



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:51 PM GMT

PDB ID : 4EGN
Title : The X-ray crystal structure of CYP199A4 in complex with veratric acid
Authors : Zhou, W.; Bell, S.G.; Yang, W.; Zhou, R.M.; Tan, A.B.H.; Wong, L.-L.
Deposited on : 2012-03-31
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

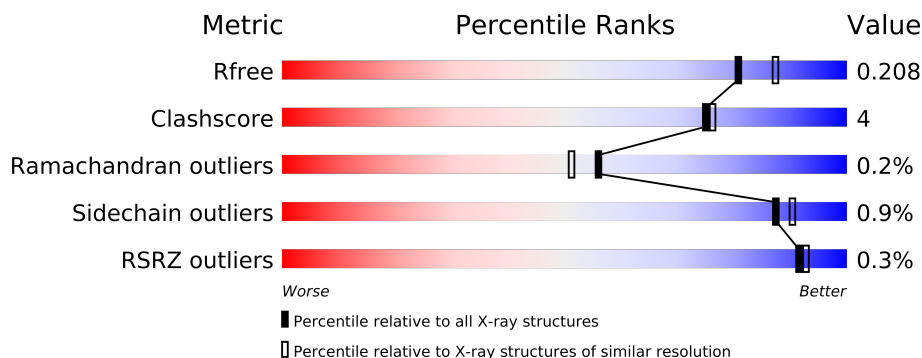
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	410	
1	B	410	
1	C	410	
1	D	410	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	C	503	-	X
3	SO4	C	504	-	X
3	SO4	D	503	-	X
3	SO4	D	504	-	X
4	GOL	B	503	-	X

2 Entry composition i

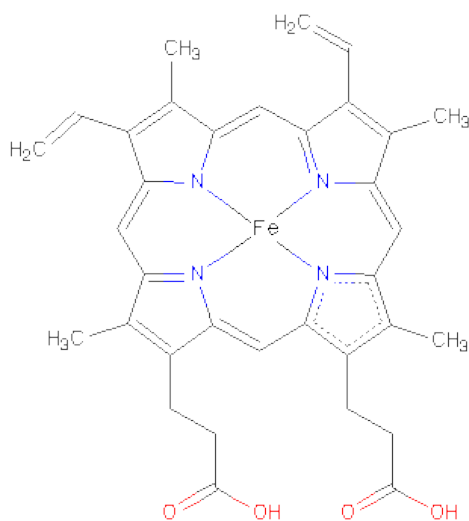
There are 7 unique types of molecules in this entry. The entry contains 13711 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	1	0
			3024	1914	534	564	12			
1	B	393	Total	C	N	O	S	0	1	0
			3024	1914	534	564	12			
1	C	393	Total	C	N	O	S	0	1	0
			3024	1914	534	564	12			
1	D	393	Total	C	N	O	S	0	1	0
			3024	1914	534	564	12			

- 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	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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

- Molecule 3 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



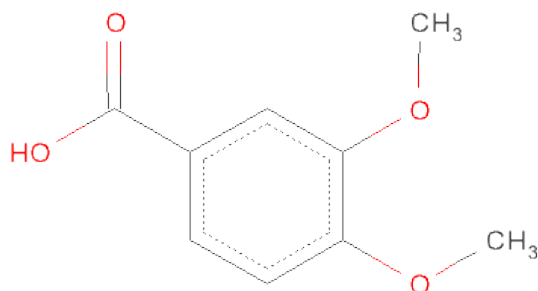
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S		
			5	4	1	0	0
3	B	1	Total	O	S		
			5	4	1	0	0
3	C	1	Total	O	S		
			5	4	1	0	0
3	C	1	Total	O	S		
			5	4	1	0	0
3	C	1	Total	O	S		
			5	4	1	0	0
3	D	1	Total	O	S		
			5	4	1	0	0
3	D	1	Total	O	S		
			5	4	1	0	0
3	D	1	Total	O	S		
			5	4	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 3,4-DIMETHOXYBENZOIC ACID (three-letter code: TWO) (formula: $C_9H_{10}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 9 4	0	0
5	B	1	Total C O 13 9 4	0	0
5	C	1	Total C O 13 9 4	0	0
5	D	1	Total C O 13 9 4	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	A	1	Total Cl 1 1	0	0
6	D	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	358	Total O 358 358	0	0
7	B	349	Total O 349 349	0	0
7	C	345	Total O 345 345	0	0
7	D	265	Total O 265 265	0	0

3 Residue-property plots

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

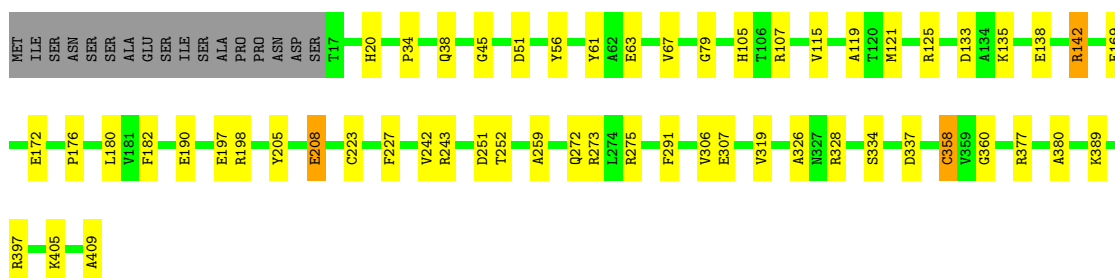
• Molecule 1: Cytochrome P450

Chain A:



• Molecule 1: Cytochrome P450

Chain B:



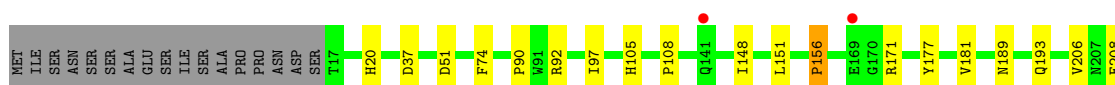
• Molecule 1: Cytochrome P450

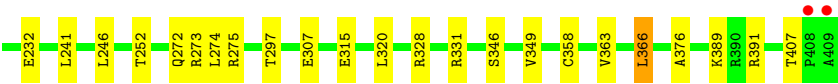
Chain C:



• Molecule 1: Cytochrome P450

Chain D:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.53Å 143.44Å 172.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.44 – 2.00 30.44 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.44-2.00) 98.0 (30.44-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.171 , 0.207 0.174 , 0.208	Depositor DCC
R_{free} test set	8799 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 32.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 176091 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13711	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.99 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5229e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, TWO, HEM, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.33	13/3099 (0.4%)	1.07	15/4217 (0.4%)
1	B	1.35	23/3099 (0.7%)	1.12	13/4217 (0.3%)
1	C	1.29	14/3099 (0.5%)	1.02	8/4217 (0.2%)
1	D	1.23	7/3099 (0.2%)	1.04	10/4217 (0.2%)
All	All	1.30	57/12396 (0.5%)	1.06	46/16868 (0.3%)

