



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:55 AM GMT

PDB ID : 3EPM  
Title : Crystal structure of Caulobacter crescentus ThiC  
Authors : Li, S.; Chatterjee, A.; Zhang, Y.; Grove, T.L.; Lee, M.; Krebs, C.; Booker, S.J.; Begley, T.P.; Ealick, S.E.  
Deposited on : 2008-09-29  
Resolution : 2.79 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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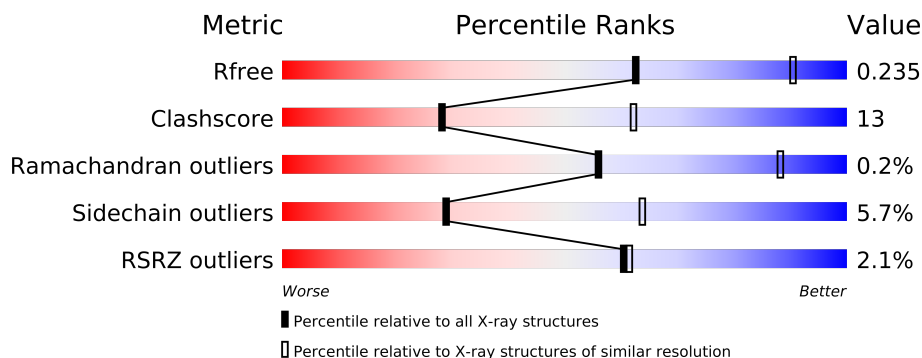
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	612	
1	B	612	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	HMH	A	1001	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8210 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.

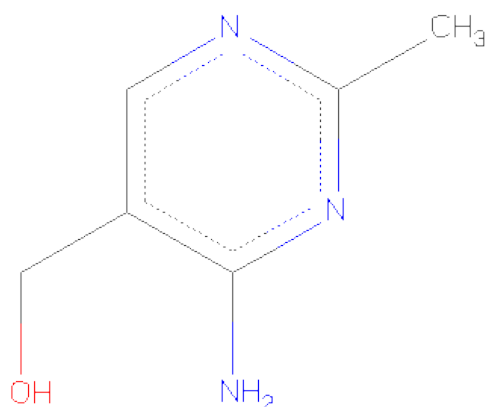
- Molecule 1 is a protein called Thiamine biosynthesis protein thiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	Se	0	0	0
			4042	2558	715	751	6	12			
1	B	512	Total	C	N	O	S	Se	0	0	0
			4018	2543	711	746	6	12			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is 4-AMINO-5-HYDROXYMETHYL-2-METHYLPYRIMIDINE (three-letter code: HMH) (formula: C<sub>6</sub>H<sub>9</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	91	Total	O	0	0
			91	91		
5	B	42	Total	O	0	0
			42	42		



THR	N426	THR
LEU		
PRO	E429	PRO
LYS	Q430	LYS
GLU	L431	GLU
ALA	K432	ALA
HIS	H433	HIS
LYS	C434	LYS
THR	H435	THR
ALA	E436	ALA
HIS		HIS
PHE	F439	PHE
CYS	V440	CYS
SER	T441	SER
MSE		MSE
CYS	P444	CYS
GLY	L445	GLY
PRO		PRO
LYS		LYS
PHE	D448	PHE
CYS		CYS
SER	T457	SER
MSE	S458	MSE
LYS	A459	LYS
ILE	T460	ILE
SER	G461	SER
GLN		GLN
GLU	M464	GLU
VAL	I465	VAL
ARG		ARG
ASP	T470	ASP
PHE		PHE
ALA	Y475	ALA
ALA	V476	ALA
GLY	T477	GLY
LYS	P478	LYS
ALA	K479	ALA
PRO	E480	PRO
ASN	H481	ASN
SER		SER
ALA	L484	ALA
GLU		GLU
LEU	R487	LEU
GLY		GLY
MSE	V490	MSE
ALA	K491	ALA
GLU		GLU
MSE	V494	MSE
SER		SER
GLU	L499	GLU
LYS		LYS
PHE	L506	PHE
ARG		ARG
GLU	D517	GLU
GLN		GLN
GLY	I520	GLY
SER		SER
GLU	H546	GLU
ILE	ASP	ILE
TYR	GLU	TYR

