



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:28 pm BST

PDB ID : 3MCN  
Title : Crystal Structure of the 6-hydroxymethyl-7,8-dihydropterin pyrophosphokinase dihydropteroate synthase bifunctional enzyme from *Francisella tularensis*  
Authors : Pemble IV, C.W.; Mehta, P.K.; Mehra, S.; Li, Z.; Lee, R.E.; White, S.W.  
Deposited on : 2010-03-29  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

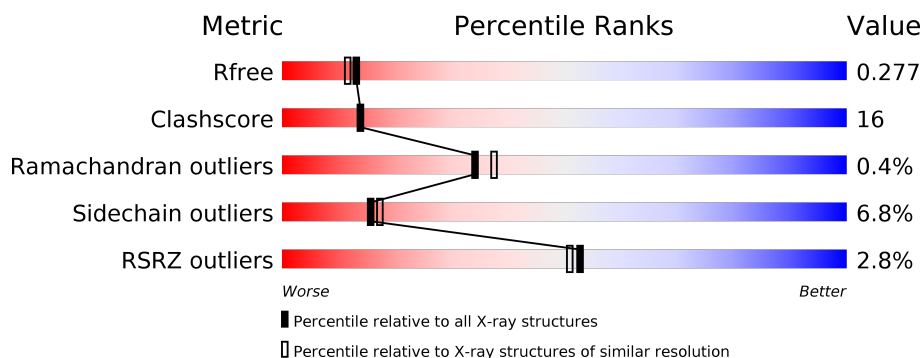
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 respectively. 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	442	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>23%</div> <div>•</div> <div>20%</div> </div> </div>
1	B	442	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>24%</div> <div>•</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6168 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 2-amino-4-hydroxy-6-hydroxymethyldihydropteridine pyrophosphokinase/dihydropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2862	1836	494	527	5			
1	B	385	Total	C	N	O	S	0	1	0
			3114	1993	538	577	6			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q2A2W3
A	-18	GLY	-	EXPRESSION TAG	UNP Q2A2W3
A	-17	SER	-	EXPRESSION TAG	UNP Q2A2W3
A	-16	SER	-	EXPRESSION TAG	UNP Q2A2W3
A	-15	HIS	-	EXPRESSION TAG	UNP Q2A2W3
A	-14	HIS	-	EXPRESSION TAG	UNP Q2A2W3
A	-13	HIS	-	EXPRESSION TAG	UNP Q2A2W3
A	-12	HIS	-	EXPRESSION TAG	UNP Q2A2W3
A	-11	HIS	-	EXPRESSION TAG	UNP Q2A2W3
A	-10	HIS	-	EXPRESSION TAG	UNP Q2A2W3
A	-9	SER	-	EXPRESSION TAG	UNP Q2A2W3
A	-8	SER	-	EXPRESSION TAG	UNP Q2A2W3
A	-7	GLY	-	EXPRESSION TAG	UNP Q2A2W3
A	-6	LEU	-	EXPRESSION TAG	UNP Q2A2W3
A	-5	VAL	-	EXPRESSION TAG	UNP Q2A2W3
A	-4	PRO	-	EXPRESSION TAG	UNP Q2A2W3
A	-3	ARG	-	EXPRESSION TAG	UNP Q2A2W3
A	-2	GLY	-	EXPRESSION TAG	UNP Q2A2W3
A	-1	SER	-	EXPRESSION TAG	UNP Q2A2W3
A	0	HIS	-	EXPRESSION TAG	UNP Q2A2W3
A	1	MET	-	EXPRESSION TAG	UNP Q2A2W3
A	2	VAL	-	EXPRESSION TAG	UNP Q2A2W3
B	-19	MET	-	EXPRESSION TAG	UNP Q2A2W3
B	-18	GLY	-	EXPRESSION TAG	UNP Q2A2W3