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	GLU	CG-CD	7.89	1.63	1.51
1	A	88	GLU	CD-OE1	7.76	1.34	1.25
1	B	138	GLU	CG-CD	7.73	1.63	1.51
1	B	182	PHE	CE1-CZ	7.68	1.51	1.37
1	C	193	GLN	CG-CD	7.14	1.67	1.51
1	B	172	GLU	CD-OE2	6.85	1.33	1.25
1	D	208	GLU	CG-CD	6.62	1.61	1.51
1	A	190	GLU	CG-CD	6.42	1.61	1.51
1	B	119	ALA	CA-CB	6.22	1.65	1.52
1	B	208	GLU	CG-CD	6.18	1.61	1.51
1	C	315	GLU	CG-CD	6.13	1.61	1.51
1	B	319	VAL	CB-CG2	6.05	1.65	1.52
1	A	172	GLU	CD-OE1	6.00	1.32	1.25
1	B	79	GLY	N-CA	5.99	1.55	1.46
1	B	242	VAL	CB-CG1	5.95	1.65	1.52
1	C	380	ALA	CA-CB	5.73	1.64	1.52
1	D	232	GLU	CG-CD	5.71	1.60	1.51
1	B	169	GLU	CD-OE1	5.63	1.31	1.25
1	C	154	ALA	CA-CB	5.62	1.64	1.52
1	A	303	THR	CB-CG2	-5.61	1.33	1.52
1	C	220	PHE	CE2-CZ	5.61	1.48	1.37
1	B	67	VAL	CB-CG1	5.59	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	177	TYR	CE1-CZ	5.58	1.45	1.38
1	A	147	ALA	C-N	-5.50	1.21	1.34
1	C	364	ALA	CA-CB	5.50	1.64	1.52
1	C	31	PHE	CE2-CZ	5.49	1.47	1.37
1	A	169	GLU	CG-CD	5.44	1.60	1.51
1	C	193	GLN	CB-CG	5.44	1.67	1.52
1	A	48	VAL	CB-CG2	5.42	1.64	1.52
1	B	291	PHE	CE1-CZ	5.40	1.47	1.37
1	B	63	GLU	CD-OE2	-5.37	1.19	1.25
1	C	351	PHE	CD2-CE2	5.33	1.50	1.39
1	D	315	GLU	CG-CD	5.33	1.59	1.51
1	C	370	VAL	CB-CG2	5.26	1.64	1.52
1	B	306	VAL	CA-CB	5.26	1.65	1.54
1	B	142	ARG	CB-CG	-5.26	1.38	1.52
1	A	33	ASP	CB-CG	5.23	1.62	1.51
1	A	63	GLU	CB-CG	5.22	1.62	1.52
1	A	311	ALA	CA-CB	5.22	1.63	1.52
1	B	227	PHE	CE2-CZ	5.22	1.47	1.37
1	D	74	PHE	CE1-CZ	5.22	1.47	1.37
1	A	169	GLU	CD-OE2	5.20	1.31	1.25
1	D	363	VAL	CB-CG2	5.16	1.63	1.52
1	C	138	GLU	CB-CG	5.16	1.61	1.52
1	B	45	GLY	N-CA	5.14	1.53	1.46
1	B	190	GLU	CG-CD	5.13	1.59	1.51
1	A	317	GLU	CB-CG	5.11	1.61	1.52
1	C	159	VAL	CB-CG2	5.09	1.63	1.52
1	C	182	PHE	CE1-CZ	5.09	1.47	1.37
1	B	197	GLU	CG-CD	5.06	1.59	1.51
1	B	397	ARG	CZ-NH2	5.06	1.39	1.33
1	A	88	GLU	C-N	-5.06	1.22	1.34
1	D	349	VAL	CB-CG2	5.05	1.63	1.52
1	B	259	ALA	CA-CB	5.04	1.63	1.52
1	B	169	GLU	CD-OE2	5.04	1.31	1.25
1	C	314	GLY	C-O	5.02	1.31	1.23
1	B	56	TYR	CD2-CE2	5.00	1.46	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ARG	NE-CZ-NH2	-15.01	112.80	120.30
1	B	273	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	D	273	ARG	NE-CZ-NH2	-9.97	115.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	D	273	ARG	NE-CZ-NH1	9.73	125.16	120.30
1	A	273	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	142	ARG	NE-CZ-NH2	8.60	124.60	120.30
1	B	243	ARG	NE-CZ-NH1	-8.50	116.05	120.30
1	A	273	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	D	171	ARG	NE-CZ-NH2	8.25	124.42	120.30
1	A	133	ASP	CB-CG-OD1	7.76	125.28	118.30
1	B	142	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	142	ARG	NE-CZ-NH1	-7.53	116.53	120.30
1	D	328	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	B	243	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	A	198	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	C	84	ASP	CB-CG-OD1	7.11	124.70	118.30
1	C	273	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	365	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	304	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	B	328	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	391	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	D	37	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	D	331	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	251	ASP	CB-CG-OD1	-6.35	112.58	118.30