LEU

LYS

THR

GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.25Å 103.44Å 95.37Å 90.00° 91.62° 90.00°	Depositor
Resolution (Å)	43.29 – 2.79 47.44 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.29-2.79) 99.5 (47.44-2.79)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.57 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.181 , 0.244 0.173 , 0.235	Depositor DCC
$R_{free}$ test set	1537 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 18.9	EDS
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30451 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, HMH, SO4

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	0.35	0/4128	0.53	0/5587
1	B	0.34	0/4104	0.52	0/5554
All	All	0.34	0/8232	0.52	0/11141

There are no bond length outliers.

There are no bond angle outliers.

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	4042	0	3962	94	0
1	B	4018	0	3936	120	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	9	1	0
4	A	5	0	0	0	0
5	A	91	0	0	2	0
5	B	42	0	0	2	0
All	All	8210	0	7907	202	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 13.

All (202) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:372:LEU:HB3	1:A:396:LEU:HD22	1.52	0.91
1:A:197:ASN:HD22	1:A:199:ASN:H	1.16	0.91
1:B:197:ASN:ND2	1:B:199:ASN:H	1.70	0.89
1:A:318:LEU:HB3	1:A:319:PRO:HD3	1.54	0.88
1:A:457:THR:HG22	1:B:499:LEU:HD13	1.58	0.84
1:B:197:ASN:HD22	1:B:199:ASN:H	1.22	0.84
1:A:197:ASN:ND2	1:A:199:ASN:H	1.76	0.83
1:A:154:ASN:HD21	1:A:178:VAL:H	1.25	0.82
1:B:350:ASN:HD21	1:B:352:LEU:HB2	1.43	0.81
1:B:313:HIS:CE1	1:B:335:GLY:HA3	2.17	0.80
1:A:194:ILE:H	1:A:409:GLN:HE22	1.29	0.78
1:B:154:ASN:HD21	1:B:178:VAL:H	1.32	0.78
1:A:350:ASN:ND2	1:A:352:LEU:H	1.83	0.77
1:A:350:ASN:C	1:A:350:ASN:HD22	1.89	0.75
1:A:499:LEU:HD13	1:B:457:THR:HG22	1.71	0.72
1:B:219:ASN:O	1:B:220:ILE:HD13	1.89	0.71
1:B:465:ILE:HG12	1:B:470:THR:OG1	1.92	0.69
1:B:350:ASN:ND2	1:B:352:LEU:H	1.92	0.68
1:A:149:VAL:HG11	1:A:207:ALA:HB2	1.76	0.67
1:B:480:GLU:O	1:B:481:HIS:HB2	1.94	0.67
1:B:199:ASN:ND2	1:B:304:GLU:HA	2.10	0.66
1:B:158:GLU:HG3	1:B:160:ASP:HB2	1.78	0.66
1:B:197:ASN:HD22	1:B:199:ASN:N	1.92	0.66
1:A:480:GLU:O	1:A:481:HIS:HB2	1.97	0.65
1:A:430:GLN:HG3	1:A:439:PHE:CE1	2.31	0.65
1:B:199:ASN:HD22	1:B:304:GLU:HA	1.63	0.64
1:B:153:GLU:HB3	5:B:631:HOH:O	1.96	0.64
1:B:25:VAL:HG23	1:B:39:PHE:HB2	1.80	0.63
1:A:313:HIS:CE1	1:A:335:GLY:HA3	2.34	0.63
1:B:242:TRP:CZ2	1:B:491:LYS:HE3	2.34	0.62
1:B:350:ASN:ND2	1:B:352:LEU:HB2	2.15	0.61
1:A:350:ASN:HD22	1:A:351:PHE:N	1.98	0.60
