



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:45 PM GMT

PDB ID : 3S38
Title : Structure of Thermus thermophilus cytochrome ba3 oxidase 30s after Xe de-pressurization
Authors : Luna, V.M.; Fee, J.A.; Deniz, A.A.; Stout, C.D.
Deposited on : 2011-05-17
Resolution : 4.20 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

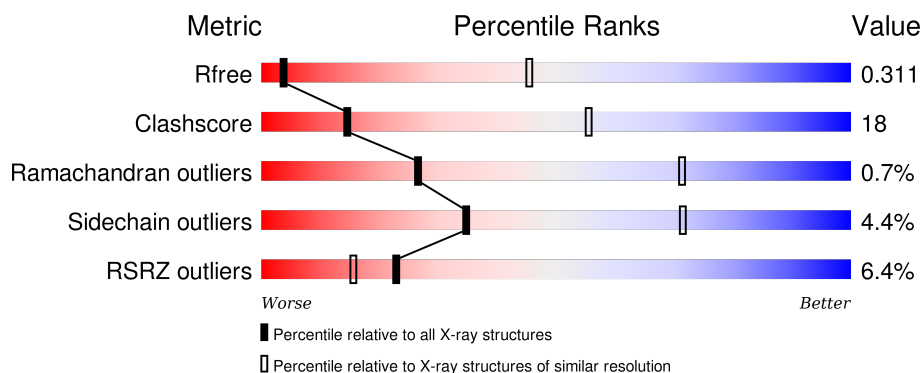
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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>5%</div> <div>61%</div> <div>33%</div> <div>• •</div> </div>
2	B	166	<div> <div>9%</div> <div>64%</div> <div>30%</div> <div>5%</div> <div>•</div> </div>
3	C	33	<div> <div>9%</div> <div>70%</div> <div>21%</div> <div>9%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	XE	A	565	-	-	X	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6056 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	554	Total	C	N	O	S	0	0	0
			4384	2971	704	693	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 (II) ION (three-letter code: CU) (formula: Cu).

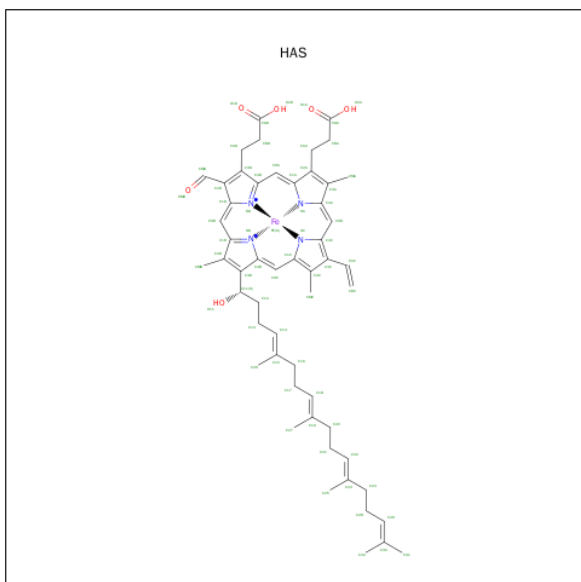
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



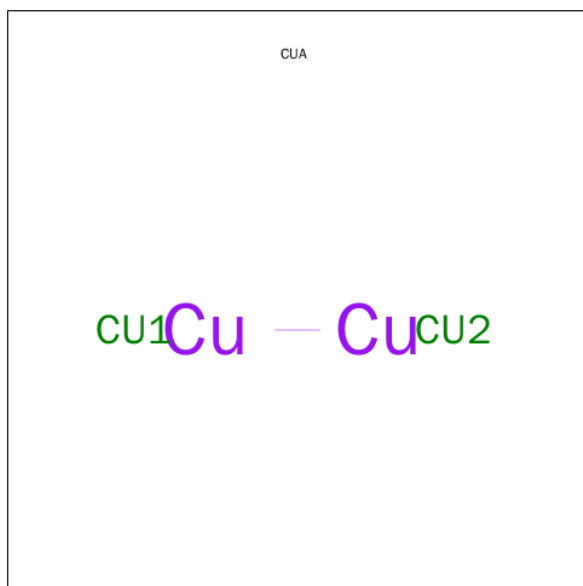
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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		

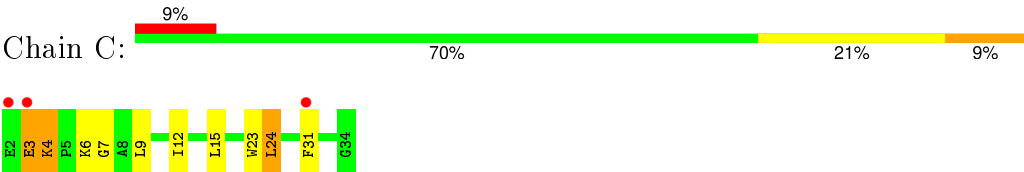
- Molecule 7 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 8 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	Xe	0	0
			4	4		



