WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 03:48 PM GMT

PDB ID : 2A1N
Title : Crystal structure of ferrous dioxygen complex of D251N cytochrome P450cam
Authors : Nagano, S.; Poulos, T.L.
Deposited on : 2005-06-20
Resolution : 1.90 Å(reported)

1 Overall quality at a glance (i)

The reported resolution of this entry is 1.90 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.
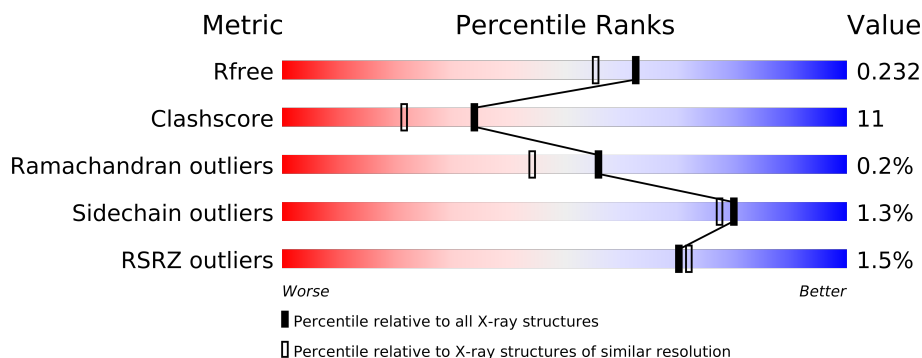
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	415	
1	B	415	

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 7055 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-cam.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3218	2040	563	598	17			
1	B	405	Total	C	N	O	S	0	0	0
			3207	2033	561	596	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	ASN	ASP	ENGINEERED	UNP P00183
A	334	ALA	CYS	ENGINEERED	UNP P00183
B	251	ASN	ASP	ENGINEERED	UNP P00183
B	334	ALA	CYS	ENGINEERED	UNP P00183

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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

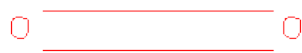- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			2	2		
4	B	1	Total	O	0	0
			2	2		

- Molecule 5 is CAMPHOR (three-letter code: CAM) (formula: $C_{10}H_{16}O$).

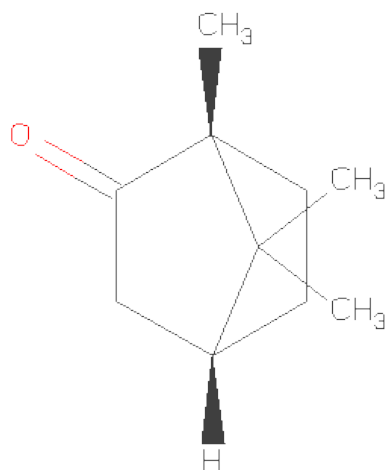| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 11	C 10	O 1	0	0
5	B	1	Total 11	C 10	O 1	0	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

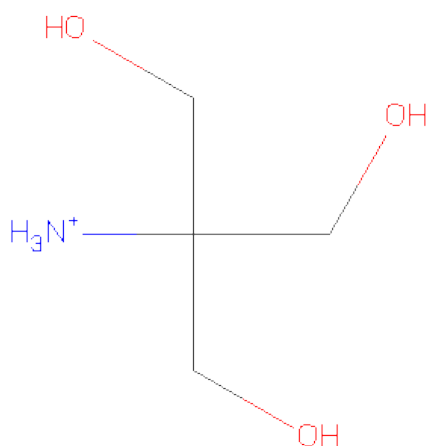| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total 8	C 4	N 1	O 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	284	Total 284	O 284	0	0
7	B	223	Total 223	O 223	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-cam