1:A:219:ASN:O	1:A:220:ILE:HD13	2.02	0.60
1:A:457:THR:HG22	1:B:499:LEU:CD1	2.31	0.60
1:B:318:LEU:HB3	1:B:319:PRO:HD3	1.85	0.59
1:B:131:VAL:O	1:B:136:TYR:HE2	1.86	0.59
1:B:96:ARG:HH21	1:B:300:ILE:HG21	1.68	0.58
1:B:430:GLN:O	1:B:434:CYS:HB2	2.02	0.58
1:B:445:LEU:HD22	1:B:458:SER:HB3	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:236:LEU:HD12	1:A:247:VAL:HG11	1.85	0.58
1:A:260:ARG:HD2	1:A:305:GLN:OE1	2.04	0.58
1:B:465:ILE:HG12	1:B:470:THR:HG1	1.68	0.57
1:B:283:VAL:O	1:B:283:VAL:HG23	2.02	0.57
1:A:280:LEU:HD22	1:A:338:ILE:HD13	1.86	0.57
1:B:149:VAL:HG11	1:B:207:ALA:HB2	1.86	0.57
1:A:197:ASN:HD22	1:A:199:ASN:N	1.97	0.57
1:B:160:ASP:HB3	1:B:161:ARG:HD2	1.87	0.57
1:A:350:ASN:HD22	1:A:352:LEU:H	1.49	0.57
1:B:160:ASP:O	1:B:162:PRO:HD3	2.05	0.57
1:A:27:GLN:OE1	1:A:156:ARG:HG2	2.05	0.56
1:B:312:ILE:HG23	1:B:352:LEU:HD13	1.88	0.56
1:A:302:GLN:HE21	1:A:310:PHE:HE1	1.54	0.56
1:A:400:THR:HG23	1:A:410:VAL:HG11	1.87	0.56
1:A:334:ARG:O	1:A:338:ILE:HG13	2.05	0.56
1:B:490:VAL:O	1:B:494:VAL:HG23	2.06	0.55
1:B:372:LEU:HB3	1:B:396:LEU:HD22	1.89	0.55
1:B:392:GLU:O	1:B:396:LEU:HG	2.07	0.55
1:B:28:ALA:HB1	1:B:36:ARG:HH21	1.71	0.55
1:B:161:ARG:HD2	1:B:161:ARG:N	2.21	0.55
1:B:70:ASP:OD2	1:B:73:LYS:HG2	2.06	0.55
1:A:246:THR:HG22	1:A:270:PRO:HD2	1.88	0.55
1:A:350:ASN:C	1:A:350:ASN:ND2	2.60	0.55
1:B:432:LYS:HD3	1:B:433:HIS:CE1	2.43	0.54
1:B:499:LEU:C	1:B:499:LEU:HD12	2.28	0.54
1:B:310:PHE:CD2	1:B:368:VAL:HG11	2.42	0.54
1:B:220:ILE:HG23	1:B:235:LYS:NZ	2.23	0.53
1:B:153:GLU:OE2	1:B:212:PHE:HB3	2.08	0.53
1:B:350:ASN:HD22	1:B:352:LEU:H	1.55	0.53
1:A:430:GLN:HG3	1:A:439:PHE:CD1	2.43	0.53
1:A:79:ARG:NH1	1:A:196:ALA:HB1	2.22	0.53
1:A:318:LEU:HB3	1:A:319:PRO:CD	2.33	0.53
1:B:350:ASN:HD22	1:B:352:LEU:N	2.07	0.53
1:A:455:HIS:CE1	1:A:456:ILE:HG13	2.44	0.53
1:B:385:ASN:H	1:B:389:GLN:HE22	1.55	0.53
1:B:460:ILE:O	1:B:464:MSE:HG3	2.08	0.53
1:A:364:ARG:HG3	5:A:2065:HOH:O	2.09	0.52
1:A:153:GLU:HB3	5:A:2060:HOH:O	2.09	0.52
1:A:167:GLY:HA2	1:B:421:HIS:CE1	2.44	0.52
1:A:467:TRP:HB2	1:B:420:MSE:HE1	1.92	0.52
1:B:444:PRO:HD2	1:B:461:GLY:C	2.29	0.52
1:B:242:TRP:CE2	1:B:491:LYS:HE3	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:421:HIS:CE1	1:B:167:GLY:HA2	2.46	0.51
1:A:302:GLN:NE2	1:A:310:PHE:CE1	2.77	0.51
1:B:115:PHE:CE1	1:B:265:ARG:HG3	2.45	0.51
1:A:254:ARG:O	1:A:255:ASN:HB2	2.10	0.51
1:A:334:ARG:H	3:A:1001:HMH:C6A	2.24	0.50
1:B:321:ILE:HB	1:B:322:PRO:HD3	1.94	0.50
1:A:467:TRP:HB2	1:B:420:MSE:CE	2.41	0.50
1:B:194:ILE:H	1:B:409:GLN:NE2	2.10	0.50
1:B:148:TYR:CE2	1:B:205:PRO:HD2	2.47	0.49