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.28 Å 108.28 Å 159.53 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.59 – 4.20 48.42 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (89.59-4.20) 99.7 (48.42-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 4.14 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.276 , 0.325 0.268 , 0.311	Depositor DCC
R_{free} test set	340 reflections (4.85%)	DCC
Wilson B-factor (Å ²)	146.3	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 24.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 7344 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6056	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, HAS, CUA, CU, XE

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	0.83	16/4541 (0.4%)	0.74	4/6232 (0.1%)
2	B	1.19	13/1335 (1.0%)	0.69	1/1822 (0.1%)
3	C	2.97	4/265 (1.5%)	0.94	2/359 (0.6%)
All	All	1.09	33/6141 (0.5%)	0.74	7/8413 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	GLU	CD-OE1	42.91	1.72	1.25
2	B	144	GLU	CD-OE2	13.38	1.40	1.25
2	B	168	GLU	CD-OE2	13.11	1.40	1.25
3	C	3	GLU	CG-CD	11.94	1.69	1.51
1	A	11	VAL	CB-CG2	11.15	1.76	1.52
1	A	13	GLU	CD-OE2	-11.12	1.13	1.25
3	C	3	GLU	CD-OE2	-10.92	1.13	1.25
2	B	144	GLU	CD-OE1	10.15	1.36	1.25
1	A	13	GLU	CD-OE1	9.96	1.36	1.25
1	A	157	TRP	CZ3-CH2	9.67	1.55	1.40
2	B	144	GLU	CB-CG	9.60	1.70	1.52
2	B	165	VAL	CB-CG1	9.15	1.72	1.52
2	B	61	GLU	CD-OE1	8.84	1.35	1.25
1	A	177	LYS	CD-CE	-8.57	1.29	1.51
1	A	15	TYR	CE2-CZ	8.26	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	130	GLY	C-O	8.05	1.36	1.23
1	A	15	TYR	CD2-CE2	-8.00	1.27	1.39
2	B	139	PHE	CB-CG	7.68	1.64	1.51
1	A	157	TRP	CD2-CE2	7.51	1.50	1.41
1	A	455	GLN	CD-OE1	7.30	1.40	1.24
1	A	11	VAL	CB-CG1	-7.13	1.37	1.52
2	B	60	GLN	CB-CG	7.03	1.71	1.52
2	B	143	GLY	N-CA	6.47	1.55	1.46
1	A	376	HIS	CG-ND1	6.42	1.52	1.38
1	A	518	ARG	CZ-NH2	6.24	1.41	1.33
1	A	15	TYR	CE1-CZ	5.70	1.46	1.38
2	B	139	PHE	C-O	5.69	1.34	1.23
1	A	531	PHE	CE1-CZ	5.59	1.48	1.37
2	B	144	GLU	C-O	5.58	1.33	1.23
1	A	283	HIS	C-O	5.40	1.33	1.23
2	B	139	PHE	CG-CD1	5.32	1.46	1.38
3	C	4	LYS	CD-CE	5.31	1.64	1.51
1	A	157	TRP	NE1-CE2	-5.10	1.30	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	GLU	OE1-CD-OE2	-19.27	100.17	123.30
1	A	13	GLU	CG-CD-OE2	11.82	141.93	118.30
1	A	518	ARG	NE-CZ-NH1	10.61	125.61	120.30
3	C	3	GLU	OE1-CD-OE2	10.02	135.32	123.30
3	C	3	GLU	CG-CD-OE1	-7.58	103.15	118.30
1	A	157	TRP	CH2-CZ2-CE2	-7.18	110.22	117.40
2	B	168	GLU	OE1-CD-OE2	-6.60	115.38	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	TYR	Sidechain
1	A	13	GLU	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4384	0	4494	157	23
2	B	1298	0	1280	55	28
3	C	259	0	279	15	5
4	A	1	0	0	0	0
5	A	43	0	30	4	0
6	A	65	0	62	11	0
7	B	2	0	0	0	0
8	A	4	0	0	3	0
All	All	6056	0	6145	218	28

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 18.

