



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:35 am GMT

PDB ID : 2J2M  
Title : CRYSTAL STRUCTURE ANALYSIS OF CATALASE FROM EXIGUOBACTERIUM OXIDOTOLERANS  
Authors : Hara, I.; Ichise, N.; Kojima, K.; Kondo, H.; Ohgiya, S.; Matsuyama, H.; Yumoto, I.  
Deposited on : 2006-08-17  
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](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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

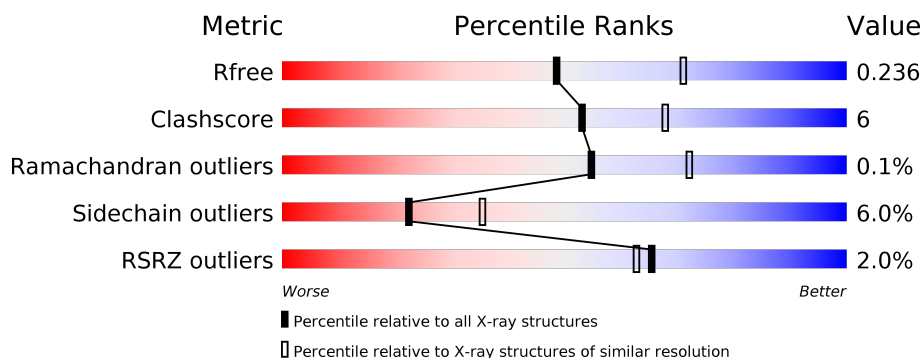
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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  $\geq 3$ , 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	491	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 83%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>83%</span> <span>13%</span> <span>...</span> </div> </div>
1	B	491	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 81%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>81%</span> <span>14%</span> <span>..</span> </div> </div>
1	C	491	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 14%, green 81%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>81%</span> <span>14%</span> <span>..</span> </div> </div>
1	D	491	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 14%, green 81%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>81%</span> <span>14%</span> <span>..</span> </div> </div>

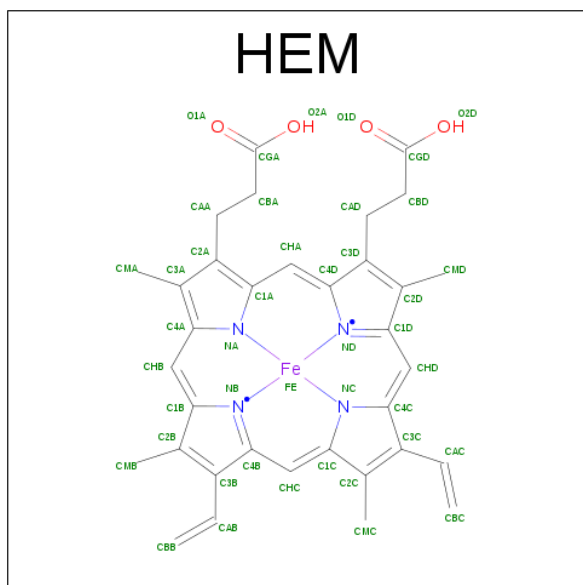


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CATALASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total 3894	C 2456	N 681	O 743	S 14	0	0	0
1	B	480	Total 3894	C 2456	N 681	O 743	S 14	0	0	0
1	C	480	Total 3894	C 2456	N 681	O 743	S 14	0	0	0
1	D	480	Total 3894	C 2456	N 681	O 743	S 14	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

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

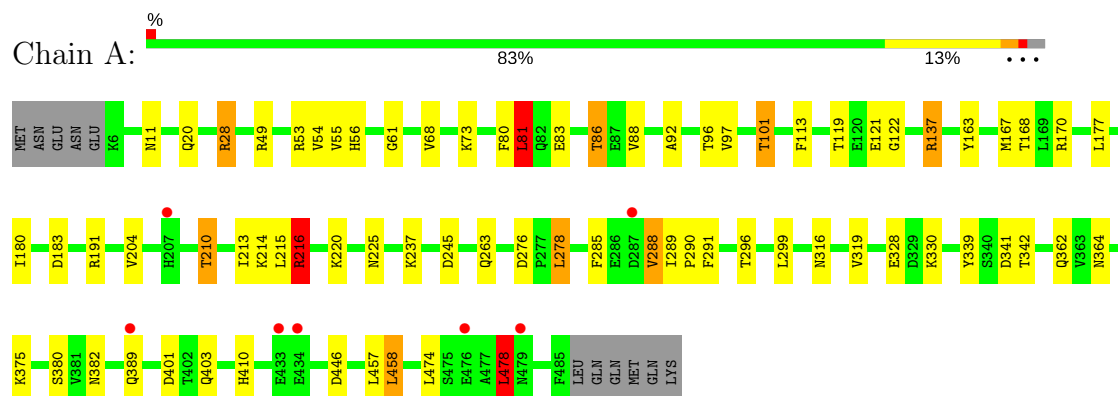
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	162	Total	O	0	0
			162	162		
3	B	155	Total	O	0	0
			155	155		
3	C	108	Total	O	0	0
			108	108		
3	D	111	Total	O	0	0
			111	111		

