



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:35 am GMT

PDB ID : 1A4E  
Title : CATALASE A FROM SACCHAROMYCES CEREVISIAE  
Authors : Mate, M.J.  
Deposited on : 1998-01-29  
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

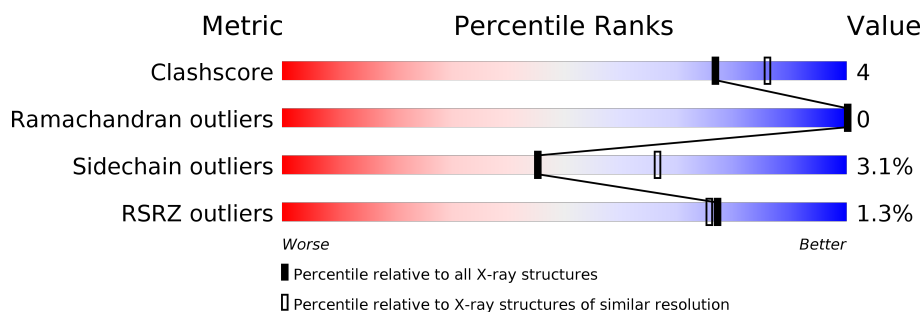
# 1 Overall quality at a glance

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))
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	488	<div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	B	488	<div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	C	488	<div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	D	488	<div> <div>2%</div> <div>84%</div> <div>14%</div> <div>.</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
2	AZI	A	504	-	-	-	X
3	SO4	A	1	-	-	-	X
3	SO4	D	2	-	-	-	X

## 2 Entry composition [i](#)

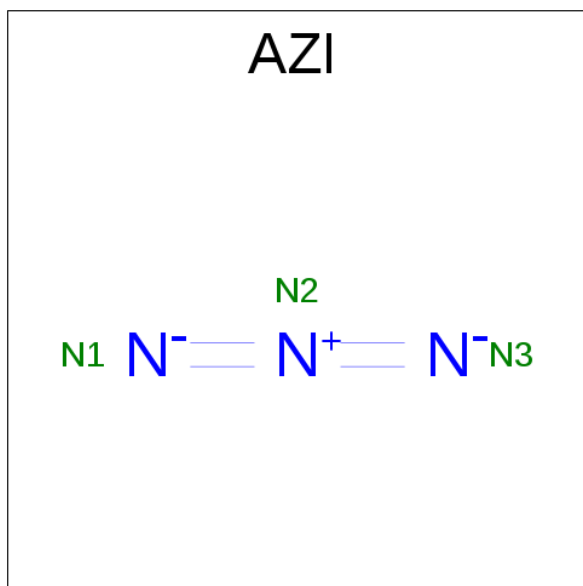
There are 5 unique types of molecules in this entry. The entry contains 16879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	29	0	0
			3932	2493	695	732	12			
1	B	488	Total	C	N	O	S	0	0	0
			3932	2493	695	732	12			
1	C	488	Total	C	N	O	S	0	0	0
			3932	2493	695	732	12			
1	D	488	Total	C	N	O	S	0	0	0
			3932	2493	695	732	12			

- Molecule 2 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N	0	0
			3	3		
2	B	1	Total	N	0	0
			3	3		

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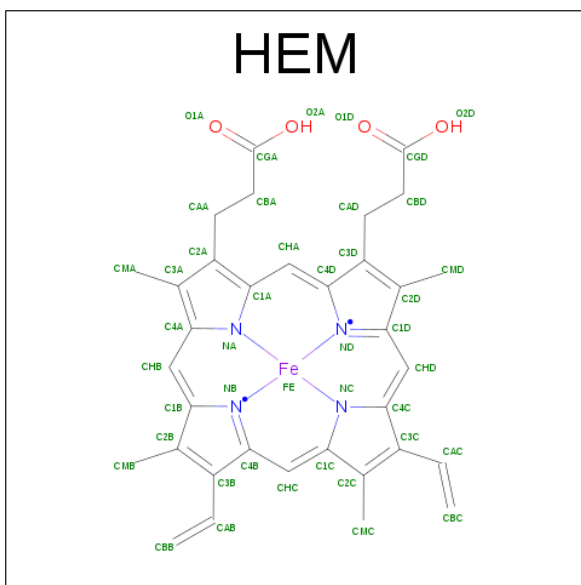
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	N	0	0
			3	3		
2	D	1	Total	N	0	0
			3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

