



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:57 AM GMT

PDB ID : 3QJU
Title : The structure of and photolytic induced changes of carbon monoxide binding to the cytochrome ba3-oxidase from *Thermus thermophilus*
Authors : Liu, B.; Zhang, Y.; Sage, J.T.; Doukov, T.; Chen, Y.; Stout, C.D.; Fee, J.A
Deposited on : 2011-01-30
Resolution : 2.90 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

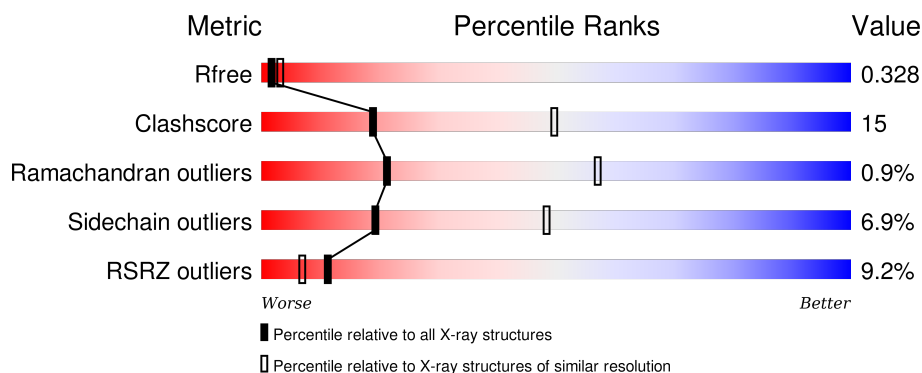
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	568	<div> <div>9%</div> <div>62%</div> <div>33%</div> <div>• •</div> </div>
2	B	168	<div> <div>7%</div> <div>68%</div> <div>26%</div> <div>5%</div> <div>•</div> </div>
3	C	34	<div> <div>12%</div> <div>56%</div> <div>38%</div> <div>• •</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6037 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 c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4367	2962	699	690	16			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP Q5SJ79
A	-4	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-3	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-2	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	0	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	1	HIS	-	EXPRESSION TAG	UNP Q5SJ79

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1298	844	216	234	4			

- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	33	Total	C	N	O	0	0	0
			259	179	39	41			

- Molecule 4 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

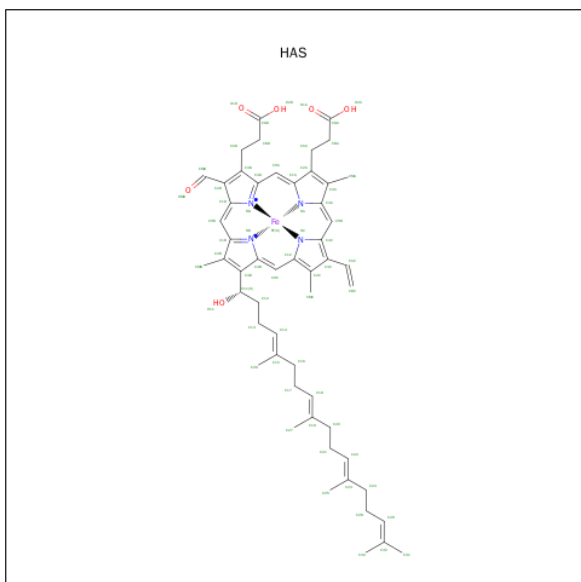
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



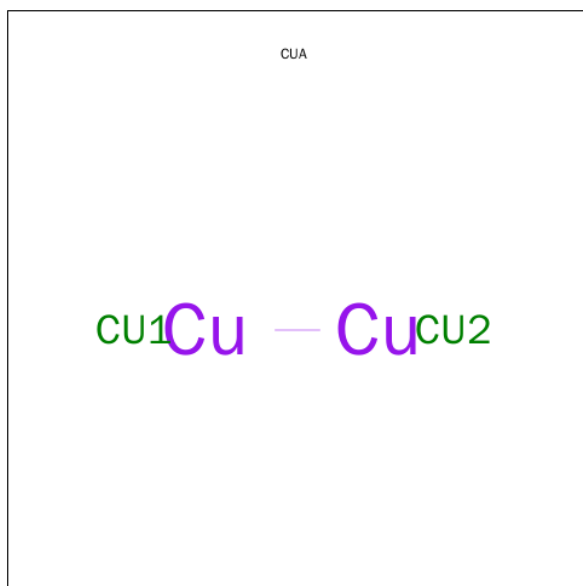
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).



