



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:46 PM GMT

PDB ID : 4EGO
Title : The X-ray crystal structure of CYP199A4 in complex with indole-6-carboxylic 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 : 1.76 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>

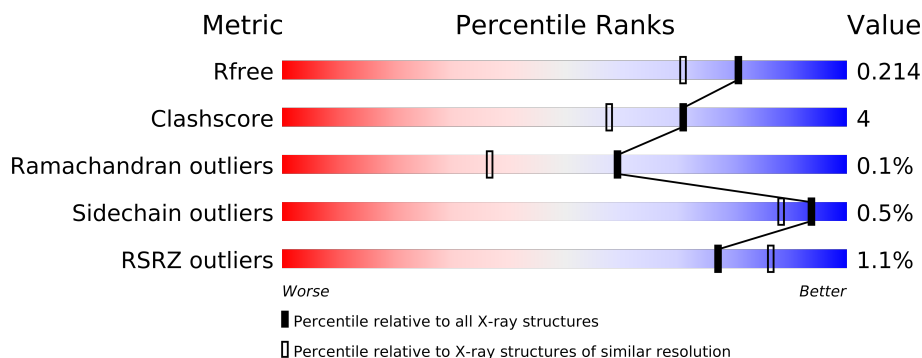
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.76 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	1134 (1.76-1.76)
Clashscore	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

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	1F1	A	503	-	X
3	1F1	A	504	-	X
3	1F1	B	503	-	X
3	1F1	C	503	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	1F1	D	501	-	X
4	SO4	A	506	-	X
4	SO4	C	505	-	X
4	SO4	C	506	-	X
5	GOL	A	508	-	X
5	GOL	B	506	-	X
5	GOL	B	507	-	X

2 Entry composition i

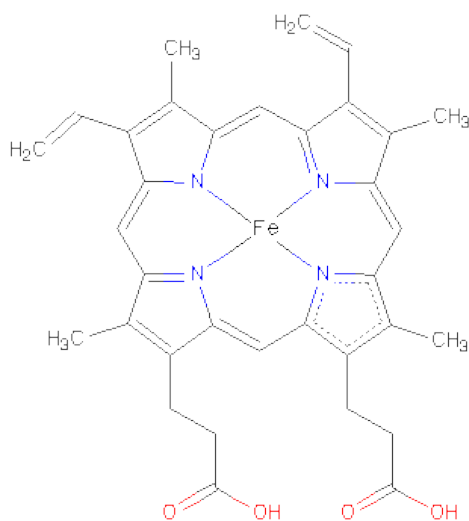
There are 7 unique types of molecules in this entry. The entry contains 13688 atoms, of which 0 are hydrogen and 0 are deuterium.

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	3	0
			3035	1922	535	566	12			
1	B	393	Total	C	N	O	S	0	1	0
			3027	1916	534	566	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: $C_{34}H_{32}FeN_4O_4$).



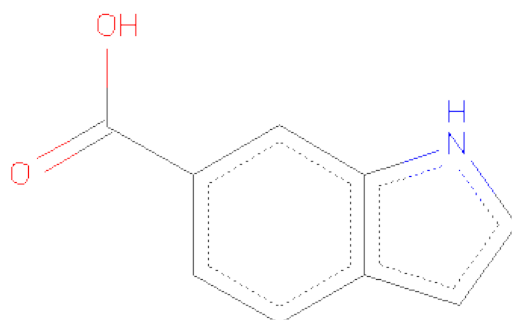
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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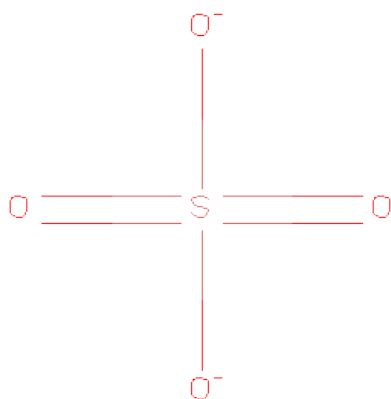
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 1H-INDOLE-6-CARBOXYLICACID (three-letter code: 1F1) (formula: $C_9H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	B	1	Total	C	N	O	0	0
			12	9	1	2		
3	B	1	Total	C	N	O	0	0
			12	9	1	2		
3	C	1	Total	C	N	O	0	0
			12	9	1	2		
3	C	1	Total	C	N	O	0	0
			12	9	1	2		
3	D	1	Total	C	N	O	0	0
			12	9	1	2		
3	D	1	Total	C	N	O	0	0
			12	9	1	2		

- 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	A	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	C	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		
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	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

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

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

- Molecule 7 is water.

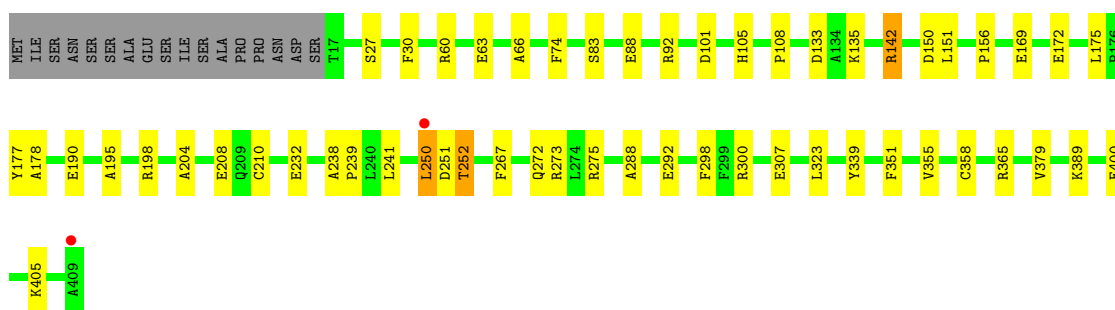
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	347	Total 347	O 347	0	0
7	B	332	Total 332	O 332	0	0
7	C	314	Total 314	O 314	0	0
7	D	225	Total 225	O 225	0	0

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.

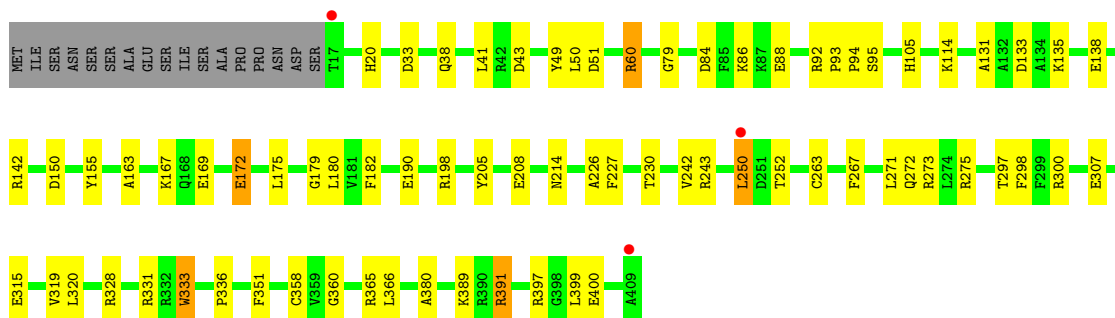
• Molecule 1: Cytochrome P450

Chain A:



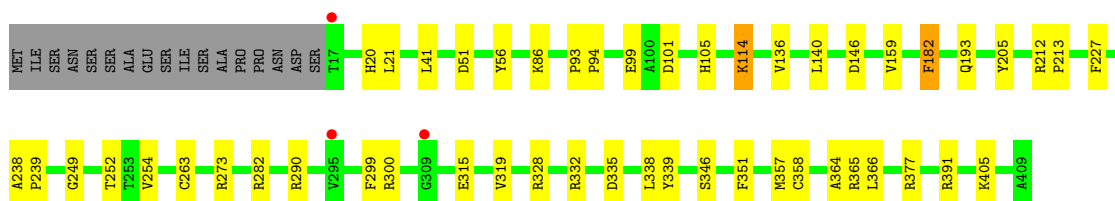
• Molecule 1: Cytochrome P450

Chain B:



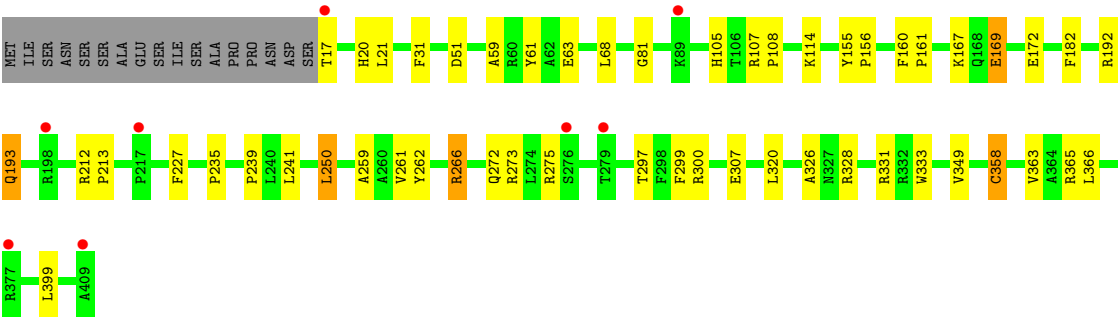
• Molecule 1: Cytochrome P450

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	106.86Å 143.67Å 172.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 1.76 39.00 – 1.76	Depositor EDS
% Data completeness (in resolution range)	90.0 (39.00-1.76) 89.9 (39.00-1.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.182 , 0.214 0.183 , 0.214	Depositor DCC
R_{free} test set	11782 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 32.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 234985 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13688	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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 49.59 % 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 7.2997e-05. 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, 1F1, 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	1.57	28/3116 (0.9%)	1.22	16/4239 (0.4%)
1	B	1.58	25/3102 (0.8%)	1.34	26/4221 (0.6%)
1	C	1.49	20/3093 (0.6%)	1.19	14/4209 (0.3%)
1	D	1.41	15/3093 (0.5%)	1.18	13/4209 (0.3%)
All	All	1.52	88/12404 (0.7%)	1.23	69/16878 (0.4%)

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	GLU	CD-OE2	11.59	1.38	1.25
1	B	169	GLU	CG-CD	11.59	1.69	1.51
1	A	210	CYS	CB-SG	8.82	1.97	1.82
1	A	172	GLU	CG-CD	8.73	1.65	1.51
1	A	307	GLU	CG-CD	8.17	1.64	1.51
1	C	193	GLN	CG-CD	8.15	1.69	1.51
1	A	74	PHE	CD2-CE2	8.14	1.55	1.39
1	B	172	GLU	CD-OE1	8.01	1.34	1.25
1	A	88	GLU	CB-CG	7.82	1.67	1.52
1	C	56	TYR	CD1-CE1	7.62	1.50	1.39
1	A	169	GLU	CG-CD	7.60	1.63	1.51
1	D	169	GLU	CG-CD	7.46	1.63	1.51
1	A	208	GLU	CG-CD	7.23	1.62	1.51
1	D	193	GLN	CB-CG	7.20	1.72	1.52
1	D	193	GLN	CG-CD	7.12	1.67	1.51
1	B	169	GLU	CD-OE1	7.06	1.33	1.25
1	A	190	GLU	CG-CD	7.05	1.62	1.51
1	A	88	GLU	CG-CD	6.94	1.62	1.51
1	C	351	PHE	CE1-CZ	6.87	1.50	1.37
1	B	315	GLU	CG-CD	6.69	1.61	1.51
1	B	88	GLU	CG-CD	6.67	1.61	1.51
1	C	315	GLU	CG-CD	6.66	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	PHE	CE1-CZ	6.50	1.49	1.37
1	B	267	PHE	CE1-CZ	6.48	1.49	1.37
1	D	61	TYR	CD1-CE1	6.46	1.49	1.39
1	B	49	TYR	CD1-CE1	6.39	1.49	1.39
1	A	177	TYR	CG-CD2	6.31	1.47	1.39
1	A	172	GLU	CD-OE1	6.25	1.32	1.25
1	D	259	ALA	CA-CB	6.21	1.65	1.52
1	D	363	VAL	CB-CG2	6.13	1.65	1.52
1	B	333	TRP	CG-CD1	6.01	1.45	1.36
1	A	63	GLU	CG-CD	5.98	1.60	1.51
1	B	79	GLY	N-CA	5.97	1.55	1.46
1	A	298	PHE	CD2-CE2	5.95	1.51	1.39
1	D	326	ALA	CA-CB	5.92	1.64	1.52
1	A	27	SER	CA-CB	5.89	1.61	1.52
1	B	380	ALA	CA-CB	5.89	1.64	1.52
1	C	339	TYR	CG-CD1	5.87	1.46	1.39
1	B	138	GLU	CG-CD	5.86	1.60	1.51
1	B	319	VAL	CB-CG2	5.84	1.65	1.52
1	B	131	ALA	CA-CB	5.83	1.64	1.52
1	D	31	PHE	CE1-CZ	5.79	1.48	1.37
1	B	250	LEU	CG-CD1	-5.78	1.30	1.51
1	C	136	VAL	CB-CG2	5.76	1.65	1.52
1	A	292	GLU	CD-OE2	5.73	1.31	1.25
1	A	379	VAL	CB-CG2	5.72	1.64	1.52
1	C	319	VAL	CB-CG1	5.71	1.64	1.52
1	D	333	TRP	CE3-CZ3	5.69	1.48	1.38
1	C	263	CYS	CB-SG	5.64	1.91	1.82
1	A	288	ALA	CA-CB	5.61	1.64	1.52
1	A	232	GLU	CB-CG	5.57	1.62	1.52
1	C	299	PHE	CD1-CE1	5.53	1.50	1.39
1	B	397	ARG	CZ-NH1	5.53	1.40	1.33
1	D	59	ALA	CA-CB	5.49	1.64	1.52
1	A	204	ALA	CA-CB	5.49	1.64	1.52
1	B	190	GLU	CG-CD	5.45	1.60	1.51
1	B	163	ALA	CA-CB	5.43	1.63	1.52
1	B	190	GLU	CD-OE1	5.40	1.31	1.25
1	A	30	PHE	CE2-CZ	5.38	1.47	1.37
1	D	349	VAL	CB-CG2	5.37	1.64	1.52
1	A	66	ALA	CA-CB	5.35	1.63	1.52
1	C	182	PHE	CD1-CE1	5.32	1.49	1.39
1	D	261	VAL	CB-CG1	5.27	1.64	1.52
1	B	351	PHE	CE2-CZ	5.25	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	227	PHE	CE2-CZ	5.24	1.47	1.37
1	D	81	GLY	N-CA	5.23	1.53	1.46
1	C	290	ARG	CB-CG	5.22	1.66	1.52
1	B	155	TYR	CD1-CE1	5.22	1.47	1.39
1	D	63	GLU	CD-OE1	-5.19	1.20	1.25
1	C	193	GLN	CB-CG	5.19	1.66	1.52
1	A	351	PHE	CE1-CZ	5.18	1.47	1.37
1	C	159	VAL	CB-CG2	5.17	1.63	1.52
1	A	355	VAL	CB-CG2	-5.17	1.42	1.52
1	C	99	GLU	CB-CG	5.15	1.61	1.52
1	C	299	PHE	CE1-CZ	5.14	1.47	1.37
1	B	227	PHE	CE2-CZ	5.12	1.47	1.37
1	B	226	ALA	N-CA	5.12	1.56	1.46
1	C	205	TYR	CD1-CE1	5.11	1.47	1.39
1	B	263	CYS	CB-SG	5.10	1.91	1.82
1	C	346	SER	CB-OG	-5.09	1.35	1.42
1	A	339	TYR	CG-CD2	5.08	1.45	1.39
1	A	195	ALA	CA-CB	5.08	1.63	1.52
1	D	172	GLU	CG-CD	5.08	1.59	1.51
1	C	364	ALA	CA-CB	5.06	1.63	1.52
1	B	242	VAL	CB-CG1	5.05	1.63	1.52
1	A	83	SER	CB-OG	5.04	1.48	1.42
1	C	254	VAL	CB-CG1	5.03	1.63	1.52
1	B	95	SER	CB-OG	5.00	1.48	1.42

