Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:27 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 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

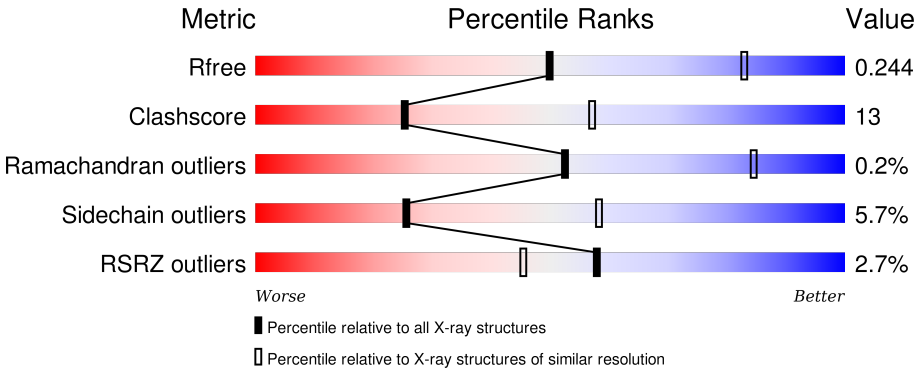
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 <=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	2% 64% 18% • 16%
1	B	612	3% 58% 24% • 16%

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

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.

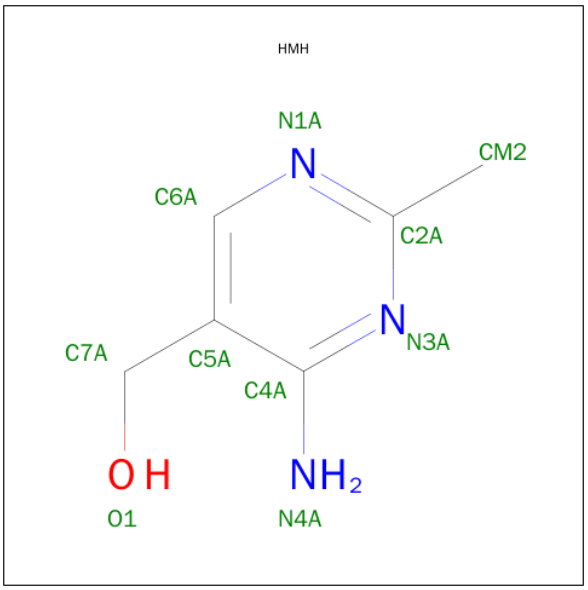
- Molecule 1 is a protein called Thiamine biosynthesis protein thiC.

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).

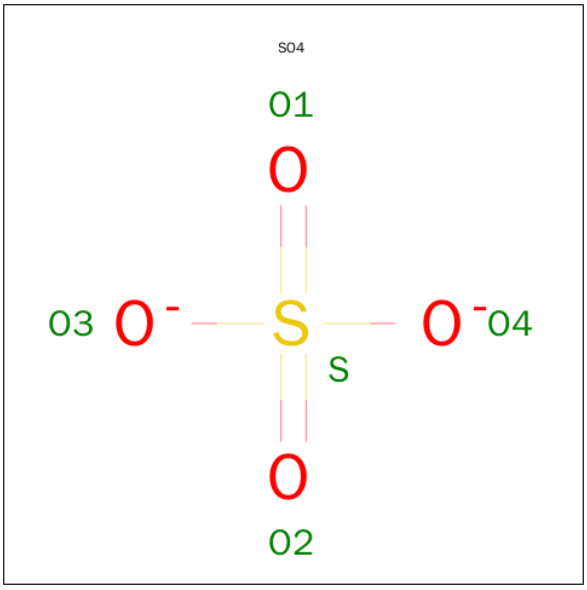
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 4-AMINO-5-HYDROXYMETHYL-2-METHYLPYRIMIDINE (three-letter code: HMH) (formula: $C_6H_9N_3O$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