All (218) 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:11:VAL:CB	1:A:11:VAL:CG2	1.76	1.60
3:C:3:GLU:CD	3:C:3:GLU:OE1	1.72	1.28
3:C:3:GLU:CG	3:C:4:LYS:H	1.57	1.17
3:C:3:GLU:HG3	3:C:4:LYS:N	1.73	1.02
3:C:3:GLU:HG3	3:C:4:LYS:H	0.87	1.01
1:A:11:VAL:CG1	1:A:11:VAL:CG2	2.49	0.90
2:B:164:ILE:HG22	2:B:166:VAL:HG13	1.53	0.89
1:A:388:GLN:HB2	6:A:801:HAS:HAC	1.54	0.89
1:A:233:HIS:NE2	1:A:237:TYR:CE2	2.45	0.85
1:A:401:LEU:O	1:A:405:LEU:HB2	1.77	0.83
2:B:95:ILE:O	2:B:165:VAL:N	2.13	0.81
1:A:233:HIS:NE2	1:A:237:TYR:HE2	1.79	0.80
2:B:145:TYR:CE1	2:B:166:VAL:HG21	2.15	0.80
3:C:9:LEU:HD23	3:C:12:ILE:HD11	1.66	0.78
2:B:97:VAL:O	2:B:166:VAL:HA	1.83	0.77
1:A:9:SER:OG	1:A:497:ARG:NH2	2.19	0.76
2:B:94:PRO:HB2	2:B:165:VAL:HG23	1.66	0.76
1:A:149:ALA:CB	8:A:565:XE:XE	3.12	0.75
1:A:149:ALA:HB3	8:A:565:XE:XE	2.64	0.75
2:B:97:VAL:HG23	2:B:166:VAL:HG12	1.68	0.74
1:A:379:ALA:HB1	1:A:439:LEU:HD12	1.72	0.72
2:B:118:VAL:HG22	2:B:147:ILE:HG12	1.72	0.71
2:B:114:HIS:CE1	2:B:153:CYS:HB2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:TYR:CD1	2:B:166:VAL:HG21	2.26	0.70
2:B:97:VAL:N	2:B:165:VAL:O	2.24	0.69
1:A:232:GLY:O	1:A:235:ILE:HG22	1.92	0.69
1:A:388:GLN:HB2	6:A:801:HAS:CAC	2.22	0.69
3:C:3:GLU:CG	3:C:4:LYS:N	2.36	0.69
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.28	0.69
1:A:401:LEU:HB3	1:A:405:LEU:HD22	1.75	0.69
1:A:179:THR:O	1:A:266:ARG:NH2	2.21	0.68
1:A:11:VAL:CA	1:A:11:VAL:CG2	2.71	0.67
1:A:335:TRP:O	1:A:339:LEU:HD22	1.95	0.67
1:A:233:HIS:O	1:A:236:VAL:HG22	1.94	0.67
1:A:314:PHE:CD1	2:B:15:GLU:OE2	2.48	0.66
1:A:298:HIS:CE1	1:A:541:ALA:HB1	2.29	0.66
1:A:149:ALA:HB1	8:A:565:XE:XE	2.73	0.66
2:B:9:LYS:HE2	2:B:9:LYS:HA	1.78	0.65
1:A:487:GLY:O	1:A:491:VAL:HG23	1.96	0.65
2:B:88:PHE:HA	2:B:160:MET:HB2	1.79	0.65
1:A:122:LEU:HB2	1:A:123:PRO:HD3	1.79	0.64
1:A:230:TRP:HZ3	1:A:546:LEU:HD11	1.63	0.64
1:A:441:TRP:HZ3	1:A:469:PHE:HE2	1.45	0.63
2:B:139:PHE:HD2	2:B:145:TYR:CZ	2.17	0.63
1:A:435:MET:HG2	1:A:439:LEU:CD2	2.29	0.63
2:B:145:TYR:HE1	2:B:166:VAL:HG21	1.64	0.62
1:A:258:LYS:HG2	1:A:510:GLU:HB2	1.81	0.62
1:A:30:LEU:O	1:A:34:VAL:HG23	2.01	0.61
1:A:394:THR:O	1:A:398:MET:HG3	1.99	0.61
1:A:127:ASN:OD1	1:A:130:THR:OG1	2.18	0.61
1:A:307:VAL:HA	1:A:310:LEU:HD12	1.83	0.60
1:A:465:VAL:HG23	1:A:466:PRO:HD3	1.81	0.60
1:A:233:HIS:HE2	1:A:237:TYR:HE2	1.44	0.60
1:A:262:ASP:HB2	1:A:511:VAL:HG11	1.84	0.60