1:A:440:TYR:CD1	1:A:472:MSE:HG2	2.47	0.49
1:A:197:ASN:C	1:A:197:ASN:HD22	2.16	0.49
1:B:420:MSE:HA	1:B:423:ILE:HD12	1.94	0.49
1:B:197:ASN:ND2	1:B:199:ASN:N	2.51	0.49
1:A:56:TYR:CE1	1:A:152:ARG:HG2	2.47	0.49
1:A:96:ARG:HE	1:A:300:ILE:HG21	1.78	0.49
1:B:350:ASN:HD21	1:B:352:LEU:CB	2.21	0.49
1:A:507:ALA:HA	1:B:421:HIS:CD2	2.48	0.49
1:A:364:ARG:HD2	1:A:406:HIS:O	2.13	0.49
1:B:91:GLU:OE2	1:B:121:LYS:HD3	2.13	0.49
1:B:350:ASN:ND2	1:B:352:LEU:N	2.59	0.49
1:B:420:MSE:HG3	5:B:617:HOH:O	2.12	0.48
1:A:520:ILE:HG12	1:A:535:LEU:CB	2.43	0.48
1:A:435:HIS:O	1:A:436:GLU:HB2	2.13	0.48
1:B:310:PHE:CE2	1:B:368:VAL:HG11	2.49	0.48
1:B:282:LYS:NZ	1:B:301:GLU:OE1	2.45	0.48
1:B:260:ARG:O	1:B:264:ILE:HG13	2.14	0.47
1:A:520:ILE:HG12	1:A:535:LEU:HB3	1.96	0.47
1:B:198:ILE:HG23	1:B:366:TYR:O	2.13	0.47
1:A:45:HIS:CD2	1:A:46:PRO:HD2	2.50	0.47
1:A:220:ILE:HG23	1:A:235:LYS:NZ	2.30	0.47
1:A:385:ASN:N	1:A:385:ASN:HD22	2.14	0.46
1:B:395:THR:O	1:B:399:LEU:HG	2.15	0.46
1:A:219:ASN:HB3	1:A:250:LEU:HD12	1.97	0.46
1:A:260:ARG:HH22	1:A:278:GLN:NE2	2.12	0.46
1:A:274:VAL:HG12	1:A:276:ILE:HG22	1.97	0.46
1:A:475:TYR:CD2	1:A:475:TYR:C	2.89	0.46
1:B:435:HIS:O	1:B:436:GLU:HB2	2.14	0.46
1:B:441:THR:HG21	1:B:465:ILE:HD13	1.97	0.46
1:B:194:ILE:H	1:B:409:GLN:HE22	1.62	0.46
1:B:479:LYS:HD2	1:B:484:LEU:O	2.16	0.46
1:A:126:LYS:HB2	1:A:129:LYS:HG3	1.96	0.45
1:A:248:MSE:HB3	1:A:248:MSE:HE2	1.87	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:197:ASN:C	1:B:197:ASN:HD22	2.20	0.45
1:A:231:ASP:O	1:A:235:LYS:HG3	2.16	0.45
1:A:326:LYS:HD2	1:A:326:LYS:H	1.82	0.45
1:A:445:LEU:HD22	1:A:458:SER:HB3	1.98	0.45
1:B:320:PHE:CE1	1:B:391:SER:HB3	2.52	0.45
1:A:350:ASN:HD21	1:A:352:LEU:HB2	1.82	0.45
1:B:149:VAL:CG1	1:B:207:ALA:HB2	2.46	0.45
1:B:417:HIS:ND1	1:B:448:ASP:OD2	2.39	0.45
1:A:197:ASN:HD22	1:A:198:ILE:N	2.16	0.44
1:B:364:ARG:HD2	1:B:406:HIS:O	2.17	0.44
1:B:363:MSE:HE1	1:B:370:PHE:CD1	2.52	0.44
1:A:484:LEU:HA	1:A:485:PRO:HD3	1.76	0.44
1:A:62:TYR:OH	1:A:266:ASN:HB3	2.17	0.44
1:B:256:ILE:HD11	1:B:278:GLN:HA	1.98	0.44
1:B:169:ASP:HB2	1:B:172:ALA:HB3	1.99	0.44
1:B:174:ILE:HA	1:B:175:PRO:HD3	1.84	0.44
1:A:276:ILE:HD12	1:A:276:ILE:HA	1.76	0.44
1:B:350:ASN:HD22	1:B:350:ASN:C	2.21	0.44
1:B:165:ARG:NH2	1:B:174:ILE:O	2.50	0.44
1:A:490:VAL:O	1:A:494:VAL:HG23	2.18	0.44
1:B:303:CYS:SG	1:B:368:VAL:HG21	2.58	0.44
1:A:535:LEU:HA	1:A:535:LEU:HD23	1.82	0.44
1:B:232:GLU:OE2	1:B:235:LYS:HE3	2.18	0.43
1:B:258:ASN:O	1:B:261:ASP:HB2	2.18	0.43
1:B:220:ILE:HG23	1:B:235:LYS:HZ1	1.82	0.43
1:B:376:LEU:HD12	1:B:392:GLU:HB2	1.99	0.43