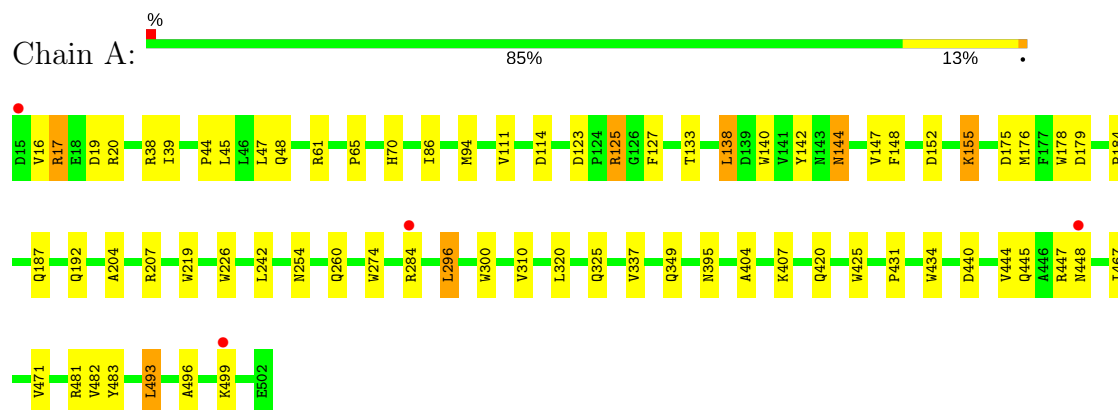
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	221	Total O 221 221	0	0
5	B	262	Total O 262 262	0	0
5	C	242	Total O 242 242	0	0
5	D	232	Total O 232 232	0	0

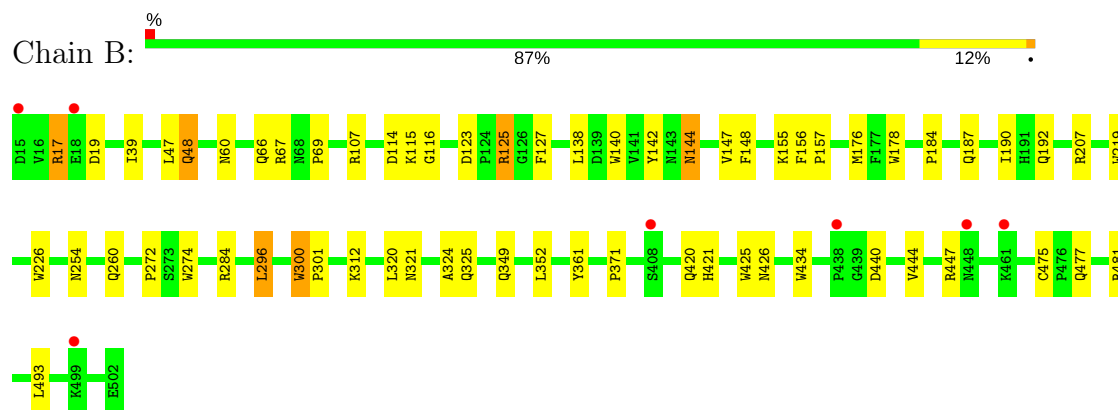
### 3 Residue-property plots [i](#)

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.