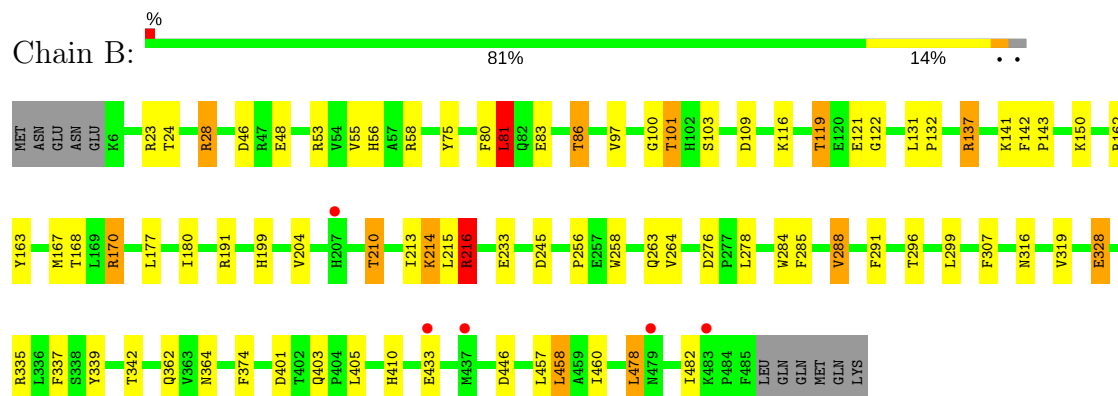
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

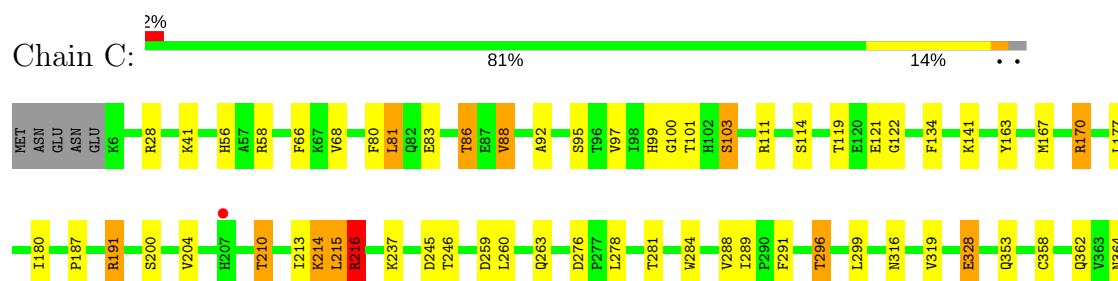
#### • Molecule 1: CATALASE

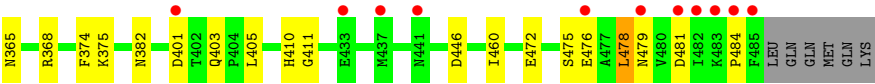


#### • Molecule 1: CATALASE

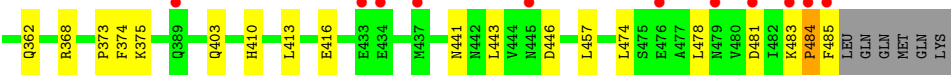
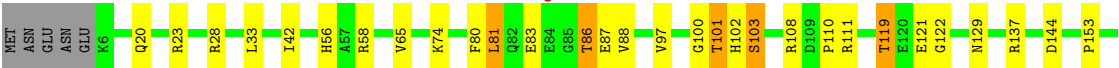
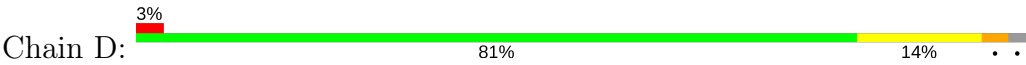


#### • Molecule 1: CATALASE





● Molecule 1: CATALASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.27Å 131.94Å 110.64Å 90.00° 107.61° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.40) 99.1 (19.99-2.40)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.66 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.199 , 0.230 0.204 , 0.236	Depositor DCC
$R_{free}$ test set	4994 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16284	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.66	0/3997	0.73	6/5424 (0.1%)
1	B	0.67	0/3997	0.73	7/5424 (0.1%)
1	C	0.62	0/3997	0.70	3/5424 (0.1%)
1	D	0.61	0/3997	0.67	1/5424 (0.0%)
All	All	0.64	0/15988	0.71	17/21696 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	B	137	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	C	216	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	B	216	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	278	LEU	CA-CB-CG	6.17	129.49	115.30
1	A	216	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	81	LEU	CA-CB-CG	5.90	128.88	115.30
1	C	170	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	216	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	28	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	D	137	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	81	LEU	CA-CB-CG	5.41	127.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	A	28	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	137	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	B	478	LEU	N-CA-C	5.13	124.86	111.00
1	B	170	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	478	LEU	Peptide