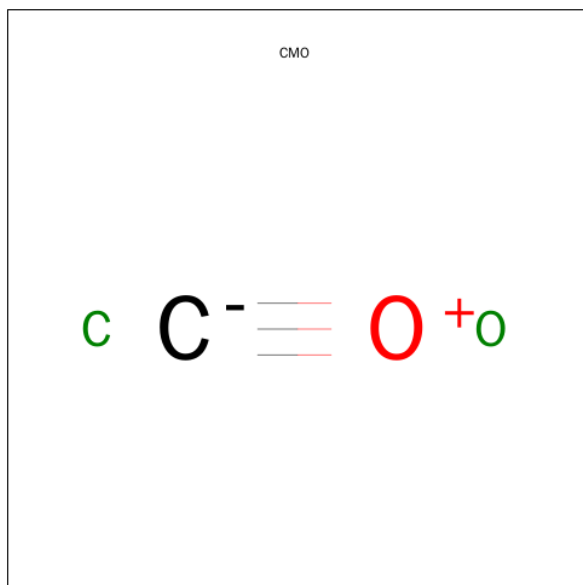
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 7 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cu	0	0
			2	2		

- Molecule 8 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).

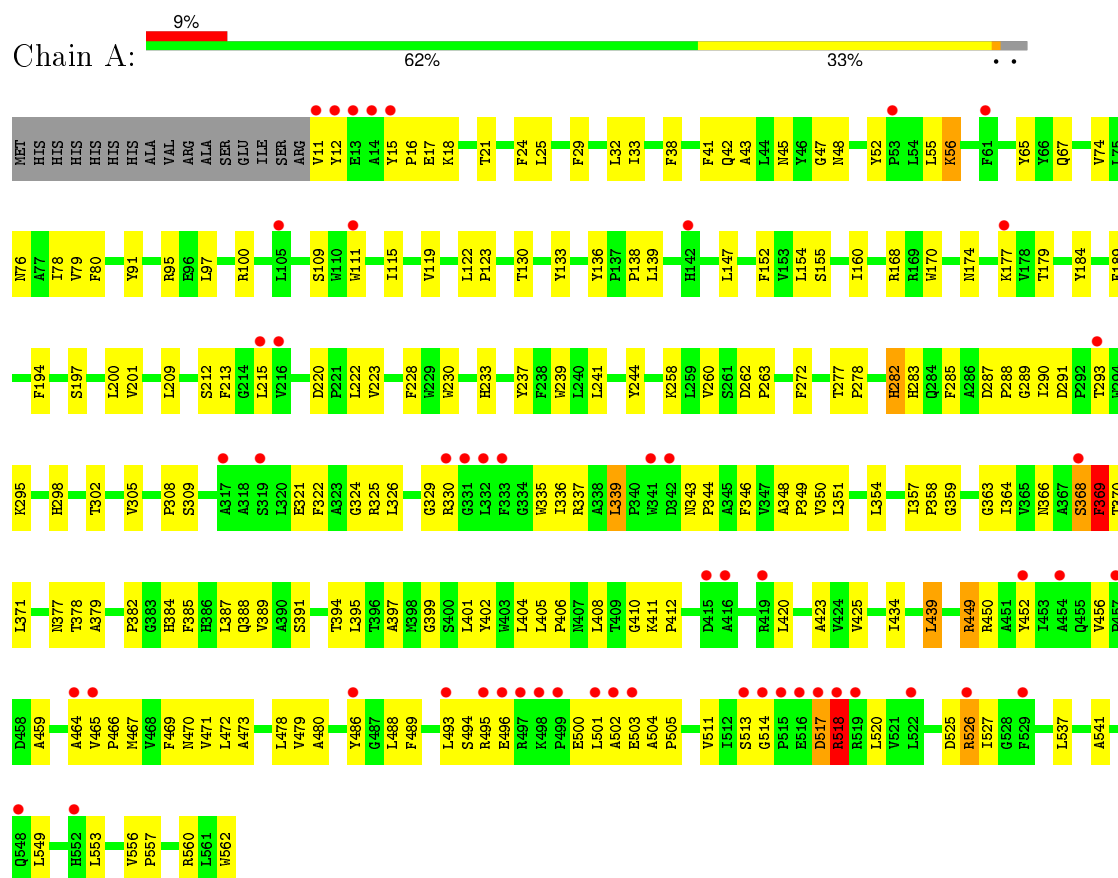


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			2	1	1		

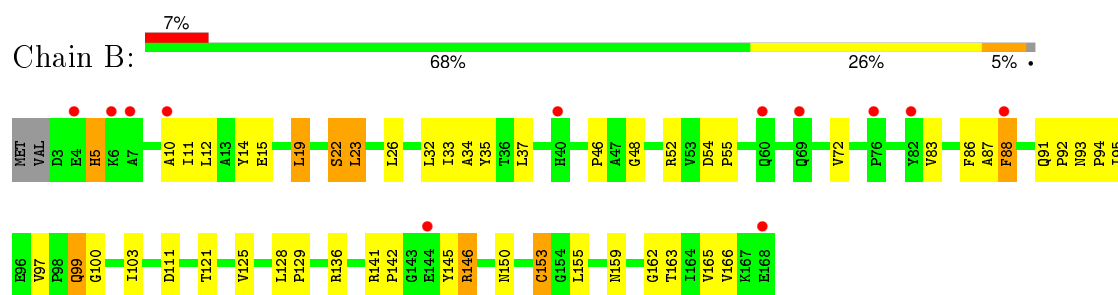
3 Residue-property plots [i](#)

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.

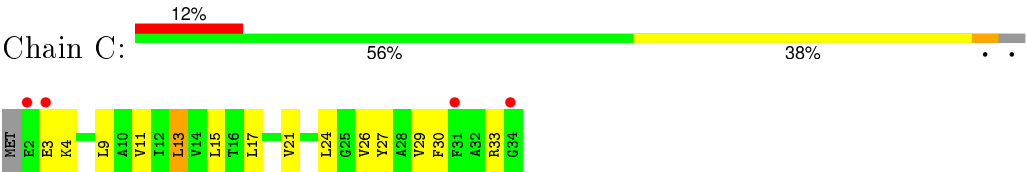
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 3: Cytochrome c oxidase polypeptide 2A



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.75Å 109.75Å 164.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.90 19.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (19.91-2.90) 95.7 (19.91-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.286 , 0.329 0.284 , 0.328	Depositor DCC
R_{free} test set	1127 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	82.3	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 28.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	1 of 21912 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6037	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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: CMO, HEM, HAS, CUA, CU1

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	0.71	2/4524 (0.0%)	0.75	0/6210
2	B	0.70	1/1335 (0.1%)	0.72	0/1822
3	C	0.94	0/265	0.89	0/359
All	All	0.72	3/6124 (0.0%)	0.75	0/8391

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	153	CYS	CB-SG	-7.04	1.70	1.82
1	A	500	GLU	CD-OE1	6.30	1.32	1.25
1	A	189	PHE	CE1-CZ	5.65	1.48	1.37

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	4367	0	4476	156	0
2	B	1298	0	1280	33	0
3	C	259	0	279	8	0
4	A	1	0	0	0	0
5	A	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	65	0	62	10	0
7	B	2	0	0	0	0
8	A	2	0	0	0	0
All	All	6037	0	6127	186	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 15.

