



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:19 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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

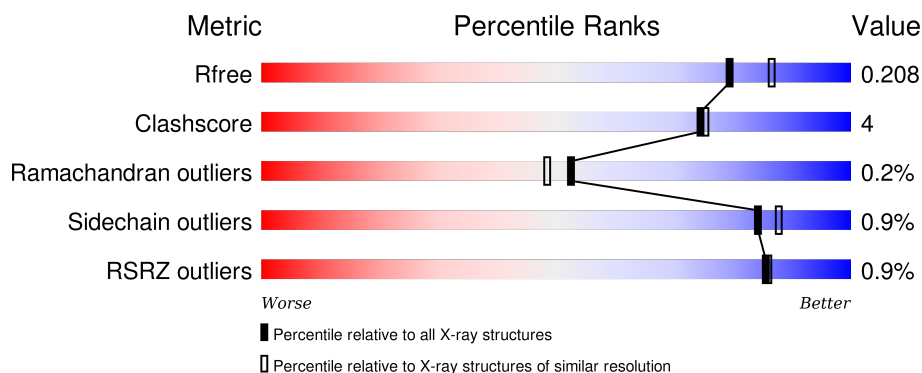
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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	410	 87% 8% . .
1	B	410	 82% 13% . .
1	C	410	 84% 10% . .
1	D	410	 86% 10% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	C	503	-	-	-	X
3	SO4	C	504	-	-	-	X
3	SO4	D	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 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 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	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 SULFATE ION (three-letter code: SO₄) (formula: O₄S).



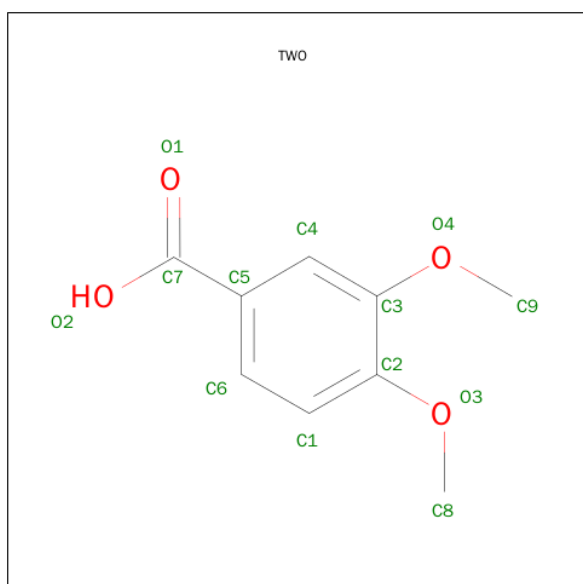
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- 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: C₉H₁₀O₄).



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

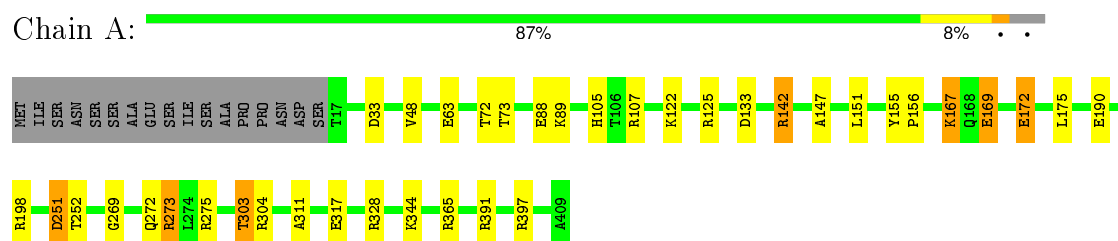
- Molecule 7 is water.