2:B:96:GLU:HA	2:B:165:VAL:O	2.01	0.60
1:A:188:VAL:HG21	1:A:269:PHE:HB3	1.83	0.59
1:A:227:LEU:O	1:A:230:TRP:HB3	2.03	0.58
1:A:357:ILE:HB	1:A:358:PRO:HD3	1.85	0.58
1:A:482:LEU:HA	1:A:485:ILE:HD12	1.86	0.57
2:B:164:ILE:CG2	2:B:166:VAL:HG13	2.30	0.57
2:B:71:VAL:HG13	2:B:81:VAL:HG22	1.86	0.57
1:A:127:ASN:ND2	1:A:562:TRP:HD1	2.02	0.57
1:A:286:ALA:HB1	2:B:125:VAL:HA	1.86	0.57
2:B:101:ALA:O	2:B:103:ILE:HD12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ASP:HB2	1:A:511:VAL:CG1	2.34	0.57
1:A:189:PHE:CE1	1:A:242:PRO:HD3	2.38	0.57
2:B:156:GLY:HA2	2:B:158:GLN:HE22	1.68	0.57
1:A:388:GLN:CB	6:A:801:HAS:CAC	2.83	0.57
1:A:359:GLY:HA3	1:A:388:GLN:NE2	2.20	0.56
1:A:376:HIS:ND1	6:A:801:HAS:O1D	2.37	0.56
1:A:410:GLY:CA	1:A:502:ALA:HB2	2.35	0.56
1:A:467:MET:O	1:A:471:VAL:HG23	2.06	0.55
2:B:147:ILE:HD11	2:B:164:ILE:HG13	1.88	0.55
1:A:230:TRP:CZ3	1:A:546:LEU:HD11	2.42	0.55
1:A:138:PRO:HG2	2:B:111:ASP:O	2.07	0.55
1:A:472:LEU:O	1:A:476:VAL:HG23	2.06	0.54
1:A:322:PHE:O	1:A:326:LEU:HD13	2.07	0.54
1:A:241:LEU:HA	1:A:244:TYR:HB2	1.89	0.54
1:A:209:LEU:O	1:A:213:PHE:HD1	1.90	0.54
2:B:94:PRO:HB2	2:B:165:VAL:CG2	2.37	0.54
2:B:92:PRO:HG2	2:B:95:ILE:HG12	1.88	0.54
2:B:18:TRP:CE3	3:C:12:ILE:HD12	2.43	0.54
1:A:218:GLY:HA3	1:A:555:PRO:HB2	1.90	0.54
1:A:361:ALA:O	1:A:365:VAL:HG23	2.08	0.53
2:B:92:PRO:HD2	2:B:95:ILE:HG12	1.90	0.53
2:B:69:GLN:HA	2:B:69:GLN:NE2	2.22	0.53
2:B:145:TYR:CD1	2:B:166:VAL:CG2	2.91	0.53
2:B:97:VAL:O	2:B:167:LYS:N	2.36	0.53
1:A:90:VAL:O	1:A:93:PRO:HG2	2.09	0.53
1:A:389:VAL:HG13	1:A:390:ALA:N	2.25	0.52
1:A:335:TRP:HE1	3:C:7:GLY:HA3	1.75	0.52
1:A:381:VAL:HB	1:A:382:PRO:HD3	1.91	0.52
1:A:157:TRP:HA	1:A:160:ILE:HD12	1.92	0.52
1:A:52:TYR:N	1:A:53:PRO:HD2	2.25	0.52
2:B:8:HIS:CD2	2:B:9:LYS:HE3	2.45	0.51
2:B:99:GLN:C	2:B:101:ALA:H	2.13	0.51
2:B:145:TYR:HD1	2:B:166:VAL:CG2	2.24	0.51
1:A:357:ILE:HG23	3:C:15:LEU:HD12	1.93	0.51
1:A:233:HIS:N	1:A:234:PRO:HD2	2.26	0.51
1:A:76:ASN:HB3	5:A:800:HEM:CBC	2.40	0.50
1:A:441:TRP:CZ3	1:A:469:PHE:HE2	2.26	0.50
1:A:314:PHE:HD1	2:B:15:GLU:OE2	1.93	0.50
1:A:165:ASP:OD1	1:A:169:ARG:NH2	2.45	0.50
1:A:449:ARG:HH12	6:A:801:HAS:CGA	2.24	0.50
3:C:23:TRP:HE3	3:C:24:LEU:HD12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:HIS:CD2	1:A:237:TYR:HE2	2.28	0.49
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.47	0.49