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	397	ARG	NE-CZ-NH2	-12.38	114.11	120.30
1	B	391	ARG	NE-CZ-NH1	-11.94	114.33	120.30
1	D	273	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	D	328	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	D	273	ARG	NE-CZ-NH1	10.75	125.68	120.30
1	B	142	ARG	NE-CZ-NH1	-10.36	115.12	120.30
1	A	273	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	B	142	ARG	NE-CZ-NH2	9.65	125.13	120.30
1	D	328	ARG	NE-CZ-NH2	-9.41	115.60	120.30
1	B	198	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	A	142	ARG	NE-CZ-NH2	9.23	124.92	120.30
1	A	273	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	C	273	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	B	273	ARG	NE-CZ-NH1	8.66	124.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	B	243	ARG	NE-CZ-NH1	-8.39	116.11	120.30
1	C	273	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	300	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	B	133	ASP	CB-CG-OD1	8.02	125.52	118.30
1	B	397	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	A	198	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	D	300	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	D	266	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	B	273	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	D	107	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	377	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	B	243	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	C	101	ASP	CB-CG-OD1	-6.96	112.03	118.30
1	C	365	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	B	92	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	B	328	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	C	328	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	C	282	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	331	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	C	114	LYS	CD-CE-NZ	-6.30	97.22	111.70
1	C	300	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	D	365	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	B	60	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	B	328	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	D	266	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	D	331	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	198	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	60	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	B	180	LEU	CB-CG-CD2	-6.03	100.76	111.00
1	D	21	LEU	CB-CG-CD1	-5.97	100.84	111.00
1	A	133	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	198	ARG	CB-CG-CD	5.90	126.94	111.60
1	A	142	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	A	101	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	B	84	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	299	PHE	CB-CG-CD1	-5.73	116.79	120.80
1	C	332	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	365	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	298	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	B	86	LYS	CD-CE-NZ	-5.51	99.02	111.70
1	B	365	ARG	NE-CZ-NH1	5.45	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	391	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	B	198	ARG	CB-CG-CD	5.27	125.29	111.60
1	A	198	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	101	ASP	OD1-CG-OD2	5.20	133.18	123.30
1	B	300	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	266	ARG	CG-CD-NE	5.18	122.68	111.80
1	A	92	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	B	43	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	391	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	252	THR	CA-CB-CG2	-5.09	105.28	112.40
1	B	33	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	C	146	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	299	PHE	CB-CG-CD2	-5.03	117.28	120.80

