



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:51 PM GMT

PDB ID : 4DO1
Title : The crystal structures of 4-methoxybenzoate bound CYP199A4
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Zhang, A.; Rao, Z.; Wong, L.-L.
Deposited on : 2012-02-09
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

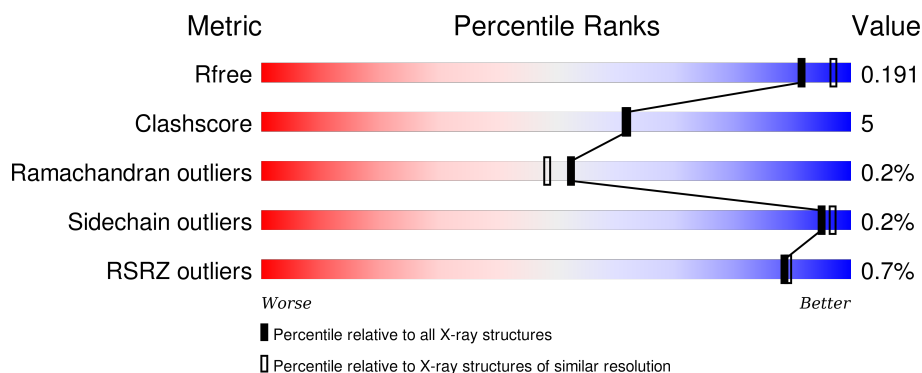
1 Overall quality at a glance

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	<div> <div>83%</div> <div>11% . .</div> </div>
1	B	410	<div> <div>84%</div> <div>10% . .</div> </div>
1	C	410	<div> <div>%</div> <div>87%</div> <div>8% .</div> </div>
1	D	410	<div> <div>%</div> <div>83%</div> <div>12% . .</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
4	SO4	B	504	-	-	-	X

2 Entry composition [i](#)

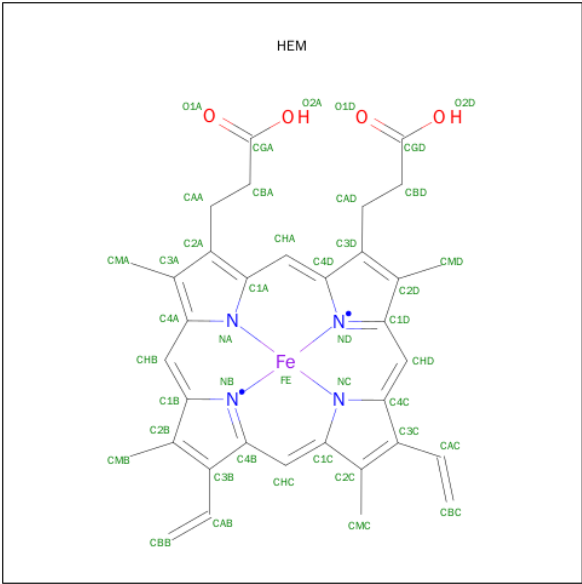
There are 7 unique types of molecules in this entry. The entry contains 14553 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	0	0
			3021	1912	534	564	11			
1	C	393	Total	C	N	O	S	0	0	0
			3021	1912	534	564	11			
1	D	393	Total	C	N	O	S	0	0	0
			3021	1912	534	564	11			

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



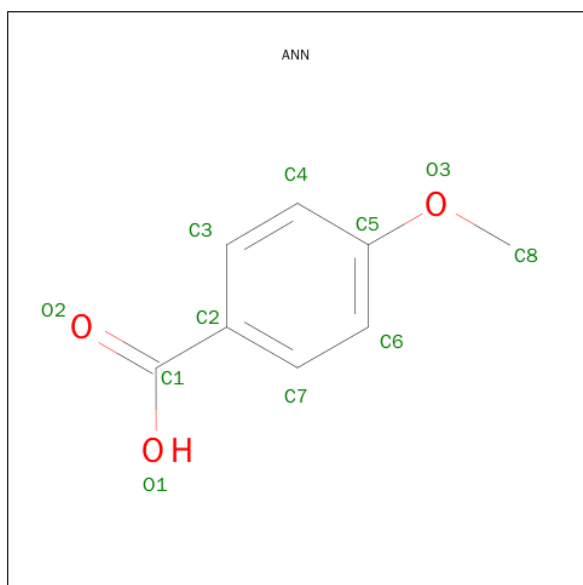
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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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 4-METHOXYBENZOIC ACID (three-letter code: ANN) (formula: C₈H₈O₃).



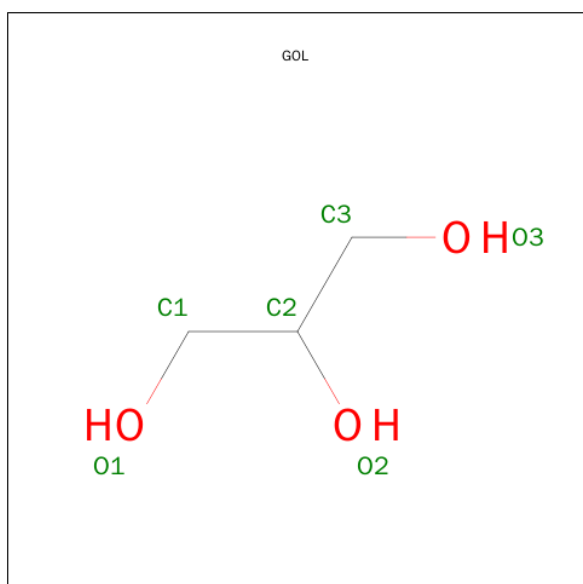
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	8	3		
3	B	1	Total	C	O	0	0
			11	8	3		
3	C	1	Total	C	O	0	0
			11	8	3		
3	D	1	Total	C	O	0	0
			11	8	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