Chain A:
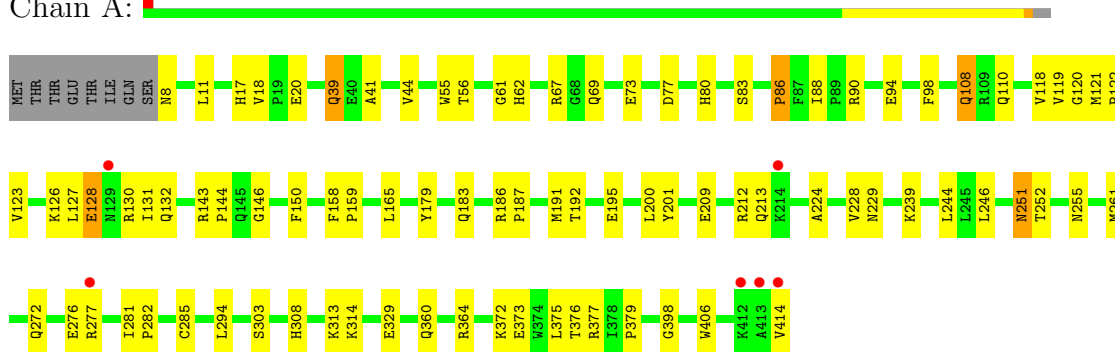
- Molecule 1: Cytochrome P450-cam

Chain B:

4 Data and refinement statistics (i)

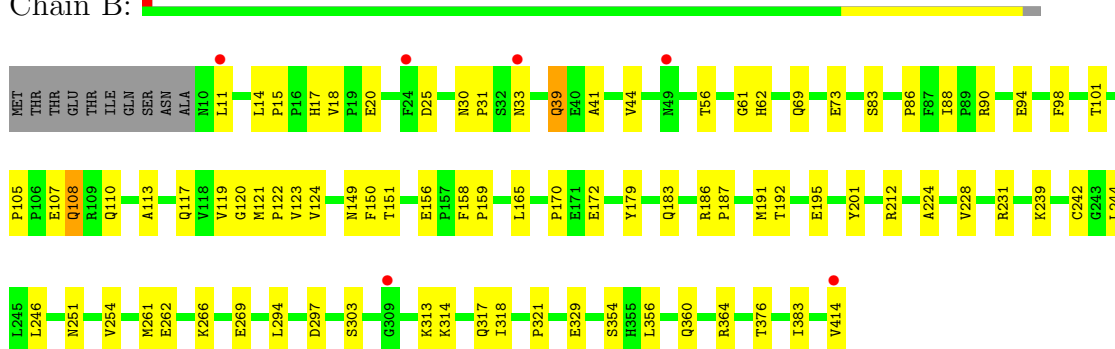| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.01Å 62.13Å 95.06Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	33.51 – 1.90 33.50 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.3 (33.51-1.90) 94.4 (33.50-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.235 0.190 , 0.232	Depositor DCC
R_{free} test set	2936 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 37.1	EDS
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
L-test for twinning	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 60811 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7055	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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: TRS, HEM, K, OXY, CAM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.32	0/3297	0.60	0/4479
1	B	0.30	0/3286	0.56	1/4464 (0.0%)
All	All	0.31	0/6583	0.58	1/8943 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	149	ASN	N-CA-C	-5.12	97.18	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts (i)

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	3218	0	3167	74	0
1	B	3207	0	3158	64	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	43	0	30	1	0
3	B	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	2	0
4	B	2	0	0	1	0
5	A	11	0	16	1	0
5	B	11	0	16	1	0
6	B	8	0	12	0	0
7	A	284	0	0	1	0
7	B	223	0	0	2	0
All	All	7055	0	6429	141	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 11.

