



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:00 PM GMT

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

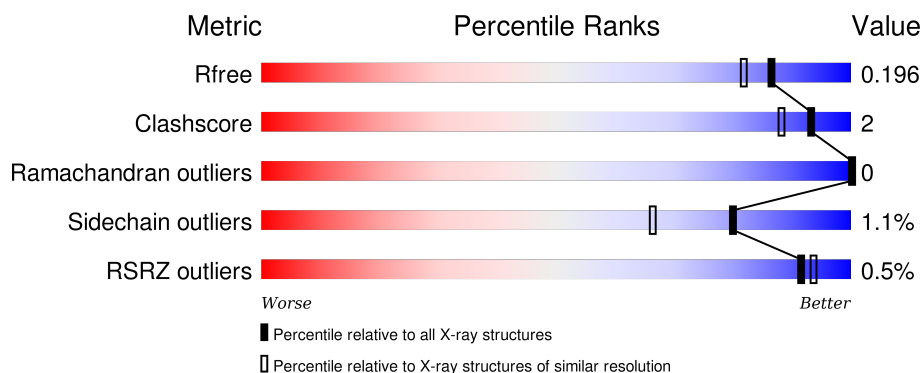
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	515	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 96%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="position: absolute; right: 0; top: 0;">%</div> <div style="position: absolute; left: 50%; top: 0;">96%</div> <div style="position: absolute; right: 5%; top: 0;">5%</div> <div style="position: absolute; right: 0; top: 0;">.</div> </div>
1	B	515	<div> <div style="width: 95%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="position: absolute; right: 0; top: 0;">%</div> <div style="position: absolute; left: 50%; top: 0;">95%</div> <div style="position: absolute; right: 5%; top: 0;">5%</div> </div>
1	C	515	<div> <div style="width: 95%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="position: absolute; right: 0; top: 0;">%</div> <div style="position: absolute; left: 50%; top: 0;">95%</div> <div style="position: absolute; right: 5%; top: 0;">5%</div> </div>
1	D	515	<div> <div style="width: 95%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="position: absolute; right: 0; top: 0;">%</div> <div style="position: absolute; left: 50%; top: 0;">95%</div> <div style="position: absolute; right: 5%; top: 0;">5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NDP	A	1518	-	-	-	X
3	NDP	B	1517	-	-	-	X
3	NDP	C	1517	-	-	-	X
3	NDP	D	1518	-	-	-	X
4	NO	A	1519	-	-	X	X
4	NO	B	1520	-	-	-	X
4	NO	C	1519	-	-	-	X
4	NO	D	1520	-	-	X	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 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 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).

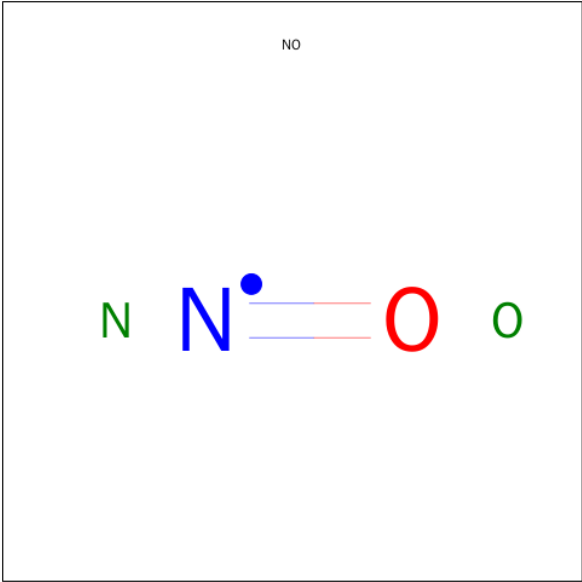
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



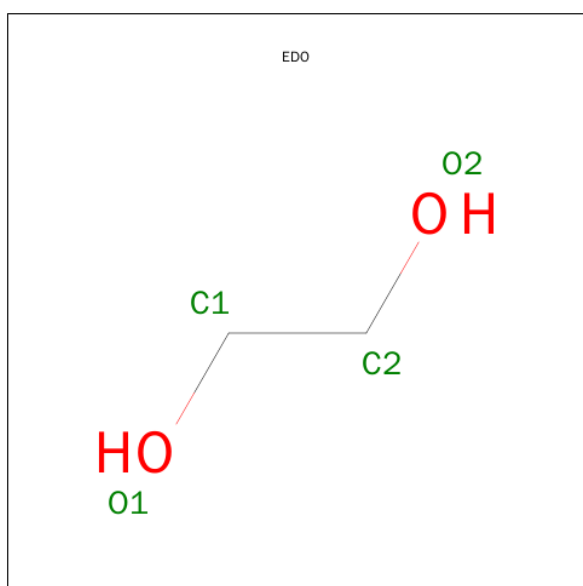
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- 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