1:A:427:MSE:HG2	1:A:468:PHE:HB3	2.00	0.43
1:A:506:LEU:HA	1:A:506:LEU:HD23	1.75	0.43
1:B:34:GLU:H	1:B:34:GLU:CD	2.21	0.43
1:A:450:ALA:N	1:A:451:PRO:HD3	2.34	0.43
1:A:37:VAL:HA	1:A:38:PRO:HD3	1.75	0.43
1:A:507:ALA:HA	1:B:421:HIS:HD2	1.84	0.43
1:B:242:TRP:CD1	1:B:491:LYS:HG3	2.54	0.43
1:B:390:PHE:CZ	1:B:429:GLU:HG3	2.53	0.43
1:A:169:ASP:HB2	1:A:172:ALA:HB3	2.00	0.42
1:A:312:ILE:HG23	1:A:352:LEU:HD13	2.01	0.42
1:B:475:TYR:C	1:B:475:TYR:CD2	2.92	0.42
1:A:174:ILE:HA	1:A:175:PRO:HD3	1.77	0.42
1:B:185:GLN:O	1:B:189:ARG:HG2	2.19	0.42
1:B:74:GLY:HA2	1:B:266:ASN:OD1	2.20	0.42
1:B:276:ILE:HA	1:B:276:ILE:HD12	1.93	0.42
1:A:506:LEU:HD23	1:A:513:ALA:CB	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:480:GLU:O	1:B:481:HIS:CB	2.66	0.42
1:A:427:MSE:HE2	1:A:469:GLY:HA3	2.01	0.42
1:A:220:ILE:HG22	1:A:221:GLY:N	2.34	0.42
1:A:421:HIS:ND1	1:B:167:GLY:HA2	2.35	0.42
1:A:440:TYR:CE1	1:A:472:MSE:HG2	2.55	0.42
1:B:477:THR:HB	1:B:478:PRO:HD2	2.02	0.42
1:B:79:ARG:NH1	1:B:196:ALA:HB1	2.35	0.42
1:B:125:ALA:HB2	1:B:131:VAL:HG21	2.02	0.41
1:A:167:GLY:HA2	1:B:421:HIS:ND1	2.34	0.41
1:A:421:HIS:HE1	1:B:166:ASP:OD1	2.03	0.41
1:B:317:ARG:HB3	1:B:319:PRO:HD2	2.02	0.41
1:B:260:ARG:HH12	1:B:278:GLN:HE22	1.68	0.41
1:B:229:VAL:HG23	1:B:230:ALA:H	1.86	0.41
1:A:258:ASN:O	1:A:261:ASP:HB2	2.21	0.41
1:A:218:ALA:O	1:A:247:VAL:HA	2.20	0.41
1:B:149:VAL:HG12	1:B:150:ALA:N	2.36	0.41
1:A:270:PRO:HA	1:A:308:ASP:OD2	2.20	0.41
1:A:115:PHE:HA	1:A:116:PRO:HD3	1.79	0.41
1:B:37:VAL:HA	1:B:38:PRO:HD3	1.80	0.41
1:A:374:ASP:OD1	1:A:374:ASP:N	2.53	0.41
1:B:126:LYS:HB2	1:B:129:LYS:HG3	2.01	0.41
1:A:399:LEU:HD23	1:A:399:LEU:HA	1.91	0.41
1:B:415:PRO:HA	1:B:416:GLY:HA3	1.91	0.41
1:B:131:VAL:O	1:B:136:TYR:CE2	2.69	0.41
1:B:397:GLY:HA3	1:B:433:HIS:O	2.21	0.41
1:A:170:PHE:HE2	1:A:467:TRP:CE2	2.39	0.41
1:B:79:ARG:O	1:B:83:VAL:HG23	2.21	0.41
1:B:303:CYS:HB3	1:B:366:TYR:CD2	2.56	0.41
1:B:320:PHE:HB3	1:B:376:LEU:HD11	2.03	0.40
1:B:253:GLY:O	1:B:256:ILE:HG23	2.21	0.40
1:B:94:ASP:HA	1:B:95:PRO:HD3	1.79	0.40
1:B:56:TYR:CE1	1:B:152:ARG:HG2	2.57	0.40
1:B:220:ILE:HG22	1:B:221:GLY:N	2.36	0.40
1:A:430:GLN:O	1:A:434:CYS:HB2	2.21	0.40
1:B:274:VAL:HG12	1:B:276:ILE:HG22	2.04	0.40
1:A:537:LEU:HA	1:A:537:LEU:HD23	1.82	0.40
1:A:143:THR:OG1	1:A:146:MSE:HE3	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	509/612 (83%)	483 (95%)	25 (5%)	1 (0%)	56	88
1	B	506/612 (83%)	479 (95%)	26 (5%)	1 (0%)	56	88
All	All	1015/1224 (83%)	962 (95%)	51 (5%)	2 (0%)	56	88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	160	ASP
1	A	131	VAL

