



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:35 AM GMT

PDB ID : 3NXU  
Title : Crystal structure of human cytochrome P4503A4 bound to an inhibitor ritonavir  
Authors : Sevrioukova, I.F.; Poulos, T.L.  
Deposited on : 2010-07-14  
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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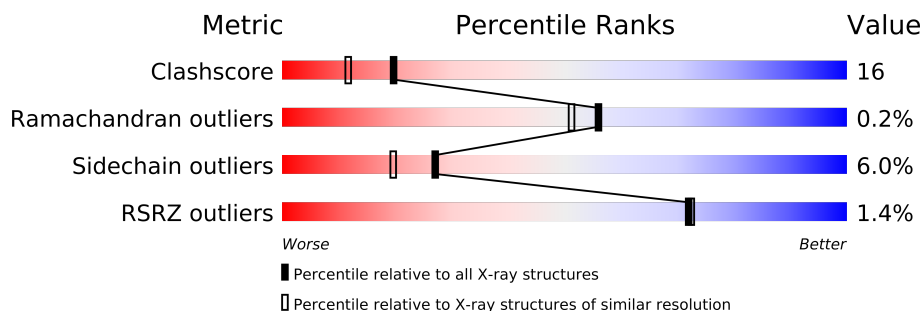
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	485	
1	B	485	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	DMS	A	703	-	X
2	DMS	B	705	-	X
4	RIT	B	600	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7955 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 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3678	2394	603	657	24			
1	B	457	Total	C	N	O	S	0	0	0
			3678	2394	603	657	24			

There are 12 discrepancies between the modelled and reference sequences:

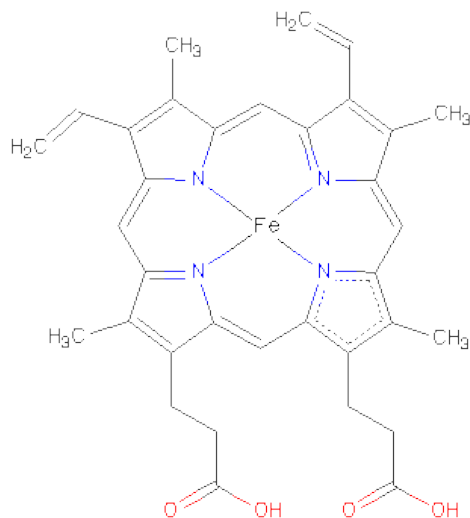
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	SEE REMARK 999	UNP P08684
A	24	ALA	-	SEE REMARK 999	UNP P08684
A	504	HIS	-	EXPRESSION TAG	UNP P08684
A	505	HIS	-	EXPRESSION TAG	UNP P08684
A	506	HIS	-	EXPRESSION TAG	UNP P08684
A	507	HIS	-	EXPRESSION TAG	UNP P08684
B	23	MET	-	SEE REMARK 999	UNP P08684
B	24	ALA	-	SEE REMARK 999	UNP P08684
B	504	HIS	-	EXPRESSION TAG	UNP P08684
B	505	HIS	-	EXPRESSION TAG	UNP P08684
B	506	HIS	-	EXPRESSION TAG	UNP P08684
B	507	HIS	-	EXPRESSION TAG	UNP P08684

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



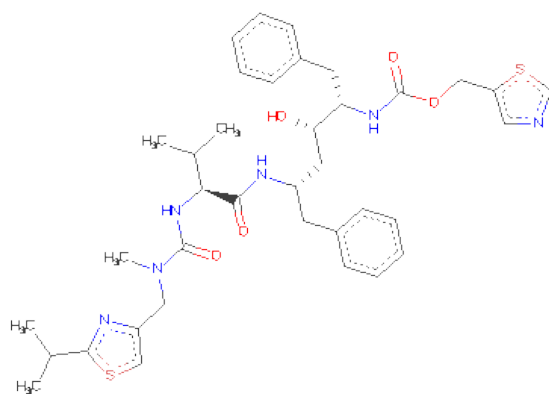
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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 RITONAVIR (three-letter code: RIT) (formula:  $C_{37}H_{48}N_6O_5S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			50	37	6	5	2		
4	B	1	Total	C	N	O	S	0	0
			50	37	6	5	2		

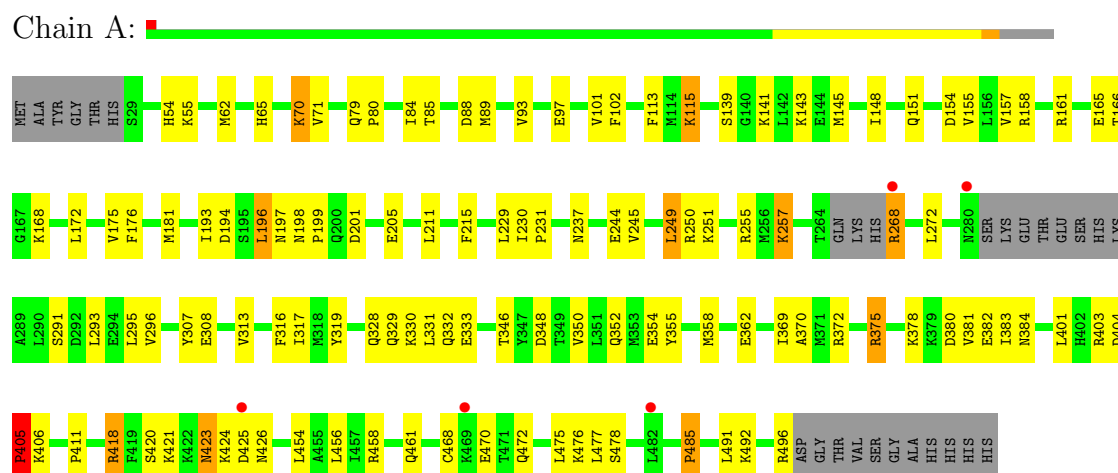
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	217	Total 217	O 217	0	0
5	B	172	Total 172	O 172	0	0