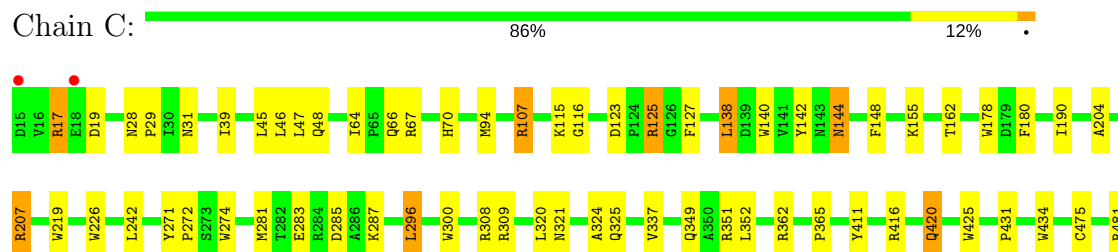
#### • Molecule 1: CATALASE A

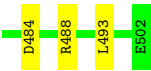


#### • Molecule 1: CATALASE A

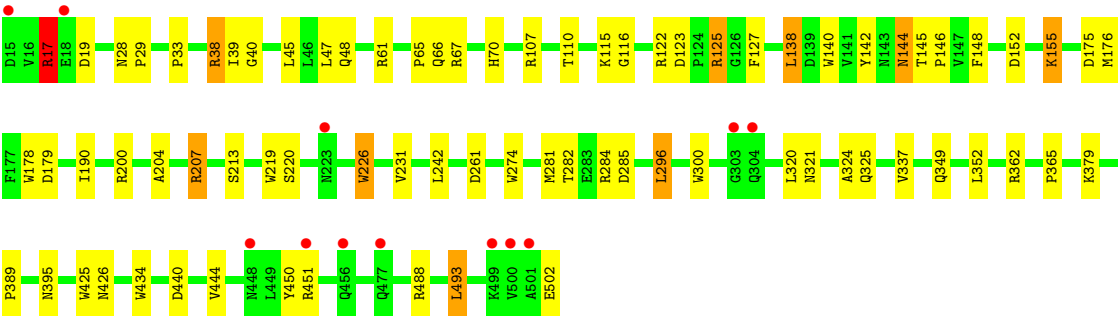
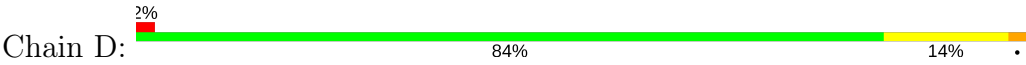


#### • Molecule 1: CATALASE A





● Molecule 1: CATALASE A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.17Å 184.17Å 304.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 30.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.9 (20.00-2.40) 97.4 (30.00-2.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.84 (at 2.36Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.154 , 0.198 0.186 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	33.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: AZI, SO4, 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	0.67	0/4047	1.19	33/5505 (0.6%)
1	B	0.66	0/4047	1.21	33/5505 (0.6%)
1	C	0.67	0/4047	1.22	41/5505 (0.7%)
1	D	0.66	0/4047	1.19	42/5505 (0.8%)
All	All	0.67	0/16188	1.20	149/22020 (0.7%)

There are no bond length outliers.