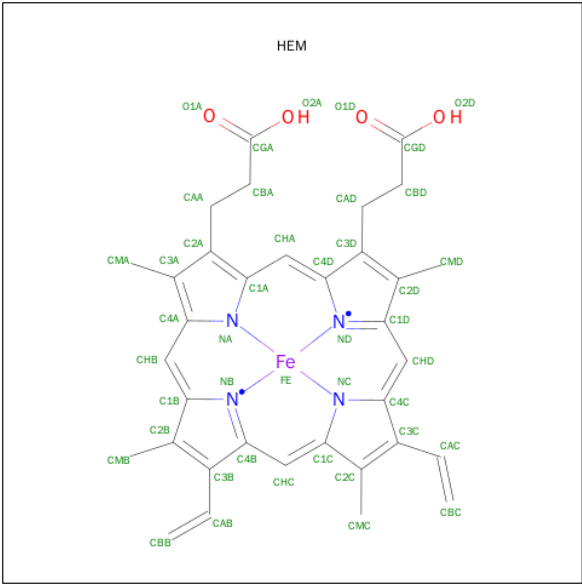
- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

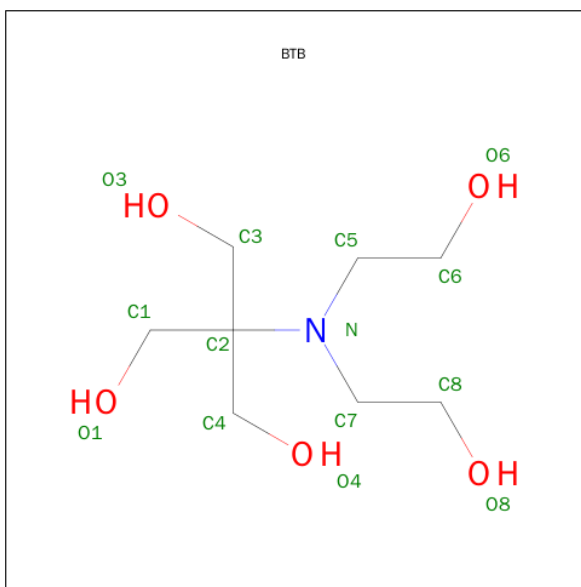
- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 7 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



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

- Molecule 8 is water.

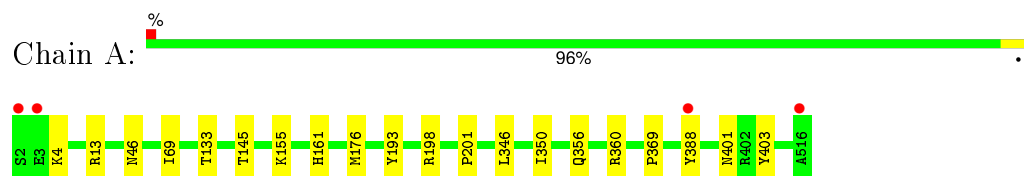
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	378	Total	O	0	0
			378	378		
8	B	276	Total	O	0	0
			276	276		
8	C	265	Total	O	0	0
			265	265		
8	D	196	Total	O	0	0
			196	196		



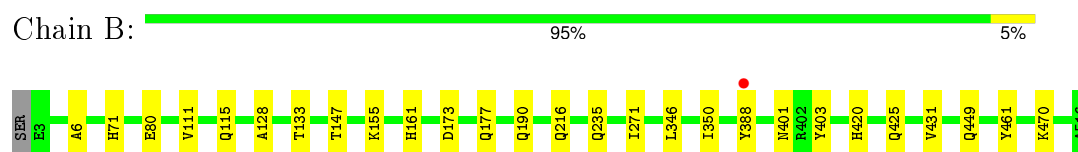
### 3 Residue-property plots [i](#)