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

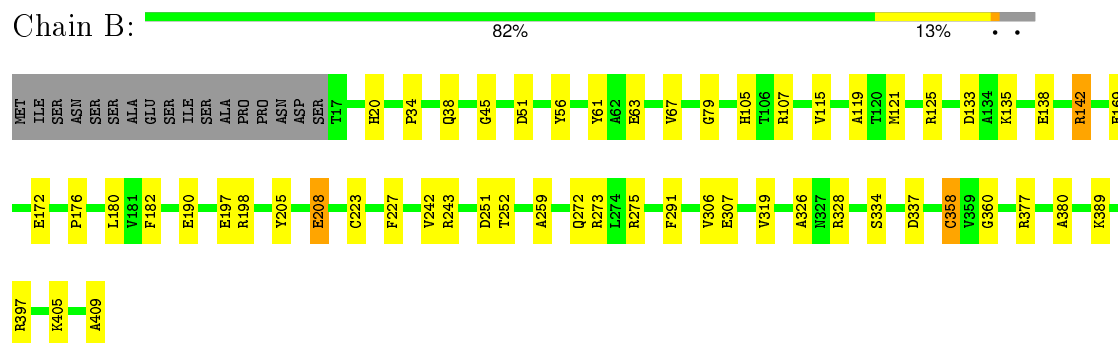
3 Residue-property plots

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.

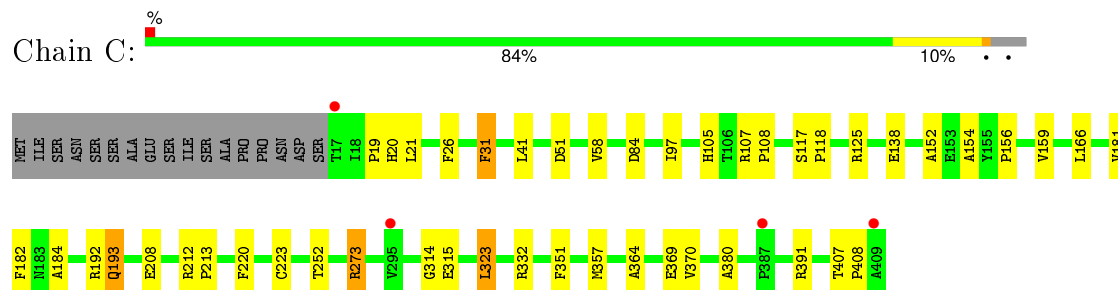
• Molecule 1: Cytochrome P450



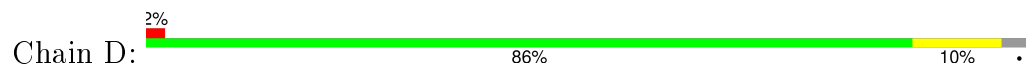
• Molecule 1: Cytochrome P450

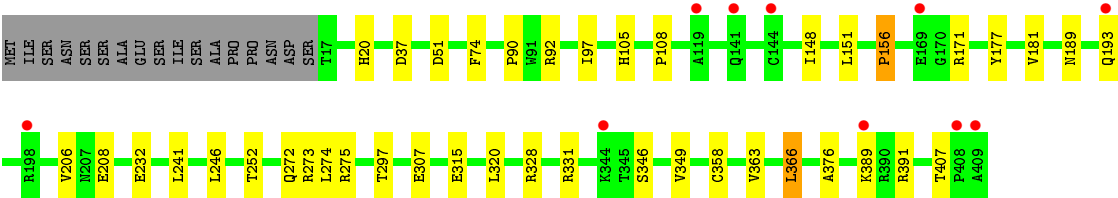


• Molecule 1: Cytochrome P450



• Molecule 1: Cytochrome P450





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	8806 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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 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	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
7	C	345	0	0	11	0
7	D	265	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13711	0	12187	99	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 (99) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:THR:CA	1:A:303:THR:HG21	2.47	0.44
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	392/410 (96%)	384 (98%)	7 (2%)	1 (0%)	46	41
1	C	392/410 (96%)	386 (98%)	6 (2%)	0	100	100
1	D	392/410 (96%)	382 (97%)	8 (2%)	2 (0%)	34	26
All	All	1568/1640 (96%)	1538 (98%)	27 (2%)	3 (0%)	52	48