### 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	423/486 (87%)	398 (94%)	25 (6%)	28	62
1	B	420/486 (86%)	397 (94%)	23 (6%)	30	65
All	All	843/972 (87%)	795 (94%)	48 (6%)	29	64

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	15	SER
1	A	97	GLN
1	A	131	VAL
1	A	197	ASN
1	A	217	ASN
1	A	228	THR

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Mol	Chain	Res	Type
1	A	229	VAL
1	A	248	MSE
1	A	254	ARG
1	A	276	ILE
1	A	326	LYS
1	A	350	ASN
1	A	377	ARG
1	A	385	ASN
1	A	426	ASN
1	A	430	GLN
1	A	439	PHE
1	A	445	LEU
1	A	447	THR
1	A	475	TYR
1	A	487	ARG
1	A	506	LEU
1	A	517	ASP
1	A	520	ILE
1	B	96	ARG
1	B	131	VAL
1	B	161	ARG
1	B	197	ASN
1	B	198	ILE
1	B	217	ASN
1	B	228	THR
1	B	236	LEU
1	B	254	ARG
1	B	326	LYS
1	B	350	ASN
1	B	377	ARG
1	B	381	THR
1	B	426	ASN
1	B	430	GLN
1	B	439	PHE
1	B	445	LEU
1	B	475	TYR
1	B	487	ARG
1	B	499	LEU
1	B	506	LEU
1	B	517	ASP
1	B	520	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	97	GLN
1	A	154	ASN
1	A	159	GLN
1	A	197	ASN
1	A	217	ASN
1	A	255	ASN
1	A	257	HIS
1	A	278	GLN
1	A	302	GLN
1	A	350	ASN
1	A	385	ASN
1	A	389	GLN
1	A	409	GLN
1	A	421	HIS
1	A	430	GLN
1	A	532	GLN
1	A	546	HIS
1	B	45	HIS
1	B	154	ASN
1	B	159	GLN
1	B	197	ASN
1	B	255	ASN
1	B	278	GLN
1	B	302	GLN
1	B	313	HIS
1	B	350	ASN
1	B	385	ASN
1	B	389	GLN
1	B	409	GLN
1	B	421	HIS
1	B	430	GLN
1	B	433	HIS
1	B	546	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.