All (141) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:186:ARG:HH22	1:A:251:ASN:HD21	0.96	0.92
1:A:130:ARG:HD2	1:A:165:LEU:HD11	1.61	0.83
1:A:120:GLY:O	1:A:123:VAL:HG22	1.82	0.80
1:A:186:ARG:NH2	1:A:251:ASN:HD21	1.79	0.76
1:A:360:GLN:HE21	1:A:364:ARG:HH22	1.32	0.76
1:A:8:ASN:HB3	1:A:11:LEU:HD13	1.67	0.76
1:B:360:GLN:HE21	1:B:364:ARG:HH22	1.36	0.73
1:B:120:GLY:O	1:B:123:VAL:HG22	1.90	0.72
1:A:146:GLY:HA2	1:A:406:TRP:NE1	2.04	0.72
1:B:121:MET:O	1:B:124:VAL:HG12	1.90	0.71
1:A:186:ARG:HH22	1:A:251:ASN:ND2	1.81	0.71
1:A:255:ASN:HD22	1:A:398:GLY:HA3	1.56	0.71
1:B:33:ASN:HD22	1:B:44:VAL:HG11	1.55	0.71
1:B:303:SER:HA	1:B:314:LYS:HB2	1.75	0.68
1:B:90:ARG:O	1:B:94:GLU:HG3	1.93	0.68
1:A:252:THR:HG21	4:A:420:OXY:O2	1.95	0.66
1:B:110:GLN:HB2	1:B:228:VAL:HG12	1.78	0.65
1:B:56:THR:O	1:B:61:GLY:HA2	1.99	0.63
1:A:69:GLN:O	1:A:73:GLU:HG3	1.98	0.63
1:B:20:GLU:H	1:B:20:GLU:CD	2.03	0.62
1:A:377:ARG:HG2	1:A:414:VAL:HG23	1.82	0.62
1:A:146:GLY:HA2	1:A:406:TRP:CD1	2.35	0.62
1:B:121:MET:SD	1:B:124:VAL:HG11	2.42	0.60
1:A:77:ASP:OD2	1:A:80:HIS:HD2	1.85	0.59
1:B:183:GLN:O	1:B:187:PRO:HG3	2.02	0.59
1:B:121:MET:N	1:B:122:PRO:HD2	2.18	0.59
1:A:20:GLU:H	1:A:20:GLU:CD	2.06	0.59
1:B:294:LEU:H	1:B:294:LEU:HD23	1.68	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:165:LEU:HD23	1:A:165:LEU:C	2.24	0.58
1:A:212:ARG:HG3	1:A:224:ALA:HB1	1.85	0.58
1:B:41:ALA:O	1:B:44:VAL:HG22	2.04	0.58
1:A:209:GLU:O	1:A:213:GLN:HG2	2.05	0.57
1:A:255:ASN:ND2	7:A:1968:HOH:O	2.36	0.57
1:A:126:LYS:NZ	1:A:130:ARG:HH22	2.03	0.56
1:A:150:PHE:CZ	1:A:261:MET:HG3	2.39	0.56
1:A:255:ASN:ND2	1:A:398:GLY:HA3	2.20	0.56
1:B:159:PRO:HG2	1:B:254:VAL:HG22	1.87	0.56
1:B:165:LEU:HD23	1:B:165:LEU:C	2.27	0.55
1:B:360:GLN:NE2	1:B:364:ARG:HH22	2.04	0.54
1:B:179:TYR:O	1:B:183:GLN:HG2	2.08	0.54
1:B:151:THR:O	1:B:156:GLU:HG3	2.08	0.54
1:B:11:LEU:N	1:B:11:LEU:HD12	2.23	0.54
1:A:73:GLU:OE2	1:A:308:HIS:HE1	1.91	0.54
1:B:113:ALA:O	1:B:117:GLN:HG3	2.07	0.54
1:A:191:MET:HG2	1:A:195:GLU:HB2	1.91	0.53
1:A:123:VAL:O	1:A:127:LEU:HD23	2.09	0.53
1:A:146:GLY:HA2	1:A:406:TRP:CE2	2.44	0.52
1:A:67:ARG:HH12	1:A:329:GLU:CD	2.13	0.52