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%)	94	96
1	B	320/334 (96%)	316 (99%)	4 (1%)	76	79
1	C	320/334 (96%)	318 (99%)	2 (1%)	90	93
1	D	320/334 (96%)	315 (98%)	5 (2%)	70	73
All	All	1280/1336 (96%)	1268 (99%)	12 (1%)	84	88

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

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Mol	Chain	Res	Type
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 molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	30,50,50	2.52	8 (26%)	24,82,82	2.72	10 (41%)
3	SO4	A	502	-	4,4,4	0.74	0	6,6,6	0.89	0
4	GOL	A	503	-	5,5,5	0.39	0	5,5,5	0.82	0
5	TWO	A	504	-	10,13,13	0.98	0	13,17,17	1.78	2 (15%)
2	HEM	B	501	1	30,50,50	2.53	11 (36%)	24,82,82	2.82	12 (50%)
3	SO4	B	502	-	4,4,4	0.50	0	6,6,6	1.40	2 (33%)
4	GOL	B	503	-	5,5,5	0.78	0	5,5,5	1.89	2 (40%)
4	GOL	B	504	-	5,5,5	0.48	0	5,5,5	0.62	0
5	TWO	B	505	-	10,13,13	0.87	0	13,17,17	2.40	9 (69%)
2	HEM	C	501	1	30,50,50	2.11	9 (30%)	24,82,82	2.63	12 (50%)
3	SO4	C	502	-	4,4,4	0.79	0	6,6,6	0.92	1 (16%)
3	SO4	C	503	-	4,4,4	1.02	0	6,6,6	1.29	1 (16%)
3	SO4	C	504	-	4,4,4	0.60	0	6,6,6	0.52	0
4	GOL	C	505	-	5,5,5	0.85	0	5,5,5	1.05	1 (20%)
5	TWO	C	506	-	10,13,13	0.98	0	13,17,17	2.30	6 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	D	501	1	30,50,50	2.42	10 (33%)	24,82,82	2.85	14 (58%)
3	SO4	D	502	-	4,4,4	0.48	0	6,6,6	0.70	0
3	SO4	D	503	-	4,4,4	0.45	0	6,6,6	1.20	1 (16%)
3	SO4	D	504	-	4,4,4	0.23	0	6,6,6	0.59	0
4	GOL	D	505	-	5,5,5	0.45	0	5,5,5	0.88	0
5	TWO	D	506	-	10,13,13	1.28	2 (20%)	13,17,17	1.40	2 (15%)