1	C	125	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	323	LEU	CB-CG-CD1	6.19	121.53	111.00
1	C	323	LEU	CB-CG-CD2	5.96	121.13	111.00
1	B	251	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	D	391	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	332	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	133	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	107	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	377	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	198	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	167	LYS	CD-CE-NZ	5.37	124.04	111.70
1	A	328	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	107	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	328	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	125	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	315	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	C	391	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	273	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	198	ARG	CB-CG-CD	5.09	124.83	111.60
1	B	121	MET	CG-SD-CE	5.04	108.27	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	366	LEU	CB-CG-CD2	5.01	119.51	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3024	0	2997	26	0
1	B	3024	0	2998	21	0
1	C	3024	0	2998	28	0
1	D	3024	0	2998	21	0
2	A	43	0	30	3	0
2	B	43	0	30	6	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
4	A	6	0	8	0	0
4	B	12	0	16	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	13	0	9	0	0
5	B	13	0	9	0	0
5	C	13	0	9	3	0
5	D	13	0	9	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	358	0	0	5	0
7	B	349	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	345	0	0	11	0
7	D	265	0	0	7	0
All	All	13711	0	12187	99	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (99) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:273:ARG:HB3	7:C:847:HOH:O	1.40	1.22
1:D:206:VAL:HG13	7:D:793:HOH:O	1.38	1.21
1:B:405:LYS:HD3	7:B:879:HOH:O	1.41	1.18
1:A:73:THR:O	1:A:303:THR:HG22	1.48	1.13
1:B:208:GLU:HG2	7:B:678:HOH:O	1.50	1.11
1:C:97:ILE:HB	7:C:911:HOH:O	1.52	1.08
1:A:72:THR:O	1:A:303:THR:HG21	1.53	1.08
1:C:108:PRO:HB2	7:C:911:HOH:O	1.52	1.08
1:C:369:GLU:HA	7:C:873:HOH:O	1.76	0.84
1:D:246:LEU:CD1	7:D:793:HOH:O	2.26	0.82
1:D:246:LEU:HD12	7:D:793:HOH:O	1.81	0.80
1:A:73:THR:HA	1:A:303:THR:CG2	2.13	0.78
1:D:105:HIS:HD2	7:D:605:HOH:O	1.67	0.76
1:D:156:PRO:HG3	7:D:803:HOH:O	1.86	0.76
1:B:272:GLN:HE22	1:B:275:ARG:HH11	1.36	0.73
1:A:344:LYS:HE3	7:A:862:HOH:O	1.89	0.72
1:B:105:HIS:HD2	7:B:602:HOH:O	1.74	0.71
1:A:105:HIS:HD2	7:A:606:HOH:O	1.72	0.71
2:B:501:HEM:HBC2	2:B:501:HEM:HMC1	1.73	0.70
1:D:407:THR:HG23	7:D:782:HOH:O	1.93	0.69
1:A:272:GLN:HE22	1:A:275:ARG:HH11	1.41	0.69
1:C:105:HIS:HD2	7:C:613:HOH:O	1.75	0.68
1:D:20:HIS:HD2	1:D:51:ASP:OD1	1.76	0.67
1:D:181:VAL:HG11	5:D:506:TWO:H4	1.76	0.66
1:A:73:THR:C	1:A:303:THR:HG22	2.15	0.66
1:C:105:HIS:HE1	2:C:501:HEM:O1D	1.80	0.65
1:D:105:HIS:HE1	2:D:501:HEM:O1D	1.80	0.65
1:C:208:GLU:HG2	7:C:638:HOH:O	1.96	0.65
1:B:105:HIS:HE1	2:B:501:HEM:O1D	1.79	0.64
1:B:307:GLU:HG2	7:B:948:HOH:O	1.97	0.63
1:C:20:HIS:HD2	1:C:51:ASP:OD1	1.83	0.61
1:B:125:ARG:NH1	7:B:886:HOH:O	2.34	0.60