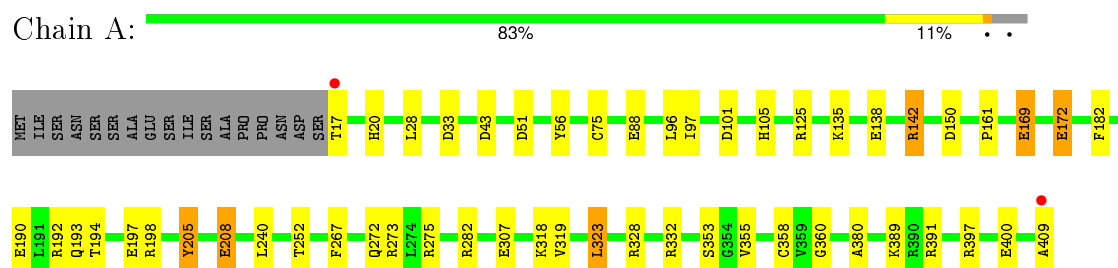
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	567	Total O 567 567	0	0
7	B	542	Total O 542 542	0	0
7	C	563	Total O 563 563	0	0
7	D	525	Total O 525 525	0	0

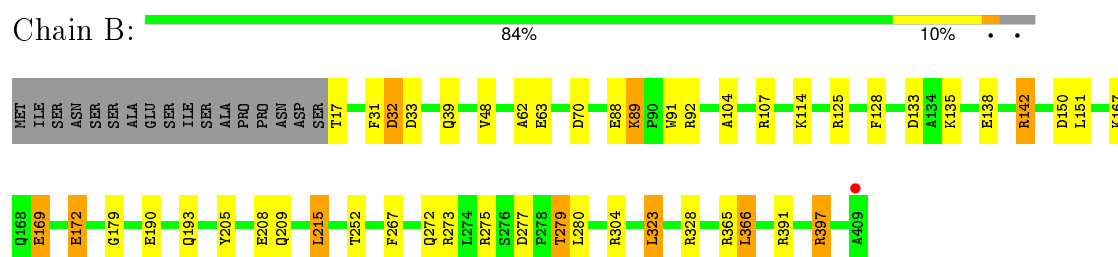
3 Residue-property plots [i](#)

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

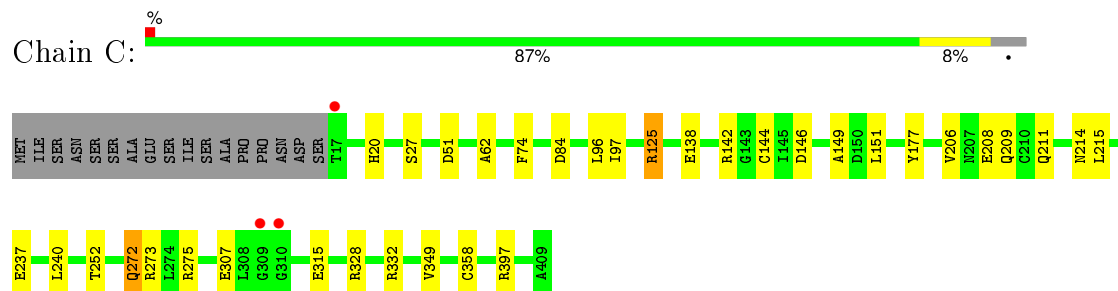
• Molecule 1: Cytochrome P450



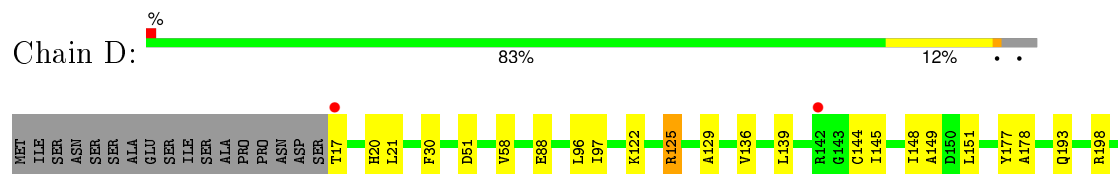
• Molecule 1: Cytochrome P450



• 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	107.02Å 143.48Å 172.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.67 – 2.00 43.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.67-2.00) 99.4 (43.66-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.11 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.154 , 0.189 0.157 , 0.191	Depositor DCC
R_{free} test set	8967 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.4	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 178754 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14553	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 40.69 % 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 2.6363e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ANN, SO4, 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	1.51	15/3099 (0.5%)	1.10	14/4217 (0.3%)
1	B	1.43	16/3093 (0.5%)	1.08	17/4209 (0.4%)
1	C	1.38	11/3093 (0.4%)	1.06	11/4209 (0.3%)
1	D	1.43	14/3093 (0.5%)	1.14	16/4209 (0.4%)
All	All	1.44	56/12378 (0.5%)	1.10	58/16844 (0.3%)

