128.46
3	A	1518	NDP	N3A-C4A-N9A	3.41	131.24	125.39
3	B	1517	NDP	PN-O3-PA	-3.40	122.53	131.93
6	A	3000	HEM	CBD-CAD-C3D	-3.32	107.31	114.51
3	B	1517	NDP	N3A-C4A-N9A	3.25	130.97	125.39
3	D	1518	NDP	PN-O3-PA	-3.14	123.25	131.93
3	A	1518	NDP	O4B-C1B-N9A	3.13	114.91	108.10
6	B	3001	HEM	CBA-CAA-C2A	-3.12	107.44	112.63
3	C	1517	NDP	O4B-C1B-N9A	3.12	114.89	108.10
6	D	3003	HEM	CBD-CAD-C3D	-3.12	107.74	114.51
3	C	1517	NDP	P2B-O2B-C2B	-2.94	114.98	121.77
6	C	3002	HEM	CBA-CAA-C2A	-2.88	107.84	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3003	HEM	C3A-C4A-NA	-2.83	107.61	109.50
3	C	1517	NDP	PN-O3-PA	-2.78	124.24	131.93
6	C	3002	HEM	CMA-C3A-C4A	-2.64	124.41	128.46
3	D	1518	NDP	O4B-C1B-N9A	2.62	113.81	108.10
6	A	3000	HEM	CBA-CAA-C2A	-2.62	108.27	112.63
6	C	3002	HEM	C3A-C4A-NA	-2.53	107.81	109.50
6	B	3001	HEM	CMA-C3A-C4A	-2.52	124.59	128.46
6	D	3003	HEM	CBA-CAA-C2A	-2.46	108.54	112.63
6	D	3003	HEM	CAD-C3D-C4D	2.40	128.98	125.60
3	D	1518	NDP	C2A-N3A-C4A	2.36	120.07	113.27
3	B	1517	NDP	C3D-C2D-C1D	2.33	106.03	101.38
3	C	1517	NDP	C1D-N1N-C2N	-2.33	116.99	121.03
6	B	3001	HEM	C4A-C3A-C2A	2.33	108.62	107.00
3	C	1517	NDP	C2A-N3A-C4A	2.32	119.96	113.27
3	B	1517	NDP	C1B-N9A-C4A	-2.25	122.74	126.64
3	A	1518	NDP	PN-O3-PA	-2.24	125.72	131.93
3	B	1517	NDP	O4B-C1B-N9A	2.22	112.93	108.10
3	B	1517	NDP	C2A-N3A-C4A	2.20	119.62	113.27
6	B	3001	HEM	C3A-C4A-NA	-2.20	108.03	109.50
3	D	1518	NDP	C3D-C2D-C1D	2.20	105.76	101.38
7	D	1517	BTB	C7-N-C5	-2.20	109.52	111.22
3	A	1518	NDP	C2A-N3A-C4A	2.15	119.45	113.27
3	C	1517	NDP	C3D-C2D-C1D	2.14	105.64	101.38
6	D	3003	HEM	C4A-C3A-C2A	2.12	108.47	107.00
6	A	3000	HEM	CMA-C3A-C4A	-2.11	125.22	128.46
3	D	1518	NDP	P2B-O2B-C2B	-2.10	116.91	121.77
6	A	3000	HEM	C4A-C3A-C2A	2.06	108.43	107.00
3	B	1517	NDP	C4A-C5A-N7A	-2.03	107.44	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	515/515 (100%)	-0.49	3 (0%) 86 92	9, 14, 24, 65	0
1	B	514/515 (99%)	-0.44	2 (0%) 90 94	9, 16, 26, 55	0
1	C	514/515 (99%)	-0.46	1 (0%) 93 95	9, 14, 24, 52	0
1	D	514/515 (99%)	-0.38	4 (0%) 83 90	9, 15, 26, 56	0
All	All	2057/2060 (99%)	-0.44	10 (0%) 86 92	9, 15, 25, 65	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	GLU	4.3
1	A	2	SER	4.1
1	D	4	LYS	3.7
1	B	516	ALA	3.3
1	C	516	ALA	2.8
1	D	388[A]	TYR	2.7
1	D	516	ALA	2.6
1	B	388	TYR	2.4
1	A	388[A]	TYR	2.3
1	A	516	ALA	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NDP	C	1517	48/48	0.22	12.11	21,36,52,57	0
7	BTB	D	1517	14/14	0.29	5.18	30,51,64,71	0
4	NO	C	1519	2/2	0.10	5.08	20,20,20,20	0
3	NDP	B	1517	48/48	0.14	4.27	20,29,37,40	0
3	NDP	D	1518	48/48	0.18	4.26	25,35,49,58	0
5	EDO	B	1522	4/4	0.11	3.83	14,15,17,18	0
3	NDP	A	1518	48/48	0.11	3.25	20,26,32,37	0
4	NO	D	1520	2/2	0.08	2.32	20,20,20,20	0
5	EDO	B	1521	4/4	0.08	1.13	16,17,17,18	0
6	HEM	D	3003	43/43	0.07	1.12	7,11,13,16	0
6	HEM	A	3000	43/43	0.07	1.02	7,10,13,14	0
6	HEM	C	3002	43/43	0.07	0.45	8,10,13,15	0
6	HEM	B	3001	43/43	0.07	0.44	8,12,15,17	0
5	EDO	D	1519	4/4	0.07	0.13	12,12,15,16	0
4	NO	A	1519	2/2	0.07	0.09	20,20,20,20	0
5	EDO	B	1519	4/4	0.07	0.07	12,13,16,17	0
5	EDO	D	1521	4/4	0.06	-0.77	15,17,21,22	0
4	NO	B	1520	2/2	0.06	-0.80	20,20,20,20	0
5	EDO	A	1520	4/4	0.06	-0.87	11,11,12,13	0
2	CL	A	1517	1/1	0.04	-4.93	15,15,15,15	0
5	EDO	C	1518	4/4	0.04	-5.04	11,13,13,13	0
2	CL	B	1518	1/1	0.04	-6.10	16,16,16,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.