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	3035	0	3015	25	0
1	B	3027	0	2999	38	0
1	C	3021	0	2993	20	0
1	D	3021	0	2993	24	0
2	A	43	0	30	4	0
2	B	43	0	30	5	0
2	C	43	0	30	5	0
2	D	43	0	30	3	0
3	A	36	0	18	0	0
3	B	24	0	12	3	0
3	C	24	0	12	3	0
3	D	24	0	12	2	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	15	0	0	0	0
4	D	10	0	0	0	0
5	A	12	0	16	0	0
5	B	18	0	24	2	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	347	0	0	3	0
7	B	332	0	0	5	0
7	C	314	0	0	5	0
7	D	225	0	0	5	0
All	All	13688	0	12230	111	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 (111) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:60:ARG:HH12	5:B:506:GOL:H32	1.09	1.10
1:D:272:GLN:HE22	1:D:275:ARG:HH11	1.14	0.91
1:A:272:GLN:HE22	1:A:275:ARG:HH11	1.21	0.86
1:B:307:GLU:HG2	7:B:670:HOH:O	1.75	0.84
1:B:135:LYS:CE	1:B:150:ASP:O	2.27	0.82
1:B:272:GLN:HE22	1:B:275:ARG:HH11	1.27	0.82
1:B:60:ARG:NH1	5:B:506:GOL:H32	1.93	0.79
1:D:307:GLU:HG2	7:D:717:HOH:O	1.85	0.75
1:D:105:HIS:HD2	7:D:613:HOH:O	1.70	0.73
2:D:502:HEM:HBC2	2:D:502:HEM:HMC1	1.70	0.73
1:D:262:TYR:CE2	1:D:266:ARG:HD3	2.24	0.72
1:D:105:HIS:HE1	2:D:502:HEM:O1D	1.73	0.71
1:C:105:HIS:HD2	7:C:607:HOH:O	1.74	0.70
1:D:262:TYR:CZ	1:D:266:ARG:HD3	2.27	0.69
1:A:105:HIS:HD2	7:A:626:HOH:O	1.75	0.69
1:B:208[B]:GLU:HG2	7:B:826:HOH:O	1.92	0.68
1:B:250:LEU:C	1:B:250:LEU:HD13	2.15	0.67
1:B:135:LYS:HE3	1:B:150:ASP:O	1.95	0.66
1:B:105:HIS:HE1	2:B:501:HEM:O1D	1.79	0.64
1:A:135:LYS:CE	1:A:150:ASP:O	2.46	0.64
1:B:114:LYS:HE3	7:B:804:HOH:O	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:323:LEU:HD12	1:A:323:LEU:N	2.12	0.63
1:A:135:LYS:HE3	1:A:150:ASP:O	1.97	0.63
1:C:105:HIS:HE1	2:C:501:HEM:O1D	1.81	0.62
1:B:135:LYS:NZ	1:B:150:ASP:O	2.32	0.62
1:B:272:GLN:HE22	1:B:275:ARG:NH1	1.97	0.62
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.83	0.61
1:D:167:LYS:HE3	1:D:169:GLU:HG2	1.81	0.61
1:A:105:HIS:HE1	2:A:501:HEM:O1D	1.83	0.61
1:A:323:LEU:H	1:A:323:LEU:HD12	1.67	0.60
1:B:167:LYS:NZ	1:B:214:ASN:ND2	2.49	0.60
3:C:503:1F1:H6	7:C:734:HOH:O	2.01	0.60
2:B:501:HEM:HBC2	2:B:501:HEM:HMC1	1.83	0.59
1:C:114:LYS:NZ	7:C:727:HOH:O	2.35	0.59
1:C:405:LYS:HE3	7:D:749:HOH:O	2.01	0.59
1:A:405:LYS:HE3	7:A:779:HOH:O	2.01	0.59
1:D:20:HIS:HD2	1:D:51:ASP:OD1	1.86	0.58
1:D:17:THR:O	1:D:17:THR:OG1	2.21	0.58
1:B:167:LYS:HZ2	1:B:214:ASN:ND2	2.02	0.57
1:D:272:GLN:HE22	1:D:275:ARG:NH1	1.95	0.56
1:D:114:LYS:HD3	1:D:227:PHE:CZ	2.43	0.53
1:D:114:LYS:HD3	1:D:227:PHE:HZ	1.73	0.53
1:B:179:GLY:HA3	3:B:503:1F1:C2	2.38	0.53
1:B:230:THR:O	1:B:230:THR:HG22	2.10	0.52
1:B:389:LYS:HE3	1:B:400:GLU:OE2	2.09	0.52
1:C:20:HIS:HD2	1:C:51:ASP:OD1	1.91	0.52
1:A:142:ARG:HD3	1:B:205:TYR:HA	1.92	0.51
1:B:358:CYS:HA	2:B:501:HEM:CHA	2.41	0.51
1:C:21:LEU:HD12	1:C:41:LEU:HD23	1.93	0.51
1:D:250:LEU:HD12	1:D:250:LEU:O	2.12	0.50
1:C:335:ASP:HB3	1:C:338:LEU:HD22	1.94	0.49
1:B:172:GLU:HG2	7:B:747:HOH:O	2.12	0.49
1:C:252:THR:HB	2:C:501:HEM:C3B	2.48	0.49
1:B:230:THR:O	1:B:230:THR:CG2	2.60	0.49
1:A:272:GLN:HE22	1:A:275:ARG:NH1	2.01	0.48
1:A:358:CYS:HA	2:A:501:HEM:CHA	2.44	0.48
3:D:501:1F1:H6	7:D:713:HOH:O	2.14	0.48
1:C:358:CYS:HA	2:C:501:HEM:CHA	2.43	0.48
1:B:20:HIS:HD2	1:B:51:ASP:OD1	1.97	0.47
1:B:297:THR:HB	1:B:320:LEU:HD11	1.97	0.47
1:C:182:PHE:CE2	3:C:502:1F1:H8	2.50	0.47
1:A:175:LEU:HD23	1:A:251[B]:ASP:OD1	2.15	0.47
1:D:399:LEU:HD12	7:D:694:HOH:O	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:235:PRO:O	1:D:239:PRO:HD3	2.16	0.46
1:B:271:LEU:O	1:B:275:ARG:HG3	2.16	0.46
1:A:156:PRO:HB2	1:A:250:LEU:HD11	1.96	0.46
1:B:182:PHE:CZ	3:B:502:1F1:H8	2.51	0.46
1:D:108:PRO:HB3	1:D:241:LEU:HD21	1.99	0.45
1:D:160:PHE:HB3	1:D:161:PRO:HD3	1.99	0.44
1:A:323:LEU:CD1	1:A:323:LEU:H	2.29	0.44
1:A:405:LYS:CE	7:A:779:HOH:O	2.63	0.44
1:A:108:PRO:HB3	1:A:241:LEU:HD21	1.98	0.44
1:D:297:THR:HB	1:D:320:LEU:HD11	1.99	0.44
1:B:167:LYS:NZ	1:B:214:ASN:HD22	2.14	0.44
1:A:252:THR:HB	2:A:501:HEM:C3B	2.52	0.44
1:D:358:CYS:HA	2:D:502:HEM:CHA	2.47	0.44
1:B:175:LEU:HB3	3:B:503:1F1:C8	2.48	0.44
1:B:399:LEU:HD12	7:B:885:HOH:O	2.18	0.43
1:C:140:LEU:HA	1:C:140:LEU:HD23	1.87	0.43
1:A:272:GLN:HE22	1:A:275:ARG:HD3	1.83	0.43
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.90	0.43
1:C:238:ALA:HB3	1:C:239:PRO:HD3	1.99	0.43
1:A:272:GLN:NE2	1:A:275:ARG:HD3	2.33	0.43
1:C:182:PHE:CZ	3:C:502:1F1:H8	2.54	0.43
1:C:114:LYS:CE	7:C:727:HOH:O	2.66	0.43
1:A:323:LEU:CD1	1:A:323:LEU:N	2.82	0.42
1:B:360:GLY:HA3	2:B:501:HEM:C3C	2.54	0.42
1:D:192:ARG:HH21	1:D:193:GLN:HE22	1.68	0.42
1:B:391:ARG:HH11	1:B:391:ARG:HD2	1.48	0.42
2:C:501:HEM:CMC	2:C:501:HEM:HBC2	2.50	0.42
1:D:68:LEU:HA	1:D:68:LEU:HD23	1.92	0.42
1:C:249:GLY:HA2	2:C:501:HEM:C2C	2.54	0.42
1:C:93:PRO:HA	1:C:94:PRO:HD3	1.81	0.42
1:C:357:MET:O	1:C:358:CYS:C	2.58	0.42
1:C:212:ARG:N	1:C:213:PRO:CD	2.83	0.42
1:B:333:TRP:O	1:B:336:PRO:HD3	2.19	0.42
1:A:178:ALA:HB3	1:A:251[B]:ASP:CG	2.40	0.41
1:B:38:GLN:HA	1:B:41:LEU:HD12	2.02	0.41
1:D:155:TYR:HB3	1:D:156:PRO:HD3	2.02	0.41
1:B:252:THR:HB	2:B:501:HEM:C3B	2.55	0.41
1:A:142:ARG:HG3	1:B:208[A]:GLU:OE1	2.21	0.41
1:A:151:LEU:C	1:A:151:LEU:HD23	2.41	0.41
1:A:238:ALA:HB3	1:A:239:PRO:HD3	2.02	0.41
1:B:50:LEU:HA	1:B:50:LEU:HD23	1.86	0.41
1:A:389:LYS:NZ	1:A:400:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:167:LYS:HZ1	1:B:214:ASN:HD22	1.69	0.40
1:C:20:HIS:CD2	1:C:51:ASP:OD1	2.73	0.40
1:B:175:LEU:HD23	1:B:250:LEU:HD12	2.02	0.40
1:C:86:LYS:NZ	7:C:767:HOH:O	2.34	0.40
1:D:212:ARG:N	1:D:213:PRO:CD	2.84	0.40
1:D:182:PHE:CE2	3:D:503:1F1:H8	2.56	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	394/410 (96%)	386 (98%)	8 (2%)	0	100	100
1	B	392/410 (96%)	384 (98%)	8 (2%)	0	100	100
1	C	391/410 (95%)	383 (98%)	8 (2%)	0	100	100
1	D	391/410 (95%)	384 (98%)	6 (2%)	1 (0%)	50	28
All	All	1568/1640 (96%)	1537 (98%)	30 (2%)	1 (0%)	59	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	358	CYS