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	ARG	NE-CZ-NH1	12.19	126.40	120.30
1	C	425	TRP	CD1-CG-CD2	9.76	114.11	106.30
1	B	125	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	C	425	TRP	CE2-CD2-CG	-9.46	99.73	107.30
1	B	125	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	D	425	TRP	CD1-CG-CD2	8.78	113.32	106.30
1	B	107	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	A	125	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	A	226	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	D	226	TRP	CD1-CG-CD2	8.42	113.04	106.30
1	C	178	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	C	362	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	C	125	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	D	178	TRP	CD1-CG-CD2	8.32	112.96	106.30
1	A	178	TRP	CD1-CG-CD2	8.24	112.90	106.30
1	B	178	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	B	425	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	A	125	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	C	362	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	C	226	TRP	CD1-CG-CD2	8.09	112.77	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	A	300	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	A	178	TRP	CE2-CD2-CG	-7.98	100.91	107.30
1	B	226	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	C	125	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	C	178	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	D	178	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	D	300	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	D	425	TRP	CE2-CD2-CG	-7.77	101.09	107.30
1	B	274	TRP	CE2-CD2-CG	-7.72	101.13	107.30
1	B	178	TRP	CE2-CD2-CG	-7.71	101.13	107.30
1	B	300	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	C	300	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	D	274	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	A	274	TRP	CD1-CG-CD2	7.63	112.41	106.30
1	C	274	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	C	207	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	A	226	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	B	274	TRP	CD1-CG-CD2	7.52	112.32	106.30
1	D	107	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	B	434	TRP	CD1-CG-CD2	7.48	112.28	106.30
1	A	425	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	D	434	TRP	CD1-CG-CD2	7.42	112.24	106.30
1	C	274	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	D	226	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	D	274	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	D	451	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	274	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	C	226	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	B	425	TRP	CE2-CD2-CG	-7.33	101.43	107.30
1	D	219	TRP	CD1-CG-CD2	7.25	112.10	106.30
1	A	300	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	C	434	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	C	219	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	C	434	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	D	219	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	A	140	TRP	CD1-CG-CD2	7.16	112.03	106.30
1	B	226	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	C	140	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	B	434	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	A	38	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	B	140	TRP	CD1-CG-CD2	7.11	111.99	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	A	434	TRP	CD1-CG-CD2	7.08	111.96	106.30
1	C	219	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	C	140	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	C	300	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	D	434	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	D	300	TRP	CE2-CD2-CG	-6.93	101.75	107.30
1	B	219	TRP	CE2-CD2-CG	-6.87	101.80	107.30
1	D	140	TRP	CE2-CD2-CG	-6.86	101.82	107.30
1	B	140	TRP	CE2-CD2-CG	-6.85	101.82	107.30
1	A	434	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	A	140	TRP	CE2-CD2-CG	-6.82	101.84	107.30
1	B	219	TRP	CD1-CG-CD2	6.77	111.72	106.30
1	C	488	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	B	17	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	D	122	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	D	140	TRP	CD1-CG-CD2	6.70	111.66	106.30
1	A	219	TRP	CE2-CD2-CG	-6.69	101.94	107.30
1	C	425	TRP	CG-CD2-CE3	6.67	139.90	133.90
1	D	125	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	D	125	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	176	MET	CA-CB-CG	6.31	124.03	113.30
1	C	107	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	D	207	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	67	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	142	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	B	142	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	A	219	TRP	CD1-CG-CD2	6.14	111.21	106.30
1	C	484	ASP	CB-CG-OD1	6.14	123.82	118.30
1	A	17	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	178	TRP	CG-CD2-CE3	6.13	139.42	133.90
1	C	207	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	D	17	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	178	TRP	CG-CD2-CE3	5.94	139.24	133.90
1	C	416	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	447	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	284	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	C	178	TRP	CG-CD2-CE3	5.76	139.09	133.90
1	C	309	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	178	TRP	CG-CD2-CE3	5.70	139.03	133.90
1	A	481	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	C	351	ARG	NE-CZ-NH1	5.59	123.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	MET	CA-CB-CG	5.59	122.80	113.30
1	D	38	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	48	GLN	CA-CB-CG	5.57	125.65	113.40
1	D	488	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	284	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	274	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	D	425	TRP	CG-CD1-NE1	-5.47	104.63	110.10
1	A	274	TRP	CG-CD2-CE3	5.46	138.82	133.90
1	C	142	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	D	67	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	219	TRP	CG-CD2-CE3	5.43	138.79	133.90
1	A	274	TRP	CB-CG-CD1	-5.39	120.00	127.00
1	B	361	TYR	CB-CG-CD2	-5.38	117.78	121.00
1	A	61	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	434	TRP	CG-CD2-CE3	5.34	138.70	133.90
1	B	274	TRP	CB-CG-CD1	-5.30	120.10	127.00
1	D	122	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	178	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	C	274	TRP	CB-CG-CD1	-5.24	120.19	127.00
1	D	207	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	362	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	308	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	142	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	C	481	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	226	TRP	CG-CD1-NE1	-5.19	104.91	110.10
1	B	447	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	274	TRP	CG-CD2-CE3	5.14	138.53	133.90
1	D	425	TRP	CG-CD2-CE3	5.13	138.52	133.90
1	D	178	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	C	425	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	C	67	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	D	200	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	D	274	TRP	CB-CG-CD1	-5.09	120.38	127.00
1	C	274	TRP	CG-CD2-CE3	5.08	138.47	133.90
1	A	226	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	D	425	TRP	CB-CG-CD1	-5.05	120.43	127.00
1	A	207	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	67	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	226	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	A	483	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	A	493	LEU	CA-CB-CG	5.02	126.85	115.30
1	D	176	MET	CA-CB-CG	5.02	121.83	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	362	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	B	178	TRP	CG-CD1-NE1	-5.01	105.09	110.10
1	C	488	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	3932	0	3749	33	0
1	B	3932	0	3749	28	0
1	C	3932	0	3749	32	0
1	D	3932	0	3749	38	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	43	0	30	0	0
4	B	43	0	30	0	0
4	C	43	0	30	0	0
4	D	43	0	30	0	0
5	A	221	0	0	0	0
5	B	262	0	0	0	0
5	C	242	0	0	1	0
5	D	232	0	0	0	0
All	All	16879	0	15116	109	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 4.

