



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:04 AM UTC

PDB ID : 3MCN / pdb_00003mcn
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

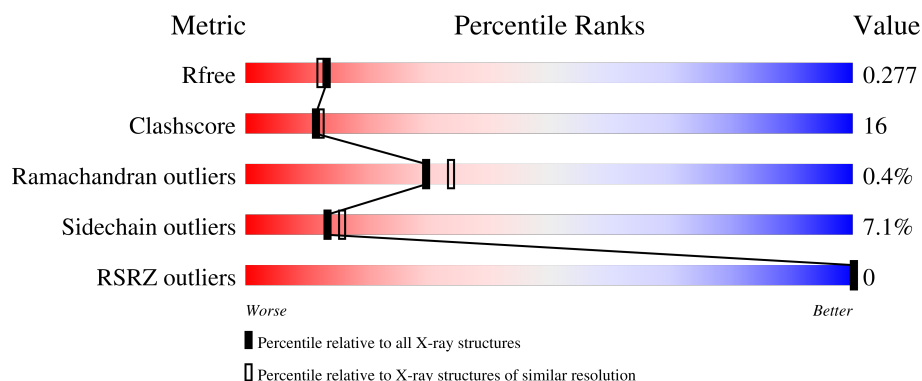
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	B	442	

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

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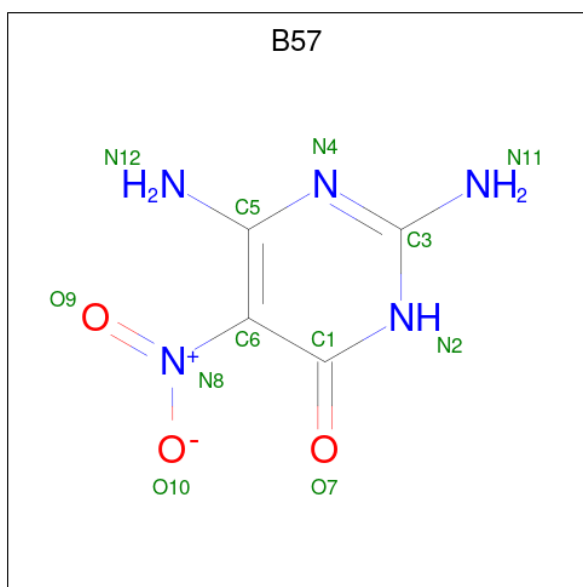
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP Q2A2W3
B	-16	SER	-	expression tag	UNP Q2A2W3
B	-15	HIS	-	expression tag	UNP Q2A2W3
B	-14	HIS	-	expression tag	UNP Q2A2W3
B	-13	HIS	-	expression tag	UNP Q2A2W3
B	-12	HIS	-	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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is 2,6-diamino-5-nitropyrimidin-4(3H)-one (CCD ID: B57) (formula: C₄H₅N₅O₃).



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		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.90Å 58.19Å 105.08Å 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
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.220 , 0.280 0.219 , 0.277	Depositor DCC
R_{free} test set	2194 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.106 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6168	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: B57, MG

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	0.53	0/2898	0.88	4/3893 (0.1%)
1	B	0.55	0/3157	0.85	1/4243 (0.0%)
All	All	0.54	0/6055	0.86	5/8136 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	GLU	N-CA-C	7.08	125.88	110.80
1	A	193	GLN	N-CA-C	5.49	117.27	111.28
1	B	274	TRP	N-CA-C	-5.47	106.66	113.55
1	A	34	ILE	CB-CA-C	-5.20	104.66	110.96
1	A	406	SER	N-CA-C	-5.20	105.52	111.14