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

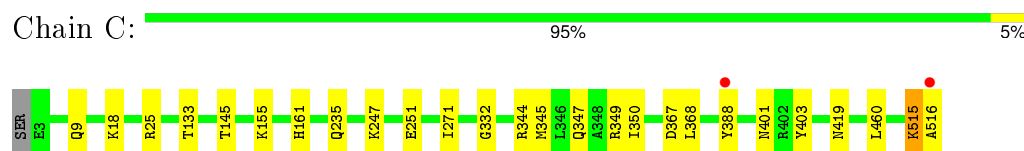
#### • Molecule 1: CATALASE



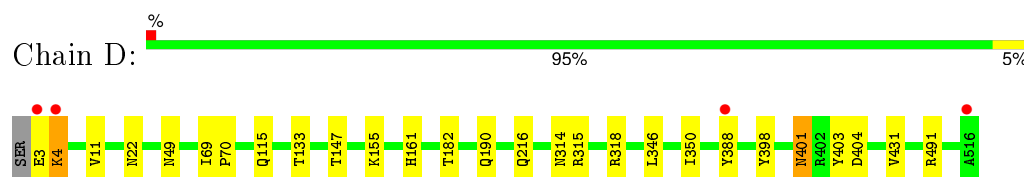
#### • Molecule 1: CATALASE



#### • Molecule 1: CATALASE



#### • Molecule 1: CATALASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 1.76Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, $R_{free}$	0.158 , 0.194 0.161 , 0.196	Depositor DCC
$R_{free}$ test set	9387 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 41.2	EDS
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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

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 2.

All (60) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:O	1:A:350:ILE:HG12	2.19	0.43
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:182:THR:HB	1:D:491:ARG:HG2	2.03	0.41
1:D:147:THR:HG23	1:D:190:GLN:HE21	1.85	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%)	80	66
1	B	440/436 (101%)	436 (99%)	4 (1%)	84	72
1	C	442/436 (101%)	437 (99%)	5 (1%)	80	66
1	D	440/436 (101%)	435 (99%)	5 (1%)	80	66
All	All	1766/1744 (101%)	1747 (99%)	19 (1%)	80	66

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
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 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 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	-	42,52,52	1.50	4 (9%)	55,80,80	1.78	4 (7%)
4	NO	A	1519	6	0,1,1	0.00	-	0,0,0	0.00	-
5	EDO	A	1520	-	3,3,3	0.51	0	2,2,2	0.50	0
6	HEM	A	3000	1,4	30,50,50	2.19	8 (26%)	24,82,82	2.50	12 (50%)
3	NDP	B	1517	-	42,52,52	1.51	4 (9%)	55,80,80	1.84	6 (10%)
5	EDO	B	1519	-	3,3,3	0.52	0	2,2,2	0.47	0
4	NO	B	1520	6	0,1,1	0.00	-	0,0,0	0.00	-
5	EDO	B	1521	-	3,3,3	0.62	0	2,2,2	0.17	0
5	EDO	B	1522	-	3,3,3	0.46	0	2,2,2	0.44	0
6	HEM	B	3001	1,4	30,50,50	2.19	9 (30%)	24,82,82	2.45	11 (45%)
3	NDP	C	1517	-	42,52,52	1.53	4 (9%)	55,80,80	1.87	6 (10%)
5	EDO	C	1518	-	3,3,3	0.54	0	2,2,2	0.38	0
4	NO	C	1519	6	0,1,1	0.00	-	0,0,0	0.00	-
6	HEM	C	3002	1,4	30,50,50	2.11	7 (23%)	24,82,82	2.46	11 (45%)
7	BTB	D	1517	-	12,13,13	0.92	0	8,16,16	0.56	0
3	NDP	D	1518	-	42,52,52	1.53	5 (11%)	55,80,80	1.89	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	D	1519	-	3,3,3	0.59	0	2,2,2	0.42	0
4	NO	D	1520	6	0,1,1	0.00	-	0,0,0	0.00	-
5	EDO	D	1521	-	3,3,3	0.57	0	2,2,2	0.35	0
6	HEM	D	3003	1,4	30,50,50	2.15	9 (30%)	24,82,82	2.51	11 (45%)