All (109) 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:39:ILE:HG13	1:C:39:ILE:HG13	1.68	0.74
1:A:444:VAL:HG12	1:A:448:ASN:HD21	1.52	0.73
1:B:39:ILE:HG13	1:D:39:ILE:HG13	1.73	0.71
1:B:321:ASN:HD22	1:B:324:ALA:H	1.41	0.68
1:A:320:LEU:H	1:A:325:GLN:HE22	1.41	0.68
1:B:320:LEU:H	1:B:325:GLN:HE22	1.45	0.64
1:C:148:PHE:HB3	1:C:296:LEU:HD13	1.79	0.62
1:A:445:GLN:HA	1:A:448:ASN:HD22	1.66	0.61
1:C:320:LEU:H	1:C:325:GLN:HE22	1.49	0.61
1:B:147:VAL:HG23	1:B:192:GLN:HE21	1.66	0.61
1:D:320:LEU:H	1:D:325:GLN:HE22	1.48	0.60
1:D:321:ASN:HD22	1:D:324:ALA:H	1.48	0.59
1:A:349:GLN:HE22	1:B:48:GLN:HE21	1.50	0.59
1:B:148:PHE:HB3	1:B:296:LEU:HD13	1.86	0.58
1:C:321:ASN:HD22	1:C:324:ALA:H	1.51	0.58
1:D:148:PHE:HB3	1:D:296:LEU:HD13	1.85	0.57
1:A:148:PHE:HB3	1:A:296:LEU:HD13	1.86	0.57
1:C:48:GLN:HE21	1:D:349:GLN:HE22	1.53	0.56
1:A:48:GLN:HE21	1:B:349:GLN:HE22	1.54	0.56
1:D:17:ARG:HD3	1:D:19:ASP:OD1	2.06	0.55
1:C:66:GLN:NE2	1:C:115:LYS:H	2.04	0.55
1:C:349:GLN:HE22	1:D:48:GLN:HE21	1.55	0.55
1:B:17:ARG:HD3	1:B:19:ASP:OD1	2.07	0.55
1:D:125:ARG:H	1:D:144:ASN:ND2	2.06	0.54
1:B:207:ARG:HG2	1:B:272:PRO:HB3	1.90	0.53
1:C:94:MET:SD	1:C:138:LEU:HD12	2.49	0.52
1:C:125:ARG:H	1:C:144:ASN:ND2	2.07	0.52
1:A:431:PRO:HD2	1:C:420:GLN:HG3	1.91	0.52
1:D:282:THR:HG22	1:D:284:ARG:H	1.74	0.52
1:B:66:GLN:NE2	1:B:115:LYS:H	2.07	0.51
1:B:426:ASN:HD22	1:D:426:ASN:HD22	1.58	0.51
1:A:125:ARG:H	1:A:144:ASN:ND2	2.08	0.51
1:D:138:LEU:HG	1:D:337:VAL:HG22	1.92	0.51
1:D:152:ASP:HB2	1:D:155:LYS:HE2	1.93	0.50
1:D:204:ALA:HA	1:D:242:LEU:HG	1.93	0.50
1:A:440:ASP:O	1:A:444:VAL:HG23	2.12	0.50
1:B:125:ARG:H	1:B:144:ASN:ND2	2.10	0.50
1:B:66:GLN:HE22	1:B:115:LYS:H	1.60	0.50
1:D:213:SER:HB2	1:D:231:VAL:H	1.77	0.50
1:C:17:ARG:HB3	1:D:379:LYS:HE2	1.93	0.49
1:D:66:GLN:NE2	1:D:115:LYS:H	2.10	0.49
1:A:114:ASP:HB2	1:D:116:GLY:HA3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LEU:HG	1:C:337:VAL:HG22	1.93	0.49
1:C:66:GLN:HE22	1:C:115:LYS:H	1.59	0.49
1:D:320:LEU:N	1:D:325:GLN:HE22	2.10	0.49
1:B:321:ASN:ND2	1:B:324:ALA:H	2.10	0.48
1:C:204:ALA:HA	1:C:242:LEU:HG	1.94	0.48
1:A:404:ALA:HB3	1:A:407:LYS:HG3	1.96	0.48
1:A:420:GLN:HG3	1:C:431:PRO:HD2	1.95	0.48
1:D:281:MET:HG2	1:D:285:ASP:HB2	1.96	0.47
1:A:16:VAL:HG11	1:A:20:ARG:NH1	2.29	0.47
1:D:321:ASN:H	1:D:325:GLN:NE2	2.12	0.47
1:C:281:MET:HG2	1:C:285:ASP:HB2	1.98	0.46
1:A:444:VAL:HG12	1:A:448:ASN:ND2	2.23	0.46
1:C:321:ASN:ND2	1:D:395:ASN:HD22	2.14	0.46
1:B:116:GLY:H	1:C:116:GLY:H	1.64	0.45
1:C:365:PRO:HG3	1:D:61:ARG:HD3	1.97	0.45
1:A:395:ASN:HD22	1:B:321:ASN:HD21	1.64	0.45
1:D:365:PRO:HG2	1:D:389:PRO:HD2	1.99	0.45
1:A:204:ALA:HA	1:A:242:LEU:HG	1.99	0.45