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	-	0/10/54/54	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	-	-	0/4/8/8	0/1/1/1
2	HEM	B	501	1	-	0/10/54/54	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	-	-	0/4/8/8	0/1/1/1
2	HEM	C	501	1	-	0/10/54/54	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	-	-	0/4/8/8	0/1/1/1
2	HEM	D	501	1	-	0/10/54/54	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	-	-	0/4/8/8	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3B-C4B	-9.98	1.42	1.51
2	A	501	HEM	C3B-C4B	-9.00	1.43	1.51
2	D	501	HEM	C3B-C4B	-8.33	1.44	1.51
2	C	501	HEM	C3B-C4B	-6.22	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C2C-C1C	-4.82	1.43	1.52
2	A	501	HEM	C3D-C4D	-4.76	1.45	1.51
2	C	501	HEM	C3D-C4D	-4.72	1.45	1.51
2	D	501	HEM	C3D-C4D	-3.86	1.46	1.51
2	C	501	HEM	C2C-C1C	-3.25	1.46	1.52
2	B	501	HEM	C3D-C4D	-2.82	1.48	1.51
5	D	506	TWO	C3-C2	-2.61	1.35	1.40
2	B	501	HEM	C2C-C1C	-2.52	1.47	1.52
2	A	501	HEM	C2D-C3D	-2.50	1.47	1.54
2	D	501	HEM	C2C-C1C	-2.24	1.48	1.52
2	C	501	HEM	C2B-C1B	-2.24	1.44	1.51
2	B	501	HEM	C2A-C3A	-2.21	1.31	1.37
2	B	501	HEM	C2D-C3D	-2.21	1.48	1.54
2	C	501	HEM	C2D-C3D	-2.15	1.48	1.54
2	A	501	HEM	C2D-C1D	-2.11	1.44	1.51
2	B	501	HEM	C2D-C1D	-2.11	1.44	1.51
2	D	501	HEM	CMC-C2C	2.03	1.57	1.53
5	D	506	TWO	C4-C3	2.03	1.42	1.38
2	D	501	HEM	CAD-C3D	2.09	1.58	1.54
2	B	501	HEM	FE-NB	2.12	2.08	1.97
2	D	501	HEM	C4C-NC	2.30	1.38	1.36
2	C	501	HEM	C3B-CAB	2.41	1.55	1.51
2	D	501	HEM	C3B-CAB	2.53	1.56	1.51
2	C	501	HEM	C3C-CAC	2.55	1.56	1.51
2	B	501	HEM	CAD-C3D	2.56	1.59	1.54
2	A	501	HEM	C3B-CAB	2.58	1.56	1.51
2	A	501	HEM	C1C-NC	2.60	1.39	1.36
2	B	501	HEM	CAA-C2A	2.66	1.56	1.52
2	C	501	HEM	FE-NC	2.74	2.06	1.95
2	B	501	HEM	C1C-NC	2.76	1.39	1.36
2	C	501	HEM	CMA-C3A	2.92	1.57	1.51
2	D	501	HEM	FE-ND	3.09	2.13	1.97
2	B	501	HEM	FE-NC	3.56	2.09	1.95
2	A	501	HEM	FE-NC	3.87	2.11	1.95
2	D	501	HEM	CAA-C2A	4.13	1.59	1.52
2	D	501	HEM	FE-NC	4.43	2.13	1.95