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	322/334 (96%)	321 (100%)	1 (0%)	96	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	320/334 (96%)	318 (99%)	2 (1%)	92	85
1	C	319/334 (96%)	318 (100%)	1 (0%)	96	93
1	D	319/334 (96%)	317 (99%)	2 (1%)	92	85
All	All	1280/1336 (96%)	1274 (100%)	6 (0%)	94	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	LEU
1	B	298	PHE
1	B	366	LEU
1	C	366	LEU
1	D	250	LEU
1	D	366	LEU

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	211	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	207	ASN
1	B	211	GLN
1	B	214	ASN
1	B	255	ASN
1	B	272	GLN
1	B	283	ASN
1	B	296	GLN
1	C	20	HIS
1	C	105	HIS
1	C	211	GLN
1	C	214	ASN
1	C	283	ASN
1	C	296	GLN

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Mol	Chain	Res	Type
1	D	20	HIS
1	D	105	HIS
1	D	168	GLN
1	D	193	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 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 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	3.80	15 (30%)	46,82,82	2.58	15 (32%)
3	1F1	A	502	-	13,13,13	2.52	5 (38%)	18,18,18	2.15	7 (38%)
3	1F1	A	503	-	13,13,13	1.98	4 (30%)	18,18,18	2.56	6 (33%)
3	1F1	A	504	-	13,13,13	1.97	4 (30%)	18,18,18	1.45	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	505	-	4,4,4	0.64	0	6,6,6	2.26	1 (16%)
4	SO4	A	506	-	4,4,4	1.47	1 (25%)	6,6,6	0.42	0
5	GOL	A	507	-	5,5,5	0.27	0	5,5,5	1.20	0
5	GOL	A	508	-	5,5,5	0.42	0	5,5,5	1.59	1 (20%)
2	HEM	B	501	1	49,50,50	3.21	20 (40%)	46,82,82	2.37	12 (26%)
3	1F1	B	502	-	13,13,13	2.09	5 (38%)	18,18,18	1.58	4 (22%)
3	1F1	B	503	-	13,13,13	2.64	7 (53%)	18,18,18	1.79	4 (22%)
4	SO4	B	504	-	4,4,4	0.63	0	6,6,6	0.62	0
5	GOL	B	505	-	5,5,5	0.62	0	5,5,5	1.16	0
5	GOL	B	506	-	5,5,5	0.74	0	5,5,5	3.50	3 (60%)
5	GOL	B	507	-	5,5,5	0.45	0	5,5,5	0.99	0
2	HEM	C	501	1	49,50,50	3.93	18 (36%)	46,82,82	2.22	19 (41%)
3	1F1	C	502	-	13,13,13	1.82	3 (23%)	18,18,18	1.85	4 (22%)
3	1F1	C	503	-	13,13,13	2.55	3 (23%)	18,18,18	1.49	4 (22%)
4	SO4	C	504	-	4,4,4	0.50	0	6,6,6	0.59	0
4	SO4	C	505	-	4,4,4	0.42	0	6,6,6	0.98	1 (16%)
4	SO4	C	506	-	4,4,4	0.92	0	6,6,6	0.56	0
5	GOL	C	507	-	5,5,5	0.43	0	5,5,5	0.90	0
3	1F1	D	501	-	13,13,13	2.65	6 (46%)	18,18,18	2.16	7 (38%)
2	HEM	D	502	1	49,50,50	2.95	20 (40%)	46,82,82	3.39	17 (36%)
3	1F1	D	503	-	13,13,13	2.09	5 (38%)	18,18,18	1.42	3 (16%)
4	SO4	D	504	-	4,4,4	0.49	0	6,6,6	0.71	0
4	SO4	D	505	-	4,4,4	0.49	0	6,6,6	1.47	2 (33%)
5	GOL	D	506	-	5,5,5	0.29	0	5,5,5	1.03	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	-	0/14/114/114	0/0/8/8
3	1F1	A	502	-	-	0/4/4/4	0/0/2/2
3	1F1	A	503	-	-	0/4/4/4	0/0/2/2
3	1F1	A	504	-	-	0/4/4/4	0/0/2/2
4	SO4	A	505	-	-	0/0/0/0	0/0/0/0
4	SO4	A	506	-	-	0/0/0/0	0/0/0/0
5	GOL	A	507	-	-	0/4/4/4	0/0/0/0
5	GOL	A	508	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	501	1	-	0/14/114/114	0/0/8/8
3	1F1	B	502	-	-	0/4/4/4	0/0/2/2
3	1F1	B	503	-	-	0/4/4/4	0/0/2/2
4	SO4	B	504	-	-	0/0/0/0	0/0/0/0
5	GOL	B	505	-	-	0/4/4/4	0/0/0/0
5	GOL	B	506	-	-	0/4/4/4	0/0/0/0
5	GOL	B	507	-	-	0/4/4/4	0/0/0/0
2	HEM	C	501	1	-	0/14/114/114	0/0/8/8
3	1F1	C	502	-	-	0/4/4/4	0/0/2/2
3	1F1	C	503	-	-	0/4/4/4	0/0/2/2
4	SO4	C	504	-	-	0/0/0/0	0/0/0/0
4	SO4	C	505	-	-	0/0/0/0	0/0/0/0
4	SO4	C	506	-	-	0/0/0/0	0/0/0/0
5	GOL	C	507	-	-	0/4/4/4	0/0/0/0
3	1F1	D	501	-	-	0/4/4/4	0/0/2/2
2	HEM	D	502	1	-	0/14/114/114	0/0/8/8
3	1F1	D	503	-	-	0/4/4/4	0/0/2/2
4	SO4	D	504	-	-	0/0/0/0	0/0/0/0
4	SO4	D	505	-	-	0/0/0/0	0/0/0/0
5	GOL	D	506	-	-	0/4/4/4	0/0/0/0