1:C:19:PRO:HG2	7:C:892:HOH:O	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:108:PRO:HB3	1:D:241:LEU:HD21	1.84	0.59
1:A:73:THR:CA	1:A:303:THR:CG2	2.81	0.59
1:A:105:HIS:HE1	2:A:501:HEM:O1D	1.86	0.58
1:C:192:ARG:HH21	1:C:193:GLN:HE22	1.50	0.57
1:C:357:MET:HE1	7:C:901:HOH:O	2.05	0.57
1:D:189:ASN:O	1:D:193:GLN:HG2	2.07	0.55
1:D:181:VAL:CG1	5:D:506:TWO:H4	2.38	0.54
1:D:272:GLN:HE22	1:D:275:ARG:HH11	1.55	0.53
1:B:20:HIS:HD2	1:B:51:ASP:OD1	1.92	0.53
1:B:389:LYS:HE2	7:B:836:HOH:O	2.07	0.53
1:A:73:THR:HA	1:A:303:THR:HG21	1.92	0.52
1:A:172:GLU:HG2	7:A:951:HOH:O	2.07	0.52
1:A:252:THR:HB	2:A:501:HEM:C3B	2.44	0.52
1:A:142:ARG:HD3	1:B:205:TYR:HA	1.91	0.52
1:C:212:ARG:HB3	1:C:213:PRO:HD3	1.92	0.52
1:A:89:LYS:HE3	7:A:732:HOH:O	2.09	0.52
1:D:20:HIS:CD2	1:D:51:ASP:OD1	2.62	0.51
1:B:337:ASP:HB2	7:B:643:HOH:O	2.10	0.51
1:A:272:GLN:HE22	1:A:275:ARG:NH1	2.07	0.51
1:C:252:THR:HB	2:C:501:HEM:C3B	2.45	0.51
1:D:246:LEU:HD13	7:D:793:HOH:O	2.01	0.51
1:A:167:LYS:HE3	1:A:169:GLU:HB3	1.92	0.50
1:C:181:VAL:CG1	5:C:506:TWO:H4	2.42	0.50
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.92	0.50
1:C:58:VAL:HG13	7:C:893:HOH:O	2.12	0.49
1:C:21:LEU:HD12	1:C:41:LEU:HD23	1.93	0.49
1:A:73:THR:C	1:A:303:THR:CG2	2.81	0.49
1:D:274:LEU:HG	1:D:376:ALA:HB2	1.94	0.49
1:B:360:GLY:HA3	2:B:501:HEM:C3C	2.48	0.48
1:B:252:THR:HB	2:B:501:HEM:C3B	2.47	0.48
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.43	0.48
1:A:175:LEU:HD23	1:A:251:ASP:OD1	2.13	0.48
1:C:223[A]:CYS:SG	7:C:918:HOH:O	2.28	0.48
1:C:20:HIS:CD2	1:C:51:ASP:OD1	2.66	0.46
1:D:252:THR:HB	2:D:501:HEM:C3B	2.51	0.46
1:C:184:ALA:HA	1:C:192:ARG:HG3	1.97	0.46
1:C:152:ALA:O	1:C:156:PRO:HD2	2.16	0.46
1:D:97:ILE:HG12	2:D:501:HEM:CGD	2.46	0.45
1:C:181:VAL:HG12	5:C:506:TWO:H4	1.98	0.45
1:C:107:ARG:HB3	1:C:108:PRO:HD3	1.98	0.44
1:C:407:THR:HG23	1:C:408:PRO:HD2	1.99	0.44
1:A:73:THR:CA	1:A:303:THR:HG21	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:90:PRO:HB2	1:D:92:ARG:O	2.17	0.43
1:C:21:LEU:HG	7:C:892:HOH:O	2.18	0.43
1:D:151:LEU:C	1:D:151:LEU:HD23	2.38	0.43
1:C:97:ILE:HD13	1:C:97:ILE:HG21	1.69	0.43
1:A:269:GLY:O	1:A:273:ARG:HG3	2.19	0.42
1:A:151:LEU:HD23	1:A:151:LEU:C	2.39	0.42
1:A:155:TYR:HB3	1:A:156:PRO:HD3	2.00	0.42
1:B:34:PRO:O	1:B:38:GLN:HG3	2.20	0.42
1:B:135:LYS:HD3	1:B:135:LYS:HA	1.93	0.42
1:B:20:HIS:CD2	1:B:51:ASP:OD1	2.71	0.41
1:B:380:ALA:HB2	1:B:409:ALA:HA	2.02	0.41
1:B:115:VAL:HG22	1:B:223[A]:CYS:SG	2.60	0.41
1:A:272:GLN:NE2	1:A:275:ARG:HD3	2.36	0.41
1:A:397:ARG:NH1	7:A:950:HOH:O	2.25	0.41
1:C:26:PHE:HA	1:C:31:PHE:CZ	2.56	0.41
1:B:272:GLN:HE22	1:B:275:ARG:NH1	2.11	0.41
1:C:117:SER:HB2	1:C:118:PRO:HD2	2.03	0.41
1:B:61:TYR:HA	1:B:326:ALA:HB1	2.02	0.41
1:A:303:THR:HG22	1:A:303:THR:H	1.64	0.40
2:C:501:HEM:C4D	5:C:506:TWO:H9	2.56	0.40
1:D:297:THR:HB	1:D:320:LEU:HD11	2.03	0.40
1:C:192:ARG:NH2	1:C:193:GLN:HE22	2.18	0.40
1:A:73:THR:O	1:A:303:THR:CG2	2.41	0.40
1:B:358:CYS:HA	2:B:501:HEM:CHA	2.52	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	392/410 (96%)	386 (98%)	6 (2%)	0	100	100
1	B	392/410 (96%)	384 (98%)	7 (2%)	1 (0%)	50	44
1	C	392/410 (96%)	386 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	392/410 (96%)	382 (97%)	8 (2%)	2 (0%)	38	29
All	All	1568/1640 (96%)	1538 (98%)	27 (2%)	3 (0%)	56	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	CYS
1	D	358	CYS
1	D	148	ILE