All (186) 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:A:233:HIS:NE2	1:A:237:TYR:CE2	1.88	1.38
1:A:233:HIS:NE2	1:A:237:TYR:HE2	1.26	1.28
1:A:449:ARG:HD2	1:A:450:ARG:HG3	1.35	1.09
1:A:518:ARG:HG2	1:A:518:ARG:HH21	1.11	1.08
1:A:233:HIS:CD2	1:A:237:TYR:HE2	1.84	0.96
1:A:518:ARG:CG	1:A:518:ARG:HH21	1.79	0.95
1:A:357:ILE:HB	1:A:358:PRO:HD3	1.51	0.93
1:A:47:GLY:HA3	1:A:471:VAL:HG23	1.52	0.92
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.58	0.91
1:A:321:GLU:O	1:A:325:ARG:HG2	1.76	0.85
1:A:410:GLY:CA	1:A:502:ALA:HB2	2.08	0.84
1:A:518:ARG:NH2	1:A:518:ARG:HG2	1.83	0.82
1:A:262:ASP:HB2	1:A:511:VAL:HG11	1.66	0.77
1:A:449:ARG:HH12	6:A:801:HAS:CGA	1.97	0.77
6:A:801:HAS:H253	3:C:11:VAL:HG11	1.66	0.76
1:A:357:ILE:HB	1:A:358:PRO:CD	2.16	0.75
1:A:410:GLY:HA3	1:A:502:ALA:HB2	1.71	0.73
1:A:76:ASN:HB3	5:A:800:HEM:CAC	2.20	0.72
1:A:291:ASP:OD2	1:A:293:THR:HB	1.91	0.71
1:A:76:ASN:O	1:A:80:PHE:HB3	1.92	0.69
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.74	0.69
1:A:262:ASP:HB3	1:A:263:PRO:HD3	1.75	0.69
2:B:141:ARG:O	2:B:145:TYR:OH	2.04	0.69
1:A:379:ALA:HB1	1:A:439:LEU:HD12	1.76	0.68
1:A:272:PHE:CZ	1:A:308:PRO:HB2	2.29	0.67
1:A:465:VAL:HG23	1:A:466:PRO:HD3	1.76	0.67
1:A:38:PHE:O	1:A:42:GLN:HG3	1.95	0.67
2:B:97:VAL:O	2:B:166:VAL:HA	1.95	0.67
1:A:197:SER:O	1:A:201:VAL:HG23	1.95	0.66
1:A:411:LYS:HG2	1:A:496:GLU:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:TRP:O	1:A:115:ILE:HG13	1.97	0.65
2:B:142:PRO:HA	2:B:166:VAL:CG2	2.26	0.64
2:B:46:PRO:HG3	2:B:125:VAL:HG23	1.78	0.64
1:A:220:ASP:HB3	1:A:223:VAL:HG22	1.80	0.64
1:A:174:ASN:HB3	1:A:177:LYS:HD3	1.78	0.64
2:B:166:VAL:HG23	2:B:166:VAL:O	2.00	0.62
1:A:115:ILE:O	1:A:119:VAL:HG23	2.01	0.61
1:A:239:TRP:HE3	6:A:801:HAS:CBC	2.14	0.60
1:A:395:LEU:HD22	1:A:425:VAL:HG13	1.84	0.60
1:A:562:TRP:HA	2:B:155:LEU:HG	1.84	0.59
2:B:54:ASP:OD1	2:B:55:PRO:HD2	2.03	0.59
2:B:19:LEU:HD22	2:B:23:LEU:HD22	1.85	0.59
1:A:371:LEU:HD11	3:C:27:TYR:HD1	1.68	0.58
1:A:298:HIS:HE1	1:A:541:ALA:O	1.86	0.58
1:A:263:PRO:HB3	1:A:520:LEU:HD23	1.86	0.58
2:B:94:PRO:HB2	2:B:165:VAL:CG2	2.34	0.58
1:A:348:ALA:HA	1:A:425:VAL:HG11	1.86	0.58
1:A:368:SER:HB3	2:B:33:ILE:HD11	1.84	0.58
1:A:282:HIS:CD2	1:A:283:HIS:CD2	2.92	0.58
1:A:24:PHE:HZ	1:A:109:SER:HG	1.51	0.58
2:B:86:PHE:O	2:B:88:PHE:N	2.38	0.57
1:A:465:VAL:HG23	1:A:466:PRO:CD	2.35	0.56
1:A:122:LEU:HB2	1:A:123:PRO:CD	2.36	0.56
1:A:122:LEU:HB2	1:A:123:PRO:HD3	1.87	0.56
2:B:10:ALA:O	2:B:14:TYR:HD1	1.89	0.55
1:A:366:ASN:HB3	6:A:801:HAS:CMD	2.36	0.55
1:A:366:ASN:HB3	6:A:801:HAS:C2D	2.37	0.55
1:A:518:ARG:CG	1:A:518:ARG:NH2	2.50	0.55
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.41	0.54
1:A:11:VAL:HG22	1:A:503:GLU:HG3	1.88	0.54
1:A:200:LEU:HD12	1:A:200:LEU:O	2.07	0.54
1:A:282:HIS:HA	1:A:285:PHE:CZ	2.42	0.54