*Continued on next page...*

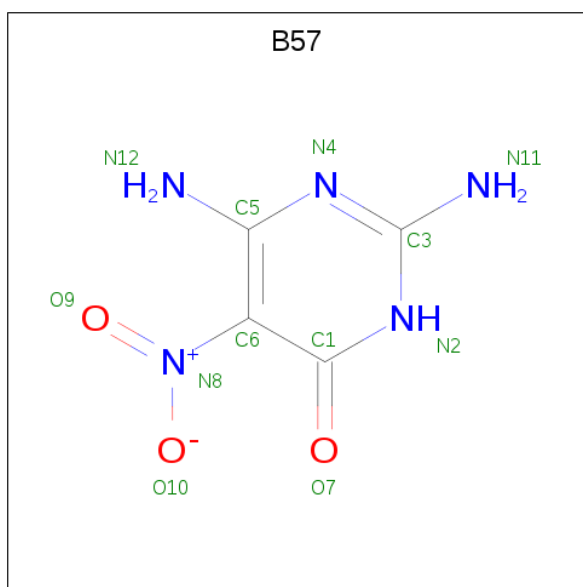
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	EXPRESSION TAG	UNP Q2A2W3
B	-16	SER	-	EXPRESSION TAG	UNP Q2A2W3
B	-15	HIS	-	EXPRESSION TAG	UNP Q2A2W3
B	-14	HIS	-	EXPRESSION TAG	UNP Q2A2W3
B	-13	HIS	-	EXPRESSION TAG	UNP Q2A2W3
B	-12	HIS	-	EXPRESSION TAG	UNP Q2A2W3
B	-11	HIS	-	EXPRESSION TAG	UNP Q2A2W3
B	-10	HIS	-	EXPRESSION TAG	UNP Q2A2W3
B	-9	SER	-	EXPRESSION TAG	UNP Q2A2W3
B	-8	SER	-	EXPRESSION TAG	UNP Q2A2W3
B	-7	GLY	-	EXPRESSION TAG	UNP Q2A2W3
B	-6	LEU	-	EXPRESSION TAG	UNP Q2A2W3
B	-5	VAL	-	EXPRESSION TAG	UNP Q2A2W3
B	-4	PRO	-	EXPRESSION TAG	UNP Q2A2W3
B	-3	ARG	-	EXPRESSION TAG	UNP Q2A2W3
B	-2	GLY	-	EXPRESSION TAG	UNP Q2A2W3
B	-1	SER	-	EXPRESSION TAG	UNP Q2A2W3
B	0	HIS	-	EXPRESSION TAG	UNP Q2A2W3
B	1	MET	-	EXPRESSION TAG	UNP Q2A2W3
B	2	VAL	-	EXPRESSION TAG	UNP Q2A2W3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is 2,6-diamino-5-nitropyrimidin-4(3H)-one (three-letter code: B57) (formula: C<sub>4</sub>H<sub>5</sub>N<sub>5</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			12	4	5	3		
3	B	1	Total	C	N	O	0	0
			12	4	5	3		

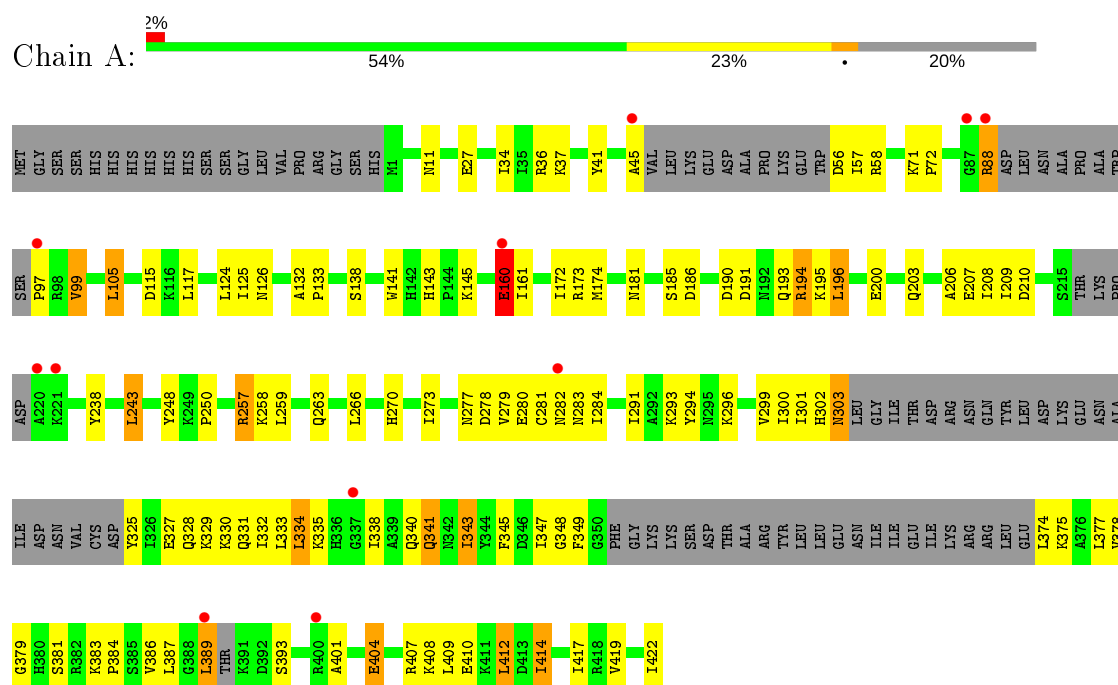
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total	O	0	0
			76	76		
4	B	89	Total	O	0	0
			89	89		