## 5.2 Too-close contacts [i](#)

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	3894	0	3706	45	0
1	B	3894	0	3706	56	0
1	C	3894	0	3706	55	0
1	D	3894	0	3706	58	0
2	A	43	0	30	2	0
2	B	43	0	30	0	0
2	C	43	0	30	4	0
2	D	43	0	30	2	0
3	A	162	0	0	3	0
3	B	155	0	0	3	0
3	C	108	0	0	3	0
3	D	111	0	0	5	0
All	All	16284	0	14944	190	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 6.

All (190) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:THR:HG22	1:B:121:GLU:H	1.30	0.95
1:C:210:THR:HG21	1:C:403:GLN:HE22	1.35	0.91
1:C:119:THR:HG22	1:C:121:GLU:H	1.34	0.91
1:B:119:THR:HB	1:B:122:GLY:O	1.72	0.90
1:A:210:THR:HG21	1:A:403:GLN:HE22	1.38	0.88
2:C:501:HEM:HBC2	2:C:501:HEM:HMC1	1.56	0.86
1:B:210:THR:HG21	1:B:403:GLN:HE22	1.39	0.85
1:D:119:THR:HG22	1:D:121:GLU:H	1.39	0.85
1:A:119:THR:HG22	1:A:121:GLU:H	1.42	0.84
1:C:358:CYS:SG	1:C:375:LYS:NZ	2.52	0.83
1:D:210:THR:HG21	1:D:403:GLN:HE22	1.46	0.80
1:D:259:ASP:OD2	1:D:296:THR:HG22	1.83	0.79
1:A:119:THR:HG21	3:A:2035:HOH:O	1.83	0.79
1:C:119:THR:HB	1:C:122:GLY:O	1.84	0.78
1:C:83:GLU:O	1:C:86:THR:HG23	1.83	0.77
1:A:119:THR:HB	1:A:122:GLY:O	1.85	0.77
1:D:191:ARG:HD3	1:D:245:ASP:OD2	1.87	0.74
1:A:83:GLU:O	1:A:86:THR:HG23	1.89	0.73
1:D:119:THR:CG2	1:D:121:GLU:H	2.02	0.73
1:B:86:THR:HG21	3:B:2032:HOH:O	1.89	0.72
1:C:99:HIS:HB2	1:C:103:SER:OG	1.90	0.72
1:C:100:GLY:O	1:C:103:SER:HB2	1.90	0.71
1:B:100:GLY:O	1:B:103:SER:HB2	1.91	0.71
1:B:119:THR:HG21	3:B:2034:HOH:O	1.91	0.70
2:C:501:HEM:CMC	2:C:501:HEM:HBC2	2.22	0.69
1:B:285:PHE:HB2	1:B:288:VAL:HG13	1.73	0.69
1:B:119:THR:HG22	1:B:121:GLU:N	2.06	0.69
1:D:216:ARG:HG2	1:D:291:PHE:CE2	2.27	0.68
1:B:83:GLU:O	1:B:86:THR:HG22	1.93	0.68
1:D:100:GLY:O	1:D:103:SER:HB2	1.93	0.68
2:D:501:HEM:HMB1	2:D:501:HEM:HBB2	1.76	0.67
1:C:374:PHE:CE2	3:C:2092:HOH:O	2.48	0.67
1:B:83:GLU:O	1:B:86:THR:CG2	2.43	0.67
1:A:86:THR:HG21	3:A:2034:HOH:O	1.95	0.67
1:B:119:THR:CG2	1:B:121:GLU:H	2.05	0.67
1:A:276:ASP:OD1	1:B:28:ARG:HD2	1.96	0.65
1:A:101:THR:O	1:B:101:THR:O	2.15	0.64
1:D:210:THR:HG22	3:D:2056:HOH:O	1.97	0.64
1:D:170:ARG:CG	1:D:170:ARG:HH11	2.11	0.63
1:C:191:ARG:HD3	1:C:245:ASP:OD2	1.99	0.62
1:D:200:SER:OG	1:D:278:LEU:HD12	2.00	0.62
1:A:204:VAL:HG22	1:A:210:THR:HB	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:VAL:HG22	1:B:210:THR:HB	1.82	0.62