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	-	-	0/30/77/77	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	-	0/10/54/54	0/0/8/8
3	NDP	B	1517	-	-	0/30/77/77	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	-	0/10/54/54	0/0/8/8
3	NDP	C	1517	-	-	0/30/77/77	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	-	0/10/54/54	0/0/8/8
7	BTB	D	1517	-	-	0/21/21/21	0/0/0/0
3	NDP	D	1518	-	-	0/30/77/77	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	-	0/10/54/54	0/0/8/8

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3000	HEM	C3B-C4B	-7.56	1.45	1.51
6	D	3003	HEM	C3B-C4B	-7.51	1.45	1.51
6	B	3001	HEM	C3B-C4B	-7.18	1.45	1.51
6	C	3002	HEM	C3B-C4B	-6.62	1.46	1.51
6	C	3002	HEM	C3D-C4D	-5.53	1.44	1.51
6	B	3001	HEM	C3D-C4D	-5.27	1.44	1.51
6	A	3000	HEM	C3D-C4D	-5.15	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3003	HEM	C3D-C4D	-4.96	1.45	1.51
6	B	3001	HEM	C2C-C1C	-3.76	1.45	1.52
6	A	3000	HEM	C2C-C1C	-3.65	1.45	1.52
6	C	3002	HEM	C2C-C1C	-3.40	1.46	1.52
6	D	3003	HEM	C2C-C1C	-3.27	1.46	1.52
6	C	3002	HEM	C2D-C1D	-2.36	1.44	1.51
6	D	3003	HEM	C2D-C1D	-2.34	1.44	1.51
6	A	3000	HEM	C2D-C1D	-2.29	1.44	1.51
6	A	3000	HEM	C2B-C1B	-2.28	1.44	1.51
6	B	3001	HEM	C2D-C1D	-2.25	1.44	1.51
6	D	3003	HEM	C2B-C1B	-2.13	1.44	1.51
6	B	3001	HEM	CAA-C2A	2.04	1.55	1.52
6	A	3000	HEM	C3B-CAB	2.05	1.55	1.51
6	D	3003	HEM	C3C-CAC	2.06	1.55	1.51
3	D	1518	NDP	C2N-C3N	2.07	1.39	1.34
6	B	3001	HEM	C3C-CAC	2.09	1.55	1.51
6	B	3001	HEM	C1C-NC	2.11	1.38	1.36
6	D	3003	HEM	C3B-CAB	2.17	1.55	1.51
6	A	3000	HEM	C3C-CAC	2.19	1.55	1.51
6	D	3003	HEM	C1C-NC	2.22	1.38	1.36
6	B	3001	HEM	C3B-CAB	2.22	1.55	1.51
6	C	3002	HEM	C3C-CAC	2.23	1.55	1.51
6	C	3002	HEM	C4C-NC	2.27	1.38	1.36
6	C	3002	HEM	C3B-CAB	2.30	1.55	1.51
6	D	3003	HEM	C4C-NC	2.34	1.38	1.36
6	A	3000	HEM	C1C-NC	2.39	1.39	1.36
3	A	1518	NDP	C2A-N1A	2.54	1.38	1.33
3	D	1518	NDP	C2A-N1A	2.55	1.38	1.33
3	C	1517	NDP	C2A-N1A	2.58	1.38	1.33
3	B	1517	NDP	C2A-N1A	2.66	1.39	1.33
6	B	3001	HEM	FE-NC	2.67	2.06	1.95
3	B	1517	NDP	C2A-N3A	3.45	1.38	1.32
3	D	1518	NDP	C6N-C5N	3.52	1.40	1.33
3	A	1518	NDP	C6N-C5N	3.55	1.40	1.33
3	B	1517	NDP	C6N-C5N	3.56	1.40	1.33
3	C	1517	NDP	C6N-C5N	3.61	1.40	1.33
3	A	1518	NDP	C2A-N3A	3.67	1.38	1.32
3	C	1517	NDP	C2A-N3A	3.72	1.38	1.32
3	D	1518	NDP	C2A-N3A	3.77	1.38	1.32
3	A	1518	NDP	O7N-C7N	6.46	1.40	1.24
3	B	1517	NDP	O7N-C7N	6.48	1.40	1.24
3	C	1517	NDP	O7N-C7N	6.52	1.40	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1518	NDP	O7N-C7N	6.57	1.41	1.24