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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
3	HMH	A	1001	-	10,10,10	0.89	0	13,13,13	1.99	5 (38%)
4	SO4	A	2001	-	4,4,4	0.13	0	6,6,6	0.09	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	HMH	A	1001	-	-	0/2/2/2	0/1/1/1
4	SO4	A	2001	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	HMH	C6A-N1A-C2A	3.43	121.70	115.68
3	A	1001	HMH	N1A-C2A-N3A	-3.34	119.63	125.65
3	A	1001	HMH	N4A-C4A-N3A	2.68	120.77	116.88
3	A	1001	HMH	C5A-C4A-N4A	-2.22	118.92	122.23
3	A	1001	HMH	CM2-C2A-N1A	2.21	119.65	117.02

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	515/612 (84%)	-0.09	10 (1%) 64 64	21, 39, 67, 121	0
1	B	512/612 (83%)	-0.11	12 (2%) 57 58	22, 41, 66, 119	0
All	All	1027/1224 (83%)	-0.10	22 (2%) 60 61	21, 40, 67, 121	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	THR	4.2
1	A	15	SER	4.0
1	B	94	ASP	3.7
1	A	162	PRO	3.7
1	A	164	VAL	3.3
1	B	163	CYS	3.1
1	A	14	ILE	2.9
1	B	128	GLY	2.8
1	A	474	CYS	2.7
1	B	162	PRO	2.6
1	B	164	VAL	2.6
1	A	254	ARG	2.5
1	B	262	TRP	2.3
1	B	116	PRO	2.3
1	B	252	THR	2.3
1	B	289	ASP	2.3
1	B	288	GLU	2.2
1	B	113	PRO	2.2
1	A	163	CYS	2.1
1	A	529	TRP	2.1
1	A	543	ARG	2.0
1	B	294	VAL	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
3	HMH	A	1001	10/10	0.42	5.23	55,80,88,94	0
4	SO4	A	2001	5/5	0.15	-0.05	59,68,96,111	0
2	ZN	A	613	1/1	0.12	-1.39	56,56,56,56	0
2	ZN	B	613	1/1	0.08	-6.43	69,69,69,69	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.