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	320/334 (96%)	319 (100%)	1 (0%)	96	97
1	B	320/334 (96%)	316 (99%)	4 (1%)	80	82
1	C	320/334 (96%)	318 (99%)	2 (1%)	92	94
1	D	320/334 (96%)	315 (98%)	5 (2%)	75	77
All	All	1280/1336 (96%)	1268 (99%)	12 (1%)	87	90

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LYS
1	B	142	ARG
1	B	176	PRO
1	B	180	LEU
1	B	334	SER
1	C	166	LEU
1	C	323	LEU
1	D	156	PRO
1	D	307	GLU
1	D	346	SER
1	D	366	LEU
1	D	389	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	209	GLN
1	A	214	ASN
1	A	272	GLN
1	A	283	ASN
1	A	296	GLN
1	B	20	HIS
1	B	105	HIS
1	B	209	GLN
1	B	211	GLN
1	B	214	ASN
1	B	272	GLN
1	B	283	ASN
1	B	296	GLN
1	C	20	HIS
1	C	38	GLN
1	C	105	HIS
1	C	193	GLN
1	C	211	GLN
1	C	214	ASN
1	C	283	ASN
1	C	296	GLN
1	D	20	HIS
1	D	105	HIS
1	D	141	GLN
1	D	168	GLN
1	D	211	GLN
1	D	214	ASN
1	D	272	GLN
1	D	283	ASN
1	D	296	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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$
2	HEM	A	501	1	49,50,50	2.58	17 (34%)	46,82,82	2.51	12 (26%)
3	SO4	A	502	-	4,4,4	0.79	0	6,6,6	0.88	0
4	GOL	A	503	-	5,5,5	0.38	0	5,5,5	0.79	0
5	TWO	A	504	-	13,13,13	1.09	1 (7%)	17,17,17	1.57	2 (11%)
2	HEM	B	501	1	49,50,50	3.14	22 (44%)	46,82,82	2.72	15 (32%)
3	SO4	B	502	-	4,4,4	0.55	0	6,6,6	1.34	2 (33%)
4	GOL	B	503	-	5,5,5	0.76	0	5,5,5	1.81	2 (40%)
4	GOL	B	504	-	5,5,5	0.47	0	5,5,5	0.54	0
5	TWO	B	505	-	13,13,13	1.08	1 (7%)	17,17,17	2.17	8 (47%)
2	HEM	C	501	1	49,50,50	2.29	18 (36%)	46,82,82	1.94	12 (26%)
3	SO4	C	502	-	4,4,4	0.81	0	6,6,6	0.89	1 (16%)
3	SO4	C	503	-	4,4,4	1.05	0	6,6,6	1.25	1 (16%)
3	SO4	C	504	-	4,4,4	0.65	0	6,6,6	0.52	0
4	GOL	C	505	-	5,5,5	0.82	0	5,5,5	1.03	0
5	TWO	C	506	-	13,13,13	0.91	0	17,17,17	2.23	8 (47%)
2	HEM	D	501	1	49,50,50	4.28	20 (40%)	46,82,82	2.68	14 (30%)
3	SO4	D	502	-	4,4,4	0.53	0	6,6,6	0.69	0
3	SO4	D	503	-	4,4,4	0.49	0	6,6,6	1.16	1 (16%)
3	SO4	D	504	-	4,4,4	0.23	0	6,6,6	0.58	0
4	GOL	D	505	-	5,5,5	0.45	0	5,5,5	0.80	0
5	TWO	D	506	-	13,13,13	1.34	2 (15%)	17,17,17	1.27	2 (11%)

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	-	0/14/114/114	0/0/8/8
3	SO4	A	502	-	-	0/0/0/0	0/0/0/0
4	GOL	A	503	-	-	0/4/4/4	0/0/0/0
5	TWO	A	504	-	-	0/8/8/8	0/1/1/1
2	HEM	B	501	1	-	0/14/114/114	0/0/8/8
3	SO4	B	502	-	-	0/0/0/0	0/0/0/0
4	GOL	B	503	-	-	0/4/4/4	0/0/0/0
4	GOL	B	504	-	-	0/4/4/4	0/0/0/0
5	TWO	B	505	-	-	0/8/8/8	0/1/1/1
2	HEM	C	501	1	-	0/14/114/114	0/0/8/8
3	SO4	C	502	-	-	0/0/0/0	0/0/0/0
3	SO4	C	503	-	-	0/0/0/0	0/0/0/0
3	SO4	C	504	-	-	0/0/0/0	0/0/0/0
4	GOL	C	505	-	-	0/4/4/4	0/0/0/0
5	TWO	C	506	-	-	0/8/8/8	0/1/1/1
2	HEM	D	501	1	-	0/14/114/114	0/0/8/8
3	SO4	D	502	-	-	0/0/0/0	0/0/0/0
3	SO4	D	503	-	-	0/0/0/0	0/0/0/0
3	SO4	D	504	-	-	0/0/0/0	0/0/0/0
4	GOL	D	505	-	-	0/4/4/4	0/0/0/0
5	TWO	D	506	-	-	0/8/8/8	0/1/1/1