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3D-C4D	18.45	1.49	1.44
2	C	501	HEM	C2D-C1D	15.99	1.48	1.44
2	C	501	HEM	C2B-C1B	15.67	1.48	1.44
2	B	501	HEM	C2B-C1B	11.86	1.47	1.44
2	D	502	HEM	C2B-C1B	10.67	1.47	1.44
2	B	501	HEM	C2D-C1D	-9.88	1.42	1.44
2	A	501	HEM	C4A-C3A	9.22	1.51	1.40
2	C	501	HEM	C3D-C4D	8.71	1.46	1.44
2	D	502	HEM	C2D-C1D	7.68	1.46	1.44
2	A	501	HEM	C2B-C1B	-6.86	1.42	1.44
3	C	503	1F1	C9-C8	6.56	1.59	1.36
2	A	501	HEM	CHB-C1B	5.91	1.44	1.35
2	A	501	HEM	C3B-CAB	5.56	1.58	1.40
2	A	501	HEM	C3B-C2B	-5.56	1.34	1.43
2	B	501	HEM	C3D-C4D	5.54	1.45	1.44
3	B	503	1F1	C9-C8	5.45	1.55	1.36
3	D	501	1F1	C9-C8	5.41	1.55	1.36
2	A	501	HEM	C3C-C2C	-5.37	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	HEM	C3C-CAC	5.35	1.57	1.40
3	A	503	1F1	C9-C8	5.29	1.55	1.36
3	A	502	1F1	C5-C4	5.29	1.48	1.39
3	C	503	1F1	C9-N10	5.26	1.53	1.37
2	D	502	HEM	C3B-CAB	5.12	1.56	1.40
3	A	504	1F1	C9-C8	5.04	1.54	1.36
2	C	501	HEM	C3C-C2C	-4.96	1.35	1.43
2	D	502	HEM	C3C-C2C	-4.72	1.35	1.43
2	B	501	HEM	C3C-C2C	-4.67	1.35	1.43
2	D	502	HEM	C1A-C2A	4.64	1.51	1.43
2	B	501	HEM	C4A-C3A	4.64	1.46	1.40
2	C	501	HEM	C3B-CAB	4.59	1.54	1.40
2	B	501	HEM	C3B-CAB	4.57	1.54	1.40
2	C	501	HEM	C3B-C2B	-4.56	1.35	1.43
2	B	501	HEM	C3C-CAC	4.54	1.54	1.40
2	B	501	HEM	FE-NA	4.50	2.11	1.92
2	B	501	HEM	CHB-C1B	4.46	1.42	1.35
3	A	502	1F1	C9-C8	4.35	1.51	1.36
2	D	502	HEM	FE-NA	4.34	2.11	1.92
3	C	502	1F1	C9-C8	4.31	1.51	1.36
3	D	501	1F1	C12-C4	4.23	1.44	1.37
2	A	501	HEM	CMC-C2C	4.19	1.60	1.47
3	B	502	1F1	C9-C8	4.16	1.51	1.36
2	C	501	HEM	C3C-CAC	4.06	1.53	1.40
3	B	503	1F1	O1-C2	4.00	1.35	1.23
3	D	503	1F1	C9-C8	3.97	1.50	1.36
2	A	501	HEM	C3C-CAC	3.88	1.52	1.40
3	B	503	1F1	C9-N10	3.78	1.49	1.37
3	D	501	1F1	C9-N10	3.77	1.49	1.37
3	A	502	1F1	C12-C4	3.72	1.44	1.37
2	D	502	HEM	C3B-C2B	-3.60	1.37	1.43
3	B	503	1F1	C12-C4	3.52	1.43	1.37
3	D	501	1F1	C4-C2	3.51	1.56	1.49
3	D	503	1F1	C12-C4	3.40	1.43	1.37
3	D	503	1F1	C5-C4	3.33	1.45	1.39
3	B	502	1F1	C5-C4	3.22	1.44	1.39
2	D	502	HEM	CAA-C2A	3.19	1.57	1.52
2	C	501	HEM	CHB-C1B	3.14	1.40	1.35
3	C	502	1F1	C5-C4	3.12	1.44	1.39
2	B	501	HEM	CMC-C2C	3.09	1.57	1.47
2	A	501	HEM	CMD-C2D	3.04	1.56	1.47
2	B	501	HEM	C3B-C2B	-3.02	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	1F1	C9-N10	3.02	1.46	1.37
2	D	502	HEM	FE-NC	3.02	2.09	1.97
2	C	501	HEM	C4A-C3A	2.97	1.43	1.40
2	B	501	HEM	C1D-ND	2.91	1.44	1.37
2	C	501	HEM	CMB-C2B	2.90	1.56	1.47
2	B	501	HEM	CHD-C4C	2.90	1.41	1.36
2	D	502	HEM	C3D-C2D	2.89	1.48	1.43
2	D	502	HEM	FE-NB	2.85	2.08	1.97
2	B	501	HEM	CAA-C2A	2.84	1.57	1.52
2	C	501	HEM	FE-NB	2.83	2.08	1.97
2	B	501	HEM	CAD-CBD	2.83	1.60	1.52
2	B	501	HEM	C2C-C1C	2.80	1.51	1.43
2	D	502	HEM	CMD-C2D	2.79	1.56	1.47
2	B	501	HEM	C4C-NC	-2.78	1.34	1.38
3	D	503	1F1	C9-N10	2.78	1.46	1.37
3	B	502	1F1	C9-N10	2.75	1.46	1.37
2	C	501	HEM	CAD-CBD	2.75	1.60	1.52
3	A	504	1F1	C9-N10	2.74	1.46	1.37
2	D	502	HEM	CMA-C3A	2.67	1.57	1.51
2	D	502	HEM	CMC-C2C	2.60	1.55	1.47
2	B	501	HEM	CHA-C4D	2.60	1.39	1.35
2	D	502	HEM	CMB-C2B	2.54	1.55	1.47
2	A	501	HEM	FE-NA	2.53	2.03	1.92
3	D	503	1F1	C6-C5	2.50	1.41	1.36
3	D	501	1F1	C6-C5	2.50	1.41	1.36
2	D	502	HEM	CAD-CBD	2.43	1.59	1.52
2	A	501	HEM	C3D-C2D	2.40	1.48	1.43
3	B	503	1F1	C4-C2	2.39	1.54	1.49
2	A	501	HEM	CAA-C2A	2.37	1.56	1.52
2	D	502	HEM	CHD-C4C	2.35	1.40	1.36
2	D	502	HEM	C4C-NC	2.33	1.41	1.38
3	A	502	1F1	C6-C7	-2.32	1.36	1.41
2	C	501	HEM	O1D-CGD	2.27	1.30	1.22
3	C	502	1F1	C9-N10	2.26	1.44	1.37
3	A	504	1F1	C12-C4	2.25	1.41	1.37
3	B	502	1F1	C12-C11	-2.24	1.34	1.39
2	A	501	HEM	CAD-CBD	2.18	1.58	1.52
3	C	503	1F1	C12-C4	2.16	1.41	1.37
3	A	503	1F1	C12-C4	2.15	1.41	1.37
3	A	504	1F1	C5-C4	2.14	1.43	1.39
2	A	501	HEM	CMB-C2B	2.10	1.53	1.47
3	D	501	1F1	C5-C4	2.10	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	1F1	C6-C5	2.09	1.41	1.36
2	D	502	HEM	CHC-C4B	2.08	1.44	1.39
3	A	502	1F1	C12-C11	-2.08	1.34	1.39
3	A	503	1F1	C5-C4	2.08	1.42	1.39
2	C	501	HEM	CMC-C2C	2.07	1.53	1.47
3	B	503	1F1	C5-C4	2.05	1.42	1.39
2	C	501	HEM	C1A-NA	2.05	1.40	1.36
2	B	501	HEM	CMB-C2B	2.04	1.53	1.47
2	C	501	HEM	CHC-C1C	2.04	1.39	1.36
2	C	501	HEM	CHD-C4C	2.03	1.39	1.36
2	B	501	HEM	C1C-NC	2.01	1.40	1.38
4	A	506	SO4	O1-S	-2.01	1.40	1.47
3	B	503	1F1	C6-C5	2.01	1.40	1.36
2	C	501	HEM	CMD-C2D	2.00	1.53	1.47