1:D:365:PRO:CG	1:D:389:PRO:HD2	2.46	0.45
1:D:440:ASP:O	1:D:444:VAL:HG23	2.17	0.44
1:C:207:ARG:HG2	1:C:272:PRO:HB3	1.99	0.44
1:B:321:ASN:H	1:B:325:GLN:HE21	1.66	0.44
1:A:44:PRO:HB2	1:C:46:LEU:HD22	2.00	0.44
1:A:467:ILE:O	1:A:471:VAL:HG23	2.18	0.44
1:C:17:ARG:HD3	1:C:19:ASP:OD1	2.17	0.44
1:A:65:PRO:HG3	1:D:65:PRO:HD3	2.00	0.43
1:A:94:MET:SD	1:A:138:LEU:HD12	2.58	0.43
1:B:477:GLN:O	1:B:481:ARG:HG3	2.18	0.43
1:C:28:ASN:HA	1:C:29:PRO:HD3	1.91	0.43
1:C:64:ILE:HG22	1:D:389:PRO:HG3	1.99	0.43
1:A:17:ARG:HD3	1:A:19:ASP:OD1	2.18	0.43
1:D:220:SER:HB3	1:D:226:TRP:HB3	2.01	0.43
1:A:496:ALA:HA	1:A:499:LYS:HD2	2.01	0.43
1:B:184:PRO:HA	1:B:187:GLN:NE2	2.34	0.42
1:C:162:THR:HG21	1:C:180:PHE:HB2	2.01	0.42
1:C:411:TYR:CZ	1:D:33:PRO:HB3	2.55	0.42
1:D:145:THR:HA	1:D:146:PRO:HD3	1.94	0.42
1:A:175:ASP:O	1:A:179:ASP:HB2	2.20	0.42
1:D:175:ASP:O	1:D:179:ASP:HB2	2.20	0.42
1:B:254:ASN:HD21	1:B:260:GLN:NE2	2.17	0.41
1:C:321:ASN:HD21	1:D:395:ASN:HD22	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LEU:N	1:A:325:GLN:HE22	2.12	0.41
1:B:321:ASN:H	1:B:325:GLN:NE2	2.17	0.41
1:C:271:TYR:HA	1:C:272:PRO:HD2	1.94	0.41
1:C:320:LEU:N	1:C:325:GLN:HE22	2.17	0.41
1:D:207:ARG:HD3	1:D:261:ASP:OD2	2.20	0.41
1:D:450:TYR:CE1	1:D:493:LEU:HG	2.55	0.41
1:B:421:HIS:H	1:B:421:HIS:CD2	2.37	0.41
1:C:283:GLU:HG2	1:C:287:LYS:HE3	2.02	0.41
1:A:147:VAL:HG23	1:A:192:GLN:HE21	1.85	0.41
1:D:28:ASN:HA	1:D:29:PRO:HD3	1.91	0.41
1:B:114:ASP:HB2	1:C:116:GLY:CA	2.51	0.41
1:A:86:ILE:HG21	1:A:310:VAL:HG22	2.03	0.41
1:B:426:ASN:HD22	1:D:426:ASN:ND2	2.18	0.41
1:A:138:LEU:HG	1:A:337:VAL:HG22	2.02	0.41
1:B:440:ASP:O	1:B:444:VAL:HG23	2.21	0.41
1:C:70:HIS:O	1:C:107:ARG:NH2	2.54	0.41
1:A:70:HIS:CE1	1:A:111:VAL:HG22	2.56	0.41
1:B:60:ASN:HA	5:C:568:HOH:O	2.21	0.41
1:D:38:ARG:HG3	1:D:40:GLY:O	2.21	0.41
1:B:156:PHE:HB3	1:B:157:PRO:HD3	2.03	0.41
1:A:152:ASP:HB2	1:A:155:LYS:HE2	2.02	0.40
1:B:300:TRP:HA	1:B:301:PRO:HD3	1.92	0.40
1:D:70:HIS:HA	1:D:110:THR:O	2.22	0.40
1:A:184:PRO:HA	1:A:187:GLN:NE2	2.37	0.40
1:A:254:ASN:HD21	1:A:260:GLN:NE2	2.19	0.40
1:A:471:VAL:HG21	1:A:482:VAL:HG11	2.02	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	486/488 (100%)	471 (97%)	15 (3%)	0	100	100
1	B	486/488 (100%)	472 (97%)	14 (3%)	0	100	100
1	C	486/488 (100%)	472 (97%)	14 (3%)	0	100	100
1	D	486/488 (100%)	470 (97%)	16 (3%)	0	100	100
All	All	1944/1952 (100%)	1885 (97%)	59 (3%)	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	422/422 (100%)	412 (98%)	10 (2%)	54	74
1	B	422/422 (100%)	407 (96%)	15 (4%)	40	60
1	C	422/422 (100%)	407 (96%)	15 (4%)	40	60
1	D	422/422 (100%)	409 (97%)	13 (3%)	45	66
All	All	1688/1688 (100%)	1635 (97%)	53 (3%)	45	66