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	PRO	N-CD	-14.60	1.27	1.47
1	D	370	VAL	CB-CG2	-9.77	1.32	1.52
1	B	88	GLU	CD-OE1	9.63	1.36	1.25
1	A	172	GLU	CG-CD	8.86	1.65	1.51
1	B	172	GLU	CG-CD	8.41	1.64	1.51
1	B	169	GLU	CG-CD	8.00	1.64	1.51
1	A	88	GLU	CG-CD	7.59	1.63	1.51
1	C	208	GLU	CD-OE2	7.49	1.33	1.25
1	C	208	GLU	CG-CD	7.40	1.63	1.51
1	D	292	GLU	CG-CD	7.29	1.62	1.51
1	A	267	PHE	CE1-CZ	7.10	1.50	1.37
1	A	169	GLU	CG-CD	7.08	1.62	1.51
1	B	323	LEU	CG-CD2	-6.84	1.26	1.51
1	A	208	GLU	CG-CD	6.81	1.62	1.51
1	B	62	ALA	CA-CB	6.68	1.66	1.52
1	A	323	LEU	CG-CD2	-6.61	1.27	1.51
1	B	397	ARG	CZ-NH2	-6.56	1.24	1.33
1	A	319	VAL	CB-CG2	6.44	1.66	1.52
1	C	27	SER	CB-OG	6.44	1.50	1.42
1	D	318	LYS	CD-CE	6.44	1.67	1.51
1	B	169	GLU	CD-OE2	6.38	1.32	1.25
1	B	104	ALA	CA-CB	6.37	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	315	GLU	CG-CD	6.26	1.61	1.51
1	B	267	PHE	CE1-CZ	6.26	1.49	1.37
1	C	272	GLN	CG-CD	6.19	1.65	1.51
1	A	125	ARG	CZ-NH2	6.12	1.41	1.33
1	A	125	ARG	CG-CD	6.04	1.67	1.51
1	B	48	VAL	CB-CG2	6.03	1.65	1.52
1	C	315	GLU	CG-CD	5.95	1.60	1.51
1	D	232	GLU	CB-CG	5.73	1.63	1.52
1	B	88	GLU	CG-CD	5.63	1.60	1.51
1	C	149	ALA	CA-CB	5.54	1.64	1.52
1	D	30	PHE	CD2-CE2	5.50	1.50	1.39
1	B	63	GLU	CB-CG	5.47	1.62	1.52
1	C	237	GLU	CG-CD	5.46	1.60	1.51
1	D	88	GLU	CG-CD	5.46	1.60	1.51
1	D	178	ALA	CA-CB	-5.44	1.41	1.52
1	B	31	PHE	CE1-CZ	5.44	1.47	1.37
1	D	177	TYR	CE1-CZ	5.43	1.45	1.38
1	B	179	GLY	N-CA	5.35	1.54	1.46
1	A	205	TYR	CE1-CZ	5.34	1.45	1.38
1	D	58	VAL	CA-CB	5.32	1.66	1.54
1	B	215	LEU	CG-CD2	-5.31	1.32	1.51
1	C	349	VAL	CB-CG2	5.30	1.64	1.52
1	D	149	ALA	CA-CB	5.25	1.63	1.52
1	C	74	PHE	CE2-CZ	5.24	1.47	1.37
1	A	56	TYR	CD2-CE2	5.21	1.47	1.39
1	D	122	LYS	CD-CE	5.18	1.64	1.51
1	A	182	PHE	CE1-CZ	5.17	1.47	1.37
1	A	353	SER	CA-CB	5.13	1.60	1.52
1	B	33	ASP	CB-CG	5.13	1.62	1.51
1	A	318	LYS	CE-NZ	5.12	1.61	1.49
1	D	359	VAL	CB-CG2	5.10	1.63	1.52
1	C	62	ALA	CA-CB	5.07	1.63	1.52
1	C	138	GLU	CG-CD	5.04	1.59	1.51
1	D	363	VAL	CB-CG2	5.01	1.63	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	D	273	ARG	NE-CZ-NH2	-11.17	114.71	120.30
1	D	328	ARG	NE-CZ-NH2	-11.01	114.79	120.30
1	D	125	ARG	NE-CZ-NH2	-10.22	115.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	D	273	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	B	33	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	C	273	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	A	273	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	D	215	LEU	CD1-CG-CD2	-8.37	85.39	110.50
1	D	125	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	C	332	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	B	304	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	C	328	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	A	142	ARG	NE-CZ-NH1	-7.29	116.66	120.30
1	C	273	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	B	142	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	A	328	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	D	328	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	328	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	282	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	33	ASP	CB-CG-OD1	6.47	124.12	118.30
1	B	133	ASP	CB-CG-OD1	6.45	124.11	118.30
1	D	315	GLU	OE1-CD-OE2	-6.42	115.59	123.30
1	D	275	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	273	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	323	LEU	CD1-CG-CD2	-6.07	92.28	110.50
1	C	146	ASP	CB-CG-OD2	6.00	123.70	118.30
1	D	198	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	125	ARG	CG-CD-NE	-5.96	99.28	111.80
1	D	331	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	328	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	D	290	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	391	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	198	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	43	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	D	240	LEU	CB-CG-CD1	5.74	120.76	111.00