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CBD-CAD-C3D	-5.20	98.43	113.55
2	B	501	HEM	CBD-CAD-C3D	-4.60	100.18	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CBD-CAD-C3D	-4.35	100.88	113.55
2	D	501	HEM	CAA-CBA-CGA	-3.97	105.47	112.75
2	D	501	HEM	CMA-C3A-C4A	-3.72	122.20	128.36
5	B	505	TWO	O3-C2-C1	-3.56	118.36	124.35
2	B	501	HEM	CMA-C3A-C4A	-3.37	122.79	128.36
2	A	501	HEM	CMA-C3A-C4A	-3.25	122.99	128.36
2	B	501	HEM	C2C-C1C-NC	-3.22	104.78	110.21
2	C	501	HEM	CAA-C2A-C1A	-3.04	123.71	127.01
4	B	503	GOL	O1-C1-C2	-2.94	95.95	110.18
5	B	505	TWO	C6-C1-C2	-2.88	114.45	120.03
2	C	501	HEM	CBD-CAD-C3D	-2.83	105.33	113.55
5	C	506	TWO	C5-C4-C3	-2.82	116.34	120.17
3	C	503	SO4	O2-S-O1	-2.77	100.72	109.50
3	D	503	SO4	O2-S-O1	-2.74	100.82	109.50
2	A	501	HEM	CAA-C2A-C1A	-2.66	124.11	127.01
2	B	501	HEM	C3B-C4B-NB	-2.66	106.54	111.63
4	B	503	GOL	O3-C3-C2	-2.65	97.31	110.18
3	B	502	SO4	O2-S-O1	-2.54	101.44	109.50
5	C	506	TWO	C6-C1-C2	-2.42	115.36	120.03
2	B	501	HEM	CAA-C2A-C1A	-2.38	124.43	127.01
5	B	505	TWO	O4-C3-C4	-2.28	120.31	124.21
2	A	501	HEM	C3B-C4B-NB	-2.28	107.27	111.63
5	B	505	TWO	C5-C4-C3	-2.26	117.09	120.17
2	C	501	HEM	C2C-C1C-NC	-2.25	106.41	110.21
2	D	501	HEM	C3B-C4B-NB	-2.24	107.35	111.63
2	D	501	HEM	CAA-C2A-C1A	-2.19	124.63	127.01
3	C	502	SO4	O2-S-O1	-2.18	102.59	109.50
5	C	506	TWO	O3-C2-C1	-2.13	120.76	124.35
4	C	505	GOL	O1-C1-C2	-2.03	100.34	110.18
2	D	501	HEM	CMA-C3A-C2A	2.03	129.47	125.24
3	B	502	SO4	O4-S-O3	2.16	117.76	108.98
2	C	501	HEM	CBA-CAA-C2A	2.17	116.42	112.53
2	A	501	HEM	C2C-C1C-CHC	2.22	127.06	123.68
5	D	506	TWO	O3-C2-C3	2.34	118.74	115.40
5	C	506	TWO	C1-C2-C3	2.36	122.92	119.74
2	D	501	HEM	C2D-C3D-C4D	2.40	105.58	101.50
2	C	501	HEM	C3B-C4B-CHC	2.55	126.75	123.16
5	B	505	TWO	C8-O3-C2	2.55	121.41	117.54
5	B	505	TWO	C6-C5-C4	2.58	121.60	118.17
2	C	501	HEM	CMD-C2D-C3D	2.59	125.81	114.35
5	B	505	TWO	O4-C3-C2	2.66	119.19	115.40
2	D	501	HEM	C1D-CHD-C4C	2.73	130.39	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CMD-C2D-C3D	2.79	126.71	114.35
2	C	501	HEM	C3B-CAB-CBB	2.82	128.79	124.46
5	C	506	TWO	C6-C5-C4	2.90	122.01	118.17
2	B	501	HEM	CMD-C2D-C3D	2.90	127.17	114.35
2	C	501	HEM	C2D-C3D-C4D	2.92	106.45	101.50
5	D	506	TWO	C4-C3-C2	2.93	123.73	119.79
2	D	501	HEM	CMD-C2D-C3D	2.95	127.38	114.35
5	B	505	TWO	C9-O4-C3	2.97	122.05	117.54
2	B	501	HEM	C2C-C1C-CHC	3.30	128.71	123.68
2	D	501	HEM	C2C-C1C-CHC	3.44	128.91	123.68
5	A	504	TWO	O4-C3-C2	3.46	120.33	115.40
2	B	501	HEM	C3B-C4B-CHC	3.60	128.23	123.16
5	B	505	TWO	C1-C2-C3	3.63	124.64	119.74
5	A	504	TWO	C9-O4-C3	3.92	123.49	117.54
2	D	501	HEM	CAD-C3D-C4D	4.19	127.25	112.47
2	D	501	HEM	CMC-C2C-C3C	4.24	127.11	116.53
2	A	501	HEM	CMB-C2B-C3B	4.31	127.28	116.53
2	C	501	HEM	CAD-C3D-C4D	4.34	127.77	112.47