2:B:12:LEU:O	2:B:16:LYS:HG3	2.12	0.49
1:A:12:TYR:O	1:A:16:PRO:HB3	2.11	0.49
1:A:282:HIS:HA	1:A:285:PHE:CZ	2.47	0.49
1:A:82:GLN:HG2	1:A:86:GLN:OE1	2.13	0.49
1:A:79:VAL:HA	1:A:152:PHE:CZ	2.48	0.49
1:A:191:LEU:HD22	1:A:531:PHE:CD2	2.48	0.48
1:A:431:GLY:HA2	1:A:434:ILE:HD12	1.95	0.48
2:B:8:HIS:HD2	2:B:9:LYS:HE3	1.77	0.48
1:A:209:LEU:O	1:A:213:PHE:CD1	2.67	0.48
2:B:69:GLN:HA	2:B:69:GLN:HE21	1.78	0.47
1:A:389:VAL:CA	6:A:801:HAS:HBC2	2.45	0.47
1:A:229:TRP:CE3	1:A:232:GLY:HA3	2.50	0.47
1:A:51:ALA:O	1:A:54:LEU:HB3	2.14	0.47
1:A:321:GLU:O	1:A:325:ARG:HG2	2.15	0.47
2:B:66:ASP:HB3	2:B:69:GLN:HB2	1.97	0.47
1:A:260:VAL:HA	1:A:512:ILE:HD12	1.96	0.47
1:A:389:VAL:HB	6:A:801:HAS:CBC	2.45	0.46
2:B:141:ARG:HB3	2:B:145:TYR:OH	2.15	0.46
1:A:76:ASN:HB3	5:A:800:HEM:CAC	2.45	0.46
2:B:113:ILE:HG23	2:B:128:LEU:HD12	1.96	0.46
2:B:139:PHE:CD2	2:B:145:TYR:CE1	3.03	0.46
1:A:330:ARG:HB2	1:A:334:GLY:HA3	1.96	0.46
2:B:158:GLN:CD	2:B:158:GLN:H	2.19	0.46
1:A:420:LEU:HD21	1:A:487:GLY:HA2	1.98	0.46
1:A:170:TRP:CH2	1:A:180:PRO:HD3	2.50	0.46
3:C:9:LEU:HA	3:C:12:ILE:HG12	1.98	0.46
1:A:386:HIS:CE1	5:A:800:HEM:NA	2.84	0.45
3:C:4:LYS:HE3	3:C:6:LYS:HG2	1.97	0.45
1:A:230:TRP:C	1:A:230:TRP:CD1	2.89	0.45
1:A:430:LEU:O	1:A:434:ILE:HG13	2.17	0.45
1:A:361:ALA:HA	1:A:364:ILE:HD12	1.99	0.45
1:A:386:HIS:HE1	5:A:800:HEM:C1A	2.35	0.45
1:A:352:GLY:HA3	1:A:392:LEU:HA	1.98	0.45
1:A:130:THR:HB	1:A:562:TRP:CG	2.52	0.45
1:A:272:PHE:CZ	1:A:308:PRO:HB2	2.52	0.45
1:A:134:THR:O	1:A:135:PHE:C	2.55	0.44
2:B:27:PHE:HA	2:B:30:ILE:HD12	1.98	0.44
6:A:801:HAS:HBD1	6:A:801:HAS:HHA	1.99	0.44
1:A:402:TYR:CD1	1:A:413:ILE:HD13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:O	1:A:229:TRP:HD1	2.00	0.44
1:A:417:GLN:HA	1:A:420:LEU:HB3	1.99	0.44
1:A:261:SER:OG	1:A:263:PRO:HD2	2.18	0.44
1:A:186:ALA:O	1:A:190:TRP:CD1	2.71	0.44
2:B:139:PHE:H	2:B:139:PHE:HD1	1.65	0.44
2:B:139:PHE:N	2:B:139:PHE:CD1	2.86	0.44
1:A:369:PHE:C	1:A:369:PHE:CD2	2.90	0.44
1:A:184:TYR:CD1	1:A:527:ILE:HD11	2.53	0.44
2:B:89:GLY:N	2:B:160:MET:HG3	2.34	0.43
1:A:506:LEU:HB2	1:A:508:PHE:CE1	2.53	0.43
2:B:83:VAL:HB	2:B:107:ILE:HG12	2.00	0.43
3:C:4:LYS:HG2	3:C:6:LYS:HG2	2.00	0.43
1:A:389:VAL:HA	6:A:801:HAS:HBC2	2.00	0.43
1:A:92:LEU:N	1:A:93:PRO:HD2	2.33	0.43
1:A:424:VAL:HG11	1:A:484:PHE:HD1	1.83	0.43
1:A:391:SER:O	1:A:395:LEU:HG	2.19	0.43
1:A:279:VAL:O	1:A:282:HIS:ND1	2.52	0.43