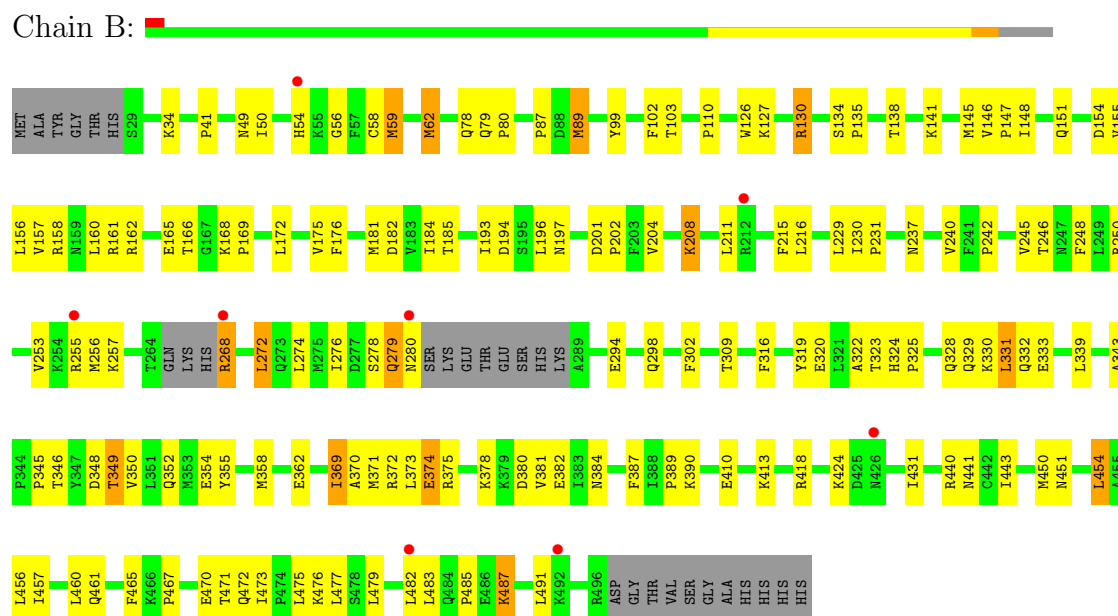
### 3 Residue-property plots

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 3A4



#### • Molecule 1: Cytochrome P450 3A4



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.12Å 94.69Å 93.13Å 90.00° 124.25° 90.00°	Depositor
Resolution (Å)	40.40 – 2.00 77.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.40-2.00) 97.6 (77.33-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.09 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.232 , 0.262 0.231 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.4	EDS
Estimated twinning fraction	0.006 for -1/2*h+3/2*k-l,1/2*h+1/2*k+l,1/2*h-1/2*k 0.003 for 1/2*h-1/2*k+2*l,-1/2*h+1/2*k,-1/2*h-1/2*k-l 0.009 for -h-k-l,l,k 0.016 for -h+k-l,-l,-k 0.003 for -1/2*h-3/2*k-l,-1/2*h+1/2*k-l,1/2*h+1/2*k 0.005 for 1/2*h+1/2*k+2*l,1/2*h+1/2*k,-1/2*h+1/2*k-l 0.010 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.016 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k 0.012 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.015 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.018 for -h-2*l,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 76658 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7955	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

<sup>1</sup>Intensities estimated from amplitudes.



Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, RIT, DMS

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	0.40	0/3766	0.63	1/5094 (0.0%)
1	B	0.37	0/3766	0.61	0/5094
All	All	0.39	0/7532	0.62	1/10188 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	ARG	NE-CZ-NH2	-5.44	117.58	120.30

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	3678	0	3764	99	0
1	B	3678	0	3764	140	0
2	A	16	0	24	1	0
2	B	8	0	12	3	0
3	A	43	0	30	7	0
3	B	43	0	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	50	0	47	6	0
4	B	50	0	46	4	0
5	A	217	0	0	13	0
5	B	172	0	0	15	0
All	All	7955	0	7717	246	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 16.

