



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2017 – 05:17 PM EDT

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 : unknown
Resolution : 2.79 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

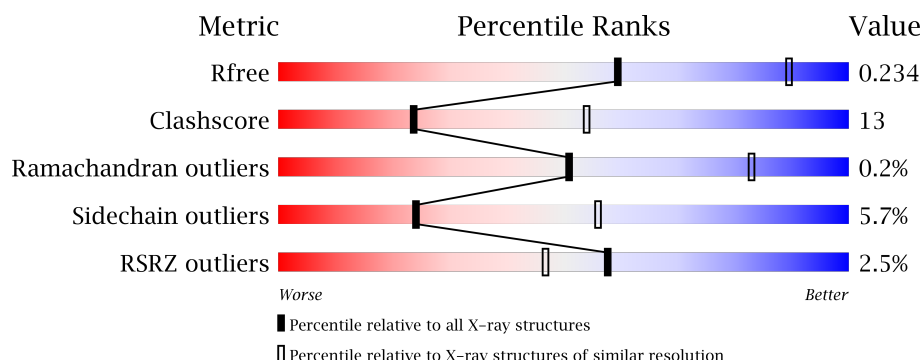
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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 ≥ 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	612	<div> <div>2%</div> <div>64%</div> <div>18%</div> <div>•</div> <div>16%</div> </div>
1	B	612	<div> <div>2%</div> <div>58%</div> <div>24%</div> <div>•</div> <div>16%</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
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 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.

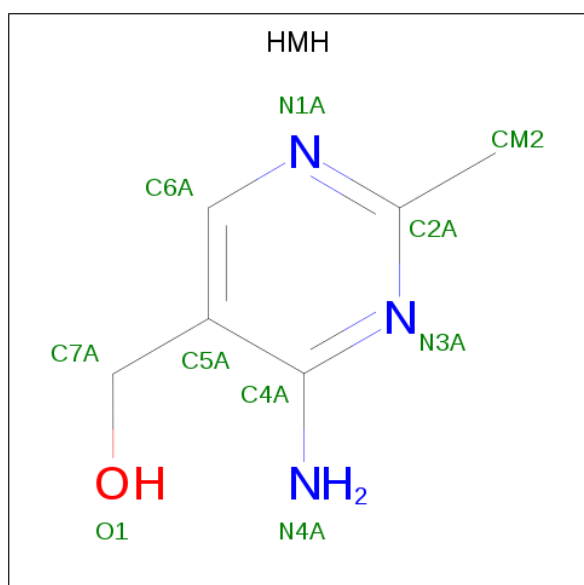
- Molecule 1 is a protein called Thiamine biosynthesis protein thiC.

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: C₆H₉N₃O).



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: O₄S).



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

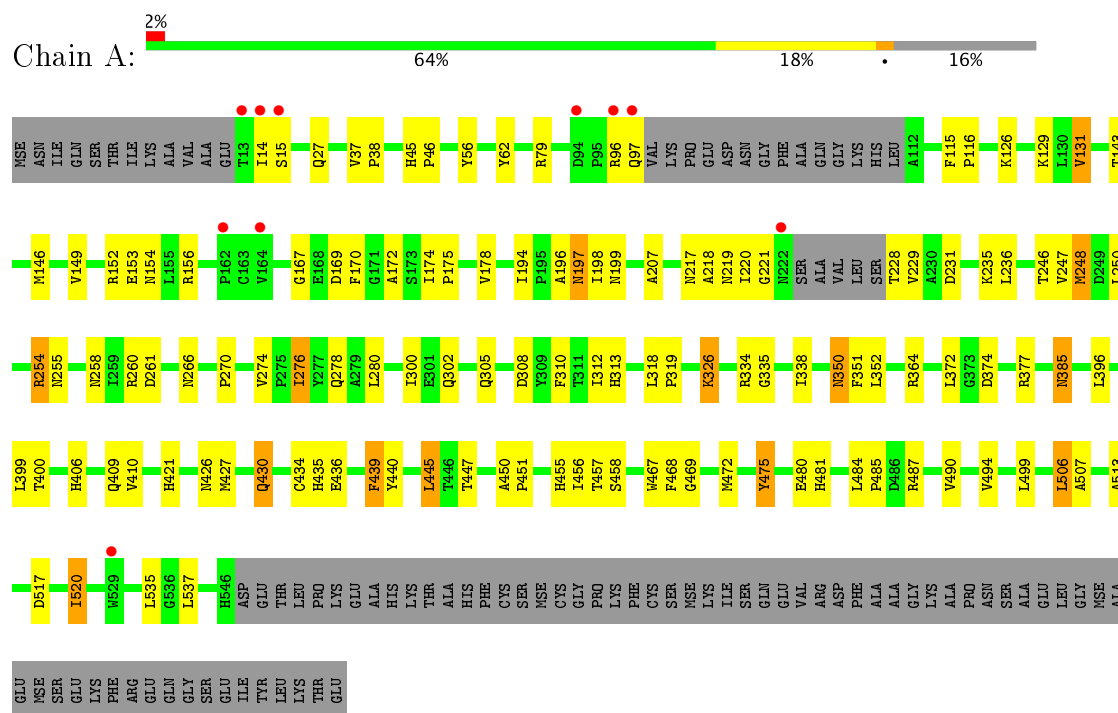
- Molecule 5 is water.