1:C:362:GLN:HG3	1:C:364:ASN:ND2	2.15	0.62
1:D:170:ARG:HH11	1:D:170:ARG:HG3	1.65	0.62
1:A:119:THR:HG22	1:A:121:GLU:N	2.13	0.61
1:D:119:THR:HG22	1:D:121:GLU:N	2.13	0.61
1:D:204:VAL:HG22	1:D:210:THR:HB	1.82	0.61
1:D:80:PHE:CE2	1:D:81:LEU:HD13	2.35	0.61
1:D:170:ARG:NH1	1:D:172:GLU:OE1	2.34	0.61
1:B:119:THR:CG2	3:B:2034:HOH:O	2.50	0.60
1:C:99:HIS:CB	1:C:103:SER:OG	2.49	0.60
1:D:216:ARG:HG2	1:D:291:PHE:CZ	2.37	0.59
1:C:476:GLU:O	1:C:479:ASN:HB3	2.03	0.59
1:D:119:THR:HB	1:D:122:GLY:O	2.03	0.59
1:D:170:ARG:NH1	1:D:170:ARG:HG3	2.18	0.58
1:A:339:TYR:O	1:A:342:THR:HG22	2.03	0.58
1:D:358:CYS:SG	1:D:375:LYS:NZ	2.71	0.58
1:A:330:LYS:HD3	1:B:24:THR:HG21	1.85	0.57
1:C:66:PHE:HB3	1:C:88:VAL:HG13	1.85	0.57
1:A:80:PHE:CE2	1:A:81:LEU:HD13	2.39	0.57
1:C:362:GLN:HG3	1:C:364:ASN:HD21	1.70	0.57
1:D:214:LYS:HE2	1:D:284:TRP:CG	2.39	0.57
1:D:216:ARG:NH2	3:D:2057:HOH:O	2.37	0.57
1:A:216:ARG:HG2	1:A:291:PHE:CE2	2.40	0.56
1:D:56:HIS:CE1	1:D:97:VAL:HG22	2.41	0.56
1:B:278:LEU:HD21	1:B:328:GLU:HG2	1.88	0.56
1:C:353:GLN:O	1:C:375:LYS:HE2	2.06	0.56
1:A:210:THR:HG21	1:A:403:GLN:NE2	2.15	0.56
1:A:216:ARG:HG2	1:A:291:PHE:CZ	2.40	0.55
1:D:119:THR:HG21	3:D:2031:HOH:O	2.05	0.55
1:C:216:ARG:HG2	1:C:291:PHE:CE2	2.42	0.55
1:A:380:SER:HA	1:D:153:PRO:HG2	1.89	0.55
1:A:119:THR:CG2	1:A:121:GLU:H	2.16	0.55
1:D:282:LYS:HE2	3:D:2106:HOH:O	2.07	0.54
1:C:215:LEU:HG	1:C:260:LEU:HD11	1.88	0.54
2:D:501:HEM:CMB	2:D:501:HEM:HBB2	2.38	0.54
1:C:119:THR:HG22	1:C:121:GLU:N	2.12	0.54
1:A:213:ILE:HA	1:A:263:GLN:O	2.07	0.53
1:A:403:GLN:HB2	1:D:410:HIS:CE1	2.44	0.53
1:C:80:PHE:CE2	1:C:81:LEU:HD13	2.43	0.53
1:C:111:ARG:HG3	1:C:187:PRO:HG2	1.91	0.53
1:C:210:THR:HG21	1:C:403:GLN:NE2	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:LYS:HE2	1:C:284:TRP:CG	2.45	0.52
1:A:278:LEU:HD21	1:A:328:GLU:HB2	1.91	0.52
1:D:97:VAL:HG21	1:D:110:PRO:HG2	1.89	0.52
1:C:204:VAL:HG22	1:C:210:THR:HB	1.92	0.52
1:C:374:PHE:CD2	3:C:2092:HOH:O	2.63	0.52
1:A:191:ARG:HD3	1:A:245:ASP:OD2	2.10	0.51
1:C:101:THR:O	1:D:101:THR:O	2.29	0.51
1:A:28:ARG:O	1:B:328:GLU:HG3	2.11	0.51
1:B:337:PHE:HB2	1:D:33:LEU:HD11	1.93	0.51
1:C:119:THR:HG21	3:C:2030:HOH:O	2.12	0.50
1:B:210:THR:HG21	1:B:403:GLN:NE2	2.18	0.50
1:B:307:PHE:CE1	1:D:373:PRO:HG3	2.47	0.49
1:C:141:LYS:HD3	1:D:20:GLN:HA	1.94	0.49
1:B:216:ARG:HG2	1:B:291:PHE:CZ	2.48	0.49