All (246) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:251:LYS:HG2	1:A:255:ARG:HH21	1.21	1.06
1:A:70:LYS:HD2	1:A:71:VAL:HG23	1.41	0.98
1:A:369:ILE:HG12	3:A:508:HEM:HMB1	1.52	0.90
1:B:472:GLN:HE21	1:B:476:LYS:H	1.16	0.90
1:A:370:ALA:HA	4:A:600:RIT:H50	1.50	0.90
1:B:472:GLN:NE2	1:B:476:LYS:H	1.75	0.85
1:A:251:LYS:HG2	1:A:255:ARG:NH2	1.94	0.82
1:B:329:GLN:O	1:B:333:GLU:HG2	1.83	0.78
1:A:70:LYS:CD	1:A:71:VAL:HG23	2.12	0.77
1:A:148:ILE:HD13	1:A:268:ARG:NH2	2.00	0.77
1:A:375:ARG:NH2	3:A:508:HEM:O1A	2.17	0.76
1:A:251:LYS:CG	1:A:255:ARG:HH21	1.98	0.76
1:A:369:ILE:HD12	4:A:600:RIT:H51	1.68	0.75
1:A:403:ARG:O	1:A:405:PRO:HD3	1.86	0.74
1:B:89:MET:HA	1:B:384:ASN:ND2	2.02	0.74
1:B:257:LYS:NZ	1:B:279:GLN:HE22	1.84	0.74
1:B:204:VAL:HG23	5:B:646:HOH:O	1.88	0.73
1:B:477:LEU:HA	1:B:485:PRO:HA	1.71	0.72
1:B:126:TRP:CZ2	1:B:440:ARG:HG2	2.24	0.72
1:B:155:VAL:HB	1:B:196:LEU:HD23	1.70	0.72
1:B:369:ILE:HG12	3:B:508:HEM:HMB1	1.70	0.71
1:A:70:LYS:HD2	1:A:71:VAL:CG2	2.20	0.70
1:A:423:ASN:OD1	1:A:423:ASN:N	2.24	0.70
1:B:475:LEU:HD21	1:B:485:PRO:HB3	1.74	0.70
1:A:404:ASP:OD1	1:A:406:LYS:HG3	1.91	0.70
1:A:250:ARG:HG2	1:A:296:VAL:HG11	1.74	0.69
1:A:468:CYS:HB3	1:A:492:LYS:HD2	1.74	0.69
1:B:59:MET:HE1	5:B:526:HOH:O	1.92	0.69
1:A:148:ILE:HD13	1:A:268:ARG:HH21	1.59	0.68
1:A:115:LYS:HD2	5:A:673:HOH:O	1.94	0.68
1:A:346:THR:O	1:A:350:VAL:HG23	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:97:GLU:HB3	1:A:101:VAL:HG12	1.77	0.67
1:B:161:ARG:O	1:B:165:GLU:HG2	1.95	0.67
1:B:346:THR:O	1:B:350:VAL:HG23	1.94	0.67
1:B:110:PRO:HD2	1:B:240:VAL:HG13	1.77	0.66
1:B:482:LEU:HD23	1:B:483:LEU:N	2.11	0.66
1:B:246:THR:O	1:B:250:ARG:HB2	1.96	0.66
1:B:257:LYS:NZ	1:B:279:GLN:NE2	2.43	0.66
1:A:316:PHE:CZ	1:A:485:PRO:HD3	2.31	0.66
1:A:369:ILE:HG12	3:A:508:HEM:CMB	2.25	0.65
1:B:323:THR:HG23	1:B:324:HIS:ND1	2.12	0.64
1:A:161:ARG:O	1:A:165:GLU:HG2	1.97	0.64
1:B:475:LEU:HD23	1:B:476:LYS:N	2.12	0.64
1:B:319:TYR:CZ	1:B:475:LEU:HB2	2.34	0.63
1:A:97:GLU:HB3	1:A:101:VAL:CG1	2.28	0.63
1:B:172:LEU:HD22	1:B:176:PHE:HE1	1.62	0.63
1:B:472:GLN:HE21	1:B:476:LYS:N	1.94	0.63
1:B:370:ALA:HB2	3:B:508:HEM:HMA2	1.81	0.63
1:B:54:HIS:O	1:B:479:LEU:HD13	1.99	0.63
1:A:155:VAL:HB	1:A:196:LEU:HD23	1.81	0.62
1:A:370:ALA:HB2	3:A:508:HEM:HMA2	1.82	0.62
1:B:148:ILE:HD13	1:B:268:ARG:NH2	2.15	0.62
1:B:257:LYS:HZ2	1:B:279:GLN:HE22	1.48	0.62
1:B:148:ILE:CD1	1:B:268:ARG:NH2	2.62	0.62
1:B:372:ARG:HB2	4:B:600:RIT:H951	1.81	0.62
1:B:355:TYR:HA	1:B:358:MET:HE2	1.82	0.62
1:B:278:SER:C	1:B:280:ASN:H	2.03	0.62
1:A:230:ILE:HB	1:A:231:PRO:HD3	1.82	0.61
1:B:156:LEU:O	1:B:160:LEU:HD13	2.00	0.61
1:A:257:LYS:HE3	1:A:295:LEU:HD13	1.83	0.61
1:B:181:MET:HG3	1:B:193:ILE:HD11	1.83	0.61
1:B:370:ALA:HB2	3:B:508:HEM:CMA	2.31	0.61
1:B:134:SER:OG	1:B:135:PRO:HD3	2.00	0.60
1:B:204:VAL:O	1:B:208:LYS:HG2	2.01	0.60
1:B:99:TYR:OH	1:B:127:LYS:HE2	2.02	0.60
1:A:154:ASP:O	1:A:157:VAL:HG22	2.01	0.60
1:A:172:LEU:HD11	1:A:491:LEU:HD12	1.83	0.60
1:A:331:LEU:HD23	1:A:331:LEU:O	2.02	0.60
1:A:181:MET:HG3	1:A:193:ILE:HD11	1.83	0.60
1:B:348:ASP:O	1:B:352:GLN:HG3	2.02	0.59
1:B:339:LEU:HB3	1:B:343:ALA:HB3	1.82	0.59
1:B:355:TYR:HA	1:B:358:MET:CE	2.32	0.59
1:B:58:CYS:SG	1:B:371:MET:CE	2.91	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:101:VAL:HG13	1:A:102:PHE:CD1	2.37	0.59
1:B:182:ASP:OD1	1:B:196:LEU:HB2	2.03	0.59
1:B:380:ASP:HB2	5:B:578:HOH:O	2.02	0.59
1:A:145:MET:HA	1:A:148:ILE:HD12	1.85	0.59
1:A:113:PHE:CD2	1:A:293:LEU:HD22	2.38	0.58
1:B:89:MET:HE3	5:B:659:HOH:O	2.03	0.58
1:B:457:ILE:O	1:B:461:GLN:HG2	2.03	0.58
1:B:330:LYS:HA	1:B:333:GLU:HG3	1.85	0.58
1:B:194:ASP:OD2	1:B:197:ASN:HB2	2.02	0.58
1:A:375:ARG:HD2	5:A:510:HOH:O	2.04	0.58
1:B:138:THR:OG1	1:B:141:LYS:HG2	2.04	0.57
1:B:354:GLU:HG2	1:B:358:MET:HE2	1.88	0.56
1:B:41:PRO:HB2	1:B:49:ASN:ND2	2.20	0.56
1:B:58:CYS:H	2:B:704:DMS:H21	1.71	0.56
1:B:354:GLU:HG2	1:B:358:MET:CE	2.36	0.55
1:B:58:CYS:SG	1:B:371:MET:HE2	2.46	0.55
1:A:89:MET:CE	5:A:4:HOH:O	2.54	0.55
1:A:375:ARG:HH22	3:A:508:HEM:CGA	2.17	0.55
4:B:600:RIT:C10	4:B:600:RIT:H141	2.37	0.55
1:B:134:SER:HA	1:B:443:ILE:HD11	1.87	0.55
1:A:330:LYS:HE3	1:A:355:TYR:CE2	2.42	0.55
1:A:372:ARG:HB2	4:A:600:RIT:H951	1.89	0.55
1:A:370:ALA:HB2	3:A:508:HEM:CMA	2.35	0.55
1:A:470:GLU:OE1	1:A:470:GLU:N	2.38	0.55
1:B:169:PRO:HG3	1:B:470:GLU:OE2	2.06	0.55
1:A:458:ARG:HG3	1:A:458:ARG:HH21	1.71	0.55
1:B:204:VAL:HG12	1:B:208:LYS:HE3	1.88	0.54
1:B:390:LYS:NZ	5:B:651:HOH:O	2.40	0.54
1:B:355:TYR:HD2	1:B:358:MET:HE3	1.73	0.54
1:A:65:HIS:HD2	5:A:16:HOH:O	1.90	0.54
4:A:600:RIT:H141	4:A:600:RIT:C10	2.37	0.54
1:B:471:THR:HG22	1:B:473:ILE:HG13	1.90	0.54
1:B:472:GLN:OE1	1:B:487:LYS:CE	2.55	0.53
1:B:320:GLU:HA	1:B:323:THR:HG22	1.90	0.53
1:A:166:THR:OG1	1:A:168:LYS:HG3	2.08	0.53
1:B:322:ALA:O	1:B:467:PRO:HD3	2.09	0.53
1:A:84:ILE:HB	1:A:89:MET:HE3	1.89	0.53
1:A:458:ARG:HD3	1:A:461:GLN:HE21	1.73	0.53
1:A:161:ARG:HG3	1:A:161:ARG:HH11	1.72	0.53
1:B:380:ASP:OD2	1:B:387:PHE:CE2	2.62	0.53
1:B:475:LEU:HD21	1:B:485:PRO:CB	2.38	0.53
1:B:201:ASP:HB3	5:B:646:HOH:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:103:THR:O	1:B:440:ARG:HD2	2.10	0.52
1:B:381:VAL:HG22	1:B:382:GLU:N	2.25	0.52
1:B:58:CYS:HB2	2:B:704:DMS:H23	1.91	0.52
1:B:230:ILE:HB	1:B:231:PRO:HD3	1.92	0.52
1:B:257:LYS:HZ1	1:B:279:GLN:HE22	1.55	0.51
1:B:354:GLU:O	1:B:358:MET:HG3	2.10	0.51
1:B:175:VAL:HG23	1:B:176:PHE:H	1.75	0.51
1:B:278:SER:C	1:B:280:ASN:N	2.63	0.51
1:B:58:CYS:SG	1:B:371:MET:HE3	2.50	0.51
1:B:154:ASP:O	1:B:157:VAL:HG22	2.10	0.51
1:A:316:PHE:HZ	1:A:485:PRO:HD3	1.72	0.51
1:B:369:ILE:HG12	3:B:508:HEM:CMB	2.39	0.51