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	HEM	C3B-C4B-NB	-12.25	105.24	114.00
2	D	502	HEM	C1B-NB-C4B	8.23	113.58	105.16
2	D	502	HEM	CHC-C4B-NB	7.20	130.57	124.58
2	B	501	HEM	CHC-C4B-NB	-6.83	118.91	124.58
2	A	501	HEM	C3A-C4A-NA	-6.71	104.34	109.41
2	C	501	HEM	CBD-CAD-C3D	-6.36	100.48	114.37
5	B	506	GOL	C3-C2-C1	-6.26	83.61	111.26
2	D	502	HEM	CHD-C1D-ND	6.17	129.71	124.58
2	B	501	HEM	C4C-NC-C1C	5.97	111.74	105.53
2	D	502	HEM	CMA-C3A-C4A	-5.96	119.45	128.62
2	B	501	HEM	CHC-C1C-NC	5.88	129.84	124.73
3	A	503	1F1	C5-C6-C7	-5.63	111.98	120.83
2	C	501	HEM	C3B-C4B-NB	-5.58	110.01	114.00
2	A	501	HEM	C4C-NC-C1C	5.49	111.24	105.53
2	D	502	HEM	C4A-C3A-C2A	5.47	110.81	107.00
2	A	501	HEM	C1B-NB-C4B	-5.44	99.59	105.16
2	A	501	HEM	CHD-C4C-NC	5.32	129.36	124.73
4	A	505	SO4	O2-S-O1	5.30	127.06	109.53
2	D	502	HEM	C4D-ND-C1D	5.27	110.56	105.16
2	B	501	HEM	CHD-C4C-NC	4.96	129.04	124.73
2	D	502	HEM	C2D-C1D-ND	-4.94	107.10	112.93
2	D	502	HEM	CBD-CAD-C3D	-4.91	103.67	114.37
2	B	501	HEM	CBD-CAD-C3D	-4.83	103.84	114.37
2	A	501	HEM	C4A-CHB-C1B	-4.73	121.25	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CBD-CAD-C3D	-4.56	104.41	114.37
2	C	501	HEM	O2D-CGD-O1D	-4.46	111.95	123.30
3	C	502	1F1	C5-C6-C7	-4.42	113.89	120.83
2	A	501	HEM	CHB-C4A-NA	4.32	131.80	124.58
2	A	501	HEM	C4A-C3A-C2A	4.25	109.95	107.00
3	D	501	1F1	O3-C2-C4	4.18	126.08	115.01
3	A	503	1F1	C4-C12-C11	-4.18	111.67	117.90
3	A	502	1F1	C8-C7-C6	-4.07	122.46	136.72
2	B	501	HEM	CMA-C3A-C4A	-4.06	122.38	128.62
2	A	501	HEM	CMA-C3A-C4A	-4.04	122.41	128.62
3	A	503	1F1	C5-C4-C12	4.00	125.10	119.22
3	D	501	1F1	C12-C4-C2	3.98	126.84	121.06
3	A	503	1F1	C8-C7-C6	-3.74	123.61	136.72
3	B	503	1F1	C8-C7-C6	-3.74	123.65	136.72
3	B	503	1F1	C5-C6-C7	-3.73	114.97	120.83
2	C	501	HEM	O2D-CGD-CBD	3.71	127.32	114.22
2	D	502	HEM	C1A-C2A-C3A	-3.54	103.25	106.92
5	B	506	GOL	O2-C2-C3	3.52	124.27	108.22
3	A	503	1F1	C12-C4-C2	-3.50	115.97	121.06
2	C	501	HEM	C4A-C3A-C2A	3.49	109.42	107.00
3	A	502	1F1	C6-C7-C11	3.42	127.30	119.94
2	A	501	HEM	CHC-C1C-NC	3.31	127.60	124.73
3	A	502	1F1	O3-C2-C4	3.30	123.73	115.01
2	A	501	HEM	CHC-C4B-NB	-3.28	121.86	124.58
3	D	501	1F1	O3-C2-O1	-3.28	115.91	123.35
2	C	501	HEM	CHD-C1D-ND	3.24	127.28	124.58
2	D	502	HEM	C4C-NC-C1C	3.14	108.80	105.53
2	B	501	HEM	C4D-ND-C1D	-3.12	101.97	105.16
3	A	502	1F1	C6-C5-C4	-3.11	117.27	120.82
3	A	502	1F1	O3-C2-O1	-3.09	116.34	123.35
3	C	503	1F1	C8-C7-C6	-3.03	126.11	136.72
3	C	502	1F1	C8-C7-C6	-3.03	126.12	136.72
3	A	503	1F1	C6-C7-C11	3.02	126.44	119.94
3	D	501	1F1	C6-C5-C4	2.96	124.20	120.82
2	B	501	HEM	CMA-C3A-C2A	2.92	130.45	124.94
3	C	502	1F1	C4-C12-C11	-2.92	113.54	117.90
2	C	501	HEM	CAD-C3D-C4D	2.83	129.62	124.53
2	C	501	HEM	CAD-CBD-CGD	-2.82	104.67	113.48
3	A	502	1F1	C5-C6-C7	-2.82	116.40	120.83
2	C	501	HEM	C4A-CHB-C1B	-2.81	123.77	127.47
2	B	501	HEM	C1D-CHD-C4C	-2.80	119.19	126.57
3	B	502	1F1	C5-C6-C7	-2.76	116.49	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	1F1	C8-C7-C6	-2.75	127.10	136.72
2	C	501	HEM	C2D-C1D-ND	-2.74	109.69	112.93
3	A	504	1F1	C8-C7-C6	-2.72	127.19	136.72
3	C	503	1F1	C8-C9-N10	-2.71	103.59	108.17
2	D	502	HEM	O1A-CGA-CBA	-2.67	113.83	123.03
3	D	503	1F1	C8-C7-C6	-2.65	127.43	136.72
3	D	503	1F1	C8-C9-N10	-2.62	103.74	108.17
3	B	502	1F1	O3-C2-O1	-2.62	117.41	123.35
2	D	502	HEM	O2D-CGD-CBD	2.58	123.32	114.22
2	C	501	HEM	CHD-C4C-NC	2.55	126.95	124.73
2	D	502	HEM	CMA-C3A-C2A	2.54	129.73	124.94
2	B	501	HEM	C3B-C4B-NB	-2.51	112.20	114.00
5	B	506	GOL	O1-C1-C2	-2.51	97.48	109.71
2	A	501	HEM	O2D-CGD-CBD	2.49	123.03	114.22
2	B	501	HEM	CAD-C3D-C4D	2.48	128.99	124.53
4	D	505	SO4	O4-S-O3	-2.48	98.59	109.08
3	A	502	1F1	C8-C9-N10	-2.47	103.98	108.17
3	D	503	1F1	C6-C5-C4	-2.44	118.04	120.82
3	D	501	1F1	C5-C4-C2	-2.44	115.97	120.44
3	A	504	1F1	O3-C2-C4	2.43	121.44	115.01
2	C	501	HEM	C4C-NC-C1C	2.41	108.04	105.53
2	C	501	HEM	C1A-CHA-C4D	-2.41	124.30	127.47
4	D	505	SO4	O2-S-O1	-2.40	101.59	109.53
2	C	501	HEM	CHB-C4A-NA	2.40	128.58	124.58
3	D	501	1F1	C8-C7-C11	2.39	113.00	106.70
3	B	502	1F1	C8-C7-C6	-2.38	128.38	136.72
2	D	502	HEM	CHB-C1B-NB	2.37	127.56	124.31
2	C	501	HEM	C4D-ND-C1D	2.35	107.57	105.16
2	A	501	HEM	C4A-NA-C1A	2.35	109.86	106.76
3	B	503	1F1	C4-C12-C11	-2.34	114.42	117.90
2	C	501	HEM	O2A-CGA-O1A	-2.30	117.45	123.30
2	D	502	HEM	CAD-C3D-C4D	2.28	128.63	124.53
2	A	501	HEM	CMC-C2C-C3C	2.27	131.51	126.16
3	B	503	1F1	C6-C7-C11	2.20	124.68	119.94
2	A	501	HEM	CAD-CBD-CGD	-2.20	106.63	113.48
3	C	502	1F1	C5-C4-C12	2.19	122.43	119.22
2	C	501	HEM	CHC-C1C-NC	2.17	126.62	124.73
2	C	501	HEM	C3A-C4A-CHB	-2.15	121.92	126.00
2	B	501	HEM	O1D-CGD-CBD	-2.14	115.68	123.03
4	C	505	SO4	O2-S-O1	2.14	116.60	109.53
3	C	503	1F1	C7-C11-N10	2.12	112.36	105.61
2	C	501	HEM	O2A-CGA-CBA	2.11	121.69	114.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	1F1	C5-C6-C7	-2.10	117.53	120.83
2	D	502	HEM	O2A-CGA-O1A	2.10	128.64	123.30
3	A	504	1F1	C5-C6-C7	-2.10	117.54	120.83
3	B	502	1F1	O3-C2-C4	2.02	120.35	115.01
5	A	508	GOL	O2-C2-C1	2.00	117.33	108.22