1:A:230:TRP:HZ3	1:A:546:LEU:CD1	2.30	0.43
2:B:93:ASN:HA	2:B:94:PRO:HA	1.82	0.43
2:B:99:GLN:C	2:B:101:ALA:N	2.72	0.43
1:A:15:TYR:HB2	1:A:18:LYS:HD2	2.00	0.43
1:A:410:GLY:HA2	1:A:502:ALA:HB2	2.00	0.43
1:A:47:GLY:HA3	1:A:471:VAL:HG23	2.00	0.43
1:A:200:LEU:N	1:A:231:THR:OG1	2.51	0.43
1:A:46:TYR:HA	1:A:453:ILE:HD11	2.01	0.43
1:A:277:THR:N	1:A:278:PRO:CD	2.82	0.43
1:A:120:ALA:HB2	1:A:148:GLY:HA3	2.00	0.42
1:A:450:ARG:NH2	2:B:151:GLN:OE1	2.50	0.42
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.54	0.42
1:A:500:GLU:HG2	1:A:501:LEU:N	2.34	0.42
1:A:537:LEU:HD23	1:A:540:LEU:HD12	2.01	0.42
1:A:339:LEU:HB3	1:A:346:PHE:CZ	2.54	0.42
1:A:313:ALA:HB2	6:A:801:HAS:H273	2.01	0.42
1:A:42:GLN:HG3	1:A:52:TYR:OH	2.19	0.42
1:A:109:SER:HB3	1:A:158:VAL:HB	2.02	0.42
1:A:189:PHE:HE1	1:A:242:PRO:HD3	1.83	0.42
1:A:178:VAL:HG11	1:A:521:VAL:HG11	2.02	0.42
1:A:434:ILE:HG22	1:A:469:PHE:HB3	2.01	0.41
2:B:36:THR:HG22	3:C:31:PHE:CZ	2.55	0.41
1:A:274:LEU:HA	1:A:534:ALA:HB2	2.02	0.41
1:A:378:THR:HB	1:A:443:GLY:HA2	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HG11	1:A:117:LEU:HD13	2.02	0.41
1:A:351:LEU:O	1:A:354:LEU:HB2	2.20	0.41
1:A:197:SER:O	1:A:201:VAL:HG23	2.19	0.41
1:A:379:ALA:O	1:A:439:LEU:HB3	2.20	0.41
2:B:114:HIS:CE1	2:B:153:CYS:CB	3.00	0.41
2:B:69:GLN:CA	2:B:69:GLN:HE21	2.32	0.41
1:A:427:LEU:HB3	1:A:480:ALA:HB2	2.02	0.41
1:A:368:SER:HB2	1:A:371:LEU:HB2	2.02	0.41
1:A:342:ASP:O	1:A:418:ARG:NH2	2.53	0.41
1:A:389:VAL:HB	6:A:801:HAS:HBC2	2.02	0.41
2:B:26:LEU:O	2:B:30:ILE:HG13	2.21	0.41
1:A:186:ALA:O	1:A:190:TRP:HD1	2.04	0.41
2:B:145:TYR:O	2:B:164:ILE:N	2.51	0.41
1:A:59:LEU:HA	1:A:60:PRO:HD2	1.97	0.41
1:A:229:TRP:HA	1:A:232:GLY:HA3	2.02	0.41
1:A:225:ARG:O	1:A:229:TRP:CD1	2.74	0.41
1:A:188:VAL:CG2	1:A:269:PHE:HB3	2.50	0.41
1:A:178:VAL:HG11	1:A:521:VAL:CG1	2.50	0.41
1:A:348:ALA:HB3	1:A:349:PRO:HD3	2.03	0.41
1:A:445:LEU:O	1:A:446:ASN:HB2	2.21	0.41
1:A:369:PHE:C	1:A:369:PHE:HD2	2.24	0.41
1:A:534:ALA:O	1:A:538:VAL:HG23	2.21	0.41
1:A:343:ASN:HB3	1:A:346:PHE:HB3	2.04	0.40
1:A:380:TRP:CE3	1:A:440:HIS:HD2	2.39	0.40
1:A:335:TRP:NE1	3:C:7:GLY:HA3	2.37	0.40
1:A:88:ILE:HD13	1:A:88:ILE:HA	1.77	0.40
1:A:220:ASP:HA	1:A:221:PRO:HD3	1.88	0.40
1:A:192:MET:HG3	1:A:273:LEU:HA	2.03	0.40
1:A:378:THR:OG1	1:A:380:TRP:HB3	2.21	0.40
1:A:122:LEU:CB	1:A:123:PRO:HD3	2.49	0.40
1:A:403:TRP:C	1:A:406:PRO:HD2	2.42	0.40