1:A:381:VAL:HG22	1:A:382:GLU:N	2.26	0.51
1:B:34:LYS:HD3	5:B:639:HOH:O	2.11	0.50
1:A:141:LYS:O	1:A:145:MET:HG3	2.12	0.50
1:B:472:GLN:OE1	1:B:487:LYS:HE3	2.10	0.50
1:B:410:GLU:OE2	1:B:413:LYS:NZ	2.45	0.50
1:B:331:LEU:HD13	1:B:460:LEU:CD2	2.41	0.50
1:B:175:VAL:HG23	1:B:176:PHE:N	2.27	0.50
1:B:202:PRO:HB2	1:B:248:PHE:CE2	2.46	0.50
1:B:475:LEU:HD21	1:B:485:PRO:CG	2.42	0.49
2:A:703:DMS:H13	5:A:630:HOH:O	2.11	0.49
1:B:316:PHE:CZ	1:B:485:PRO:HD3	2.47	0.49
1:B:369:ILE:HG13	1:B:370:ALA:N	2.28	0.49
1:B:328:GLN:O	1:B:332:GLN:HG3	2.13	0.49
1:B:79:GLN:NE2	1:B:80:PRO:HD2	2.26	0.49
1:B:316:PHE:HZ	1:B:485:PRO:HD3	1.79	0.48
1:A:475:LEU:HD21	1:A:485:PRO:HG3	1.95	0.48
1:B:268:ARG:HH11	1:B:268:ARG:CB	2.26	0.48
1:A:362:GLU:OE1	1:A:418:ARG:NH1	2.46	0.48
1:A:54:HIS:CD2	1:A:55:LYS:HG2	2.48	0.48
1:B:257:LYS:HZ1	1:B:279:GLN:NE2	2.08	0.48
1:A:70:LYS:HD3	5:A:4:HOH:O	2.13	0.48
1:A:369:ILE:HG13	1:A:370:ALA:N	2.27	0.48
1:B:141:LYS:HE3	5:B:619:HOH:O	2.13	0.48
1:A:85:THR:HB	1:A:401:LEU:HD21	1.94	0.48
1:A:268:ARG:HH11	1:A:268:ARG:CB	2.27	0.48
1:B:302:PHE:CD2	3:B:508:HEM:HBC1	2.49	0.47
1:B:56:GLY:HA2	5:B:540:HOH:O	2.13	0.47
1:B:465:PHE:CD2	1:B:465:PHE:N	2.82	0.47
1:A:115:LYS:CE	5:A:664:HOH:O	2.62	0.47
1:B:135:PRO:HB2	1:B:274:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:244:GLU:HB2	5:A:528:HOH:O	2.13	0.47
1:B:56:GLY:HA3	2:B:704:DMS:H22	1.96	0.47
1:B:237:ASN:ND2	5:B:647:HOH:O	2.47	0.47
1:A:458:ARG:NH2	1:A:458:ARG:HG3	2.28	0.47
1:B:151:GLN:O	1:B:154:ASP:HB2	2.15	0.47
1:B:279:GLN:O	1:B:280:ASN:HB2	2.14	0.47
1:B:272:LEU:HD22	1:B:276:ILE:CD1	2.45	0.47
1:A:115:LYS:HE3	5:A:664:HOH:O	2.14	0.47
1:B:465:PHE:HD2	1:B:465:PHE:N	2.12	0.47
1:A:79:GLN:NE2	1:A:80:PRO:HD2	2.29	0.47
1:B:102:PHE:HB3	1:B:375:ARG:HB3	1.97	0.46
1:A:215:PHE:HZ	4:A:600:RIT:H862	1.80	0.46
1:A:420:SER:O	1:A:424:LYS:HB2	2.16	0.46
1:B:89:MET:CE	5:B:659:HOH:O	2.62	0.46
3:B:508:HEM:HBC2	3:B:508:HEM:HMC2	1.96	0.46
1:B:362:GLU:OE2	1:B:418:ARG:HD2	2.14	0.46
1:A:313:VAL:O	1:A:317:ILE:HG13	2.16	0.46
1:A:245:VAL:O	1:A:249:LEU:HD22	2.16	0.46
1:B:59:MET:CE	1:B:62:MET:HE2	2.46	0.46
1:A:348:ASP:O	1:A:352:GLN:HG3	2.16	0.46
1:B:172:LEU:HD11	1:B:491:LEU:HD12	1.98	0.46
1:B:87:PRO:HG3	1:B:431:ILE:HD11	1.96	0.46
1:A:198:ASN:O	1:A:201:ASP:HB2	2.16	0.46
1:A:475:LEU:HD23	1:A:475:LEU:C	2.36	0.46
1:A:477:LEU:HA	1:A:485:PRO:HA	1.98	0.46
1:B:257:LYS:HZ2	1:B:279:GLN:NE2	2.09	0.45
1:B:59:MET:HE3	1:B:62:MET:CE	2.46	0.45
1:B:172:LEU:HD22	1:B:176:PHE:CE1	2.49	0.45
1:A:102:PHE:HB3	1:A:375:ARG:HB3	1.97	0.45
1:B:242:PRO:HB2	1:B:245:VAL:HG23	1.99	0.45
1:A:405:PRO:HG3	1:A:411:PRO:HG3	1.99	0.45
1:A:89:MET:HA	1:A:384:ASN:ND2	2.32	0.45
1:A:331:LEU:HD23	1:A:331:LEU:C	2.37	0.45
1:A:472:GLN:NE2	1:A:476:LYS:H	2.14	0.45
1:B:378:LYS:HG3	5:B:3:HOH:O	2.16	0.45
1:B:323:THR:HG23	1:B:324:HIS:CE1	2.53	0.44
1:B:387:PHE:HE1	1:B:389:PRO:HG3	1.83	0.44
1:A:354:GLU:OE1	1:A:421:LYS:HD3	2.18	0.44
1:B:330:LYS:HE3	1:B:355:TYR:CE2	2.52	0.44
1:B:346:THR:H	1:B:349:THR:HG1	1.65	0.44
1:A:194:ASP:OD2	1:A:197:ASN:HB2	2.18	0.44
1:A:461:GLN:NE2	5:A:543:HOH:O	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:139:SER:O	1:A:143:LYS:HG3	2.18	0.43
1:B:215:PHE:HZ	4:B:600:RIT:H862	1.82	0.43
1:B:134:SER:N	1:B:135:PRO:CD	2.81	0.43
1:A:329:GLN:OE1	1:A:333:GLU:OE2	2.36	0.43
1:B:380:ASP:CB	5:B:578:HOH:O	2.65	0.43
1:B:59:MET:HE3	1:B:62:MET:HE2	2.00	0.43
1:B:130:ARG:NH2	1:B:441:ASN:O	2.52	0.43
1:A:319:TYR:CZ	1:A:475:LEU:HB2	2.54	0.43
1:A:354:GLU:O	1:A:358:MET:HG3	2.18	0.43
1:A:161:ARG:HG3	1:A:161:ARG:NH1	2.33	0.43
1:B:410:GLU:O	1:B:418:ARG:NH1	2.49	0.43
1:A:418:ARG:NH2	5:A:535:HOH:O	2.50	0.43
1:A:88:ASP:OD1	1:A:384:ASN:OD1	2.36	0.43
4:B:600:RIT:H683	4:B:600:RIT:H13	2.01	0.42
1:A:55:LYS:HA	1:A:55:LYS:HD3	1.76	0.42
1:B:472:GLN:OE1	1:B:487:LYS:HE2	2.19	0.42
1:A:157:VAL:HG23	1:A:158:ARG:N	2.33	0.42
1:A:496:ARG:HD3	5:A:716:HOH:O	2.18	0.42
1:B:294:GLU:O	1:B:298:GLN:HG2	2.20	0.42
1:B:450:MET:O	1:B:454:LEU:HB2	2.19	0.42
1:B:162:ARG:O	1:B:166:THR:HG23	2.19	0.42
1:A:426:ASN:HD22	1:A:426:ASN:HA	1.64	0.42
1:B:59:MET:CE	1:B:62:MET:CE	2.98	0.42
3:A:508:HEM:HMC2	3:A:508:HEM:HBC2	2.02	0.42
1:A:307:TYR:CD1	1:A:308:GLU:N	2.87	0.42
1:B:141:LYS:O	1:B:145:MET:HG3	2.20	0.41
1:B:253:VAL:HA	1:B:256:MET:HE3	2.02	0.41
1:A:404:ASP:OD1	1:A:404:ASP:C	2.57	0.41
1:B:345:PRO:HB3	1:B:457:ILE:HG21	2.02	0.41
1:B:374:GLU:HG3	5:B:522:HOH:O	2.19	0.41
1:B:126:TRP:CH2	1:B:440:ARG:HG2	2.55	0.41
1:A:113:PHE:CG	1:A:293:LEU:HD22	2.55	0.41
1:B:148:ILE:HG23	5:B:585:HOH:O	2.19	0.41
1:B:354:GLU:C	1:B:358:MET:HE2	2.41	0.41
1:A:381:VAL:CG2	1:A:382:GLU:N	2.84	0.41
1:B:325:PRO:O	1:B:328:GLN:HB3	2.20	0.41
4:A:600:RIT:H682	4:A:600:RIT:H13	2.03	0.41
1:A:328:GLN:O	1:A:332:GLN:HG3	2.21	0.41
1:A:175:VAL:HG13	1:A:176:PHE:N	2.35	0.41
1:B:331:LEU:HD13	1:B:460:LEU:HD21	2.03	0.41
1:A:383:ILE:O	1:A:383:ILE:HG13	2.20	0.41
1:B:165:GLU:HA	1:B:165:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:184:ILE:CG2	1:B:185:THR:N	2.84	0.40
1:B:184:ILE:HG23	1:B:185:THR:N	2.36	0.40
1:A:151:GLN:HG3	5:A:583:HOH:O	2.21	0.40
1:B:146:VAL:N	1:B:147:PRO:HD2	2.36	0.40
1:A:101:VAL:O	1:A:378:LYS:HG2	2.21	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	451/485 (93%)	433 (96%)	17 (4%)	1 (0%)	56	51
1	B	451/485 (93%)	426 (94%)	24 (5%)	1 (0%)	56	51
All	All	902/970 (93%)	859 (95%)	41 (4%)	2 (0%)	56	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	424	LYS
1	A	405	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	418/441 (95%)	394 (94%)	24 (6%)	29	21
1	B	418/441 (95%)	392 (94%)	26 (6%)	26	18
All	All	836/882 (95%)	786 (94%)	50 (6%)	27	20