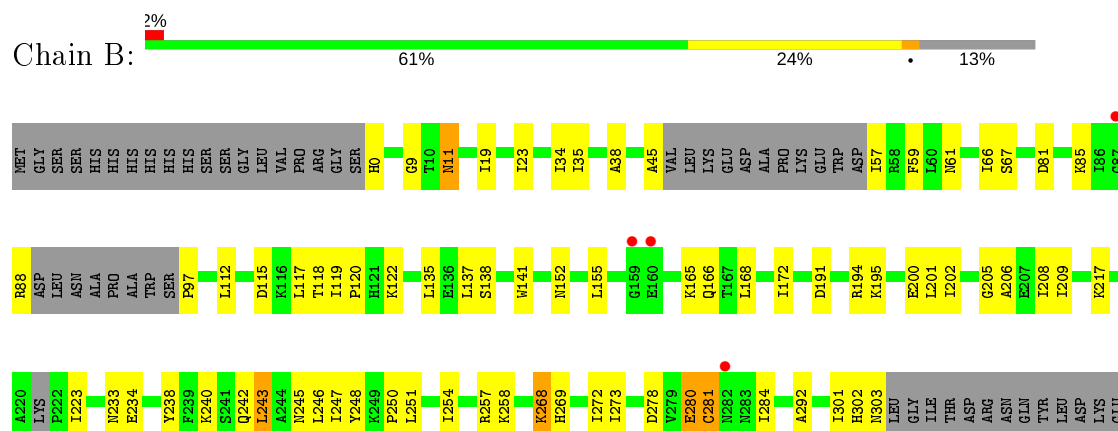
### 3 Residue-property plots [i](#)

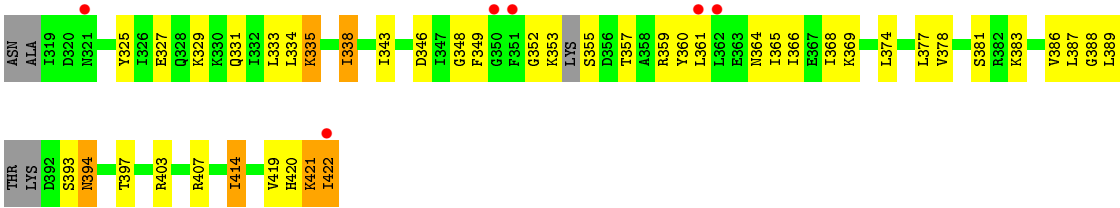
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 2-amino-4-hydroxy-6-hydroxymethyldihydropteridine pyrophosphokinase/dihydrophosphate synthase



- Molecule 1: 2-amino-4-hydroxy-6-hydroxymethyldihydropteridine pyrophosphokinase/dihydrophosphate synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.90 Å 58.19 Å 105.08 Å 91.00° 80.11° 68.29°	Depositor
Resolution (Å)	46.09 – 2.20 46.09 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.4 (46.09-2.20) 84.6 (46.09-2.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.27 (at 2.20 Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, $R_{free}$	0.220 , 0.280 0.217 , 0.277	Depositor DCC
$R_{free}$ test set	2194 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.106 for h,h-k,h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, B57

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	0.42	0/2898	0.60	1/3893 (0.0%)
1	B	0.43	0/3157	0.57	0/4243
All	All	0.42	0/6055	0.59	1/8136 (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	160	GLU	N-CA-C	5.51	125.88	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2862	0	2996	91	0
1	B	3114	0	3245	100	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	B	24	0	10	4	0
4	A	76	0	0	3	0
4	B	89	0	0	2	0
All	All	6168	0	6251	193	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 16.