1:C:119:THR:CG2	1:C:121:GLU:H	2.15	0.49
1:D:163:TYR:O	1:D:167:MET:HG2	2.11	0.49
1:B:405:LEU:HD13	1:C:405:LEU:HD13	1.95	0.48
1:B:168:THR:HB	1:B:458:LEU:HD13	1.95	0.48
1:C:134:PHE:O	1:C:281:THR:HG22	2.13	0.48
2:C:501:HEM:HMC1	2:C:501:HEM:CBC	2.37	0.48
1:B:214:LYS:HE2	1:B:284:TRP:CG	2.48	0.48
1:A:20:GLN:HA	1:B:141:LYS:HD3	1.95	0.48
1:C:214:LYS:HE2	1:C:284:TRP:CD1	2.48	0.48
1:A:285:PHE:HB2	1:A:288:VAL:HG13	1.96	0.48
1:A:316:ASN:HB3	1:A:319:VAL:HG23	1.96	0.48
1:A:382:ASN:OD1	1:D:162:ARG:NH2	2.47	0.47
1:A:168:THR:HB	1:A:458:LEU:HD13	1.95	0.47
1:D:416:GLU:OE2	1:D:416:GLU:HA	2.14	0.47
1:B:56:HIS:CE1	1:B:97:VAL:HG22	2.49	0.47
1:C:200:SER:HA	1:C:213:ILE:O	2.14	0.47
1:D:443:LEU:HD13	1:D:474:LEU:HD11	1.96	0.47
1:A:56:HIS:CE1	1:A:97:VAL:HG22	2.49	0.47
1:A:56:HIS:HA	1:A:96:THR:O	2.13	0.47
1:A:119:THR:CG2	3:A:2035:HOH:O	2.52	0.47
1:C:288:VAL:HG23	1:C:289:ILE:HG13	1.96	0.47
1:B:191:ARG:HD3	1:B:245:ASP:OD2	2.14	0.47
1:B:362:GLN:HG3	1:B:364:ASN:ND2	2.29	0.47
1:C:278:LEU:HD23	1:C:328:GLU:HG2	1.97	0.47
1:B:168:THR:HB	1:B:458:LEU:HB3	1.96	0.47
1:B:278:LEU:CD2	1:B:328:GLU:HG2	2.45	0.46
1:C:328:GLU:HG3	1:D:28:ARG:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:HIS:CE1	1:B:23:ARG:HH11	2.34	0.46
1:C:56:HIS:CE1	1:C:97:VAL:HG22	2.51	0.46
1:C:276:ASP:OD1	1:D:28:ARG:HD2	2.16	0.46
1:B:216:ARG:HG2	1:B:291:PHE:CE2	2.51	0.45
1:D:101:THR:O	1:D:102:HIS:HB2	2.17	0.45
1:D:108:ARG:HG2	1:D:180:ILE:CD1	2.47	0.45
2:C:501:HEM:HBC1	1:D:42:ILE:HD12	1.97	0.45
1:D:210:THR:HG21	1:D:403:GLN:NE2	2.23	0.45
1:A:362:GLN:HG3	1:A:364:ASN:ND2	2.33	0.44
1:C:216:ARG:HG2	1:C:291:PHE:CZ	2.53	0.44
1:A:289:ILE:HA	1:A:290:PRO:HD3	1.90	0.44
1:C:411:GLY:HA2	1:D:23:ARG:HG3	1.99	0.44
1:A:54:VAL:CG1	2:A:501:HEM:HMD1	2.47	0.44
1:B:116:LYS:HB2	1:B:116:LYS:HE2	1.85	0.44
1:D:183:ASP:O	1:D:225:ASN:HB3	2.18	0.44
1:B:75:TYR:CE2	1:B:264:VAL:HG11	2.53	0.44
1:B:339:TYR:O	1:B:342:THR:HG22	2.19	0.43
1:C:92:ALA:HA	1:C:114:SER:O	2.18	0.43
1:C:316:ASN:HB3	1:C:319:VAL:HG23	2.00	0.43
1:A:163:TYR:O	1:A:167:MET:HG2	2.19	0.43
1:A:11:ASN:ND2	1:C:365:ASN:HD21	2.15	0.43
1:A:474:LEU:O	1:A:478:LEU:HB2	2.18	0.43
1:C:163:TYR:O	1:C:167:MET:HG2	2.19	0.43
1:A:53:ARG:HB3	1:A:55:VAL:O	2.19	0.43
1:D:210:THR:CG2	3:D:2056:HOH:O	2.61	0.43
1:B:328:GLU:CD	1:B:328:GLU:H	2.22	0.42
1:D:83:GLU:O	1:D:86:THR:HG23	2.20	0.42