1	B	365	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	125	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	32	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	28	LEU	CB-CG-CD1	5.63	120.57	111.00
1	B	70	ASP	CB-CG-OD1	5.62	123.35	118.30
1	C	328	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	107	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	33	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	332	ARG	NE-CZ-NH1	5.49	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	LEU	CD1-CG-CD2	-5.47	94.08	110.50
1	C	84	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	89	LYS	CD-CE-NZ	-5.22	99.68	111.70
1	D	365	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	391	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	D	21	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	A	192	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	C	315	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	C	397	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	C	125	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	C	144	CYS	CA-CB-SG	-5.01	104.99	114.00
1	B	366	LEU	CB-CG-CD1	-5.00	102.49	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	2998	38	0
1	B	3021	0	2993	37	0
1	C	3021	0	2993	24	0
1	D	3021	0	2993	38	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	A	11	0	7	0	0
3	B	11	0	7	0	0
3	C	11	0	7	0	0
3	D	11	0	7	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	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	567	0	0	11	0
7	B	542	0	0	12	0
7	C	563	0	0	4	0
7	D	525	0	0	8	0
All	All	14553	0	12157	133	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 5.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:GLU:HG2	7:B:679:HOH:O	1.39	1.20
1:D:129:ALA:HA	1:D:370:VAL:CG1	1.74	1.17
1:D:193:GLN:HG3	7:D:1119:HOH:O	1.56	1.02
1:C:209:GLN:O	1:C:215:LEU:HD11	1.61	1.01
1:B:167:LYS:HE3	1:B:169:GLU:HG2	1.46	0.97
1:D:129:ALA:HA	1:D:370:VAL:HG11	1.46	0.97
1:C:272:GLN:HE22	1:C:275:ARG:HH11	1.18	0.91
1:B:17:THR:HG21	7:B:631:HOH:O	1.72	0.89
1:A:135:LYS:HE2	1:A:150:ASP:O	1.75	0.87
1:A:272:GLN:HE22	1:A:275:ARG:HH11	1.22	0.87
1:D:215:LEU:HD23	1:D:221:GLY:HA3	1.58	0.85
1:A:208:GLU:HG2	7:A:856:HOH:O	1.76	0.85
1:D:96:LEU:HD21	1:D:240:LEU:HD13	1.56	0.85
1:A:190:GLU:HG2	7:A:1098:HOH:O	1.79	0.83
1:A:96:LEU:HD21	1:A:240:LEU:HD13	1.61	0.82
1:B:272:GLN:HE22	1:B:275:ARG:HH21	1.22	0.82
1:D:129:ALA:HA	1:D:370:VAL:HG13	1.60	0.82
1:C:214:ASN:C	1:C:215:LEU:HD12	1.99	0.82
1:B:135:LYS:HE2	1:B:150:ASP:O	1.80	0.81
1:B:366:LEU:HD13	1:B:366:LEU:C	2.01	0.80
1:B:209:GLN:O	1:B:215:LEU:HD21	1.82	0.79
1:D:272:GLN:HE22	1:D:275:ARG:HH11	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:CYS:SG	7:D:1017:HOH:O	2.40	0.79
1:A:96:LEU:CD2	1:A:240:LEU:HD13	2.16	0.76
1:D:129:ALA:CA	1:D:370:VAL:HG11	2.16	0.75
1:C:215:LEU:HD12	1:C:215:LEU:N	2.01	0.74
1:C:215:LEU:N	1:C:215:LEU:CD1	2.51	0.74
1:D:129:ALA:CA	1:D:370:VAL:CG1	2.63	0.73
1:D:96:LEU:CD2	1:D:240:LEU:HD13	2.18	0.73
1:C:96:LEU:HD21	1:C:240:LEU:HD13	1.70	0.72
1:D:215:LEU:HD23	1:D:221:GLY:CA	2.21	0.70
1:C:272:GLN:HE22	1:C:275:ARG:NH1	1.89	0.70
1:D:96:LEU:HD21	1:D:240:LEU:CD1	2.24	0.68
1:D:209:GLN:O	1:D:215:LEU:HD11	1.94	0.66
1:B:167:LYS:CE	1:B:169:GLU:HG2	2.25	0.64
1:D:125:ARG:NH1	7:D:1104:HOH:O	2.26	0.64
1:A:138:GLU:OE1	1:B:167:LYS:NZ	2.27	0.64
2:B:501:HEM:HBC2	2:B:501:HEM:HMC1	1.81	0.63
1:B:135:LYS:CE	1:B:150:ASP:O	2.46	0.63
1:B:277:ASP:OD1	1:B:279:THR:HB	1.99	0.62
1:D:389:LYS:HE3	1:D:400:GLU:OE1	2.00	0.62
1:A:105:HIS:HE1	2:A:501:HEM:O1D	1.82	0.61
1:B:172:GLU:CD	1:B:172:GLU:H	2.04	0.61
1:A:193:GLN:HB2	7:A:910:HOH:O	2.02	0.60
1:B:17:THR:CG2	7:B:631:HOH:O	2.42	0.59
1:A:96:LEU:HD21	1:A:240:LEU:CD1	2.30	0.59
1:B:114:LYS:HG2	7:B:989:HOH:O	2.03	0.59
1:D:391:ARG:NH2	7:D:881:HOH:O	2.36	0.59
1:D:307:GLU:HG2	7:D:670:HOH:O	2.04	0.58
1:D:136:VAL:HG21	1:D:375:LEU:HD22	1.85	0.58
1:A:142:ARG:HD3	1:B:205:TYR:HA	1.86	0.58
1:A:389:LYS:HD3	1:A:400:GLU:OE1	2.03	0.58
1:D:209:GLN:O	1:D:215:LEU:CD1	2.53	0.57
1:A:105:HIS:HD2	7:A:615:HOH:O	1.87	0.57
1:D:20:HIS:HD2	1:D:51:ASP:OD1	1.87	0.56
1:B:89:LYS:HE2	7:B:1116:HOH:O	2.06	0.55