All (28) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:O	2:B:143:GLY:C[3_454]	1.15	1.05
1:A:9:SER:O	2:B:143:GLY:CA[3_454]	1.21	0.99
2:B:60:GLN:CB	3:C:3:GLU:OE1[3_554]	1.41	0.79
1:A:9:SER:O	2:B:143:GLY:O[3_454]	1.47	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:OG	2:B:142:PRO:O[3_454]	1.61	0.59
1:A:9:SER:C	2:B:143:GLY:N[3_454]	1.64	0.56
1:A:13:GLU:OE1	2:B:166:VAL:N[3_454]	1.67	0.53
1:A:10:ARG:NH1	2:B:139:PHE:CG[3_454]	1.68	0.52
1:A:9:SER:O	2:B:143:GLY:N[3_454]	1.71	0.49
1:A:11:VAL:N	2:B:143:GLY:N[3_454]	1.72	0.48
1:A:10:ARG:NH1	2:B:139:PHE:CB[3_454]	1.74	0.46
1:A:11:VAL:N	2:B:142:PRO:C[3_454]	1.78	0.42
1:A:9:SER:C	2:B:143:GLY:CA[3_454]	1.82	0.38
1:A:10:ARG:NH1	2:B:139:PHE:CD1[3_454]	1.83	0.37
1:A:10:ARG:N	2:B:143:GLY:N[3_454]	1.92	0.28
1:A:13:GLU:OE1	2:B:165:VAL:C[3_454]	1.94	0.26
2:B:60:GLN:CG	3:C:3:GLU:OE1[3_554]	1.96	0.24
1:A:13:GLU:OE2	2:B:165:VAL:CA[3_454]	1.97	0.23
1:A:10:ARG:C	2:B:143:GLY:N[3_454]	2.00	0.20
1:A:11:VAL:N	2:B:142:PRO:CB[3_454]	2.01	0.19
2:B:60:GLN:CB	3:C:3:GLU:CG[3_554]	2.04	0.16
1:A:177:LYS:NZ	2:B:5:HIS:CE1[7_465]	2.04	0.16
1:A:10:ARG:N	2:B:142:PRO:C[3_454]	2.06	0.14
1:A:9:SER:C	2:B:143:GLY:C[3_454]	2.07	0.13
1:A:11:VAL:N	2:B:142:PRO:CA[3_454]	2.08	0.12
2:B:61:GLU:OE1	3:C:4:LYS:CD[3_554]	2.08	0.12
1:A:9:SER:N	2:B:144:GLU:N[3_454]	2.14	0.06
2:B:60:GLN:CB	3:C:3:GLU:CD[3_554]	2.16	0.04