1:A:223:VAL:HG12	1:A:549:LEU:HB3	1.88	0.54
1:A:382:PRO:HB2	1:A:439:LEU:HG	1.90	0.54
1:A:41:PHE:CE2	1:A:55:LEU:HB2	2.44	0.53
1:A:357:ILE:HG23	3:C:15:LEU:HD13	1.91	0.52
1:A:389:VAL:HB	6:A:801:HAS:HBC2	1.92	0.52
1:A:464:ALA:O	1:A:467:MET:HB2	2.09	0.52
1:A:29:PHE:CE1	1:A:401:LEU:HD11	2.45	0.52
1:A:228:PHE:C	1:A:228:PHE:CD2	2.83	0.52
1:A:33:ILE:HD11	1:A:488:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:HG13	1:A:18:LYS:HD3	1.93	0.51
1:A:11:VAL:HG21	1:A:502:ALA:HB3	1.92	0.51
1:A:410:GLY:HA2	1:A:502:ALA:HB2	1.88	0.51
1:A:76:ASN:HB3	5:A:800:HEM:C3C	2.45	0.51
1:A:11:VAL:O	1:A:15:TYR:O	2.29	0.51
1:A:95:ARG:HA	1:A:95:ARG:NH2	2.26	0.51
2:B:166:VAL:CG2	2:B:166:VAL:O	2.58	0.50
1:A:277:THR:N	1:A:278:PRO:CD	2.74	0.50
1:A:364:ILE:O	1:A:368:SER:OG	2.30	0.50
1:A:209:LEU:O	1:A:213:PHE:CD1	2.65	0.50
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.47	0.49
1:A:79:VAL:HA	1:A:152:PHE:CZ	2.47	0.49
2:B:22:SER:O	2:B:26:LEU:HB2	2.13	0.49
1:A:262:ASP:HB2	1:A:511:VAL:CG1	2.41	0.49
1:A:21:THR:OG1	1:A:91:TYR:HB2	2.13	0.49
1:A:52:TYR:O	1:A:56:LYS:HB2	2.12	0.49
1:A:336:ILE:HA	1:A:339:LEU:HD22	1.94	0.48
1:A:479:VAL:O	1:A:480:ALA:C	2.52	0.48
1:A:329:GLY:HA3	1:A:335:TRP:HA	1.94	0.48
1:A:456:VAL:HG23	1:A:456:VAL:O	2.13	0.48
1:A:363:GLY:O	1:A:366:ASN:HB2	2.14	0.48
1:A:405:LEU:N	1:A:406:PRO:CD	2.77	0.47
1:A:136:TYR:O	1:A:139:LEU:HB2	2.13	0.47
2:B:94:PRO:HB2	2:B:165:VAL:HG23	1.95	0.47
1:A:456:VAL:HG23	1:A:459:ALA:HB3	1.96	0.47
1:A:43:ALA:O	1:A:470:ASN:HB3	2.13	0.47
1:A:379:ALA:O	1:A:439:LEU:HB3	2.15	0.47
1:A:459:ALA:O	2:B:146:ARG:NH1	2.38	0.47
1:A:412:PRO:HB3	1:A:501:LEU:HD21	1.96	0.47
1:A:346:PHE:CE1	1:A:350:VAL:HG21	2.50	0.47
1:A:434:ILE:HG22	1:A:473:ALA:HB2	1.96	0.47
2:B:34:ALA:HA	2:B:37:LEU:HB2	1.96	0.47
1:A:67:GLN:HA	1:A:130:THR:HG23	1.97	0.47
1:A:378:THR:O	1:A:449:ARG:HB3	2.14	0.46
1:A:449:ARG:NH1	6:A:801:HAS:CGA	2.74	0.46
1:A:12:TYR:O	1:A:16:PRO:CA	2.63	0.46
1:A:154:LEU:O	1:A:155:SER:C	2.54	0.46
1:A:295:LYS:HB2	1:A:369:PHE:CZ	2.51	0.46
1:A:556:VAL:CG1	2:B:55:PRO:HG3	2.46	0.46
1:A:290:ILE:O	1:A:295:LYS:HE3	2.15	0.46
1:A:466:PRO:HA	1:A:469:PHE:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:GLN:OE1	2:B:142:PRO:HB3	2.16	0.46
1:A:357:ILE:CB	1:A:358:PRO:CD	2.92	0.46
3:C:17:LEU:O	3:C:21:VAL:HG23	2.15	0.46
1:A:556:VAL:HG21	2:B:129:PRO:HB2	1.98	0.45
1:A:337:ARG:HA	1:A:337:ARG:HD2	1.67	0.45
1:A:525:ASP:O	1:A:527:ILE:N	2.49	0.45
6:A:801:HAS:HHB	6:A:801:HAS:OMD	2.17	0.45
1:A:97:LEU:HD22	1:A:170:TRP:CG	2.51	0.45
2:B:32:LEU:O	2:B:35:TYR:HB3	2.17	0.45
1:A:494:SER:C	1:A:496:GLU:H	2.19	0.45
1:A:287:ASP:O	1:A:295:LYS:NZ	2.47	0.45
3:C:26:VAL:O	3:C:30:PHE:N	2.41	0.44
1:A:15:TYR:HB2	1:A:18:LYS:HD2	1.99	0.44
2:B:92:PRO:HD2	2:B:95:ILE:HG12	1.98	0.44
1:A:289:GLY:HA2	2:B:48:GLY:O	2.18	0.44