All (193) 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:281:CYS:SG	1:A:284:ILE:HB	1.90	1.10
1:B:338:ILE:HD11	1:B:343:ILE:HD11	1.37	1.06
1:B:88:ARG:HH21	1:B:97:PRO:HB2	1.30	0.97
1:A:160:GLU:OE1	1:A:160:GLU:O	1.84	0.94
1:A:279:VAL:HA	1:A:301:ILE:HD12	1.52	0.88
1:A:88:ARG:HA	1:A:99:VAL:CG2	2.03	0.87
1:A:330:LYS:HG2	1:A:334:LEU:HD22	1.56	0.86
1:A:172:ILE:HG23	1:A:207:GLU:HB2	1.61	0.80
1:A:277:ASN:OD1	1:A:299:VAL:HG11	1.82	0.80
1:B:394:ASN:ND2	1:B:397:THR:H	1.79	0.80
1:A:194:ARG:HH11	1:A:194:ARG:HG3	1.51	0.74
1:A:160:GLU:CD	1:A:160:GLU:O	2.24	0.74
1:B:240:LYS:NZ	1:B:269:HIS:HD2	1.86	0.74
1:B:292:ALA:HB2	1:B:338:ILE:HG22	1.70	0.74
1:A:330:LYS:HE2	1:A:374:LEU:HD22	1.70	0.73
1:A:284:ILE:HD11	1:A:333:LEU:HD21	1.70	0.72
1:A:125:ILE:HD12	1:A:126:ASN:OD1	1.90	0.72
1:B:217:LYS:HE2	4:B:473:HOH:O	1.90	0.71
1:B:421:LYS:NZ	1:B:422:ILE:H	1.90	0.69
1:A:409:LEU:HD22	1:A:414:ILE:HG13	1.73	0.69
1:A:325:TYR:O	1:A:328:GLN:HG2	1.93	0.68
1:B:381:SER:OG	1:B:420:HIS:HD2	1.75	0.68
1:A:193:GLN:HG2	4:A:492:HOH:O	1.92	0.68
1:B:338:ILE:CD1	1:B:343:ILE:HD11	2.22	0.67
1:B:357:THR:HA	1:B:360:TYR:HB3	1.77	0.67
1:A:88:ARG:HA	1:A:99:VAL:HG21	1.77	0.67
1:A:36:ARG:NE	1:A:37:LYS:H	1.93	0.65
1:A:36:ARG:NH1	1:A:37:LYS:HE2	2.11	0.65
1:B:381:SER:HB2	1:B:419:VAL:HA	1.78	0.64
1:A:349:PHE:CD1	1:A:386:VAL:HG11	2.31	0.64
1:B:355:SER:O	1:B:359:ARG:HG3	1.97	0.64
1:B:348:GLY:O	1:B:353:LYS:HE3	1.98	0.64
1:A:349:PHE:HD2	1:A:379:GLY:O	1.81	0.63
1:B:34:ILE:HD13	1:B:66:ILE:HG22	1.80	0.63
1:B:338:ILE:HD13	1:B:338:ILE:O	1.99	0.62
1:B:377:LEU:HD23	1:B:378:VAL:N	2.14	0.62
1:A:404:GLU:O	1:A:408:LYS:HG3	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HD13	1:A:401:ALA:HB3	1.82	0.62
1:B:389:LEU:HD21	1:B:397:THR:HG22	1.80	0.62
1:B:223:ILE:O	1:B:258:LYS:NZ	2.27	0.61
1:A:330:LYS:HG2	1:A:334:LEU:CD2	2.31	0.60
1:B:61:ASN:ND2	3:B:424:B57:O10	2.22	0.60
1:A:384:PRO:CB	1:A:389:LEU:HA	2.30	0.60
1:B:365:ILE:HG21	1:B:414:ILE:HD11	1.82	0.59
1:B:268:LYS:NZ	4:B:508:HOH:O	2.35	0.59
1:A:195:LYS:HE3	4:A:472:HOH:O	2.02	0.59
1:A:257:ARG:HH11	1:A:258:LYS:HZ2	1.51	0.58
1:A:347:ILE:HD11	1:A:349:PHE:CE1	2.38	0.58
1:B:88:ARG:HH21	1:B:97:PRO:CB	2.10	0.58
1:B:242:GLN:NE2	1:B:245:ASN:HD22	2.01	0.58
1:B:112:LEU:HD23	1:B:117:LEU:HD11	1.86	0.57
1:A:328:GLN:O	1:A:332:ILE:HG13	2.05	0.57
1:A:195:LYS:HG2	1:A:238:TYR:CE2	2.40	0.57
1:B:403:ARG:NH1	1:B:422:ILE:OXT	2.37	0.57
1:B:257:ARG:HD3	1:B:280:GLU:HG3	1.87	0.57
1:B:248:TYR:CE2	1:B:250:PRO:HA	2.39	0.56
1:A:36:ARG:HE	1:A:37:LYS:H	1.54	0.56
1:A:282:ASN:O	1:A:283:ASN:HB2	2.06	0.55
1:A:381:SER:HB2	1:A:419:VAL:HA	1.87	0.55
1:B:242:GLN:HE22	1:B:245:ASN:HD22	1.54	0.54
1:B:152:ASN:N	1:B:152:ASN:HD22	2.04	0.54
1:B:421:LYS:HZ3	1:B:422:ILE:H	1.52	0.54
1:A:194:ARG:CG	1:A:194:ARG:HH11	2.19	0.54
1:A:143:HIS:CE1	1:A:145:LYS:HB2	2.42	0.54
1:A:340:GLN:O	1:A:343:ILE:HG23	2.08	0.53
1:B:81:ASP:O	1:B:85:LYS:HG3	2.08	0.53