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1518	NDP	N3A-C2A-N1A	-11.59	120.02	128.89
3	B	1517	NDP	N3A-C2A-N1A	-11.03	120.45	128.89
3	C	1517	NDP	N3A-C2A-N1A	-11.01	120.46	128.89
3	A	1518	NDP	N3A-C2A-N1A	-10.61	120.77	128.89
3	B	1517	NDP	PN-O3-PA	-3.63	122.53	132.73
3	D	1518	NDP	PN-O3-PA	-3.38	123.25	132.73
6	D	3003	HEM	CMA-C3A-C4A	-3.12	123.19	128.36
3	C	1517	NDP	PN-O3-PA	-3.02	124.24	132.73
6	B	3001	HEM	CBA-CAA-C2A	-2.84	107.44	112.53
3	B	1517	NDP	C1B-N9A-C4A	-2.78	122.74	126.94
3	C	1517	NDP	P2B-O2B-C2B	-2.74	114.98	121.56
6	A	3000	HEM	C4B-CHC-C1C	-2.70	121.31	125.82
6	C	3002	HEM	CBA-CAA-C2A	-2.61	107.84	112.53
3	A	1518	NDP	PN-O3-PA	-2.50	125.72	132.73
6	C	3002	HEM	CMA-C3A-C4A	-2.39	124.41	128.36
6	A	3000	HEM	CBA-CAA-C2A	-2.37	108.27	112.53
6	C	3002	HEM	CBD-CAD-C3D	-2.37	106.65	113.55
6	B	3001	HEM	CBD-CAD-C3D	-2.31	106.83	113.55
6	B	3001	HEM	CMA-C3A-C4A	-2.28	124.59	128.36
3	C	1517	NDP	C1D-N1N-C2N	-2.25	116.99	120.91
6	D	3003	HEM	CBA-CAA-C2A	-2.23	108.54	112.53
3	B	1517	NDP	C4A-C5A-N7A	-2.21	107.44	109.48
6	A	3000	HEM	CBD-CAD-C3D	-2.14	107.31	113.55
6	D	3003	HEM	C4B-CHC-C1C	-2.14	122.24	125.82
6	A	3000	HEM	CAD-CBD-CGD	-2.13	104.34	113.02
6	D	3003	HEM	CAD-CBD-CGD	-2.09	104.51	113.02
6	C	3002	HEM	CAA-CBA-CGA	-2.04	109.00	112.75
3	A	1518	NDP	C4A-C5A-N7A	-2.04	107.61	109.48
3	C	1517	NDP	C3D-C2D-C1D	2.11	105.64	101.40
6	B	3001	HEM	C3B-C4B-CHC	2.12	126.15	123.16
3	D	1518	NDP	C3D-C2D-C1D	2.17	105.76	101.40
6	C	3002	HEM	C2C-C1C-CHC	2.28	127.14	123.68
6	B	3001	HEM	C2C-C1C-CHC	2.28	127.15	123.68
3	B	1517	NDP	C3D-C2D-C1D	2.30	106.03	101.40
3	B	1517	NDP	O4B-C1B-N9A	2.31	112.93	108.10
6	A	3000	HEM	C3B-C4B-CHC	2.36	126.48	123.16
6	A	3000	HEM	C2C-C1C-CHC	2.55	127.56	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3003	HEM	C2C-C1C-CHC	2.57	127.59	123.68
6	B	3001	HEM	C2D-C3D-C4D	2.63	105.96	101.50
6	B	3001	HEM	CMD-C2D-C3D	2.64	126.05	114.35
3	D	1518	NDP	O4B-C1B-N9A	2.73	113.81	108.10
6	A	3000	HEM	C2D-C3D-C4D	2.75	106.16	101.50
6	D	3003	HEM	C2D-C3D-C4D	2.75	106.17	101.50
6	D	3003	HEM	CMD-C2D-C3D	2.79	126.68	114.35
6	C	3002	HEM	CMD-C2D-C3D	2.81	126.80	114.35
6	C	3002	HEM	C2D-C3D-C4D	2.82	106.28	101.50
6	A	3000	HEM	CMD-C2D-C3D	2.97	127.47	114.35
3	C	1517	NDP	O4B-C1B-N9A	3.25	114.89	108.10
3	A	1518	NDP	O4B-C1B-N9A	3.25	114.91	108.10
6	D	3003	HEM	CAD-C3D-C2D	4.05	124.85	113.22
6	C	3002	HEM	CAD-C3D-C2D	4.23	125.39	113.22
6	D	3003	HEM	CMC-C2C-C3C	4.26	127.18	116.53
6	A	3000	HEM	CAD-C3D-C4D	4.34	127.76	112.47
6	B	3001	HEM	CAD-C3D-C4D	4.35	127.81	112.47
6	A	3000	HEM	CAD-C3D-C2D	4.47	126.07	113.22
6	C	3002	HEM	CAD-C3D-C4D	4.49	128.32	112.47
6	B	3001	HEM	CAD-C3D-C2D	4.52	126.22	113.22
6	C	3002	HEM	CMC-C2C-C3C	4.59	127.98	116.53
6	A	3000	HEM	CMC-C2C-C3C	4.60	128.00	116.53
6	B	3001	HEM	CMB-C2B-C3B	4.62	128.05	116.53
6	D	3003	HEM	CAD-C3D-C4D	4.68	128.98	112.47
6	C	3002	HEM	CMB-C2B-C3B	4.76	128.41	116.53
6	B	3001	HEM	CMC-C2C-C3C	4.94	128.85	116.53
6	A	3000	HEM	CMB-C2B-C3B	4.99	128.99	116.53
6	D	3003	HEM	CMB-C2B-C3B	5.11	129.28	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1518	NDP	1	0
4	A	1519	NO	4	0
6	A	3000	HEM	4	0
6	B	3001	HEM	1	0
3	C	1517	NDP	1	0
4	D	1520	NO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	3003	HEM	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	515/515 (100%)	-0.41	4 (0%) 87 91	9, 14, 24, 65	0
1	B	514/515 (99%)	-0.37	1 (0%) 95 96	9, 16, 26, 55	0
1	C	514/515 (99%)	-0.38	2 (0%) 93 94	9, 14, 24, 52	0
1	D	514/515 (99%)	-0.30	4 (0%) 87 91	9, 15, 26, 56	0
All	All	2057/2060 (99%)	-0.37	11 (0%) 91 93	9, 15, 25, 65	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	516	ALA	4.6
1	A	2	SER	4.1
1	D	3	GLU	3.5
1	D	4	LYS	3.2
1	D	516	ALA	3.2
1	D	388[A]	TYR	3.0
1	A	388[A]	TYR	2.5
1	B	388	TYR	2.4
1	A	516	ALA	2.3
1	C	388	TYR	2.0
1	A	3	GLU	2.0