1:A:489:PHE:HD2	1:A:493:LEU:HD13	1.82	0.44
1:A:399:GLY:O	1:A:402:TYR:HD2	2.00	0.44
1:A:24:PHE:HZ	1:A:109:SER:OG	1.99	0.44
1:A:343:ASN:HA	1:A:344:PRO:HD2	1.91	0.44
2:B:142:PRO:HA	2:B:166:VAL:HG23	1.98	0.44
1:A:348:ALA:O	1:A:395:LEU:HB3	2.17	0.44
1:A:377:ASN:HB3	2:B:150:ASN:O	2.17	0.44
1:A:514:GLY:HA2	2:B:5:HIS:NE2	2.33	0.44
1:A:11:VAL:HG21	1:A:502:ALA:CB	2.47	0.44
1:A:15:TYR:HA	1:A:17:GLU:OE1	2.18	0.44
1:A:346:PHE:O	1:A:349:PRO:HD2	2.18	0.44
1:A:526:ARG:HB3	1:A:526:ARG:HE	1.59	0.44
1:A:379:ALA:C	1:A:382:PRO:HD2	2.39	0.43
1:A:138:PRO:HB3	1:A:557:PRO:O	2.19	0.43
1:A:16:PRO:HD2	1:A:100:ARG:HH11	1.83	0.43
1:A:420:LEU:O	1:A:423:ALA:HB3	2.19	0.43
2:B:83:VAL:HG13	2:B:95:ILE:HD11	2.00	0.43
3:C:3:GLU:CD	3:C:4:LYS:H	2.22	0.43
1:A:404:LEU:O	1:A:408:LEU:HG	2.18	0.43
1:A:122:LEU:CB	1:A:123:PRO:CD	2.96	0.43
1:A:517:ASP:O	1:A:518:ARG:C	2.57	0.43
1:A:504:ALA:HA	1:A:505:PRO:HD3	1.84	0.42
2:B:12:LEU:O	2:B:15:GLU:HB3	2.18	0.42
3:C:9:LEU:O	3:C:13:LEU:HB2	2.19	0.42
1:A:179:THR:HG21	1:A:184:TYR:HA	2.01	0.42
1:A:282:HIS:HA	1:A:285:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:O	1:A:391:SER:HB3	2.19	0.42
1:A:517:ASP:N	1:A:517:ASP:OD2	2.52	0.42
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.55	0.42
1:A:560:ARG:HG3	1:A:562:TRP:CZ2	2.55	0.42
1:A:420:LEU:HD21	1:A:486:TYR:HD2	1.85	0.42
1:A:241:LEU:HA	1:A:244:TYR:HB2	2.00	0.42
1:A:359:GLY:HA3	1:A:388:GLN:NE2	2.35	0.42
1:A:298:HIS:CE1	1:A:541:ALA:O	2.71	0.41
1:A:401:LEU:O	1:A:406:PRO:HD3	2.20	0.41
1:A:358:PRO:HB2	1:A:387:LEU:HD13	2.02	0.41
1:A:74:VAL:O	1:A:78:ILE:HB	2.20	0.41
2:B:93:ASN:HD21	2:B:162:GLY:HA2	1.84	0.41
1:A:495:ARG:HD3	1:A:495:ARG:HA	1.86	0.41
1:A:45:ASN:ND2	1:A:65:TYR:CZ	2.88	0.41
1:A:357:ILE:HG12	6:A:801:HAS:H212	2.01	0.41
1:A:401:LEU:O	1:A:405:LEU:HB2	2.20	0.41
2:B:91:GLN:HA	2:B:92:PRO:C	2.38	0.41
1:A:258:LYS:HG3	1:A:322:PHE:HE1	1.85	0.41
1:A:223:VAL:HG11	1:A:553:LEU:CD2	2.51	0.41
1:A:324:GLY:CA	1:A:339:LEU:CD1	2.98	0.41
1:A:537:LEU:HD23	1:A:537:LEU:HA	1.88	0.41
1:A:260:VAL:HB	2:B:11:ILE:HD13	2.02	0.41
1:A:394:THR:O	1:A:397:ALA:HB3	2.21	0.41
1:A:222:LEU:HD21	1:A:288:PRO:O	2.21	0.41
1:A:233:HIS:HE2	1:A:237:TYR:HH	1.69	0.40
1:A:119:VAL:HG11	1:A:147:LEU:HD23	2.02	0.40
1:A:405:LEU:N	1:A:406:PRO:HD2	2.36	0.40
2:B:103:ILE:O	2:B:136:ARG:HA	2.21	0.40
1:A:449:ARG:HD2	1:A:450:ARG:CG	2.26	0.40
1:A:302:THR:CG2	6:A:801:HAS:HMB2	2.51	0.40
3:C:29:VAL:HG12	3:C:33:ARG:HD2	2.02	0.40
1:A:351:LEU:HD12	1:A:425:VAL:HG12	2.03	0.40
1:A:220:ASP:OD2	2:B:52:ARG:NH1	2.50	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	550/568 (97%)	500 (91%)	46 (8%)	4 (1%)	26	63
2	B	164/168 (98%)	145 (88%)	16 (10%)	3 (2%)	11	37
3	C	31/34 (91%)	28 (90%)	3 (10%)	0	100	100
All	All	745/770 (97%)	673 (90%)	65 (9%)	7 (1%)	21	57