1:A:185:SER:OG	1:A:193:GLN:HG3	2.09	0.53
1:A:277:ASN:HA	1:A:299:VAL:HG12	1.89	0.53
1:B:112:LEU:CD2	1:B:117:LEU:HD11	2.39	0.53
1:B:135:LEU:HD12	1:B:155:LEU:HD22	1.91	0.53
1:B:333:LEU:C	1:B:338:ILE:HD12	2.28	0.53
1:B:206:ALA:HB2	1:B:422:ILE:CD1	2.39	0.53
1:A:191:ASP:N	1:A:191:ASP:OD2	2.41	0.52
1:A:88:ARG:HB2	1:A:99:VAL:HG23	1.91	0.52
1:A:11:ASN:OD1	1:A:97:PRO:HA	2.09	0.52
1:B:117:LEU:HD12	1:B:117:LEU:C	2.29	0.52
1:B:302:HIS:ND1	1:B:353:LYS:NZ	2.57	0.52
1:A:257:ARG:HH11	1:A:258:LYS:NZ	2.07	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LYS:HE2	1:A:374:LEU:CD2	2.39	0.52
1:A:341:GLN:O	1:A:375:LYS:NZ	2.43	0.52
1:A:57:ILE:N	1:A:57:ILE:HD12	2.25	0.52
1:B:349:PHE:CD2	1:B:386:VAL:HG11	2.45	0.52
1:B:208:ILE:HG12	1:B:251:LEU:HB2	1.92	0.51
1:B:240:LYS:NZ	1:B:269:HIS:CD2	2.74	0.51
1:A:259:LEU:O	1:A:263:GLN:HG3	2.10	0.51
1:A:293:LYS:HE3	1:A:294:TYR:CE2	2.45	0.51
1:B:377:LEU:HD23	1:B:377:LEU:C	2.31	0.51
1:B:301:ILE:HG13	1:B:346:ASP:HB3	1.93	0.50
1:B:11:ASN:O	1:B:57:ILE:HD11	2.11	0.50
1:B:138:SER:OG	1:B:141:TRP:HB2	2.12	0.50
1:A:27:GLU:HG3	1:A:34:ILE:HG12	1.92	0.50
1:B:234:GLU:HA	1:B:234:GLU:OE2	2.12	0.50
1:A:88:ARG:HA	1:A:99:VAL:HG23	1.92	0.50
1:A:291:ILE:HB	1:A:338:ILE:HD11	1.94	0.50
1:B:35:ILE:HD11	1:B:67:SER:HB2	1.93	0.50
1:A:208:ILE:HG22	1:A:209:ILE:N	2.27	0.50
1:B:9:GLY:HA3	3:B:424:B57:O10	2.12	0.49
1:A:281:CYS:HG	1:A:284:ILE:HB	1.69	0.49
1:B:388:GLY:O	1:B:389:LEU:HD12	2.13	0.48
1:B:191:ASP:N	1:B:191:ASP:OD2	2.46	0.48
1:A:132:ALA:HB3	1:A:133:PRO:HD3	1.95	0.47
1:A:195:LYS:HG2	1:A:238:TYR:CZ	2.49	0.47
1:B:364:ASN:O	1:B:368:ILE:HG13	2.15	0.47
1:A:329:LYS:O	1:A:333:LEU:HG	2.14	0.47
1:B:233:ASN:OD1	1:B:269:HIS:HE1	1.98	0.47
1:B:381:SER:OG	1:B:420:HIS:CD2	2.63	0.47
1:A:284:ILE:HD11	1:A:333:LEU:CD2	2.43	0.47
1:B:200:GLU:HG2	1:B:421:LYS:HE2	1.96	0.47
1:A:277:ASN:HA	1:A:299:VAL:CG1	2.45	0.47
1:A:194:ARG:NH1	1:A:194:ARG:CG	2.77	0.47
1:B:333:LEU:O	1:B:338:ILE:HD12	2.14	0.47
1:B:357:THR:O	1:B:361:LEU:HG	2.14	0.47
1:A:194:ARG:NH1	1:A:194:ARG:HG3	2.26	0.47
1:A:266:LEU:O	1:A:270:HIS:HB3	2.15	0.46
1:A:160:GLU:C	1:A:160:GLU:OE1	2.53	0.46
1:A:196:LEU:O	1:A:200:GLU:HG3	2.16	0.46
1:A:410:GLU:O	1:A:412:LEU:O	2.33	0.46
1:B:202:ILE:HD13	1:B:246:LEU:HD22	1.98	0.46
1:B:257:ARG:HB2	1:B:280:GLU:HB2	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:GLY:O	1:B:353:LYS:HG3	2.15	0.46
1:A:125:ILE:CD1	1:A:126:ASN:OD1	2.61	0.46
1:A:302:HIS:HA	1:A:303:ASN:HA	1.65	0.46
1:A:299:VAL:HG22	1:A:300:ILE:N	2.30	0.46
1:B:240:LYS:HZ2	1:B:269:HIS:HD2	1.64	0.46
1:A:248:TYR:CE2	1:A:250:PRO:HA	2.51	0.46
1:A:257:ARG:HA	1:A:278:ASP:OD1	2.16	0.46
1:B:369:LYS:HG3	1:B:374:LEU:O	2.16	0.46
1:A:387:LEU:HB3	1:A:401:ALA:HB1	1.98	0.45
1:B:240:LYS:HZ1	1:B:269:HIS:HD2	1.62	0.45
1:B:278:ASP:O	1:B:301:ILE:HD13	2.16	0.45
1:A:327:GLU:O	1:A:331:GLN:HG2	2.16	0.45
1:A:377:LEU:HD23	1:A:377:LEU:C	2.37	0.45