1:A:200:LEU:HD11	1:A:246:LEU:HD23	1.91	0.52
1:B:83:SER:O	1:B:86:PRO:HD3	2.11	0.52
1:B:186:ARG:HH12	1:B:251:ASN:HD21	1.57	0.51
1:B:62:HIS:CD2	1:B:88:ILE:HD13	2.46	0.51
1:B:201:TYR:HB3	1:B:239:LYS:HD2	1.93	0.51
1:B:15:PRO:HB2	1:B:18:VAL:HG23	1.93	0.50
1:B:62:HIS:CG	1:B:88:ILE:HD13	2.47	0.50
1:B:376:THR:HG22	1:B:414:VAL:HG21	1.94	0.50
1:A:272:GLN:HG3	1:A:276:GLU:OE2	2.12	0.50
1:A:294:LEU:H	1:A:294:LEU:HD23	1.77	0.50
1:A:110:GLN:NE2	1:A:228:VAL:HG12	2.28	0.49
1:B:150:PHE:CZ	1:B:261:MET:HG3	2.47	0.49
1:B:90:ARG:HB2	1:B:317:GLN:NE2	2.27	0.49
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.94	0.49
1:A:39:GLN:NE2	1:A:39:GLN:H	2.10	0.49
1:B:98:PHE:HB3	1:B:244:LEU:HB2	1.93	0.49
1:A:303:SER:HA	1:A:314:LYS:HB2	1.94	0.49
1:A:41:ALA:O	1:A:44:VAL:HG22	2.13	0.49
3:A:417:HEM:HBB2	3:A:417:HEM:HMB1	1.95	0.49
1:A:192:THR:OG1	1:A:195:GLU:HG3	2.13	0.49
1:A:375:LEU:O	1:A:379:PRO:HG3	2.12	0.49
1:B:294:LEU:N	1:B:294:LEU:HD23	2.27	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:277:ARG:HH11	1:A:277:ARG:HG3	1.78	0.48
4:A:420:OXY:O1	5:A:1422:CAM:H52	2.13	0.48
1:B:242:CYS:O	1:B:246:LEU:HD13	2.14	0.48
1:B:69:GLN:O	1:B:73:GLU:HG3	2.13	0.48
1:B:269:GLU:HG3	7:B:2704:HOH:O	2.14	0.47
1:B:83:SER:HB3	1:B:101:THR:O	2.14	0.47
1:B:121:MET:HA	1:B:124:VAL:HG12	1.96	0.47
1:B:228:VAL:O	1:B:231:ARG:HG3	2.14	0.47
1:B:191:MET:HG2	1:B:195:GLU:HB2	1.96	0.47
1:B:262:GLU:HG2	1:B:266:LYS:HE2	1.97	0.47
1:B:170:PRO:HB2	1:B:172:GLU:HG2	1.97	0.47
1:A:121:MET:N	1:A:122:PRO:HD2	2.30	0.46
1:A:255:ASN:HD22	1:A:398:GLY:CA	2.27	0.46
1:A:127:LEU:HD13	1:A:130:ARG:NH2	2.31	0.46
1:B:105:PRO:HG3	1:B:108:GLN:NE2	2.31	0.46
1:A:110:GLN:HE21	1:A:229:ASN:HB2	1.81	0.46
1:B:266:LYS:HD3	1:B:383:ILE:HD12	1.97	0.46
1:A:83:SER:O	1:A:86:PRO:HD3	2.15	0.46
1:A:251:ASN:O	1:A:255:ASN:OD1	2.34	0.46
1:B:192:THR:OG1	1:B:195:GLU:HG3	2.15	0.46
1:A:18:VAL:HG11	1:A:55:TRP:CG	2.52	0.45
1:A:201:TYR:HB3	1:A:239:LYS:HD2	1.98	0.45
1:B:297:ASP:OD2	3:B:417:HEM:O1A	2.33	0.45
1:B:107:GLU:H	1:B:107:GLU:CD	2.20	0.45
1:A:118:VAL:HG23	1:A:119:VAL:HG13	1.98	0.45
1:A:77:ASP:OD2	1:A:80:HIS:CD2	2.68	0.45
1:B:212:ARG:HG3	1:B:224:ALA:HB1	1.99	0.45