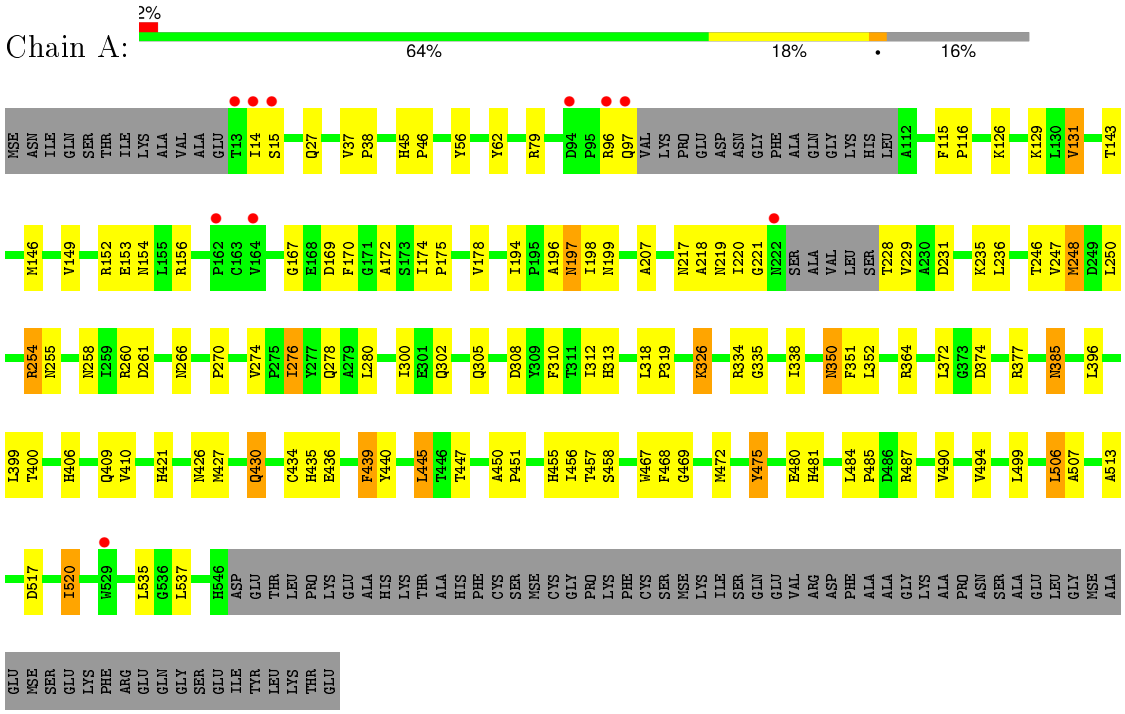
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	91	Total O 91 91	0	0
5	B	42	Total O 42 42	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

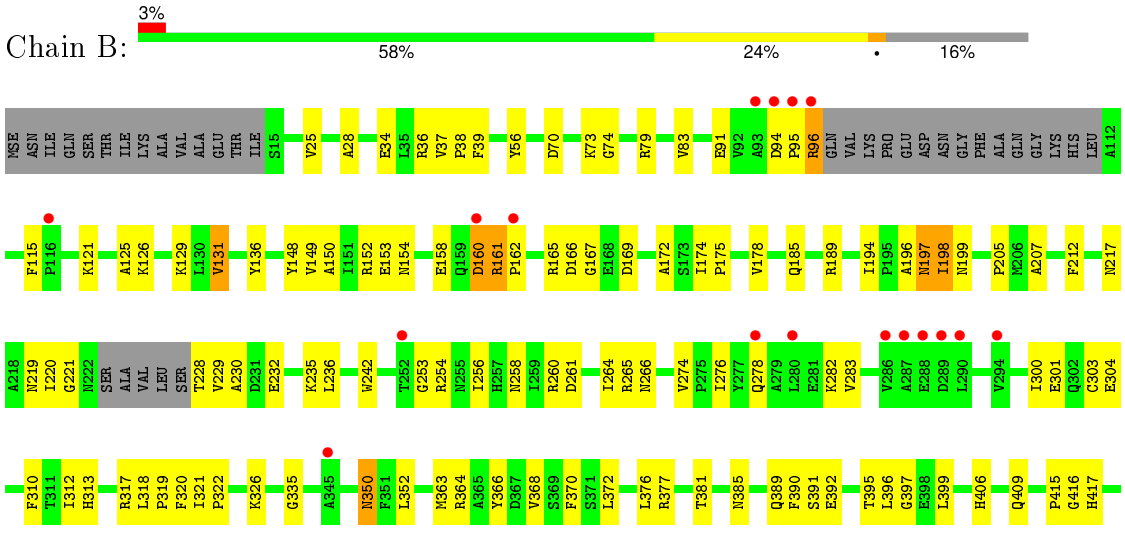
- Molecule 1: Thiamine biosynthesis protein thiC