1:B:117:LEU:HD12	1:B:117:LEU:O	2.17	0.45
1:B:152:ASN:N	1:B:152:ASN:ND2	2.65	0.45
1:A:273:ILE:O	1:A:296:LYS:HE3	2.15	0.45
3:B:424:B57:O10	3:B:424:B57:N12	2.49	0.45
1:A:409:LEU:HB3	1:A:414:ILE:HG13	1.99	0.44
1:B:115:ASP:N	1:B:115:ASP:OD1	2.49	0.44
1:B:333:LEU:HB3	1:B:338:ILE:HD12	1.99	0.44
1:A:88:ARG:CA	1:A:99:VAL:CG2	2.87	0.44
1:B:365:ILE:HG23	1:B:366:ILE:N	2.33	0.44
1:B:421:LYS:HZ2	1:B:422:ILE:H	1.62	0.44
1:B:112:LEU:O	1:B:118:THR:HA	2.17	0.44
1:A:383:LYS:HA	1:A:384:PRO:HD3	1.79	0.44
1:B:165:LYS:HB3	1:B:165:LYS:HE3	1.62	0.44
1:B:394:ASN:HD21	1:B:397:THR:H	1.60	0.44
1:B:45:ALA:HA	1:B:59:PHE:CE1	2.53	0.44
1:A:71:LYS:O	1:A:72:PRO:C	2.53	0.44
1:B:335:LYS:O	1:B:335:LYS:HG3	2.17	0.43
1:B:365:ILE:CG2	1:B:414:ILE:HD11	2.46	0.43
1:B:243:LEU:HA	1:B:243:LEU:HD12	1.80	0.43
1:A:138:SER:HB3	1:A:141:TRP:HB2	2.00	0.43
1:A:206:ALA:HB2	1:A:422:ILE:HD11	2.00	0.43
1:B:386:VAL:HG23	1:B:387:LEU:CD1	2.47	0.43
1:B:383:LYS:O	1:B:387:LEU:HD13	2.18	0.43
1:B:303:ASN:OD1	1:B:303:ASN:O	2.35	0.43
1:B:254:ILE:HG13	1:B:273:ILE:HD13	2.00	0.43
1:A:302:HIS:HB3	1:A:347:ILE:O	2.18	0.42
1:B:421:LYS:HD2	1:B:421:LYS:HA	1.35	0.42
3:B:423:B57:O9	3:B:423:B57:O7	2.37	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LEU:HA	1:A:243:LEU:HD12	1.83	0.42
1:B:208:ILE:HG22	1:B:209:ILE:N	2.33	0.42
1:A:325:TYR:CZ	1:A:329:LYS:HD2	2.55	0.42
1:B:360:TYR:O	1:B:360:TYR:CG	2.72	0.42
1:A:41:TYR:CD2	1:A:133:PRO:HG3	2.54	0.42
1:A:36:ARG:HH12	1:A:37:LYS:HE2	1.83	0.42
1:A:45:ALA:HB3	1:A:56:ASP:HB2	2.02	0.42
1:B:240:LYS:HG3	1:B:272:ILE:HD13	2.00	0.42
1:A:302:HIS:O	1:A:348:GLY:HA3	2.20	0.42
1:A:383:LYS:HB2	1:A:386:VAL:HG22	2.01	0.42
1:A:117:LEU:N	1:A:117:LEU:HD23	2.35	0.42
1:A:332:ILE:O	1:A:335:LYS:HB3	2.20	0.42
1:B:119:ILE:HA	1:B:120:PRO:C	2.39	0.42
1:B:195:LYS:HG2	1:B:238:TYR:CE2	2.55	0.42
1:A:105:LEU:HG	1:A:124:LEU:HD13	2.02	0.41
1:B:327:GLU:O	1:B:331:GLN:HG2	2.20	0.41
1:A:174:MET:SD	1:A:210:ASP:HB2	2.61	0.41
1:A:27:GLU:O	4:A:426:HOH:O	2.22	0.41
1:B:247:ILE:HG13	1:B:248:TYR:N	2.35	0.41
1:B:240:LYS:HZ1	1:B:269:HIS:CD2	2.38	0.41
1:B:386:VAL:HG23	1:B:387:LEU:HD13	2.03	0.41
1:B:381:SER:CB	1:B:420:HIS:HD2	2.34	0.41
1:B:257:ARG:HA	1:B:278:ASP:OD1	2.21	0.41
1:B:325:TYR:O	1:B:329:LYS:HG2	2.21	0.41
1:B:422:ILE:HG22	1:B:422:ILE:O	2.20	0.41
1:B:45:ALA:HA	1:B:59:PHE:CD1	2.55	0.41
1:B:88:ARG:NH2	1:B:97:PRO:HB2	2.14	0.41
1:B:281:CYS:O	1:B:284:ILE:HB	2.21	0.41
1:B:201:LEU:HA	1:B:201:LEU:HD23	1.94	0.40
1:B:38:ALA:HB2	1:B:137:LEU:HG	2.03	0.40
1:B:166:GLN:HG3	1:B:205:GLY:O	2.21	0.40
1:B:19:ILE:O	1:B:23:ILE:HG13	2.20	0.40
1:A:345:PHE:C	1:A:345:PHE:CD1	2.95	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	341/442 (77%)	317 (93%)	21 (6%)	3 (1%)	17	16
1	B	372/442 (84%)	360 (97%)	12 (3%)	0	100	100
All	All	713/884 (81%)	677 (95%)	33 (5%)	3 (0%)	34	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	GLU
1	A	161	ILE
1	A	414	ILE