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	ARG
2	B	87	ALA
2	B	88	PHE
1	A	384	HIS
1	A	330	ARG
1	A	369	PHE
2	B	100	GLY

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	448/462 (97%)	421 (94%)	27 (6%)	24	57
2	B	136/138 (99%)	123 (90%)	13 (10%)	10	31
3	C	26/27 (96%)	24 (92%)	2 (8%)	16	42
All	All	610/627 (97%)	568 (93%)	42 (7%)	19	48

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	32	LEU
1	A	48	ASN
1	A	56	LYS
1	A	133	TYR
1	A	168	ARG
1	A	212	SER
1	A	215	LEU
1	A	230	TRP
1	A	282	HIS
1	A	305	VAL
1	A	309	SER
1	A	326	LEU
1	A	339	LEU
1	A	354	LEU
1	A	368	SER
1	A	369	PHE
1	A	370	THR
1	A	439	LEU
1	A	449	ARG
1	A	452	TYR
1	A	472	LEU
1	A	478	LEU
1	A	513	SER
1	A	517	ASP
1	A	518	ARG
1	A	526	ARG
2	B	5	HIS
2	B	19	LEU
2	B	22	SER
2	B	23	LEU
2	B	72	VAL
2	B	99	GLN
2	B	111	ASP
2	B	121	THR
2	B	128	LEU
2	B	146	ARG
2	B	153	CYS
2	B	159	ASN
2	B	163	THR
3	C	13	LEU
3	C	24	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	76	ASN
1	A	254	GLN
1	A	298	HIS
1	A	366	ASN
1	A	417	GLN
2	B	8	HIS
2	B	69	GLN
2	B	93	ASN
2	B	117	HIS
2	B	122	ASN