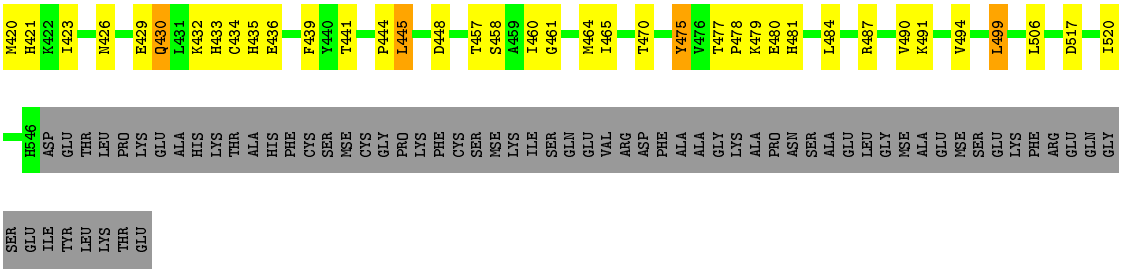
Chain A:



- Molecule 1: Thiamine biosynthesis protein thiC

Chain B:




M420
H421
K422
I423
N426
E429
Q430
L431
K432
H433
C434
H435
E436
F439
Y440
T441
P444
L445
D448
T457
S458
A459
I460
G461
M464
I465
T470
Y475
V476
T477
P478
K479
E480
H481
L484
R487
V490
K491
V494
L499
L506
D517
I520
H546
ASP
GLU
THR
LEU
PRO
LYS
GLU
ALA
HIS
LYS
THR
ALA
HIS
PHE
CYS
SER
MSE
CYS
GLY
PRO
LYS
PHE
CYS
SER
MSE
LYS
ILE
SER
GLN
GLU
VAL
ARG
ASP
PHE
ALA
ALA
GLY
LYS
ALA
PRO
ASN
SER
ALA
GLU
LEU
GLY
MSE
ALA
GLU
MSE
SER
GLU
LYS
PHE
ARG
GLU
GLN
GLY
SER
GLU
ILE
TYR
LEU
LYS
THR
GLU

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	5.57 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.181 , 0.244 0.181 , 0.244	Depositor DCC
R_{free} test set	1538 reflections (5.32%)	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
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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^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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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: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
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: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	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: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

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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: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

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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: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 (i)

5.3.1 Protein backbone (i)

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%)	52 84
1	B	506/612 (83%)	479 (95%)	26 (5%)	1 (0%)	52 84
All	All	1015/1224 (83%)	962 (95%)	51 (5%)	2 (0%)	52 84

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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%)	24 57
1	B	420/486 (86%)	397 (94%)	23 (6%)	27 59
All	All	843/972 (87%)	795 (94%)	48 (6%)	25 58

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	0.91	0	12,13,13	2.04	6 (50%)
4	SO4	A	2001	-	4,4,4	0.15	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 (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	HMH	N1A-C2A-N3A	-3.23	119.63	125.60
3	A	1001	HMH	C5A-C4A-N4A	-2.27	118.92	122.25
3	A	1001	HMH	CM2-C2A-N3A	2.07	120.72	117.20
3	A	1001	HMH	CM2-C2A-N1A	2.18	119.65	117.03
3	A	1001	HMH	N4A-C4A-N3A	2.64	120.77	116.95
3	A	1001	HMH	C6A-N1A-C2A	3.40	121.70	115.77

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, 95^{th} 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%)	-0.10	10 (1%) 68 58	21, 39, 67, 121	0
1	B	500/612 (81%)	-0.13	17 (3%) 49 36	22, 41, 67, 119	0
All	All	1003/1224 (81%)	-0.11	27 (2%) 58 45	21, 40, 67, 121	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	ASP	4.0
1	A	94	ASP	3.6
1	B	280	LEU	3.4
1	B	289	ASP	3.3
1	A	97	GLN	3.1
1	A	13	THR	3.1
1	B	294	VAL	3.1
1	A	164	VAL	3.0
1	B	252	THR	3.0
1	A	162	PRO	2.9
1	B	288	GLU	2.7
1	A	15	SER	2.5
1	A	96	ARG	2.5
1	B	286	VAL	2.4
1	B	162	PRO	2.4
1	B	96	ARG	2.4
1	B	160	ASP	2.4
1	B	93	ALA	2.3
1	A	529	TRP	2.1
1	A	14	ILE	2.1
1	A	222	ASN	2.1
1	B	278	GLN	2.1
1	B	290	LEU	2.1
1	B	345	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	116	PRO	2.1
1	B	95	PRO	2.0
1	B	287	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, 95^{th} 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.