1:A:377:ARG:C	1:A:379:PRO:HD3	2.37	0.44
1:A:179:TYR:O	1:A:183:GLN:HG2	2.16	0.44
1:B:17:HIS:CD2	1:B:313:LYS:HG2	2.52	0.44
1:A:127:LEU:O	1:A:131:ILE:HG13	2.18	0.44
1:A:143:ARG:HG2	1:A:143:ARG:HH11	1.80	0.44
1:A:56:THR:O	1:A:61:GLY:HA2	2.17	0.44
1:A:17:HIS:CD2	1:A:313:LYS:HG2	2.53	0.44
1:B:318:ILE:O	1:B:318:ILE:HG23	2.18	0.44
1:A:294:LEU:N	1:A:294:LEU:HD23	2.33	0.44
1:B:414:VAL:O	1:B:414:VAL:HG12	2.18	0.43
1:A:158:PHE:HB3	1:A:159:PRO:CD	2.48	0.43
4:B:420:OXY:O1	5:B:2422:CAM:H52	2.17	0.43
1:B:121:MET:N	1:B:122:PRO:CD	2.80	0.43
1:A:119:VAL:HA	1:A:123:VAL:HG21	1.99	0.43
1:B:110:GLN:HB2	1:B:228:VAL:CG1	2.46	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:158:PHE:HB3	1:B:159:PRO:CD	2.49	0.43
1:A:108:GLN:HE21	1:A:108:GLN:HB3	1.60	0.43
1:A:90:ARG:O	1:A:94:GLU:HG3	2.19	0.43
1:A:143:ARG:HB3	1:A:144:PRO:CD	2.48	0.43
1:A:132:GLN:HE22	1:A:373:GLU:CD	2.21	0.43
1:B:119:VAL:HA	1:B:123:VAL:HG21	2.01	0.42
1:B:39:GLN:NE2	1:B:39:GLN:H	2.16	0.42
1:A:239:LYS:HB3	1:A:239:LYS:HE2	1.86	0.42
1:A:62:HIS:CD2	1:A:88:ILE:HD13	2.54	0.42
1:B:231:ARG:O	1:B:231:ARG:HD2	2.18	0.42
1:A:183:GLN:O	1:A:187:PRO:HG3	2.19	0.42
1:A:62:HIS:CE1	1:A:88:ILE:HD13	2.54	0.42
1:A:251:ASN:HA	1:A:251:ASN:HD22	1.68	0.42
1:A:376:THR:HG22	1:A:414:VAL:HG21	2.02	0.42
1:B:31:PRO:HB2	1:B:41:ALA:HB1	2.02	0.41
1:A:277:ARG:NH1	1:A:277:ARG:HG3	2.34	0.41
1:B:329:GLU:H	1:B:329:GLU:CD	2.22	0.41
1:B:239:LYS:HE2	1:B:239:LYS:HB3	1.91	0.41
1:B:14:LEU:HD11	1:B:18:VAL:CG1	2.49	0.41
1:B:187:PRO:HG3	7:B:2585:HOH:O	2.20	0.41
1:A:282:PRO:O	1:A:285:CYS:HB3	2.21	0.41
1:B:108:GLN:HE22	1:B:354:SER:HB2	1.85	0.41
1:A:143:ARG:HB3	1:A:144:PRO:HD3	2.03	0.41
1:A:123:VAL:O	1:A:127:LEU:CD2	2.69	0.40
1:B:120:GLY:C	1:B:122:PRO:HD2	2.41	0.40
1:B:33:ASN:ND2	1:B:44:VAL:HG11	2.28	0.40
1:A:110:GLN:HB2	1:A:228:VAL:HG12	2.04	0.40
1:A:281:ILE:CD1	1:A:372:LYS:HB3	2.52	0.40
1:A:128:GLU:OE1	1:A:128:GLU:HA	2.22	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	405/415 (98%)	389 (96%)	16 (4%)	0	100	100
1	B	403/415 (97%)	388 (96%)	13 (3%)	2 (0%)	38	23
All	All	808/830 (97%)	777 (96%)	29 (4%)	2 (0%)	56	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	ASP
1	B	321	PRO