2	D	501	HEM	CMB-C2B-C3B	4.34	127.38	116.53
2	C	501	HEM	CAD-C3D-C2D	4.37	125.77	113.22
2	A	501	HEM	CAD-C3D-C2D	4.39	125.83	113.22
2	B	501	HEM	CAD-C3D-C2D	4.44	125.97	113.22
2	B	501	HEM	CMC-C2C-C3C	4.53	127.84	116.53
2	C	501	HEM	CMB-C2B-C3B	4.67	128.20	116.53
2	A	501	HEM	CAD-C3D-C4D	4.82	129.46	112.47
2	B	501	HEM	CAD-C3D-C4D	4.82	129.47	112.47
2	D	501	HEM	CAD-C3D-C2D	4.85	127.17	113.22
2	B	501	HEM	CMB-C2B-C3B	4.92	128.82	116.53
5	C	506	TWO	C9-O4-C3	5.17	125.38	117.54
2	C	501	HEM	CMC-C2C-C3C	5.79	130.98	116.53
2	A	501	HEM	CMC-C2C-C3C	6.65	133.13	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	3	0
2	B	501	HEM	6	0
2	C	501	HEM	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	506	TWO	3	0
2	D	501	HEM	3	0
5	D	506	TWO	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, 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%)	-0.40	0	100 100	12, 19, 29, 39	0
1	B	393/410 (95%)	-0.38	0	100 100	13, 19, 30, 42	0
1	C	393/410 (95%)	-0.29	4 (1%)	84 84	15, 22, 33, 43	0
1	D	393/410 (95%)	-0.04	10 (2%)	61 61	16, 26, 40, 55	0
All	All	1572/1640 (95%)	-0.28	14 (0%)	85 86	12, 21, 35, 55	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	409	ALA	4.0
1	C	295	VAL	2.9
1	D	141	GLN	2.6
1	D	169	GLU	2.6
1	C	17	THR	2.5
1	D	119	ALA	2.4
1	D	144	CYS	2.3
1	D	198	ARG	2.3
1	D	408	PRO	2.2
1	C	387	PRO	2.2
1	D	389	LYS	2.1
1	C	409	ALA	2.0
1	D	193	GLN	2.0
1	D	344	LYS	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 [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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	C	504	5/5	0.86	0.34	11.72	64,66,70,70	0
3	SO4	C	503	5/5	0.98	0.12	6.20	34,37,44,48	0
3	SO4	D	503	5/5	0.95	0.13	4.79	51,52,54,55	0
5	TWO	C	506	13/13	0.98	0.19	0.90	17,19,23,24	0
5	TWO	D	506	13/13	0.97	0.17	0.81	15,21,25,25	0
2	HEM	B	501	43/43	0.99	0.16	0.71	10,14,17,18	0
2	HEM	C	501	43/43	0.98	0.15	0.60	12,16,20,22	0
2	HEM	D	501	43/43	0.98	0.15	0.52	13,19,22,26	0
2	HEM	A	501	43/43	0.99	0.15	0.51	10,13,15,17	0
4	GOL	A	503	6/6	0.95	0.10	0.36	21,26,30,35	0
5	TWO	B	505	13/13	0.98	0.14	0.33	12,16,18,20	0
4	GOL	D	505	6/6	0.96	0.11	-0.09	27,37,42,45	0
4	GOL	B	504	6/6	0.97	0.09	-0.10	17,21,23,33	0
5	TWO	A	504	13/13	0.98	0.12	-0.22	10,14,20,20	0
4	GOL	C	505	6/6	0.97	0.09	-0.63	20,25,29,35	0
3	SO4	C	502	5/5	0.99	0.07	-	22,22,24,27	0
4	GOL	B	503	6/6	0.91	0.28	-	31,47,47,49	0
6	CL	D	507	1/1	0.97	0.06	-	36,36,36,36	0
3	SO4	B	502	5/5	1.00	0.05	-	20,21,21,24	0
6	CL	C	507	1/1	0.99	0.06	-	27,27,27,27	0
6	CL	B	506	1/1	0.98	0.07	-	21,21,21,21	0
3	SO4	D	504	5/5	0.80	0.32	-	76,77,78,79	0
3	SO4	A	502	5/5	0.98	0.09	-	28,34,38,41	0
6	CL	A	505	1/1	0.99	0.07	-	22,22,22,22	0
3	SO4	D	502	5/5	0.98	0.10	-	36,39,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.