### 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	319/396 (81%)	293 (92%)	26 (8%)	11	11
1	B	348/396 (88%)	329 (94%)	19 (6%)	21	26
All	All	667/792 (84%)	622 (93%)	45 (7%)	16	18

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	88	ARG
1	A	99	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	105	LEU
1	A	115	ASP
1	A	173	ARG
1	A	181	ASN
1	A	186	ASP
1	A	190	ASP
1	A	194	ARG
1	A	196	LEU
1	A	203	GLN
1	A	243	LEU
1	A	257	ARG
1	A	280	GLU
1	A	303	ASN
1	A	334	LEU
1	A	341	GLN
1	A	343	ILE
1	A	378	VAL
1	A	389	LEU
1	A	393	SER
1	A	404	GLU
1	A	407	ARG
1	A	412	LEU
1	A	417	ILE
1	B	0	HIS
1	B	11	ASN
1	B	122	LYS
1	B	168	LEU
1	B	172	ILE
1	B	194	ARG
1	B	243	LEU
1	B	268	LYS
1	B	280	GLU
1	B	281	CYS
1	B	334	LEU
1	B	335	LYS
1	B	338	ILE
1	B	393	SER
1	B	394	ASN
1	B	407	ARG
1	B	414	ILE
1	B	421	LYS
1	B	422	ILE