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	349/358 (98%)	344 (99%)	5 (1%)	78	75
1	B	349/358 (98%)	345 (99%)	4 (1%)	84	82
All	All	698/716 (98%)	689 (99%)	9 (1%)	80	77

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	86	PRO
1	A	108	GLN
1	A	128	GLU
1	A	251	ASN
1	B	30	ASN
1	B	39	GLN
1	B	108	GLN
1	B	356	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN

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Mol	Chain	Res	Type
1	A	33	ASN
1	A	39	GLN
1	A	46	GLN
1	A	80	HIS
1	A	108	GLN
1	A	110	GLN
1	A	117	GLN
1	A	213	GLN
1	A	251	ASN
1	A	255	ASN
1	A	272	GLN
1	A	308	HIS
1	A	317	GLN
1	A	360	GLN
1	A	400	GLN
1	B	30	ASN
1	B	33	ASN
1	B	39	GLN
1	B	46	GLN
1	B	80	HIS
1	B	108	GLN
1	B	110	GLN
1	B	117	GLN
1	B	255	ASN
1	B	308	HIS
1	B	317	GLN
1	B	360	GLN
1	B	400	GLN

5.3.3 RNA (i)

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	#$|Z| > 2$
5	CAM	A	1422	-	12,12,12	2.05	4 (33%)	21,21,21	1.95	5 (23%)
3	HEM	A	417	1,4	49,50,50	2.20	13 (26%)	46,82,82	1.26	6 (13%)
4	OXY	A	420	3	1,1,1	0.83	0	0,0,0	0.00	-
5	CAM	B	2422	-	12,12,12	2.08	4 (33%)	21,21,21	1.94	5 (23%)
6	TRS	B	2430	-	7,7,7	2.22	3 (42%)	9,9,9	3.45	5 (55%)
3	HEM	B	417	1,4	49,50,50	1.92	12 (24%)	46,82,82	1.17	4 (8%)
4	OXY	B	420	3	1,1,1	0.85	0	0,0,0	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CAM	A	1422	-	-	0/0/31/31	0/0/2/2
3	HEM	A	417	1,4	-	0/14/114/114	0/0/8/8
4	OXY	A	420	3	-	0/0/0/0	0/0/0/0
5	CAM	B	2422	-	-	0/0/31/31	0/0/2/2
6	TRS	B	2430	-	-	0/9/9/9	0/0/0/0
3	HEM	B	417	1,4	-	0/14/114/114	0/0/8/8
4	OXY	B	420	3	-	0/0/0/0	0/0/0/0