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C2D-C1D	17.40	1.48	1.44
2	D	501	HEM	C2B-C1B	15.48	1.48	1.44
2	B	501	HEM	C3D-C4D	13.66	1.48	1.44
2	A	501	HEM	C2B-C1B	8.39	1.46	1.44
2	D	501	HEM	C3D-C4D	8.28	1.46	1.44
2	B	501	HEM	C2B-C1B	7.66	1.46	1.44
2	A	501	HEM	C4A-C3A	5.86	1.47	1.40
2	C	501	HEM	C3B-C2B	-5.53	1.34	1.43
2	A	501	HEM	CHB-C1B	5.53	1.43	1.35
2	C	501	HEM	C4A-C3A	5.48	1.47	1.40
2	D	501	HEM	FE-NA	5.06	2.14	1.92
2	D	501	HEM	C4A-C3A	5.04	1.46	1.40
2	B	501	HEM	FE-NA	5.00	2.14	1.92
2	A	501	HEM	C3B-CAB	5.00	1.56	1.40
2	C	501	HEM	C3C-CAC	4.98	1.56	1.40
2	D	501	HEM	C3B-CAB	4.97	1.56	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3B-CAB	4.90	1.55	1.40
2	D	501	HEM	C3B-C2B	-4.79	1.35	1.43
2	B	501	HEM	C3C-CAC	4.59	1.54	1.40
2	D	501	HEM	C3C-C2C	-4.48	1.35	1.43
2	B	501	HEM	C3B-CAB	4.47	1.54	1.40
2	D	501	HEM	FE-ND	4.40	2.13	1.97
2	A	501	HEM	C3B-C2B	-4.20	1.36	1.43
2	B	501	HEM	C3C-C2C	-4.17	1.36	1.43
2	B	501	HEM	CHB-C1B	4.10	1.41	1.35
2	D	501	HEM	FE-NC	4.09	2.13	1.97
2	C	501	HEM	C3C-C2C	-4.08	1.36	1.43
2	D	501	HEM	CAA-C2A	4.04	1.59	1.52
2	D	501	HEM	C3D-C2D	4.01	1.50	1.43
2	D	501	HEM	C3C-CAC	4.00	1.53	1.40
2	A	501	HEM	C3C-CAC	3.95	1.52	1.40
2	C	501	HEM	C3D-C4D	3.86	1.45	1.44
2	A	501	HEM	C3D-C4D	3.67	1.45	1.44
2	A	501	HEM	FE-NA	3.61	2.07	1.92
2	C	501	HEM	C2D-C1D	3.57	1.45	1.44
2	A	501	HEM	FE-NC	3.51	2.11	1.97
2	B	501	HEM	C3B-C2B	-3.48	1.37	1.43
2	B	501	HEM	C4A-C3A	3.37	1.44	1.40
2	D	501	HEM	CMC-C2C	3.36	1.57	1.47
2	A	501	HEM	C3C-C2C	-3.23	1.38	1.43
2	B	501	HEM	FE-NC	3.19	2.09	1.97
2	C	501	HEM	CHA-C4D	3.12	1.40	1.35
2	A	501	HEM	CMD-C2D	3.05	1.56	1.47
2	D	501	HEM	CHA-C4D	3.02	1.40	1.35
2	D	501	HEM	CMD-C2D	3.00	1.56	1.47
2	B	501	HEM	FE-NB	2.98	2.08	1.97
2	B	501	HEM	CMD-C2D	2.95	1.56	1.47
2	A	501	HEM	CMC-C2C	2.92	1.56	1.47
2	C	501	HEM	CMA-C3A	2.87	1.57	1.51
2	D	501	HEM	C1A-C2A	2.84	1.48	1.43
2	C	501	HEM	FE-NA	2.83	2.04	1.92
2	C	501	HEM	CMC-C2C	2.76	1.56	1.47
2	C	501	HEM	FE-NB	2.67	2.07	1.97
2	D	501	HEM	FE-NB	2.67	2.07	1.97
5	D	506	TWO	C3-C2	-2.63	1.35	1.40
2	B	501	HEM	CMB-C2B	2.62	1.55	1.47
2	B	501	HEM	CAA-C2A	2.59	1.56	1.52
2	C	501	HEM	C3D-C2D	2.51	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CAD-CBD	2.50	1.59	1.52
2	C	501	HEM	CMD-C2D	2.49	1.55	1.47
5	B	505	TWO	O1-C7	2.46	1.30	1.23
2	B	501	HEM	C3D-C2D	2.40	1.48	1.43
2	A	501	HEM	CMB-C2B	2.35	1.54	1.47
2	D	501	HEM	CAD-CBD	2.34	1.58	1.52
2	C	501	HEM	FE-NC	2.34	2.06	1.97
2	A	501	HEM	CHD-C4C	2.32	1.40	1.36
5	A	504	TWO	C4-C5	2.28	1.42	1.39
5	D	506	TWO	O1-C7	2.27	1.30	1.23
2	D	501	HEM	CMB-C2B	2.24	1.54	1.47
2	B	501	HEM	C2A-C3A	-2.21	1.31	1.37
2	A	501	HEM	FE-NB	2.17	2.05	1.97
2	B	501	HEM	CBD-CGD	2.17	1.56	1.50
2	A	501	HEM	CHA-C4D	2.15	1.38	1.35
2	C	501	HEM	CHB-C1B	2.15	1.38	1.35
2	B	501	HEM	CHD-C4C	2.14	1.40	1.36
2	B	501	HEM	CAD-C3D	2.14	1.59	1.51
2	B	501	HEM	CMC-C2C	2.08	1.53	1.47
2	A	501	HEM	C1A-NA	2.07	1.40	1.36
2	C	501	HEM	CHC-C1C	2.07	1.40	1.36
2	B	501	HEM	FE-ND	2.03	2.05	1.97
2	C	501	HEM	CMB-C2B	2.00	1.53	1.47