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	MET
1	A	70	LYS
1	A	93	VAL
1	A	115	LYS
1	A	196	LEU
1	A	199	PRO
1	A	205	GLU
1	A	211	LEU
1	A	229	LEU
1	A	237	ASN
1	A	249	LEU
1	A	257	LYS
1	A	268	ARG
1	A	272	LEU
1	A	291	SER
1	A	380	ASP
1	A	405	PRO
1	A	418	ARG
1	A	423	ASN
1	A	425	ASP
1	A	454	LEU
1	A	456	LEU
1	A	478	SER
1	A	485	PRO
1	B	50	ILE
1	B	59	MET
1	B	62	MET
1	B	78	GLN
1	B	89	MET
1	B	130	ARG
1	B	158	ARG
1	B	168	LYS
1	B	208	LYS
1	B	211	LEU
1	B	216	LEU
1	B	229	LEU
1	B	255	ARG
1	B	268	ARG
1	B	272	LEU
1	B	279	GLN
1	B	309	THR
1	B	331	LEU

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Mol	Chain	Res	Type
1	B	349	THR
1	B	369	ILE
1	B	373	LEU
1	B	374	GLU
1	B	451	ASN
1	B	454	LEU
1	B	456	LEU
1	B	487	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	GLN
1	A	352	GLN
1	A	384	ASN
1	A	426	ASN
1	A	451	ASN
1	A	461	GLN
1	A	472	GLN
1	B	65	HIS
1	B	197	ASN
1	B	279	GLN
1	B	329	GLN
1	B	352	GLN
1	B	384	ASN
1	B	451	ASN
1	B	472	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 ⓘ