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	417	HEM	C3D-C4D	7.55	1.46	1.44
3	A	417	HEM	C2D-C1D	7.23	1.46	1.44
3	B	417	HEM	C2D-C1D	4.43	1.45	1.44
3	B	417	HEM	C4A-C3A	4.24	1.45	1.40
3	A	417	HEM	C3D-C2D	-4.18	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	417	HEM	C3B-C2B	-4.17	1.36	1.43
3	B	417	HEM	C3D-C2D	-3.99	1.36	1.43
3	B	417	HEM	C3C-C2C	-3.86	1.37	1.43
3	A	417	HEM	C3C-C2C	-3.85	1.37	1.43
3	A	417	HEM	C3B-C2B	-3.84	1.37	1.43
5	B	2422	CAM	C5-C4	3.70	1.63	1.53
3	B	417	HEM	C3D-C4D	3.66	1.45	1.44
5	A	1422	CAM	C5-C4	3.48	1.62	1.53
6	B	2430	TRS	O3-C3	3.41	1.53	1.42
5	A	1422	CAM	C1-C2	3.28	1.57	1.53
3	A	417	HEM	CHA-C4D	3.21	1.40	1.35
3	B	417	HEM	CHB-C1B	3.21	1.40	1.35
5	B	2422	CAM	C1-C2	3.06	1.57	1.53
6	B	2430	TRS	O1-C1	3.02	1.51	1.42
3	B	417	HEM	CHD-C4C	2.95	1.41	1.36
3	A	417	HEM	C4A-C3A	2.88	1.43	1.40
5	B	2422	CAM	C3-C4	2.87	1.61	1.53
6	B	2430	TRS	O2-C2	2.80	1.51	1.42
5	A	1422	CAM	C3-C4	2.77	1.61	1.53
3	B	417	HEM	CHA-C4D	2.72	1.39	1.35
5	B	2422	CAM	C8-C7	2.71	1.61	1.53
5	A	1422	CAM	C8-C7	2.60	1.61	1.53
3	A	417	HEM	CMD-C2D	2.54	1.55	1.47
3	A	417	HEM	CHB-C1B	2.52	1.39	1.35
3	A	417	HEM	CAA-C2A	2.22	1.55	1.52
3	A	417	HEM	C4A-NA	2.20	1.40	1.36
3	B	417	HEM	FE-NA	2.17	2.01	1.92
3	B	417	HEM	CMD-C2D	2.13	1.54	1.47
3	A	417	HEM	CHC-C1C	2.07	1.40	1.36
3	A	417	HEM	FE-NA	2.04	2.01	1.92
3	B	417	HEM	C4C-NC	2.01	1.40	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2430	TRS	C3-C-C2	-6.41	100.18	110.70
6	B	2430	TRS	C2-C-C1	-4.99	102.52	110.70
5	A	1422	CAM	C4-C3-C2	-4.51	94.10	101.90
6	B	2430	TRS	C3-C-C1	4.50	118.08	110.70
5	B	2422	CAM	C4-C3-C2	-4.47	94.16	101.90
3	A	417	HEM	C3B-C4B-NB	-4.28	110.94	114.00
3	B	417	HEM	C3B-C4B-NB	-4.20	110.99	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1422	CAM	C5-C6-C1	-3.88	97.93	104.62
5	B	2422	CAM	C5-C6-C1	-3.80	98.06	104.62
6	B	2430	TRS	C3-C-N	3.65	118.23	108.30
5	A	1422	CAM	C3-C4-C7	3.15	109.42	102.84
5	B	2422	CAM	C3-C4-C7	3.11	109.32	102.84
3	A	417	HEM	CMA-C3A-C4A	-2.66	124.53	128.62
5	B	2422	CAM	C6-C1-C7	2.63	107.51	101.56
5	A	1422	CAM	C6-C1-C7	2.61	107.46	101.56
3	B	417	HEM	C3A-C4A-NA	2.52	111.31	109.41
5	A	1422	CAM	C9-C7-C1	2.51	118.39	113.13
3	A	417	HEM	C4A-NA-C1A	-2.51	103.46	106.76
5	B	2422	CAM	C9-C7-C1	2.49	118.34	113.13
3	A	417	HEM	C3A-C4A-NA	2.46	111.27	109.41
6	B	2430	TRS	O2-C2-C	-2.23	106.67	111.55
3	A	417	HEM	C1A-CHA-C4D	-2.21	124.56	127.47
3	A	417	HEM	C4A-CHB-C1B	-2.20	124.58	127.47
3	B	417	HEM	CMA-C3A-C4A	-2.06	125.45	128.62
3	B	417	HEM	C4A-NA-C1A	-2.04	104.08	106.76

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(Å²)	Q<0.9
1	A	407/415 (98%)	-0.05	6 (1%)	70	72	9, 17, 36, 55	0
1	B	405/415 (97%)	0.14	6 (1%)	70	72	12, 22, 43, 57	0
All	All	812/830 (97%)	0.04	12 (1%)	70	72	9, 20, 40, 57	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	ASN	4.6
1	A	414	VAL	3.7
1	B	414	VAL	3.3
1	B	309	GLY	3.0
1	A	413	ALA	2.6
1	A	277	ARG	2.5
1	B	24	PHE	2.3
1	B	33	ASN	2.3
1	A	412	LYS	2.3
1	A	214	LYS	2.3
1	A	129	ASN	2.1
1	B	11	LEU	2.1

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
5	CAM	B	2422	11/11	0.18	1.63	17,20,22,23	0
5	CAM	A	1422	11/11	0.16	1.19	7,13,17,22	0
3	HEM	A	417	43/43	0.15	1.14	6,12,14,19	0
6	TRS	B	2430	8/8	0.10	0.43	19,20,22,25	0
3	HEM	B	417	43/43	0.13	-0.12	12,15,18,22	0
2	K	B	2515	1/1	0.09	-0.50	23,23,23,23	0
4	OXY	A	420	2/2	0.11	-1.22	19,19,19,24	2
2	K	A	1515	1/1	0.05	-1.54	12,12,12,12	0
4	OXY	B	420	2/2	0.06	-2.85	19,19,19,27	0
2	K	A	1715	1/1	0.04	-3.30	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.