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

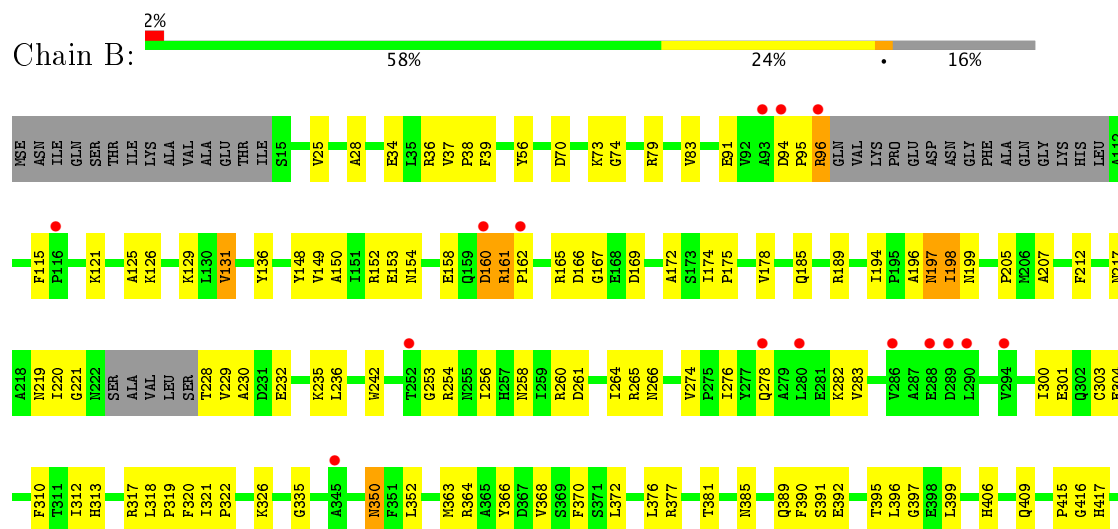
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Thiamine biosynthesis protein thiC



• Molecule 1: Thiamine biosynthesis protein thiC



SER	HE46	M420
GLU	ASP	H421
ILE	GLU	K422
THR	THR	L423
THR	LEU	
LYS	LEU	H426
GLU	PRO	
	LYS	E429
	GLU	Q430
	ALA	L431
	HIS	K432
	LYS	H433
	THR	C434
	ALA	H435
	HIS	E436
	PHE	
	CYS	F439
	SER	Y440
	NSE	T441
	CYS	
	GLY	P444
	PRO	L445
	LYS	
	PHE	D448
	CYS	
	SER	T457
	NSE	S458
	LYS	A459
	ILE	T460
	SER	G461
	GLN	
	GLU	M464
	VAL	T465
	ARG	
	ASP	T470
	PHE	
	ALA	Y475
	ALA	T476
	GLY	T477
	LYS	P478
	ALA	K479
	PRO	E480
	ASN	H481
	SER	
	ALA	L484
	GLU	
	LEU	
	GLY	R487
	NSE	
	ALA	V490
	ALA	K491
	GLU	
	NSE	V494
	SER	
	GLU	L499
	LYS	
	PHE	L506
	ARG	
	GLU	D517
	GLN	
	GLY	T520

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	5.57 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.181 , 0.244 0.171 , 0.234	Depositor DCC
R_{free} test set	1537 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8210	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

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 13.