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C3B-C4B-NB	-10.42	106.54	114.00
2	A	501	HEM	C3B-C4B-NB	-9.41	107.27	114.00
2	D	501	HEM	C3B-C4B-NB	-9.29	107.35	114.00
2	D	501	HEM	CBD-CAD-C3D	-7.30	98.43	114.37
2	C	501	HEM	C3B-C4B-NB	-6.63	109.25	114.00
2	B	501	HEM	CBD-CAD-C3D	-6.50	100.18	114.37
2	A	501	HEM	CBD-CAD-C3D	-6.18	100.88	114.37
2	B	501	HEM	C4C-NC-C1C	5.88	111.64	105.53
2	B	501	HEM	C1B-NB-C4B	5.67	110.97	105.16
2	D	501	HEM	C4D-ND-C1D	5.61	110.90	105.16
2	D	501	HEM	C4C-NC-C1C	5.53	111.28	105.53
5	C	506	TWO	C9-O4-C3	5.27	125.38	117.59
2	A	501	HEM	C4C-NC-C1C	4.93	110.67	105.53
2	B	501	HEM	C4D-ND-C1D	4.86	110.13	105.16
2	A	501	HEM	C1B-NB-C4B	4.83	110.10	105.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	C4C-NC-C1C	4.75	110.47	105.53
2	D	501	HEM	C1B-NB-C4B	4.55	109.82	105.16
2	D	501	HEM	CMA-C3A-C4A	-4.17	122.20	128.62
2	C	501	HEM	CBD-CAD-C3D	-4.14	105.33	114.37
5	A	504	TWO	C9-O4-C3	3.99	123.49	117.59
2	A	501	HEM	CHB-C1B-NB	3.92	129.69	124.31
2	B	501	HEM	CMA-C3A-C4A	-3.79	122.79	128.62
2	B	501	HEM	CHD-C1D-ND	3.72	127.67	124.58
2	A	501	HEM	CMA-C3A-C4A	-3.66	122.99	128.62
5	B	505	TWO	C1-C2-C3	3.65	124.64	119.74
5	B	505	TWO	O3-C2-C1	-3.64	118.36	124.37
2	A	501	HEM	C4A-C3A-C2A	3.60	109.50	107.00
2	A	501	HEM	C4A-CHB-C1B	-3.50	122.87	127.47
2	D	501	HEM	CHC-C4B-NB	3.42	127.42	124.58
5	A	504	TWO	O4-C3-C2	3.38	120.33	115.42
5	C	506	TWO	O2-C7-C5	3.30	123.74	115.01
2	D	501	HEM	C2D-C1D-ND	-3.20	109.16	112.93
2	B	501	HEM	C2D-C1D-ND	-3.16	109.20	112.93
5	D	506	TWO	C4-C3-C2	3.05	123.73	119.74
5	B	505	TWO	C9-O4-C3	3.02	122.05	117.59
2	A	501	HEM	CMC-C2C-C3C	2.96	133.13	126.16
2	B	501	HEM	CHB-C1B-NB	2.88	128.26	124.31
2	A	501	HEM	C3A-C4A-NA	-2.88	107.24	109.41
5	B	505	TWO	C6-C1-C2	-2.84	114.45	120.00
4	B	503	GOL	O1-C1-C2	-2.82	95.95	109.71
2	B	501	HEM	CAD-C3D-C4D	2.75	129.47	124.53
2	C	501	HEM	C4A-CHB-C1B	-2.75	123.86	127.47
2	A	501	HEM	CAD-C3D-C4D	2.74	129.46	124.53
2	C	501	HEM	CHC-C1C-NC	2.74	127.11	124.73
2	A	501	HEM	CHC-C4B-NB	2.72	126.84	124.58
3	C	503	SO4	O2-S-O1	-2.66	100.72	109.53
2	B	501	HEM	CHD-C4C-NC	2.63	127.02	124.73
3	D	503	SO4	O2-S-O1	-2.63	100.82	109.53
5	B	505	TWO	O4-C3-C2	2.60	119.19	115.42
2	D	501	HEM	C3A-C4A-NA	-2.59	107.46	109.41
5	B	505	TWO	C8-O3-C2	2.59	121.41	117.59
4	B	503	GOL	O3-C3-C2	-2.54	97.31	109.71
2	D	501	HEM	CAA-CBA-CGA	-2.49	105.47	113.47
3	B	502	SO4	O2-S-O1	-2.44	101.44	109.53
5	C	506	TWO	O1-C7-C5	-2.44	114.69	121.25
2	D	501	HEM	CMA-C3A-C2A	2.40	129.47	124.94
2	C	501	HEM	C1A-C2A-C3A	2.39	109.39	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	506	TWO	C6-C1-C2	-2.38	115.36	120.00
2	D	501	HEM	O1A-CGA-CBA	-2.37	114.88	123.03
5	C	506	TWO	C1-C2-C3	2.36	122.92	119.74
5	C	506	TWO	C5-C4-C3	-2.36	116.34	119.63
2	D	501	HEM	O2A-CGA-CBA	2.36	122.54	114.22
5	B	505	TWO	O2-C7-C5	2.35	121.22	115.01
2	B	501	HEM	O1A-CGA-CBA	-2.30	115.10	123.03
5	D	506	TWO	O3-C2-C3	2.29	118.74	115.42
5	B	505	TWO	O4-C3-C4	-2.25	120.31	124.23
2	C	501	HEM	C4D-ND-C1D	2.25	107.46	105.16
2	B	501	HEM	O2A-CGA-CBA	2.22	122.07	114.22
5	C	506	TWO	C6-C5-C4	2.20	122.01	119.24
2	D	501	HEM	C4A-NA-C1A	2.20	109.66	106.76
2	C	501	HEM	O2A-CGA-CBA	2.19	121.96	114.22
2	B	501	HEM	CMA-C3A-C2A	2.19	129.07	124.94
5	C	506	TWO	O3-C2-C1	-2.18	120.76	124.37
2	C	501	HEM	CMA-C3A-C4A	-2.12	125.36	128.62
2	C	501	HEM	CBA-CAA-C2A	2.11	116.42	112.69
3	C	502	SO4	O2-S-O1	-2.10	102.59	109.53
3	B	502	SO4	O4-S-O3	2.05	117.76	109.08
2	C	501	HEM	CMC-C2C-C3C	2.05	130.98	126.16
2	B	501	HEM	CHC-C1C-NC	2.02	126.49	124.73
2	C	501	HEM	O2A-CGA-O1A	-2.01	118.18	123.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	393/410 (95%)	-0.49	0 100 100	12, 19, 29, 39	0
1	B	393/410 (95%)	-0.49	0 100 100	13, 19, 30, 42	0
1	C	393/410 (95%)	-0.42	1 (0%) 91 93	15, 22, 33, 43	0
1	D	393/410 (95%)	-0.18	4 (1%) 79 80	16, 26, 40, 55	0
All	All	1572/1640 (95%)	-0.40	5 (0%) 91 93	12, 21, 35, 55	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	409	ALA	3.0
1	D	169	GLU	2.3
1	D	141	GLN	2.1
1	D	408	PRO	2.1
1	C	17	THR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	C	504	5/5	0.33	10.86	64,66,70,70	0
3	SO4	D	503	5/5	0.14	9.47	51,52,54,55	0
3	SO4	D	504	5/5	0.28	8.23	76,77,78,79	0
4	GOL	B	503	6/6	0.27	7.59	31,47,47,49	0
3	SO4	C	503	5/5	0.12	6.31	34,37,44,48	0
5	TWO	C	506	13/13	0.17	0.94	17,19,23,24	0
2	HEM	B	501	43/43	0.15	0.93	10,14,17,18	0
2	HEM	A	501	43/43	0.15	0.90	10,13,15,17	0
2	HEM	D	501	43/43	0.14	0.74	13,19,22,26	0
5	TWO	D	506	13/13	0.16	0.71	15,21,25,25	0
2	HEM	C	501	43/43	0.14	0.61	12,16,20,22	0
4	GOL	A	503	6/6	0.09	0.42	21,26,30,35	0
5	TWO	B	505	13/13	0.13	0.35	12,16,18,20	0
4	GOL	B	504	6/6	0.09	0.09	17,21,23,33	0
5	TWO	A	504	13/13	0.11	-0.18	10,14,20,20	0
4	GOL	D	505	6/6	0.10	-0.22	27,37,42,45	0
3	SO4	A	502	5/5	0.08	-0.49	28,34,38,41	0
4	GOL	C	505	6/6	0.08	-0.74	20,25,29,35	0
3	SO4	D	502	5/5	0.09	-1.01	36,39,44,45	0
6	CL	A	505	1/1	0.05	-1.77	22,22,22,22	0
3	SO4	B	502	5/5	0.04	-2.27	20,21,21,24	0
6	CL	D	507	1/1	0.06	-2.68	36,36,36,36	0
6	CL	C	507	1/1	0.05	-2.98	27,27,27,27	0
3	SO4	C	502	5/5	0.06	-3.48	22,22,24,27	0
6	CL	B	506	1/1	0.05	-3.89	21,21,21,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.