5.3.3 RNA [i](#)

There are no RNA molecules 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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
8	CMO	A	563	-	0,1,1	0.00	-	0,0,0	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEM	A	800	1	30,50,50	1.86	6 (20%)	24,82,82	2.61	8 (33%)
6	HAS	A	801	1	45,72,72	1.64	9 (20%)	47,109,109	2.33	13 (27%)
7	CUA	B	802	2	0,1,1	0.00	-	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
8	CMO	A	563	-	-	0/0/0/0	0/0/0/0
5	HEM	A	800	1	-	0/10/54/54	0/0/8/8
6	HAS	A	801	1	-	0/30/82/82	0/0/8/8
7	CUA	B	802	2	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C3B-C4B	-5.93	1.46	1.51
5	A	800	HEM	C3D-C4D	-3.75	1.46	1.51
5	A	800	HEM	C2C-C1C	-3.32	1.46	1.52
5	A	800	HEM	C2D-C1D	-2.28	1.44	1.51
6	A	801	HAS	C18-C19	2.07	1.37	1.33
5	A	800	HEM	C4C-NC	2.22	1.38	1.36
5	A	800	HEM	C3C-CAC	2.60	1.56	1.51
6	A	801	HAS	C1D-CHB	2.63	1.47	1.39
6	A	801	HAS	C1C-CHC	2.80	1.47	1.39
6	A	801	HAS	C4A-CHD	3.14	1.48	1.39
6	A	801	HAS	C2A-C3A	3.19	1.47	1.37
6	A	801	HAS	C14-C15	3.19	1.39	1.33
6	A	801	HAS	C1A-CHA	3.34	1.49	1.39
6	A	801	HAS	C3C-C2C	4.73	1.46	1.40
6	A	801	HAS	C2D-C3D	4.97	1.46	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	HEM	C3B-CAB-CBB	-5.93	115.36	124.46
6	A	801	HAS	CMC-C2C-C3C	-5.30	114.71	125.09
6	A	801	HAS	CAD-CBD-CGD	-4.84	103.87	112.75
5	A	800	HEM	CBA-CAA-C2A	-4.68	104.14	112.53
6	A	801	HAS	C4D-C3D-C2D	-4.63	102.43	107.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	CAA-CBA-CGA	-4.28	104.91	112.75
6	A	801	HAS	C3C-CAC-CBC	-4.27	117.58	126.32
6	A	801	HAS	OMD-CMD-C2D	-2.90	119.26	125.11
6	A	801	HAS	C32-C30-C31	2.08	119.74	114.64
5	A	800	HEM	C2C-C1C-CHC	2.29	127.16	123.68
5	A	800	HEM	CMD-C2D-C3D	2.40	124.95	114.35
6	A	801	HAS	CMC-C2C-C1C	2.64	132.74	128.36
6	A	801	HAS	C25-C23-C24	2.84	119.75	115.41
6	A	801	HAS	C2D-C1D-ND	3.06	113.17	109.21
6	A	801	HAS	CAA-C2A-C1A	3.25	130.54	127.01
6	A	801	HAS	CAD-C3D-C4D	3.55	130.86	127.01
5	A	800	HEM	CMC-C2C-C3C	4.03	126.58	116.53
5	A	800	HEM	CMB-C2B-C3B	4.17	126.93	116.53
5	A	800	HEM	CAD-C3D-C2D	4.40	125.87	113.22
5	A	800	HEM	CAD-C3D-C4D	5.19	130.76	112.47
6	A	801	HAS	C3C-C4C-NC	6.73	123.65	110.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	HEM	2	0
6	A	801	HAS	10	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	552/568 (97%)	0.46	53 (9%) 10 6	47, 66, 95, 112	0
2	B	166/168 (98%)	0.56	12 (7%) 18 12	51, 70, 103, 135	0
3	C	33/34 (97%)	0.37	4 (12%) 6 3	51, 56, 76, 82	0
All	All	751/770 (97%)	0.48	69 (9%) 11 7	47, 66, 96, 135	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ALA	7.4
2	B	7	ALA	7.1
1	A	13	GLU	7.0
1	A	502	ALA	6.4
1	A	342	ASP	6.2
1	A	503	GLU	6.2
1	A	498	LYS	6.2
2	B	168	GLU	5.9
1	A	497	ARG	5.6
1	A	11	VAL	5.3
1	A	499	PRO	5.2
3	C	2	GLU	5.2
2	B	6	LYS	5.0
1	A	496	GLU	5.0
1	A	331	GLY	4.9
1	A	330	ARG	4.9
1	A	495	ARG	4.8
2	B	4	GLU	4.7
1	A	12	TYR	4.6
1	A	493	LEU	4.2
2	B	88	PHE	4.2
3	C	3	GLU	3.8
1	A	332	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	501	LEU	3.5
1	A	552	HIS	3.4
1	A	515	PRO	3.4
1	A	464	ALA	3.4
1	A	514	GLY	3.4
1	A	333	PHE	3.3
3	C	34	GLY	3.2
2	B	60	GLN	3.2
1	A	293	THR	3.1
1	A	341	TRP	3.1
1	A	216	VAL	3.1
1	A	105	LEU	3.0
1	A	15	TYR	3.0
1	A	486	TYR	3.0
1	A	465	VAL	2.9
1	A	215	LEU	2.9
2	B	144	GLU	2.9
1	A	415	ASP	2.8
1	A	452	TYR	2.8
1	A	53	PRO	2.7
1	A	529	PHE	2.7
1	A	516	GLU	2.6
1	A	319	SER	2.6
2	B	76	PRO	2.5
1	A	111	TRP	2.5
1	A	522	LEU	2.4
1	A	177	LYS	2.4
1	A	513	SER	2.4
2	B	82	TYR	2.4
1	A	61	PHE	2.3
1	A	519	ARG	2.3
1	A	317	ALA	2.3
1	A	548	GLN	2.3
1	A	419	ARG	2.3
2	B	69	GLN	2.2
1	A	457	PRO	2.2
1	A	454	ALA	2.2
1	A	526	ARG	2.2
3	C	31	PHE	2.2
1	A	517	ASP	2.1
1	A	142	HIS	2.1
2	B	40	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	416	ALA	2.0
2	B	10	ALA	2.0
1	A	368	SER	2.0
1	A	518	ARG	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
6	HAS	A	801	65/65	0.92	0.20	-0.13	40,40,40,40	0
5	HEM	A	800	43/43	0.96	0.17	-0.68	40,40,40,40	0
7	CUA	B	802	2/2	0.94	0.05	-3.92	40,40,40,40	0
8	CMO	A	563	2/2	0.98	0.10	-	40,40,40,40	0
4	CU1	A	803	1/1	0.98	0.06	-	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.