10 ligands are modelled in this entry.

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$
3	HEM	A	508	1,4	49,50,50	2.76	12 (24%)	46,82,82	1.18	2 (4%)
4	RIT	A	600	3	53,53,53	6.29	35 (66%)	67,71,71	3.85	35 (52%)
2	DMS	A	700	-	3,3,3	0.96	0	3,3,3	0.80	0
2	DMS	A	701	-	3,3,3	0.83	0	3,3,3	0.88	0
2	DMS	A	702	-	3,3,3	0.76	0	3,3,3	0.87	0
2	DMS	A	703	-	3,3,3	0.75	0	3,3,3	0.80	0
3	HEM	B	508	1,4	49,50,50	2.64	13 (26%)	46,82,82	1.13	2 (4%)
4	RIT	B	600	3	53,53,53	6.64	37 (69%)	67,71,71	3.29	27 (40%)
2	DMS	B	704	-	3,3,3	2.08	2 (66%)	3,3,3	0.72	0
2	DMS	B	705	-	3,3,3	1.72	1 (33%)	3,3,3	0.91	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
3	HEM	A	508	1,4	-	0/14/114/114	0/0/8/8
4	RIT	A	600	3	-	0/50/53/53	0/4/4/4
2	DMS	A	700	-	-	0/0/0/0	0/0/0/0
2	DMS	A	701	-	-	0/0/0/0	0/0/0/0
2	DMS	A	702	-	-	0/0/0/0	0/0/0/0
2	DMS	A	703	-	-	0/0/0/0	0/0/0/0
3	HEM	B	508	1,4	-	0/14/114/114	0/0/8/8
4	RIT	B	600	3	-	0/50/53/53	0/4/4/4
2	DMS	B	704	-	-	0/0/0/0	0/0/0/0
2	DMS	B	705	-	-	0/0/0/0	0/0/0/0