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%)	-0.22	2 (0%) 88 92	12, 18, 30, 38	0
1	B	393/410 (95%)	-0.15	3 (0%) 83 90	11, 19, 31, 42	0
1	C	393/410 (95%)	-0.13	3 (0%) 83 90	14, 21, 33, 41	0
1	D	393/410 (95%)	0.12	8 (2%) 62 73	15, 25, 39, 54	0
All	All	1572/1640 (95%)	-0.09	16 (1%) 77 88	11, 21, 35, 54	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	409	ALA	4.0
1	D	17	THR	3.4
1	D	279	THR	3.3
1	D	89	LYS	3.2
1	C	295	VAL	3.2
1	B	17	THR	3.0
1	D	217	PRO	2.9
1	A	409	ALA	2.7
1	C	17	THR	2.5
1	C	309	GLY	2.4
1	B	409	ALA	2.2
1	D	276	SER	2.2
1	D	377	ARG	2.2
1	A	250	LEU	2.1
1	B	250	LEU	2.0
1	D	198	ARG	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
4	SO4	C	506	5/5	0.45	30.37	30,30,30,30	0
5	GOL	B	506	6/6	0.16	8.03	32,35,38,40	0
4	SO4	A	506	5/5	0.26	7.35	30,30,30,30	0
3	1F1	C	503	12/12	0.26	6.44	74,77,78,79	0
3	1F1	B	503	12/12	0.25	5.85	38,43,52,57	0
5	GOL	A	508	6/6	0.24	5.66	38,52,54,58	0
5	GOL	B	507	6/6	0.21	5.29	31,45,52,55	0
3	1F1	A	503	12/12	0.21	3.68	40,45,58,59	0
3	1F1	D	501	12/12	0.16	3.20	48,50,53,56	0
3	1F1	A	504	12/12	0.13	3.16	23,31,46,49	0
4	SO4	C	505	5/5	0.08	2.13	36,39,45,47	0
4	SO4	D	505	5/5	0.11	1.83	46,52,54,58	0
2	HEM	C	501	43/43	0.14	1.00	12,16,18,21	0
2	HEM	D	502	43/43	0.12	0.83	12,18,22,24	0
3	1F1	D	503	12/12	0.10	0.69	16,21,22,24	0
2	HEM	B	501	43/43	0.10	0.60	10,13,15,19	0
2	HEM	A	501	43/43	0.10	0.44	10,13,15,17	0
5	GOL	B	505	6/6	0.08	0.31	18,21,24,34	0
4	SO4	A	505	5/5	0.07	0.10	24,32,37,38	0
3	1F1	C	502	12/12	0.09	-0.13	15,17,19,20	0
4	SO4	D	504	5/5	0.09	-0.24	33,37,40,43	0
5	GOL	C	507	6/6	0.08	-0.31	22,25,29,35	0
3	1F1	B	502	12/12	0.09	-0.35	11,13,15,15	0
5	GOL	D	506	6/6	0.08	-0.50	21,33,36,37	0
6	CL	B	508	1/1	0.06	-0.72	18,18,18,18	0
6	CL	D	507	1/1	0.07	-0.74	32,32,32,32	0
6	CL	A	509	1/1	0.06	-0.84	17,17,17,17	0
5	GOL	A	507	6/6	0.06	-0.86	20,23,28,32	0
3	1F1	A	502	12/12	0.08	-1.14	10,14,15,17	0
4	SO4	C	504	5/5	0.06	-1.91	24,24,26,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	B	504	5/5	0.04	-3.03	22,23,27,27	0
6	CL	C	508	1/1	0.04	-3.11	27,27,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.