1:C:213:ILE:HA	1:C:263:GLN:O	2.19	0.42
1:B:163:TYR:O	1:B:167:MET:HG2	2.19	0.42
1:D:481:ASP:HB2	1:D:483:LYS:HE2	2.00	0.42
1:B:374:PHE:CZ	1:D:374:PHE:HB3	2.54	0.42
1:B:460:ILE:HG22	1:B:482:ILE:HG21	2.01	0.42
1:B:142:PHE:HB3	1:B:143:PRO:HD3	2.02	0.42
1:B:48:GLU:HG2	1:D:368:ARG:O	2.18	0.42
1:C:475:SER:O	1:C:479:ASN:HA	2.20	0.42
1:D:330:LYS:NZ	1:D:413:LEU:O	2.53	0.42
1:D:484:PRO:HB2	1:D:485:PHE:H	1.60	0.42
1:B:162:ARG:NH2	1:C:382:ASN:OD1	2.50	0.42
1:A:28:ARG:HD2	1:B:276:ASP:OD1	2.19	0.41
1:B:316:ASN:HB3	1:B:319:VAL:HG23	2.02	0.41
1:C:191:ARG:HG2	1:C:246:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:ASN:HA	1:D:317:PRO:HD2	1.94	0.41
1:B:410:HIS:CE1	1:C:403:GLN:HB2	2.55	0.41
1:D:111:ARG:O	1:D:129:ASN:HA	2.20	0.41
1:A:49:ARG:NH2	1:B:150:LYS:HE3	2.35	0.41
1:B:213:ILE:HA	1:B:263:GLN:O	2.20	0.41
1:B:256:PRO:HB2	1:B:258:TRP:CZ3	2.55	0.41
1:B:80:PHE:CE2	1:B:81:LEU:HD13	2.55	0.41
1:D:200:SER:HA	1:D:213:ILE:O	2.19	0.41
1:B:403:GLN:HB2	1:C:410:HIS:CE1	2.55	0.41
1:B:307:PHE:HE1	1:D:373:PRO:HG3	1.83	0.41
1:C:478:LEU:N	1:C:479:ASN:HA	2.36	0.41
1:A:61:GLY:HA2	1:A:92:ALA:O	2.21	0.41
1:A:54:VAL:HG11	2:A:501:HEM:HMD1	2.02	0.41
1:A:183:ASP:O	1:A:225:ASN:HB3	2.21	0.41
1:B:53:ARG:HB3	1:B:55:VAL:O	2.21	0.41
1:C:41:LYS:NZ	1:D:144:ASP:OD1	2.48	0.41
1:C:259:ASP:OD2	1:C:296:THR:HB	2.21	0.41
1:C:410:HIS:CE1	1:D:23:ARG:HH11	2.39	0.41
1:D:83:GLU:O	1:D:86:THR:CG2	2.68	0.41
1:C:95:SER:O	1:C:111:ARG:HA	2.21	0.41
1:D:65:VAL:HG21	1:D:87:GLU:OE2	2.21	0.41
1:B:199:HIS:CD2	1:B:335:ARG:HH11	2.39	0.40
1:A:341:ASP:OD2	1:B:46:ASP:OD1	2.40	0.40
1:C:460:ILE:HD11	1:C:478:LEU:HD23	2.03	0.40
1:B:131:LEU:HA	1:B:132:PRO:HD3	1.97	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	478/491 (97%)	465 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	478/491 (97%)	465 (97%)	13 (3%)	0	100	100
1	C	478/491 (97%)	465 (97%)	12 (2%)	1 (0%)	51	67
1	D	478/491 (97%)	464 (97%)	13 (3%)	1 (0%)	51	67
All	All	1912/1964 (97%)	1859 (97%)	51 (3%)	2 (0%)	55	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	484	PRO
1	D	484	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/437 (98%)	399 (94%)	27 (6%)	21	33
1	B	426/437 (98%)	401 (94%)	25 (6%)	23	36
1	C	426/437 (98%)	402 (94%)	24 (6%)	25	39
1	D	426/437 (98%)	400 (94%)	26 (6%)	22	34
All	All	1704/1748 (98%)	1602 (94%)	102 (6%)	22	35