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	61	ASN
1	A	142	HIS
1	A	182	GLN
1	A	197	ASN
1	A	203	GLN
1	A	230	ASN
1	A	242	GLN
1	A	245	ASN
1	A	282	ASN
1	A	295	ASN
1	A	331	GLN
1	A	340	GLN
1	A	342	ASN
1	B	11	ASN
1	B	152	ASN
1	B	182	GLN
1	B	188	ASN
1	B	193	GLN
1	B	203	GLN
1	B	242	GLN
1	B	269	HIS
1	B	295	ASN
1	B	342	ASN
1	B	394	ASN
1	B	420	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 5 ligands modelled in this entry, 3 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	B57	B	424	2	9,12,12	4.42	4 (44%)	11,17,17	3.04	6 (54%)
3	B57	B	423	-	9,12,12	4.31	4 (44%)	11,17,17	3.15	7 (63%)

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	B57	B	424	2	-	0/0/4/4	0/1/1/1
3	B57	B	423	-	-	0/0/4/4	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	424	B57	O9-N8	10.75	1.41	1.22
3	B	423	B57	O9-N8	10.26	1.40	1.22
3	B	423	B57	C6-N8	-6.68	1.33	1.45
3	B	424	B57	C6-N8	-6.01	1.35	1.45
3	B	424	B57	C1-N2	3.97	1.39	1.33
3	B	423	B57	C1-N2	3.37	1.38	1.33
3	B	424	B57	C3-N2	2.81	1.40	1.35
3	B	423	B57	C3-N2	2.24	1.39	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	423	B57	C1-C6-C5	6.30	119.59	114.65
3	B	424	B57	C1-C6-C5	5.41	118.89	114.65
3	B	424	B57	C6-C5-N12	-4.62	120.65	125.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	424	B57	C3-N4-C5	4.47	121.93	116.99
3	B	423	B57	C6-C5-N12	-4.16	121.09	125.08
3	B	423	B57	C3-N4-C5	3.86	121.25	116.99
3	B	423	B57	C6-C1-N2	-3.46	118.70	123.43
3	B	424	B57	N2-C3-N4	-3.36	120.15	125.42
3	B	423	B57	N2-C3-N4	-2.94	120.81	125.42
3	B	423	B57	C1-N2-C3	2.51	119.91	115.93
3	B	424	B57	C6-C1-N2	-2.47	120.06	123.43
3	B	423	B57	N11-C3-N4	2.37	120.94	117.25
3	B	424	B57	N11-C3-N4	2.28	120.80	117.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	424	B57	3	0
3	B	423	B57	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<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	355/442 (80%)	0.19	11 (3%) 49 47	22, 39, 70, 78	0
1	B	385/442 (87%)	-0.01	10 (2%) 56 53	21, 36, 63, 79	0
All	All	740/884 (83%)	0.08	21 (2%) 53 51	21, 38, 67, 79	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	GLY	5.7
1	A	97	PRO	5.4
1	B	87	GLY	3.8
1	B	361	LEU	3.5
1	A	88	ARG	3.5
1	B	422	ILE	3.0
1	B	350	GLY	2.9
1	B	160	GLU	2.8
1	B	362	LEU	2.8
1	B	282	ASN	2.7
1	A	400	ARG	2.6
1	A	160	GLU	2.6
1	A	389	LEU	2.5
1	A	220	ALA	2.4
1	A	282	ASN	2.4
1	A	337	GLY	2.3
1	A	45	ALA	2.3
1	B	321	ASN	2.2
1	B	159	GLY	2.2
1	B	351	PHE	2.2
1	A	221	LYS	2.2

## 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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	B57	B	424	12/12	0.86	0.24	37,44,51,53	0
3	B57	B	423	12/12	0.89	0.14	39,43,49,55	0
2	MG	A	423	1/1	0.92	0.08	61,61,61,61	0
2	MG	B	426	1/1	0.92	0.15	48,48,48,48	0
2	MG	B	425	1/1	0.98	0.15	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.