1:A:355:VAL:HG12	7:A:1167:HOH:O	2.06	0.55
1:B:366:LEU:CD1	1:B:366:LEU:C	2.75	0.55
1:A:194:THR:O	1:A:197:GLU:HG2	2.07	0.54
1:A:272:GLN:HE22	1:A:275:ARG:NH1	1.99	0.54
1:B:208:GLU:HB2	7:B:1104:HOH:O	2.08	0.54
1:C:20:HIS:HD2	1:C:51:ASP:OD1	1.89	0.54
1:C:96:LEU:HD22	1:C:96:LEU:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ARG:HD2	7:D:803:HOH:O	2.10	0.52
1:C:307:GLU:HG2	7:C:725:HOH:O	2.09	0.52
1:B:366:LEU:HD13	1:B:366:LEU:O	2.09	0.52
1:A:172:GLU:H	1:A:172:GLU:CD	2.13	0.51
1:A:190:GLU:CG	7:A:1098:HOH:O	2.48	0.51
1:C:252:THR:HB	2:C:501:HEM:C3B	2.46	0.50
1:A:389:LYS:HE2	1:A:400:GLU:OE2	2.11	0.50
1:C:214:ASN:C	1:C:215:LEU:CD1	2.77	0.50
1:C:97:ILE:HG12	2:C:501:HEM:CGD	2.42	0.49
1:A:193:GLN:NE2	7:A:1116:HOH:O	2.45	0.49
1:B:151:LEU:HD23	1:B:151:LEU:C	2.33	0.49
1:A:138:GLU:HG3	1:B:169:GLU:HG3	1.94	0.48
1:D:407:THR:HG23	7:D:806:HOH:O	2.14	0.48
1:A:252:THR:HB	2:A:501:HEM:C3B	2.48	0.48
1:C:142:ARG:NH1	7:C:897:HOH:O	2.46	0.48
1:D:252:THR:HB	2:D:501:HEM:C3B	2.49	0.47
1:A:397:ARG:NH2	7:A:893:HOH:O	2.43	0.47
1:D:17:THR:CG2	7:D:1113:HOH:O	2.62	0.47
1:C:96:LEU:HD23	1:C:240:LEU:HB3	1.96	0.47
1:C:214:ASN:O	1:C:215:LEU:HD12	2.14	0.47
1:C:211:GLN:O	1:C:215:LEU:HD13	2.15	0.47
1:D:389:LYS:HE3	1:D:400:GLU:CD	2.35	0.46
1:D:97:ILE:HG12	2:D:501:HEM:CGD	2.46	0.46
1:A:135:LYS:CE	1:A:150:ASP:O	2.57	0.46
1:D:129:ALA:N	1:D:370:VAL:HG11	2.31	0.46
1:B:167:LYS:NZ	1:B:208:GLU:OE1	2.49	0.46
1:B:193:GLN:HB2	7:B:1085:HOH:O	2.15	0.46
1:A:97:ILE:HG12	2:A:501:HEM:CGD	2.46	0.45
1:C:125:ARG:NH1	7:C:1132:HOH:O	2.48	0.45
1:B:397:ARG:NH2	7:B:970:HOH:O	2.43	0.45
1:A:17:THR:HG21	7:A:1159:HOH:O	2.16	0.45
1:B:128:PHE:CD2	1:B:366:LEU:HD12	2.51	0.45
1:A:360:GLY:HA3	2:A:501:HEM:C3C	2.52	0.45
1:B:39:GLN:HG2	7:B:769:HOH:O	2.17	0.45
1:D:129:ALA:CA	1:D:370:VAL:HG13	2.39	0.44
1:C:358:CYS:HA	2:C:501:HEM:CHA	2.47	0.44
1:B:91:TRP:CZ2	1:B:92:ARG:HD3	2.53	0.44
1:D:215:LEU:HD23	1:D:221:GLY:C	2.38	0.44
1:A:96:LEU:HD23	1:A:240:LEU:HB3	2.00	0.44
1:A:169:GLU:HG3	1:B:138:GLU:HG3	1.99	0.44
1:B:167:LYS:HD3	7:B:930:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:TYR:HA	1:B:142:ARG:HD3	2.00	0.44
1:B:17:THR:HG23	7:B:1025:HOH:O	2.18	0.44
1:A:20:HIS:HD2	1:A:51:ASP:OD1	2.01	0.43
1:C:177:TYR:CD2	1:C:206:VAL:HG21	2.53	0.43
1:C:142:ARG:NH2	7:C:826:HOH:O	2.30	0.43
1:C:20:HIS:CD2	1:C:51:ASP:OD1	2.70	0.43
1:D:96:LEU:HA	1:D:96:LEU:HD13	1.74	0.43
1:B:252:THR:HB	2:B:501:HEM:C3B	2.54	0.43
1:B:323:LEU:HD22	1:B:323:LEU:N	2.33	0.43
1:B:272:GLN:HE22	1:B:275:ARG:HD3	1.84	0.43
1:D:151:LEU:C	1:D:151:LEU:HD23	2.39	0.43
1:A:75:CYS:HB2	1:A:101:ASP:OD2	2.19	0.42
1:D:327:ASN:HD21	1:D:350:GLY:N	2.16	0.42
1:C:151:LEU:C	1:C:151:LEU:HD23	2.39	0.42
1:A:389:LYS:CE	1:A:400:GLU:OE2	2.67	0.42
1:D:139:LEU:HD13	1:D:145:ILE:HD13	2.01	0.42
1:A:307:GLU:HG2	7:A:622:HOH:O	2.20	0.42
1:D:136:VAL:CG2	1:D:375:LEU:HD22	2.50	0.42
1:B:272:GLN:HE22	1:B:275:ARG:NH2	2.02	0.41
1:D:97:ILE:HD13	1:D:97:ILE:HG21	1.66	0.41
1:A:17:THR:HB	7:A:1159:HOH:O	2.20	0.41
1:B:128:PHE:CD2	1:B:366:LEU:CD1	3.03	0.41
1:B:280:LEU:HD11	7:B:901:HOH:O	2.20	0.41
1:A:380:ALA:HB2	1:A:409:ALA:HA	2.03	0.41
1:A:323:LEU:HD22	1:A:323:LEU:N	2.36	0.41
1:C:215:LEU:N	1:C:215:LEU:HD13	2.33	0.41
1:D:371:MET:SD	1:D:375:LEU:CD2	3.09	0.40
1:A:96:LEU:HD13	1:A:96:LEU:HA	1.94	0.40
1:D:364:ALA:HB2	2:D:501:HEM:HHC	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	392/410 (96%)	384 (98%)	7 (2%)	1 (0%)	46	41
1	B	391/410 (95%)	383 (98%)	8 (2%)	0	100	100
1	C	391/410 (95%)	384 (98%)	7 (2%)	0	100	100
1	D	391/410 (95%)	386 (99%)	3 (1%)	2 (0%)	34	26
All	All	1565/1640 (95%)	1537 (98%)	25 (2%)	3 (0%)	52	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	358	CYS
1	A	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%)	320 (100%)	0	100	100
1	B	319/334 (96%)	317 (99%)	2 (1%)	90	93
1	C	319/334 (96%)	319 (100%)	0	100	100
1	D	319/334 (96%)	319 (100%)	0	100	100
All	All	1277/1336 (96%)	1275 (100%)	2 (0%)	95	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	32	ASP
1	B	279	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS

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Mol	Chain	Res	Type
1	A	105	HIS
1	A	209	GLN
1	A	211	GLN
1	A	214	ASN
1	A	272	GLN
1	A	283	ASN
1	A	296	GLN
1	B	211	GLN
1	B	272	GLN
1	B	283	ASN
1	B	296	GLN
1	C	20	HIS
1	C	214	ASN
1	C	272	GLN
1	C	283	ASN
1	C	296	GLN
1	D	20	HIS
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 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	2.51	12 (40%)	24,82,82	2.64	13 (54%)
3	ANN	A	502	-	8,11,11	1.25	1 (12%)	11,14,14	1.85	3 (27%)
4	SO4	A	503	-	4,4,4	0.70	0	6,6,6	1.09	0
5	GOL	A	504	-	5,5,5	0.68	0	5,5,5	1.03	0
2	HEM	B	501	1	30,50,50	2.61	8 (26%)	24,82,82	2.43	10 (41%)
3	ANN	B	502	-	8,11,11	1.32	1 (12%)	11,14,14	1.07	1 (9%)
4	SO4	B	503	-	4,4,4	0.88	0	6,6,6	1.22	1 (16%)
4	SO4	B	504	-	4,4,4	1.52	1 (25%)	6,6,6	0.51	0
5	GOL	B	505	-	5,5,5	0.60	0	5,5,5	1.39	1 (20%)
2	HEM	C	501	1	30,50,50	2.35	9 (30%)	24,82,82	2.49	11 (45%)
3	ANN	C	502	-	8,11,11	1.46	1 (12%)	11,14,14	1.37	2 (18%)
4	SO4	C	503	-	4,4,4	0.36	0	6,6,6	0.50	0
5	GOL	C	504	-	5,5,5	0.57	0	5,5,5	1.08	1 (20%)
2	HEM	D	501	1	30,50,50	2.46	14 (46%)	24,82,82	2.78	13 (54%)
3	ANN	D	502	-	8,11,11	1.13	0	11,14,14	1.43	2 (18%)
4	SO4	D	503	-	4,4,4	0.49	0	6,6,6	0.28	0
5	GOL	D	504	-	5,5,5	0.31	0	5,5,5	1.00	0