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	47	LEU
1	A	123	ASP
1	A	127	PHE
1	A	133	THR
1	A	138	LEU
1	A	144	ASN
1	A	155	LYS
1	A	296	LEU
1	A	493	LEU
1	B	47	LEU
1	B	69	PRO
1	B	123	ASP

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Mol	Chain	Res	Type
1	B	127	PHE
1	B	138	LEU
1	B	144	ASN
1	B	155	LYS
1	B	190	ILE
1	B	296	LEU
1	B	312	LYS
1	B	352	LEU
1	B	371	PRO
1	B	420	GLN
1	B	475	CYS
1	B	493	LEU
1	C	17	ARG
1	C	31	ASN
1	C	45	LEU
1	C	47	LEU
1	C	123	ASP
1	C	127	PHE
1	C	138	LEU
1	C	144	ASN
1	C	155	LYS
1	C	190	ILE
1	C	296	LEU
1	C	352	LEU
1	C	420	GLN
1	C	475	CYS
1	C	493	LEU
1	D	17	ARG
1	D	45	LEU
1	D	47	LEU
1	D	123	ASP
1	D	127	PHE
1	D	138	LEU
1	D	144	ASN
1	D	155	LYS
1	D	190	ILE
1	D	296	LEU
1	D	352	LEU
1	D	493	LEU
1	D	502	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	48	GLN
1	A	63	ASN
1	A	144	ASN
1	A	192	GLN
1	A	223	ASN
1	A	260	GLN
1	A	325	GLN
1	A	421	HIS
1	A	448	ASN
1	B	37	GLN
1	B	48	GLN
1	B	66	GLN
1	B	144	ASN
1	B	192	GLN
1	B	260	GLN
1	B	304	GLN
1	B	321	ASN
1	B	325	GLN
1	B	421	HIS
1	C	31	ASN
1	C	37	GLN
1	C	48	GLN
1	C	66	GLN
1	C	144	ASN
1	C	170	ASN
1	C	192	GLN
1	C	260	GLN
1	C	321	ASN
1	C	325	GLN
1	C	421	HIS
1	D	31	ASN
1	D	37	GLN
1	D	48	GLN
1	D	66	GLN
1	D	144	ASN
1	D	192	GLN
1	D	260	GLN
1	D	321	ASN
1	D	325	GLN
1	D	421	HIS
1	D	426	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 ⓘ

10 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	$\# Z  > 2$
3	SO4	A	1	-	4,4,4	0.65	0	6,6,6	0.36	0
4	HEM	A	503	1,2	28,50,50	1.60	6 (21%)	17,82,82	1.40	1 (5%)
2	AZI	A	504	4	0,2,2	0.00	-	0,1,1	0.00	-
4	HEM	B	503	1,2	28,50,50	1.60	5 (17%)	17,82,82	1.46	2 (11%)
2	AZI	B	504	4	0,2,2	0.00	-	0,1,1	0.00	-
4	HEM	C	503	1,2	28,50,50	1.59	6 (21%)	17,82,82	1.46	2 (11%)
2	AZI	C	504	4	0,2,2	0.00	-	0,1,1	0.00	-
3	SO4	D	2	-	4,4,4	0.66	0	6,6,6	0.26	0
4	HEM	D	503	1,2	28,50,50	1.58	5 (17%)	17,82,82	1.49	1 (5%)
2	AZI	D	504	4	0,2,2	0.00	-	0,1,1	0.00	-