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	A	73	LYS
1	A	81	LEU
1	A	86	THR
1	A	88	VAL
1	A	101	THR
1	A	113	PHE
1	A	137	ARG
1	A	170	ARG

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Mol	Chain	Res	Type
1	A	177	LEU
1	A	180	ILE
1	A	210	THR
1	A	214	LYS
1	A	215	LEU
1	A	216	ARG
1	A	220	LYS
1	A	237	LYS
1	A	288	VAL
1	A	296	THR
1	A	299	LEU
1	A	375	LYS
1	A	389	GLN
1	A	401	ASP
1	A	446	ASP
1	A	457	LEU
1	A	458	LEU
1	A	478	LEU
1	B	58	ARG
1	B	81	LEU
1	B	86	THR
1	B	101	THR
1	B	109	ASP
1	B	119	THR
1	B	137	ARG
1	B	170	ARG
1	B	177	LEU
1	B	180	ILE
1	B	210	THR
1	B	214	LYS
1	B	215	LEU
1	B	216	ARG
1	B	233	GLU
1	B	288	VAL
1	B	296	THR
1	B	299	LEU
1	B	328	GLU
1	B	401	ASP
1	B	433	GLU
1	B	446	ASP
1	B	457	LEU
1	B	458	LEU

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Mol	Chain	Res	Type
1	B	478	LEU
1	C	58	ARG
1	C	68	VAL
1	C	81	LEU
1	C	86	THR
1	C	88	VAL
1	C	103	SER
1	C	170	ARG
1	C	177	LEU
1	C	180	ILE
1	C	191	ARG
1	C	210	THR
1	C	214	LYS
1	C	215	LEU
1	C	216	ARG
1	C	237	LYS
1	C	296	THR
1	C	299	LEU
1	C	328	GLU
1	C	368	ARG
1	C	401	ASP
1	C	446	ASP
1	C	472	GLU
1	C	478	LEU
1	C	481	ASP
1	D	58	ARG
1	D	74	LYS
1	D	81	LEU
1	D	86	THR
1	D	88	VAL
1	D	101	THR
1	D	103	SER
1	D	119	THR
1	D	170	ARG
1	D	177	LEU
1	D	180	ILE
1	D	191	ARG
1	D	210	THR
1	D	214	LYS
1	D	215	LEU
1	D	216	ARG
1	D	237	LYS

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Mol	Chain	Res	Type
1	D	246	THR
1	D	278	LEU
1	D	286	GLU
1	D	299	LEU
1	D	362	GLN
1	D	441	ASN
1	D	446	ASP
1	D	457	LEU
1	D	478	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	225	ASN
1	A	364	ASN
1	B	11	ASN
1	B	225	ASN
1	B	364	ASN
1	B	441	ASN
1	C	11	ASN
1	C	207	HIS
1	C	209	ASN
1	C	225	ASN
1	C	364	ASN
1	D	11	ASN
1	D	225	ASN
1	D	235	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

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	HEM	A	501	1	28,50,50	2.18	9 (32%)	17,82,82	1.93	5 (29%)
2	HEM	B	501	1	28,50,50	2.25	9 (32%)	17,82,82	1.91	5 (29%)
2	HEM	C	501	1	28,50,50	2.21	10 (35%)	17,82,82	1.88	5 (29%)
2	HEM	D	501	1	28,50,50	2.22	8 (28%)	17,82,82	1.88	5 (29%)

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
2	HEM	A	501	1	-	0/6/54/54	0/0/8/8
2	HEM	B	501	1	-	0/6/54/54	0/0/8/8
2	HEM	C	501	1	-	0/6/54/54	0/0/8/8
2	HEM	D	501	1	-	0/6/54/54	0/0/8/8