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	ANN	A	502	-	-	0/2/6/6	0/1/1/1
4	SO4	A	503	-	-	0/0/0/0	0/0/0/0
5	GOL	A	504	-	-	0/4/4/4	0/0/0/0
2	HEM	B	501	1	-	0/10/54/54	0/0/8/8
3	ANN	B	502	-	-	0/2/6/6	0/1/1/1
4	SO4	B	503	-	-	0/0/0/0	0/0/0/0
4	SO4	B	504	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	505	-	-	0/4/4/4	0/0/0/0
2	HEM	C	501	1	-	0/10/54/54	0/0/8/8
3	ANN	C	502	-	-	0/2/6/6	0/1/1/1
4	SO4	C	503	-	-	0/0/0/0	0/0/0/0
5	GOL	C	504	-	-	0/4/4/4	0/0/0/0
2	HEM	D	501	1	-	0/10/54/54	0/0/8/8
3	ANN	D	502	-	-	0/2/6/6	0/1/1/1
4	SO4	D	503	-	-	0/0/0/0	0/0/0/0
5	GOL	D	504	-	-	0/4/4/4	0/0/0/0

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-C4B	-8.61	1.44	1.51
2	B	501	HEM	C3B-C4B	-8.09	1.44	1.51
2	C	501	HEM	C3B-C4B	-7.73	1.45	1.51
2	B	501	HEM	C3D-C4D	-6.77	1.42	1.51
2	D	501	HEM	C3B-C4B	-6.44	1.46	1.51
2	C	501	HEM	C2C-C1C	-4.20	1.44	1.52
2	A	501	HEM	C3D-C4D	-4.17	1.46	1.51
2	B	501	HEM	C2C-C1C	-4.09	1.44	1.52
2	C	501	HEM	C3D-C4D	-4.01	1.46	1.51
2	D	501	HEM	C3D-C4D	-3.83	1.46	1.51
2	A	501	HEM	C2C-C1C	-2.97	1.46	1.52
2	A	501	HEM	C2D-C1D	-2.82	1.42	1.51
2	D	501	HEM	C2C-C1C	-2.60	1.47	1.52
2	A	501	HEM	C2D-C3D	-2.43	1.47	1.54
2	B	501	HEM	C2B-C1B	-2.40	1.44	1.51
2	C	501	HEM	C2B-C1B	-2.29	1.44	1.51
2	D	501	HEM	C2D-C3D	-2.20	1.48	1.54
2	B	501	HEM	C2D-C1D	-2.14	1.44	1.51
3	B	502	ANN	O3-C5	-2.12	1.32	1.37
2	D	501	HEM	CMC-C2C	2.01	1.57	1.53
2	A	501	HEM	CMD-C2D	2.06	1.57	1.53
2	D	501	HEM	CAD-CBD	2.12	1.63	1.52
2	A	501	HEM	C1C-NC	2.14	1.38	1.36
2	D	501	HEM	FE-ND	2.19	2.09	1.97
2	C	501	HEM	CMC-C2C	2.30	1.58	1.53
2	C	501	HEM	FE-NB	2.30	2.09	1.97
2	C	501	HEM	CHC-C1C	2.36	1.42	1.36
2	D	501	HEM	C3B-CAB	2.38	1.55	1.51
2	A	501	HEM	C3B-CAB	2.40	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3B-CAB	2.50	1.56	1.51
2	D	501	HEM	CAA-C2A	2.51	1.56	1.52
4	B	504	SO4	O1-S	2.53	1.55	1.47
3	C	502	ANN	C4-C3	2.54	1.43	1.38
2	D	501	HEM	CMA-C3A	2.60	1.57	1.51
2	A	501	HEM	C3C-CAC	2.75	1.56	1.51
3	A	502	ANN	C4-C5	2.97	1.44	1.38
2	A	501	HEM	FE-ND	2.97	2.13	1.97
2	D	501	HEM	FE-NB	2.97	2.13	1.97
2	B	501	HEM	CMA-C3A	2.99	1.57	1.51
2	A	501	HEM	FE-NC	2.99	2.07	1.95
2	A	501	HEM	CMA-C3A	3.11	1.58	1.51
2	D	501	HEM	C3C-CAC	3.35	1.57	1.51
2	C	501	HEM	CMA-C3A	3.58	1.59	1.51
2	D	501	HEM	C4C-NC	4.02	1.41	1.36
2	C	501	HEM	FE-NC	4.04	2.11	1.95
2	B	501	HEM	FE-NC	4.18	2.12	1.95
2	D	501	HEM	FE-NC	4.37	2.13	1.95