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	552/568 (97%)	510 (92%)	38 (7%)	4 (1%)	26	71
2	B	164/166 (99%)	153 (93%)	10 (6%)	1 (1%)	30	74
3	C	31/33 (94%)	29 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	747/767 (97%)	692 (93%)	50 (7%)	5 (1%)	26 71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	PHE
1	A	135	PHE
2	B	87	ALA
1	A	330	ARG
1	A	102	ASN

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	450/462 (97%)	432 (96%)	18 (4%)	38 73
2	B	136/136 (100%)	128 (94%)	8 (6%)	24 64
3	C	26/26 (100%)	25 (96%)	1 (4%)	40 75
All	All	612/624 (98%)	585 (96%)	27 (4%)	35 71

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	48	ASN
1	A	133	TYR
1	A	168	ARG
1	A	230	TRP
1	A	274	LEU
1	A	277	THR
1	A	339	LEU
1	A	354	LEU
1	A	369	PHE
1	A	380	TRP

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Mol	Chain	Res	Type
1	A	401	LEU
1	A	430	LEU
1	A	439	LEU
1	A	441	TRP
1	A	449	ARG
1	A	472	LEU
1	A	513	SER
2	B	19	LEU
2	B	23	LEU
2	B	37	LEU
2	B	88	PHE
2	B	97	VAL
2	B	111	ASP
2	B	139	PHE
2	B	159	ASN
3	C	24	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	76	ASN
1	A	254	GLN
1	A	298	HIS
1	A	388	GLN
1	A	440	HIS
2	B	8	HIS
2	B	69	GLN
2	B	77	ASN
2	B	117	HIS
2	B	122	ASN
2	B	158	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	HEM	A	800	1	30,50,50	2.17	7 (23%)	24,82,82	2.31	7 (29%)
6	HAS	A	801	1	45,72,72	2.36	13 (28%)	47,109,109	2.63	17 (36%)
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
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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C3B-C4B	-6.97	1.45	1.51
5	A	800	HEM	C3D-C4D	-5.77	1.44	1.51
5	A	800	HEM	C2C-C1C	-3.85	1.45	1.52
6	A	801	HAS	C1B-NB	-2.64	1.33	1.36
5	A	800	HEM	C2D-C1D	-2.12	1.44	1.51
6	A	801	HAS	C4C-NC	-2.11	1.33	1.36
6	A	801	HAS	OMD-CMD	2.04	1.28	1.21
5	A	800	HEM	C3C-CAC	2.05	1.55	1.51
5	A	800	HEM	C3B-CAB	2.10	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	CAA-C2A	2.28	1.55	1.52
6	A	801	HAS	C14-C15	2.48	1.37	1.33
6	A	801	HAS	C1A-CHA	2.89	1.47	1.39
6	A	801	HAS	C1C-CHC	2.90	1.47	1.39
6	A	801	HAS	C4A-CHD	2.94	1.48	1.39
6	A	801	HAS	C1D-CHB	3.09	1.48	1.39
6	A	801	HAS	C2A-C3A	3.39	1.47	1.37
6	A	801	HAS	C3C-C2C	5.03	1.46	1.40
6	A	801	HAS	C2D-C3D	5.46	1.47	1.40
6	A	801	HAS	CBC-CAC	5.67	1.70	1.28
6	A	801	HAS	C3C-CAC	8.43	1.65	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	C3C-CAC-CBC	-8.58	108.76	126.32
6	A	801	HAS	C4D-C3D-C2D	-5.12	101.95	107.07
6	A	801	HAS	CAD-CBD-CGD	-4.52	104.45	112.75
6	A	801	HAS	C13-C12-C11	-4.41	108.66	114.51
6	A	801	HAS	CMC-C2C-C3C	-3.96	117.35	125.09
5	A	800	HEM	C3B-CAB-CBB	-3.69	118.79	124.46
6	A	801	HAS	C21-C22-C23	-2.59	122.13	127.76
6	A	801	HAS	C20-C21-C22	-2.55	105.01	111.69
6	A	801	HAS	C17-C18-C19	-2.39	122.56	127.76
6	A	801	HAS	CAA-CBA-CGA	-2.34	108.46	112.75
6	A	801	HAS	C13-C14-C15	-2.24	122.90	127.76
6	A	801	HAS	OMD-CMD-C2D	-2.20	120.68	125.11
6	A	801	HAS	CBA-CAA-C2A	-2.16	108.65	112.53
6	A	801	HAS	CBD-CAD-C3D	2.08	116.26	112.53
5	A	800	HEM	C2D-C3D-C4D	2.20	105.22	101.50
6	A	801	HAS	C2D-C1D-ND	2.64	112.63	109.21
5	A	800	HEM	CMD-C2D-C3D	2.97	127.49	114.35
5	A	800	HEM	CMB-C2B-C3B	3.98	126.46	116.53
5	A	800	HEM	CAD-C3D-C4D	3.98	126.52	112.47
6	A	801	HAS	C25-C23-C24	4.02	121.54	115.41
5	A	800	HEM	CMC-C2C-C3C	4.70	128.27	116.53
6	A	801	HAS	CAD-C3D-C4D	4.77	132.19	127.01
5	A	800	HEM	CAD-C3D-C2D	5.23	128.26	113.22
6	A	801	HAS	C3C-C4C-NC	6.35	122.94	110.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	HEM	4	0
6	A	801	HAS	11	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	554/568 (97%)	0.10	30 (5%)	29 22	117, 117, 117, 117	0
2	B	166/166 (100%)	0.21	15 (9%)	12 9	117, 117, 117, 117	0
3	C	33/33 (100%)	0.34	3 (9%)	11 9	117, 117, 117, 117	0
All	All	753/767 (98%)	0.13	48 (6%)	23 15	117, 117, 117, 117	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	79	TYR	5.0
2	B	136	ARG	4.9
1	A	502	ALA	4.2
1	A	552	HIS	3.8
2	B	80	THR	3.8
1	A	514	GLY	3.6
1	A	498	LYS	3.3
2	B	102	GLU	3.2
1	A	342	ASP	3.1
2	B	134	THR	3.0
3	C	3	GLU	3.0
1	A	63	GLN	3.0
1	A	411	LYS	2.9
1	A	409	THR	2.9
3	C	2	GLU	2.8
2	B	104	VAL	2.8
1	A	62	VAL	2.7
1	A	54	LEU	2.7
1	A	58	LEU	2.6
2	B	69	GLN	2.6
3	C	31	PHE	2.6
1	A	125	LEU	2.6
1	A	553	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	122	LEU	2.5
1	A	413	ILE	2.5
1	A	388	GLN	2.4
1	A	551	GLY	2.4
1	A	123	PRO	2.4
2	B	71	VAL	2.4
2	B	63	PRO	2.4
1	A	412	PRO	2.4
2	B	61	GLU	2.4
1	A	203	GLU	2.4
2	B	6	LYS	2.4
1	A	206	LEU	2.4
2	B	72	VAL	2.4
1	A	519	ARG	2.3
1	A	207	PHE	2.3
1	A	61	PHE	2.3
2	B	70	ALA	2.3
1	A	128	GLU	2.2
2	B	135	VAL	2.2
1	A	410	GLY	2.1
1	A	59	LEU	2.1
1	A	407	ASN	2.1
1	A	518	ARG	2.1
1	A	515	PRO	2.0
2	B	103	ILE	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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	XE	A	565	1/1	0.92	0.62	1.55	116,116,116,116	1
6	HAS	A	801	65/65	0.88	0.40	0.33	116,116,116,116	0
5	HEM	A	800	43/43	0.94	0.31	0.30	116,116,116,116	0
8	XE	A	564	1/1	0.90	0.31	0.04	116,116,116,116	1
8	XE	A	563	1/1	0.91	0.30	-0.23	116,116,116,116	1
8	XE	A	566	1/1	0.84	0.24	-0.45	116,116,116,116	1
7	CUA	B	802	2/2	0.97	0.14	-1.71	116,116,116,116	0
4	CU	A	803	1/1	0.85	0.33	-	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.