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3C-C2C	-6.01	1.32	1.40
2	A	501	HEM	C3B-C2B	-5.01	1.33	1.40
2	B	501	HEM	C3C-C2C	-4.74	1.34	1.40
2	C	501	HEM	C3C-C2C	-4.32	1.34	1.40
2	D	501	HEM	C3B-C2B	-4.17	1.34	1.40
2	B	501	HEM	C3B-C2B	-4.13	1.34	1.40
2	A	501	HEM	C3C-C2C	-3.90	1.35	1.40
2	C	501	HEM	C3B-C2B	-3.82	1.35	1.40
2	D	501	HEM	CMB-C2B	2.01	1.55	1.51
2	A	501	HEM	CMB-C2B	2.05	1.56	1.51
2	D	501	HEM	C4D-ND	2.06	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	CAA-C2A	2.06	1.55	1.52
2	B	501	HEM	CMC-C2C	2.08	1.56	1.51
2	C	501	HEM	CMC-C2C	2.18	1.56	1.51
2	A	501	HEM	CMC-C2C	2.20	1.56	1.51
2	D	501	HEM	CMD-C2D	2.20	1.56	1.51
2	C	501	HEM	CMB-C2B	2.25	1.56	1.51
2	C	501	HEM	CMD-C2D	2.28	1.56	1.51
2	B	501	HEM	CMB-C2B	2.40	1.56	1.51
2	C	501	HEM	C1C-NC	2.45	1.39	1.36
2	B	501	HEM	CMD-C2D	2.53	1.56	1.51
2	C	501	HEM	C3C-CAC	2.54	1.52	1.47
2	A	501	HEM	CMD-C2D	2.65	1.57	1.51
2	B	501	HEM	C4D-ND	2.89	1.40	1.36
2	B	501	HEM	C3B-CAB	2.97	1.53	1.47
2	D	501	HEM	C3C-CAC	2.98	1.53	1.47
2	D	501	HEM	C3B-CAB	3.02	1.53	1.47
2	C	501	HEM	C4D-ND	3.05	1.40	1.36
2	A	501	HEM	C3B-CAB	3.19	1.54	1.47
2	A	501	HEM	C3C-CAC	3.74	1.55	1.47
2	C	501	HEM	C3B-CAB	3.96	1.55	1.47
2	B	501	HEM	C3C-CAC	3.99	1.55	1.47
2	D	501	HEM	C3D-C2D	5.19	1.53	1.37
2	A	501	HEM	C3D-C2D	5.26	1.53	1.37
2	B	501	HEM	C3D-C2D	5.58	1.54	1.37
2	C	501	HEM	C3D-C2D	5.86	1.55	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C1D-C2D-C3D	-3.70	104.42	107.00
2	B	501	HEM	CBD-CAD-C3D	-3.63	105.55	112.47
2	C	501	HEM	CBD-CAD-C3D	-3.61	105.58	112.47
2	D	501	HEM	CBD-CAD-C3D	-3.59	105.61	112.47
2	A	501	HEM	CAA-CBA-CGA	-3.56	106.57	112.66
2	B	501	HEM	CAA-CBA-CGA	-3.32	106.99	112.66
2	D	501	HEM	C1D-C2D-C3D	-3.30	104.70	107.00
2	B	501	HEM	C1D-C2D-C3D	-3.17	104.79	107.00
2	D	501	HEM	CAA-CBA-CGA	-2.87	107.76	112.66
2	A	501	HEM	CMA-C3A-C4A	-2.84	124.09	128.46
2	C	501	HEM	C1D-C2D-C3D	-2.77	105.07	107.00
2	A	501	HEM	CBD-CAD-C3D	-2.73	107.26	112.47
2	C	501	HEM	CAA-CBA-CGA	-2.68	108.08	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CMA-C3A-C4A	-2.57	124.51	128.46
2	B	501	HEM	CMA-C3A-C4A	-2.40	124.77	128.46
2	C	501	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
2	D	501	HEM	C4C-C3C-C2C	2.04	108.33	106.90
2	B	501	HEM	C4C-C3C-C2C	2.63	108.73	106.90
2	A	501	HEM	C4C-C3C-C2C	2.79	108.85	106.90
2	C	501	HEM	C4C-C3C-C2C	3.58	109.40	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	2	0
2	C	501	HEM	4	0
2	D	501	HEM	2	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	480/491 (97%)	-0.38	7 (1%) 74 72	4, 12, 23, 34	0
1	B	480/491 (97%)	-0.39	5 (1%) 82 80	3, 12, 23, 34	0
1	C	480/491 (97%)	-0.15	12 (2%) 58 55	4, 17, 33, 59	0
1	D	480/491 (97%)	-0.07	14 (2%) 52 50	6, 18, 33, 60	0
All	All	1920/1964 (97%)	-0.24	38 (1%) 65 63	3, 14, 30, 60	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	485	PHE	11.7
1	D	485	PHE	9.5
1	D	483	LYS	5.1
1	D	207	HIS	4.7
1	C	483	LYS	3.9
1	C	207	HIS	3.8
1	D	437	MET	3.7
1	D	484	PRO	3.6
1	C	484	PRO	3.6
1	D	479	ASN	3.5
1	C	437	MET	3.5
1	C	482	ILE	3.4
1	D	434	GLU	3.0
1	B	433	GLU	2.8
1	B	437	MET	2.8
1	A	287	ASP	2.8
1	B	479	ASN	2.7
1	A	207	HIS	2.7
1	C	433	GLU	2.7
1	A	389	GLN	2.6
1	D	433	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	479	ASN	2.6
1	A	433	GLU	2.6
1	D	445	ASN	2.6
1	D	476	GLU	2.5
1	D	84	GLU	2.5
1	C	441	ASN	2.5
1	D	389	GLN	2.4
1	B	207	HIS	2.3
1	D	481	ASP	2.2
1	A	434	GLU	2.2
1	B	483	LYS	2.2
1	C	401	ASP	2.2
1	A	479	ASN	2.2
1	A	476	GLU	2.2
1	D	287	ASP	2.1
1	C	476	GLU	2.1
1	C	481	ASP	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	HEM	C	501	43/43	0.95	0.14	1.68	5,9,12,17	0
2	HEM	D	501	43/43	0.94	0.16	1.43	4,10,13,16	0
2	HEM	A	501	43/43	0.96	0.14	0.98	2,5,7,15	0
2	HEM	B	501	43/43	0.96	0.13	0.76	2,5,8,15	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.