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CBD-CAD-C3D	-4.81	99.55	113.55
3	A	502	ANN	C3-C4-C5	-4.14	114.53	119.74
2	D	501	HEM	C3C-CAC-CBC	-3.95	118.40	124.46
2	A	501	HEM	CAA-C2A-C1A	-3.76	122.92	127.01
2	A	501	HEM	CBD-CAD-C3D	-3.75	102.64	113.55
2	B	501	HEM	CBD-CAD-C3D	-3.69	102.80	113.55
2	C	501	HEM	CBD-CAD-C3D	-3.47	103.46	113.55
2	D	501	HEM	C3B-C4B-NB	-3.38	105.16	111.63
3	C	502	ANN	C3-C4-C5	-2.81	116.21	119.74
3	D	502	ANN	C3-C4-C5	-2.57	116.51	119.74
2	B	501	HEM	C4B-CHC-C1C	-2.47	121.69	125.82
2	A	501	HEM	CAA-CBA-CGA	-2.34	108.45	112.75
2	C	501	HEM	C3B-C4B-NB	-2.33	107.17	111.63
2	D	501	HEM	CAA-CBA-CGA	-2.29	108.54	112.75
2	A	501	HEM	CMA-C3A-C4A	-2.26	124.62	128.36
2	D	501	HEM	CAD-CBD-CGD	-2.20	104.04	113.02
5	B	505	GOL	C3-C2-C1	-2.12	102.80	111.12
2	C	501	HEM	CMA-C3A-C4A	-2.08	124.92	128.36
2	A	501	HEM	C2C-C1C-NC	-2.05	106.76	110.21
5	C	504	GOL	O1-C1-C2	-2.03	100.33	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	ANN	C3-C4-C5	-2.02	117.20	119.74
3	D	502	ANN	C4-C5-C6	2.14	123.67	120.20
3	A	502	ANN	C3-C2-C7	2.26	121.83	117.55
3	C	502	ANN	C4-C5-C6	2.28	123.90	120.20
2	A	501	HEM	C3B-C4B-CHC	2.29	126.39	123.16
2	C	501	HEM	C2C-C1C-CHC	2.39	127.32	123.68
2	D	501	HEM	CMD-C2D-C3D	2.39	124.92	114.35
2	C	501	HEM	CMD-C2D-C3D	2.41	125.03	114.35
2	D	501	HEM	C3B-C4B-CHC	2.49	126.67	123.16
4	B	503	SO4	O2-S-O1	2.54	117.53	109.50
2	B	501	HEM	C2D-C3D-C4D	2.58	105.87	101.50
2	A	501	HEM	C3C-CAC-CBC	2.58	128.42	124.46
2	B	501	HEM	C2C-C1C-CHC	2.62	127.66	123.68
3	A	502	ANN	C4-C5-C6	2.62	124.46	120.20
2	B	501	HEM	CMB-C2B-C3B	2.72	123.31	116.53
2	C	501	HEM	C3B-C4B-CHC	2.73	127.01	123.16
2	D	501	HEM	C2D-C3D-C4D	2.74	106.14	101.50
2	B	501	HEM	CMD-C2D-C3D	2.88	127.11	114.35
2	A	501	HEM	CMD-C2D-C3D	3.03	127.77	114.35
2	C	501	HEM	C2D-C3D-C4D	3.06	106.69	101.50
2	D	501	HEM	CMB-C2B-C3B	3.09	124.26	116.53
2	B	501	HEM	C3B-CAB-CBB	3.23	129.41	124.46
2	D	501	HEM	C2C-C1C-CHC	3.31	128.71	123.68
2	A	501	HEM	CAD-C3D-C4D	3.35	124.30	112.47
2	A	501	HEM	C2D-C3D-C4D	3.44	107.33	101.50
2	C	501	HEM	CAD-C3D-C4D	3.51	124.84	112.47
2	B	501	HEM	CAD-C3D-C2D	4.02	124.77	113.22
2	D	501	HEM	CAD-C3D-C4D	4.05	126.76	112.47
2	A	501	HEM	CMC-C2C-C3C	4.09	126.75	116.53
2	C	501	HEM	CMB-C2B-C3B	4.25	127.14	116.53
2	C	501	HEM	CMC-C2C-C3C	4.64	128.12	116.53
2	A	501	HEM	CMB-C2B-C3B	4.69	128.25	116.53
2	B	501	HEM	CAD-C3D-C4D	4.79	129.35	112.47
2	D	501	HEM	CAD-C3D-C2D	4.82	127.08	113.22
2	A	501	HEM	CAD-C3D-C2D	5.24	128.27	113.22
2	C	501	HEM	CAD-C3D-C2D	5.29	128.44	113.22
2	B	501	HEM	CMC-C2C-C3C	5.32	129.81	116.53
2	D	501	HEM	CMC-C2C-C3C	5.45	130.13	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	4	0
2	B	501	HEM	2	0
2	C	501	HEM	3	0
2	D	501	HEM	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.50	2 (0%) 91 92	13, 19, 31, 43	0
1	B	393/410 (95%)	-0.46	1 (0%) 94 94	12, 19, 31, 41	0
1	C	393/410 (95%)	-0.51	3 (0%) 87 88	14, 19, 31, 42	0
1	D	393/410 (95%)	-0.31	5 (1%) 79 80	15, 22, 35, 48	0
All	All	1572/1640 (95%)	-0.44	11 (0%) 89 89	12, 20, 32, 48	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	17	THR	4.6
1	D	142	ARG	3.3
1	D	409	ALA	3.0
1	A	17	THR	2.8
1	D	17	THR	2.7
1	A	409	ALA	2.6
1	B	409	ALA	2.3
1	D	310	GLY	2.3
1	C	310	GLY	2.0
1	D	312	VAL	2.0
1	C	309	GLY	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, 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
4	SO4	B	504	5/5	0.97	0.14	5.05	25,33,35,38	0
2	HEM	B	501	43/43	0.99	0.13	0.83	9,13,16,16	0
5	GOL	C	504	6/6	0.98	0.10	0.74	19,21,26,33	0
2	HEM	A	501	43/43	0.99	0.13	0.65	10,13,15,16	0
5	GOL	D	504	6/6	0.96	0.11	0.50	23,32,35,40	0
3	ANN	C	502	11/11	0.98	0.12	0.49	10,13,15,16	0
5	GOL	B	505	6/6	0.98	0.10	0.48	20,28,29,37	0
2	HEM	C	501	43/43	0.99	0.11	0.29	10,14,17,19	0
3	ANN	A	502	11/11	0.98	0.12	0.20	10,13,14,14	0
3	ANN	D	502	11/11	0.98	0.12	0.18	14,17,18,19	0
2	HEM	D	501	43/43	0.99	0.11	0.12	11,16,18,19	0
5	GOL	A	504	6/6	0.96	0.10	-0.20	16,19,24,35	0
3	ANN	B	502	11/11	0.99	0.10	-0.60	12,13,15,15	0
6	CL	A	505	1/1	0.99	0.09	-	19,19,19,19	0
4	SO4	B	503	5/5	0.98	0.09	-	30,33,37,40	0
4	SO4	D	503	5/5	0.98	0.07	-	36,38,42,42	0
6	CL	C	505	1/1	1.00	0.06	-	23,23,23,23	0
6	CL	B	506	1/1	0.99	0.07	-	20,20,20,20	0
6	CL	D	505	1/1	0.98	0.06	-	27,27,27,27	0
4	SO4	A	503	5/5	1.00	0.06	-	19,19,21,22	0
4	SO4	C	503	5/5	1.00	0.06	-	18,21,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.