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	RIT	C6-C2	-38.21	1.19	1.49
4	A	600	RIT	C6-C2	-30.57	1.25	1.49
4	A	600	RIT	C82-C85	12.95	1.61	1.51
4	A	600	RIT	O24-C10	11.01	1.43	1.21
3	B	508	HEM	C2D-C1D	10.64	1.47	1.44
3	A	508	HEM	C2B-C1B	10.34	1.47	1.44
3	A	508	HEM	C3D-C4D	9.55	1.46	1.44
4	A	600	RIT	C44-C15	8.94	1.66	1.53
4	B	600	RIT	O24-C10	8.92	1.39	1.21
4	A	600	RIT	C1-C2	-8.84	1.22	1.36
4	B	600	RIT	C31-C28	8.74	1.58	1.38
3	B	508	HEM	C3D-C4D	7.92	1.46	1.44
4	B	600	RIT	C21-N20	7.49	1.53	1.35
4	A	600	RIT	C52-C45	7.20	1.55	1.38
4	A	600	RIT	C12-N11	7.19	1.59	1.46
4	A	600	RIT	O76-C21	7.18	1.37	1.23
4	A	600	RIT	C31-C28	7.10	1.55	1.38
4	B	600	RIT	C82-C85	6.91	1.56	1.51
4	A	600	RIT	C21-N20	6.87	1.51	1.35
4	A	600	RIT	C19-N20	-6.82	1.31	1.45
4	B	600	RIT	C49-C48	6.73	1.54	1.39
4	B	600	RIT	O76-C21	6.72	1.36	1.23
3	A	508	HEM	C2D-C1D	6.56	1.46	1.44
4	B	600	RIT	C12-N11	6.33	1.58	1.46
4	A	600	RIT	C14-C15	-6.07	1.32	1.52
4	A	600	RIT	C80-S81	5.99	1.80	1.70
4	B	600	RIT	C52-C45	5.99	1.52	1.38
4	A	600	RIT	C49-C48	5.89	1.52	1.39
4	B	600	RIT	C14-C15	-5.80	1.33	1.52
4	A	600	RIT	O41-C13	5.72	1.56	1.43
4	B	600	RIT	C19-N20	-5.72	1.33	1.45
4	B	600	RIT	C51-C52	5.49	1.51	1.39
4	B	600	RIT	C50-C49	5.32	1.53	1.37
3	B	508	HEM	C2B-C1B	5.15	1.45	1.44
4	B	600	RIT	C44-C15	5.08	1.61	1.53
4	A	600	RIT	C62-C19	5.04	1.68	1.54
4	A	600	RIT	C34-C33	4.94	1.52	1.37
4	B	600	RIT	C80-S81	4.76	1.78	1.70
4	B	600	RIT	C34-C35	4.70	1.49	1.39
4	A	600	RIT	C51-C52	4.52	1.49	1.39
4	A	600	RIT	C32-C31	4.50	1.49	1.39
3	B	508	HEM	C3D-C2D	-4.47	1.35	1.43
4	B	600	RIT	C34-C33	4.43	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	RIT	C48-C45	4.38	1.48	1.38
4	B	600	RIT	C1-C2	-4.35	1.29	1.36
4	B	600	RIT	C51-C50	4.29	1.50	1.37
4	A	600	RIT	C50-C49	4.24	1.50	1.37
4	A	600	RIT	C19-C18	-4.24	1.42	1.52
4	B	600	RIT	C1-N5	-4.22	1.22	1.35
3	A	508	HEM	C3D-C2D	-4.10	1.36	1.43
4	A	600	RIT	C51-C50	4.09	1.49	1.37
4	B	600	RIT	C62-C19	3.98	1.65	1.54
4	A	600	RIT	C34-C35	3.84	1.47	1.39
3	B	508	HEM	CHB-C1B	3.81	1.41	1.35
4	B	600	RIT	C10-N11	3.78	1.45	1.34
4	A	600	RIT	C33-C32	3.62	1.48	1.37
3	B	508	HEM	C4A-C3A	3.53	1.44	1.40
4	B	600	RIT	O61-C18	3.44	1.30	1.23
4	B	600	RIT	C35-C28	3.43	1.46	1.38
3	A	508	HEM	C4A-C3A	3.40	1.44	1.40
4	B	600	RIT	C33-C32	3.40	1.47	1.37
4	A	600	RIT	C21-N74	3.38	1.44	1.36
3	A	508	HEM	C3C-C2C	-3.33	1.37	1.43
4	B	600	RIT	C75-C77	3.28	1.56	1.51
3	A	508	HEM	CHD-C4C	3.23	1.42	1.36
4	B	600	RIT	C18-N58	3.19	1.41	1.34
3	B	508	HEM	C3C-C2C	-3.19	1.38	1.43
4	A	600	RIT	C75-N74	3.17	1.56	1.46
4	A	600	RIT	C35-C28	3.13	1.46	1.38
4	A	600	RIT	C48-C45	3.11	1.45	1.38
4	B	600	RIT	O7-C10	-2.99	1.28	1.35
4	B	600	RIT	C68-C62	-2.96	1.41	1.52
3	B	508	HEM	C3B-C2B	-2.89	1.38	1.43
3	B	508	HEM	CHC-C1C	2.81	1.41	1.36
2	B	704	DMS	C2-S	-2.80	1.53	1.75
4	A	600	RIT	C44-C45	-2.76	1.44	1.51
3	A	508	HEM	CHA-C4D	2.74	1.39	1.35
4	B	600	RIT	C2-S3	-2.66	1.67	1.72
4	B	600	RIT	C32-C31	2.61	1.45	1.39
4	A	600	RIT	C82-N83	-2.60	1.25	1.35
3	B	508	HEM	CHA-C4D	2.52	1.39	1.35
4	A	600	RIT	C4-S3	-2.51	1.60	1.68
3	A	508	HEM	CHB-C1B	2.48	1.39	1.35
2	B	705	DMS	O-S	-2.41	1.33	1.50
4	B	600	RIT	O41-C13	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	508	HEM	CHD-C4C	2.36	1.40	1.36
4	B	600	RIT	C82-N83	-2.35	1.26	1.35
3	A	508	HEM	C3B-C4B	2.32	1.47	1.44
3	B	508	HEM	CMB-C2B	2.31	1.54	1.47
3	A	508	HEM	FE-NB	2.27	2.06	1.97
4	A	600	RIT	C68-C62	2.24	1.60	1.52
4	A	600	RIT	C18-N58	2.22	1.39	1.34
2	B	704	DMS	O-S	-2.17	1.35	1.50
3	B	508	HEM	FE-NA	2.14	2.01	1.92
4	B	600	RIT	C4-N5	-2.12	1.29	1.36
4	B	600	RIT	C77-N83	-2.11	1.30	1.36
4	B	600	RIT	C26-C28	-2.06	1.46	1.51
3	A	508	HEM	CHC-C1C	2.03	1.39	1.36
4	A	600	RIT	C10-N11	2.01	1.40	1.34
4	A	600	RIT	C26-C12	2.01	1.58	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	RIT	C44-C15-N58	11.21	127.80	110.21
4	B	600	RIT	C44-C15-N58	10.53	126.73	110.21
4	A	600	RIT	C14-C13-C12	-10.33	99.74	113.43
4	A	600	RIT	C6-C2-C1	10.21	143.37	127.44
4	A	600	RIT	C26-C12-N11	9.26	121.00	110.20
4	B	600	RIT	C1-N5-C4	9.11	119.80	105.79
4	B	600	RIT	C26-C12-N11	8.85	120.52	110.20
4	A	600	RIT	C1-N5-C4	8.25	118.48	105.79
4	B	600	RIT	C6-C2-C1	8.00	139.92	127.44
4	B	600	RIT	C14-C13-C12	-7.60	103.36	113.43
4	A	600	RIT	C4-S3-C2	7.51	98.06	91.83
4	A	600	RIT	C1-C2-S3	-6.64	105.63	112.20
4	A	600	RIT	C6-C2-S3	-6.56	110.78	120.84
4	B	600	RIT	C12-N11-C10	-5.67	113.05	122.26
4	B	600	RIT	C6-C2-S3	-5.29	112.72	120.84
4	B	600	RIT	C19-N20-C21	-5.25	109.42	121.25
4	A	600	RIT	C19-N20-C21	-5.14	109.65	121.25
4	B	600	RIT	C1-C2-S3	-5.10	107.15	112.20
4	A	600	RIT	O7-C10-N11	4.90	122.30	110.57
3	B	508	HEM	C3B-C4B-NB	-4.80	110.56	114.00
4	B	600	RIT	C62-C19-N20	-4.51	99.90	111.37
4	A	600	RIT	C77-C80-S81	-4.51	99.16	110.63
4	B	600	RIT	C77-C80-S81	-4.47	99.27	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	RIT	C19-C18-N58	-4.42	106.74	116.48
4	A	600	RIT	N20-C21-N74	4.32	120.36	116.31
4	A	600	RIT	C64-C62-C19	4.31	123.08	111.17
4	A	600	RIT	C12-N11-C10	-4.21	115.41	122.26
4	A	600	RIT	C45-C44-C15	-4.12	107.28	114.09
4	A	600	RIT	C13-C12-N11	3.98	116.69	109.61
4	B	600	RIT	C75-C77-C80	-3.82	122.72	129.07
4	B	600	RIT	O7-C10-N11	3.82	119.72	110.57
4	A	600	RIT	C62-C19-N20	-3.80	101.72	111.37
4	B	600	RIT	N20-C21-N74	3.73	119.81	116.31
4	A	600	RIT	O24-C10-N11	-3.51	118.65	124.90
4	B	600	RIT	C13-C14-C15	3.44	122.88	115.01
4	A	600	RIT	C75-C77-C80	-3.36	123.49	129.07
3	A	508	HEM	CBD-CAD-C3D	-3.34	107.08	114.37
4	B	600	RIT	C28-C26-C12	-3.27	107.40	113.46
4	B	600	RIT	C13-C12-N11	3.14	115.19	109.61
4	A	600	RIT	C2-C1-N5	3.09	115.16	108.99
4	A	600	RIT	O61-C18-C19	3.01	127.00	120.68
4	B	600	RIT	O24-C10-N11	-3.00	119.55	124.90
4	B	600	RIT	C2-C1-N5	2.94	114.86	108.99
4	A	600	RIT	C44-C45-C52	-2.93	115.16	120.90
4	A	600	RIT	O7-C10-O24	-2.88	117.88	124.19
4	A	600	RIT	C13-C14-C15	2.84	121.50	115.01
4	A	600	RIT	C28-C26-C12	-2.83	108.22	113.46
3	A	508	HEM	C3B-C4B-NB	-2.80	111.99	114.00
4	A	600	RIT	C75-C77-N83	-2.80	118.38	124.01
4	A	600	RIT	C68-C62-C19	2.80	118.90	111.17
4	B	600	RIT	C75-C77-N83	-2.80	118.38	124.01
4	A	600	RIT	C26-C28-C31	-2.72	115.56	120.90
4	B	600	RIT	C80-C77-N83	2.48	118.89	109.44
4	A	600	RIT	C6-O7-C10	-2.48	109.67	115.98
4	B	600	RIT	C44-C45-C52	-2.47	116.06	120.90
4	A	600	RIT	C15-N58-C18	2.44	127.12	123.18
4	B	600	RIT	C77-C75-N74	-2.40	109.59	113.79
4	B	600	RIT	O41-C13-C14	-2.31	104.53	109.14
4	A	600	RIT	C80-C77-N83	2.28	118.13	109.44
4	B	600	RIT	C26-C28-C31	-2.23	116.54	120.90
4	A	600	RIT	O41-C13-C12	-2.19	104.50	109.46
4	A	600	RIT	C62-C19-C18	2.17	116.93	111.39
4	A	600	RIT	C52-C45-C48	2.09	121.68	118.16
4	B	600	RIT	O7-C10-O24	-2.08	119.63	124.19
4	B	600	RIT	C62-C19-C18	2.06	116.66	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	508	HEM	C4A-CHB-C1B	-2.01	124.83	127.47