### 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NDP	C	1517	48/48	0.83	0.23	11.84	21,36,52,57	0
4	NO	B	1520	2/2	0.98	0.12	6.24	20,20,20,20	0
3	NDP	A	1518	48/48	0.92	0.13	5.71	20,26,32,37	0
3	NDP	D	1518	48/48	0.86	0.20	5.51	25,35,49,58	0
7	BTB	D	1517	14/14	0.74	0.32	5.50	30,51,64,71	0
4	NO	A	1519	2/2	0.99	0.10	5.01	20,20,20,20	0
4	NO	D	1520	2/2	0.99	0.10	4.34	20,20,20,20	0
5	EDO	B	1522	4/4	0.96	0.10	3.92	14,15,17,18	0
4	NO	C	1519	2/2	0.99	0.11	3.49	20,20,20,20	0
3	NDP	B	1517	48/48	0.94	0.14	3.25	20,29,37,40	0
6	HEM	B	3001	43/43	0.98	0.08	1.22	8,12,15,17	0
6	HEM	A	3000	43/43	0.98	0.08	0.86	7,10,13,14	0
6	HEM	D	3003	43/43	0.98	0.08	0.70	7,11,13,16	0
5	EDO	B	1521	4/4	0.95	0.08	0.64	16,17,17,18	0
5	EDO	D	1519	4/4	0.97	0.08	0.44	12,12,15,16	0
5	EDO	B	1519	4/4	0.98	0.08	0.09	12,13,16,17	0
6	HEM	C	3002	43/43	0.99	0.07	-0.04	8,10,13,15	0
5	EDO	D	1521	4/4	0.97	0.07	-1.03	15,17,21,22	0
5	EDO	A	1520	4/4	0.99	0.07	-1.29	11,11,12,13	0
2	CL	B	1518	1/1	1.00	0.07	-2.39	16,16,16,16	0
5	EDO	C	1518	4/4	0.99	0.06	-3.26	11,13,13,13	0
2	CL	A	1517	1/1	1.00	0.05	-4.12	15,15,15,15	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.