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	SO4	A	1	-	-	0/0/0/0	0/0/0/0
4	HEM	A	503	1,2	-	0/6/54/54	0/0/8/8
2	AZI	A	504	4	-	0/0/0/0	0/0/0/0
4	HEM	B	503	1,2	-	0/6/54/54	0/0/8/8
2	AZI	B	504	4	-	0/0/0/0	0/0/0/0
4	HEM	C	503	1,2	-	0/6/54/54	0/0/8/8
2	AZI	C	504	4	-	0/0/0/0	0/0/0/0
3	SO4	D	2	-	-	0/0/0/0	0/0/0/0
4	HEM	D	503	1,2	-	0/6/54/54	0/0/8/8
2	AZI	D	504	4	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	HEM	C3C-CAC	-4.31	1.39	1.47
4	D	503	HEM	C3C-CAC	-4.01	1.39	1.47
4	C	503	HEM	C3C-CAC	-4.00	1.39	1.47
4	A	503	HEM	C3C-CAC	-3.94	1.39	1.47
4	A	503	HEM	C3B-CAB	-3.83	1.40	1.47
4	D	503	HEM	C3B-CAB	-3.82	1.40	1.47
4	C	503	HEM	C3B-CAB	-3.80	1.40	1.47
4	B	503	HEM	C3B-CAB	-3.72	1.40	1.47
4	C	503	HEM	C3C-C2C	-2.79	1.36	1.40
4	D	503	HEM	C3C-C2C	-2.79	1.36	1.40
4	A	503	HEM	C3C-C2C	-2.74	1.36	1.40
4	B	503	HEM	C3C-C2C	-2.57	1.37	1.40
4	C	503	HEM	C3B-C2B	-2.38	1.37	1.40
4	A	503	HEM	C3B-C2B	-2.37	1.37	1.40
4	B	503	HEM	CBC-CAC	2.31	1.45	1.28
4	D	503	HEM	CBC-CAC	2.34	1.45	1.28
4	C	503	HEM	CBB-CAB	2.38	1.45	1.28
4	A	503	HEM	CBB-CAB	2.41	1.45	1.28
4	A	503	HEM	CBC-CAC	2.42	1.45	1.28
4	C	503	HEM	CBC-CAC	2.43	1.45	1.28
4	D	503	HEM	CBB-CAB	2.45	1.46	1.28
4	B	503	HEM	CBB-CAB	2.66	1.47	1.28

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	HEM	C3B-C4B-NB	2.12	111.96	109.21
4	C	503	HEM	CAA-CBA-CGA	2.45	116.86	112.66
4	A	503	HEM	CMB-C2B-C3B	2.53	129.59	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	HEM	CMB-C2B-C3B	2.60	129.72	124.89
4	B	503	HEM	CMB-C2B-C3B	2.70	129.91	124.89
4	D	503	HEM	CMB-C2B-C3B	2.82	130.13	124.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	484/488 (99%)	-0.42	4 (0%) 86 84	19, 29, 53, 85	0
1	B	488/488 (100%)	-0.39	7 (1%) 75 74	19, 29, 52, 81	3 (0%)
1	C	488/488 (100%)	-0.59	2 (0%) 92 91	18, 31, 52, 90	3 (0%)
1	D	488/488 (100%)	-0.23	12 (2%) 58 55	21, 35, 56, 81	3 (0%)
All	All	1948/1952 (99%)	-0.41	25 (1%) 77 75	18, 31, 54, 90	9 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	15	ASP	7.6
1	B	15	ASP	5.0
1	A	15	ASP	4.9
1	D	451	ARG	4.3
1	C	15	ASP	3.9
1	C	18	GLU	3.7
1	D	303	GLY	3.7
1	D	223	ASN	3.1
1	D	18	GLU	3.1
1	D	477	GLN	2.8
1	D	304	GLN	2.7
1	D	448	ASN	2.7
1	B	448	ASN	2.5
1	B	461	LYS	2.5
1	B	438	PRO	2.5
1	B	408	SER	2.4
1	A	448	ASN	2.4
1	D	500	VAL	2.3
1	A	284	ARG	2.2
1	D	499	LYS	2.2
1	D	456	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	18	GLU	2.1
1	A	499	LYS	2.0
1	B	499	LYS	2.0
1	D	501	ALA	2.0

## 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
3	SO4	D	2	5/5	0.97	0.43	30.31	70,77,79,80	0
3	SO4	A	1	5/5	0.93	0.44	19.39	79,82,85,87	0
2	AZI	A	504	3/3	0.94	0.19	4.45	25,25,28,28	0
2	AZI	B	504	3/3	0.91	0.17	0.90	25,25,27,27	0
2	AZI	D	504	3/3	0.95	0.16	0.66	27,27,28,32	0
4	HEM	B	503	43/43	0.95	0.15	0.45	18,22,25,28	0
4	HEM	D	503	43/43	0.95	0.14	-0.15	21,26,28,30	0
4	HEM	A	503	43/43	0.97	0.12	-0.34	18,23,25,27	0
4	HEM	C	503	43/43	0.98	0.11	-0.59	12,22,25,29	0
2	AZI	C	504	3/3	0.98	0.10	-0.84	20,20,21,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.