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	457/485 (94%)	0.02	5 (1%) 77 78	24, 38, 64, 75	0
1	B	457/485 (94%)	0.09	8 (1%) 65 66	26, 46, 70, 83	0
All	All	914/970 (94%)	0.06	13 (1%) 72 72	24, 42, 68, 83	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	482	LEU	5.1
1	A	280	ASN	2.7
1	B	54	HIS	2.6
1	B	255	ARG	2.5
1	A	482	LEU	2.4
1	B	212	ARG	2.2
1	A	469	LYS	2.2
1	A	268	ARG	2.2
1	B	268	ARG	2.2
1	A	425	ASP	2.2
1	B	492	LYS	2.2
1	B	426	ASN	2.0
1	B	280	ASN	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	DMS	A	703	4/4	0.16	2.73	71,71,72,74	0
2	DMS	B	705	4/4	0.16	2.59	60,60,61,65	0
4	RIT	B	600	50/50	0.18	2.38	41,53,58,59	0
2	DMS	B	704	4/4	0.17	0.82	51,53,54,56	0
4	RIT	A	600	50/50	0.14	0.68	33,40,45,46	0
2	DMS	A	701	4/4	0.13	0.63	71,71,71,73	0
3	HEM	A	508	43/43	0.11	-0.14	23,26,29,31	0
2	DMS	A	702	4/4	0.12	-0.24	71,71,72,74	0
3	HEM	B	508	43/43	0.10	-0.26	30,32,34,36	0
2	DMS	A	700	4/4	0.12	-0.33	38,39,39,43	0

## 6.5 Other polymers

There are no such residues in this entry.