All (202) 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: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:153:GLU:HB3	5:B:631:HOH:O	1.96	0.64
1:B:199:ASN:HD22	1:B:304:GLU:HA	1.63	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:219:ASN:O	1:A:220:ILE:HD13	2.02	0.60
1:A:350:ASN:HD22	1:A:351:PHE:N	1.98	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:430:GLN:O	1:B:434:CYS:HB2	2.02	0.58
1:B:96:ARG:HH21	1:B:300:ILE:HG21	1.68	0.58
1:B:445:LEU:HD22	1:B:458:SER:HB3	1.85	0.58
1:A:236:LEU:HD12	1:A:247:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:312:ILE:HG23	1:B:352:LEU:HD13	1.88	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:28:ALA:HB1	1:B:36:ARG:HH21	1.71	0.55
1:B:392:GLU:O	1:B:396:LEU:HG	2.07	0.55
1:B:161:ARG:HD2	1:B:161:ARG:N	2.21	0.55
1:A:246:THR:HG22	1:A:270:PRO:HD2	1.88	0.55
1:B:70:ASP:OD2	1:B:73:LYS:HG2	2.06	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:310:PHE:CD2	1:B:368:VAL:HG11	2.42	0.54
1:B:499:LEU:C	1:B:499:LEU:HD12	2.28	0.54
1:B:153:GLU:OE2	1:B:212:PHE:HB3	2.08	0.53
1:B:220:ILE:HG23	1:B:235:LYS:NZ	2.23	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	Interatomic distance (Å)	Clash overlap (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:B:194:ILE:H	1:B:409:GLN:NE2	2.10	0.50
1:A:467:TRP:HB2	1:B:420:MSE:CE	2.41	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:A:56:TYR:CE1	1:A:152:ARG:HG2	2.47	0.49
1:B:197:ASN:ND2	1:B:199:ASN:N	2.51	0.49
1:A:96:ARG:HE	1:A:300:ILE:HG21	1.78	0.49
1:A:507:ALA:HA	1:B:421:HIS:CD2	2.48	0.49
1:B:350:ASN:HD21	1:B:352:LEU:CB	2.21	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:274:VAL:HG12	1:A:276:ILE:HG22	1.97	0.46
1:A:260:ARG:HH22	1:A:278:GLN:NE2	2.12	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:194:ILE:H	1:B:409:GLN:HE22	1.62	0.46
1:B:441:THR:HG21	1:B:465:ILE:HD13	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:MSE:HB3	1:A:248:MSE:HE2	1.87	0.45
1:A:231:ASP:O	1:A:235:LYS:HG3	2.16	0.45
1:B:197:ASN:C	1:B:197:ASN:HD22	2.20	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:A:484:LEU:HA	1:A:485:PRO:HD3	1.76	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:62:TYR:OH	1:A:266:ASN:HB3	2.17	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:B:256:ILE:HD11	1:B:278:GLN:HA	1.98	0.44
1:A:276:ILE:HA	1:A:276:ILE:HD12	1.76	0.44
1:A:490:VAL:O	1:A:494:VAL:HG23	2.18	0.44
1:B:165:ARG:NH2	1:B:174:ILE:O	2.50	0.44
1:B:350:ASN:HD22	1:B:350:ASN:C	2.21	0.44
1:A:535:LEU:HA	1:A:535:LEU:HD23	1.82	0.44
1:B:303:CYS:SG	1:B:368:VAL:HG21	2.58	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:A:427:MSE:HG2	1:A:468:PHE:HB3	2.00	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: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:37:VAL:HA	1:A:38:PRO:HD3	1.75	0.43
1:A:450:ALA:N	1:A:451:PRO:HD3	2.34	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:174:ILE:HA	1:A:175:PRO:HD3	1.77	0.42
1:A:312:ILE:HG23	1:A:352:LEU:HD13	2.01	0.42
1:B:185:GLN:O	1:B:189:ARG:HG2	2.19	0.42
1:B:475:TYR:C	1:B:475:TYR:CD2	2.92	0.42
1:B:74:GLY:HA2	1:B:266:ASN:OD1	2.20	0.42

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

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%)	23	54
1	B	420/486 (86%)	397 (94%)	23 (6%)	25	57
All	All	843/972 (87%)	795 (94%)	48 (6%)	24	56

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

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Mol	Chain	Res	Type
1	A	197	ASN
1	A	217	ASN
1	A	228	THR
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

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Mol	Chain	Res	Type
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 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 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	0.94	0	12,13,13	2.10	7 (58%)
4	SO4	A	2001	-	4,4,4	0.18	0	6,6,6	0.08	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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	1001	HMH	N1A-C2A-N3A	-3.44	119.63	125.59
3	A	1001	HMH	C5A-C4A-N4A	-2.27	118.92	122.22
3	A	1001	HMH	C5A-C6A-N1A	-2.02	120.45	123.87
3	A	1001	HMH	CM2-C2A-N3A	2.15	120.72	117.20
3	A	1001	HMH	CM2-C2A-N1A	2.29	119.65	117.06
3	A	1001	HMH	N4A-C4A-N3A	2.55	120.77	117.00
3	A	1001	HMH	C6A-N1A-C2A	3.37	121.70	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	HMH	1	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	503/612 (82%)	-0.13	10 (1%) 65 56	21, 39, 67, 121	0
1	B	500/612 (81%)	-0.16	15 (3%) 51 39	22, 41, 67, 119	0
All	All	1003/1224 (81%)	-0.15	25 (2%) 58 47	21, 40, 67, 121	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	ASP	3.9
1	A	94	ASP	3.5
1	B	280	LEU	3.3
1	B	289	ASP	3.2
1	A	97	GLN	3.1
1	A	13	THR	3.0
1	B	294	VAL	3.0
1	A	164	VAL	2.9
1	B	252	THR	2.9
1	A	162	PRO	2.8
1	B	288	GLU	2.6
1	A	15	SER	2.5
1	A	96	ARG	2.4
1	B	286	VAL	2.4
1	B	162	PRO	2.4
1	B	96	ARG	2.3
1	B	160	ASP	2.3
1	B	93	ALA	2.2
1	A	529	TRP	2.1
1	A	14	ILE	2.1
1	B	290	LEU	2.0
1	A	222	ASN	2.0
1	B	278	GLN	2.0
1	B	116	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	345	ALA	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
3	HMH	A	1001	10/10	0.74	0.39	6.19	55,80,88,94	0
4	SO4	A	2001	5/5	0.94	0.15	-0.35	59,68,96,111	0
2	ZN	A	613	1/1	0.97	0.07	-	56,56,56,56	0
2	ZN	B	613	1/1	0.97	0.04	-	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.