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	2862	0	2996	93	0
1	B	3114	0	3245	101	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	10	4	0
4	A	76	0	0	3	0
4	B	89	0	0	1	0
All	All	6168	0	6251	196	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 (196) 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:160:GLU:O	1:A:160:GLU:CD	2.24	0.79
1:A:194:ARG:HH11	1:A:194:ARG:HG3	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:333:LEU:C	1:B:338:ILE:HD12	2.28	0.57
1:A:195:LYS:HG2	1:A:238:TYR:CE2	2.40	0.57
1:B:117:LEU:C	1:B:117:LEU:HD12	2.29	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:B:377:LEU:HD23	1:B:377:LEU:C	2.31	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:HD22	1:B:152:ASN:N	2.04	0.54
1:B:421:LYS:HZ3	1:B:422:ILE:H	1.52	0.54
1:A:194:ARG:HH11	1:A:194:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:HD12	1:B:155:LEU:HD22	1.91	0.53
1:B:206:ALA:HB2	1:B:422:ILE:CD1	2.39	0.53
1:A:11:ASN:OD1	1:A:97:PRO:HA	2.09	0.52
1:A:88:ARG:HB2	1:A:99:VAL:HG23	1.91	0.52
1:A:191:ASP:OD2	1:A:191:ASP:N	2.41	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
1:A:57:ILE:N	1:A:57:ILE:HD12	2.25	0.52
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: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:160:GLU:OE1	1:A:160:GLU:C	2.53	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: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:OE2	1:B:234:GLU:HA	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:A:377:LEU:C	1:A:377:LEU:HD23	2.37	0.49
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:A:71:LYS:O	1:A:72:PRO:C	2.53	0.48
1:B:191:ASP:OD2	1:B:191:ASP:N	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:CG	1:A:194:ARG:NH1	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:A:194:ARG:NH1	2.26	0.47
1:A:266:LEU:O	1:A:270:HIS:HB3	2.15	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
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:119:ILE:HA	1:B:120:PRO:C	2.39	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:345:PHE:CD1	1:A:345:PHE:C	2.95	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:OD1	1:B:115:ASP:N	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:HE3	1:B:165:LYS:HB3	1.62	0.44
1:B:45:ALA:HA	1:B:59:PHE:CE1	2.53	0.44
1:B:394:ASN:HD21	1:B:397:THR:H	1.60	0.44
1:B:44:LYS:O	1:B:45:ALA:C	2.59	0.44
1:B:365:ILE:CG2	1:B:414:ILE:HD11	2.46	0.43
1:B:243:LEU:HD12	1:B:243:LEU:HA	1.80	0.43
1:A:138:SER:HB3	1:A:141:TRP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:388:GLY:O	1:A:389:LEU:C	2.61	0.43
1:B:303:ASN:O	1:B:303:ASN:OD1	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:HA	1:B:421:LYS:HD2	1.35	0.42
3:B:423:B57:O7	3:B:423:B57:O9	2.37	0.42
1:A:243:LEU:HD12	1:A:243:LEU:HA	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:36:ARG:HH12	1:A:37:LYS:HE2	1.83	0.42
1:A:41:TYR:CD2	1:A:133:PRO:HG3	2.54	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:HD23	1:A:117:LEU:N	2.35	0.42
1:A:332:ILE:O	1:A:335:LYS:HB3	2.20	0.42
1:B:195:LYS:HG2	1:B:238:TYR:CE2	2.55	0.42
1:A:125:ILE:HD12	1:A:125:ILE:C	2.45	0.41
1:B:1:MET:HE3	1:B:67:SER:OG	2.19	0.41
1:B:71:LYS:O	1:B:72:PRO:C	2.61	0.41
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:27:GLU:O	4:A:426:HOH:O	2.22	0.41
1:A:174:MET:SD	1:A:210:ASP:HB2	2.61	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:381:SER:CB	1:B:420:HIS:HD2	2.34	0.41
1:B:386:VAL:HG23	1:B:387:LEU:HD13	2.03	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: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:281:CYS:O	1:B:284:ILE:HB	2.21	0.41
1:B:201:LEU:HD23	1:B:201:LEU:HA	1.94	0.40
1:B:38:ALA:HB2	1:B:137:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ILE:O	1:B:23:ILE:HG13	2.20	0.40
1:B:166:GLN:HG3	1:B:205:GLY:O	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	341/442 (77%)	317 (93%)	21 (6%)	3 (1%)	14	14
1	B	372/442 (84%)	360 (97%)	12 (3%)	0	100	100
All	All	713/884 (81%)	677 (95%)	33 (5%)	3 (0%)	30	34

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 [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	319/396 (81%)	291 (91%)	28 (9%)	9	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	348/396 (88%)	329 (94%)	19 (6%)	19	24
All	All	667/792 (84%)	620 (93%)	47 (7%)	13	16

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	88	ARG
1	A	99	VAL
1	A	105	LEU
1	A	170	ASN
1	A	181	ASN
1	A	190	ASP
1	A	194	ARG
1	A	196	LEU
1	A	203	GLN
1	A	211	ILE
1	A	243	LEU
1	A	257	ARG
1	A	268	LYS
1	A	280	GLU
1	A	303	ASN
1	A	334	LEU
1	A	341	GLN
1	A	343	ILE
1	A	374	LEU
1	A	375	LYS
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	11	ASN
1	B	152	ASN
1	B	168	LEU
1	B	172	ILE
1	B	243	LEU
1	B	268	LYS
1	B	280	GLU
1	B	281	CYS

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Mol	Chain	Res	Type
1	B	284	ILE
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	408	LYS
1	B	414	ILE
1	B	421	LYS
1	B	422	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	29	GLN
1	A	61	ASN
1	A	142	HIS
1	A	182	GLN
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	341	GLN
1	A	342	ASN
1	B	11	ASN
1	B	152	ASN
1	B	182	GLN
1	B	193	GLN
1	B	203	GLN
1	B	245	ASN
1	B	269	HIS
1	B	295	ASN
1	B	303	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 oligosaccharides 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	423	-	11,12,12	3.08	1 (9%)	10,17,17	2.14	4 (40%)
3	B57	B	424	2	11,12,12	3.24	1 (9%)	10,17,17	2.51	4 (40%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	424	B57	O9-N8	10.50	1.41	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	423	B57	O9-N8	10.02	1.40	1.22

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	424	B57	C6-C1-N2	3.98	120.06	111.84
3	B	424	B57	C3-N4-C5	3.93	121.93	113.79
3	B	423	B57	C3-N4-C5	3.60	121.25	113.79
3	B	424	B57	C3-N2-C1	-3.44	118.87	125.11
3	B	423	B57	C6-C1-N2	3.32	118.70	111.84
3	B	424	B57	O7-C1-C6	-2.97	121.38	128.01
3	B	423	B57	C3-N2-C1	-2.87	119.91	125.11
3	B	423	B57	O7-C1-C6	-2.29	122.90	128.01

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	423	B57	1	0
3	B	424	B57	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	355/442 (80%)	-1.13	0 100 100	22, 39, 70, 78	0
1	B	385/442 (87%)	-1.17	0 100 100	21, 36, 63, 79	1 (0%)
All	All	740/884 (83%)	-1.15	0 100 100	21, 38, 67, 79	1 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
2	MG	A	423	1/1	0.98	0.03	61,61,61,61	0
2	MG	B	426	1/1	0.98	0.04	48,48,48,48	0
3	B57	B	424	12/12	0.98	0.04	37,44,51,53	0
3	B57	B	423	12/12	0.99	0.04	39,43,49,55	0
2	MG	B	425	1/1	0.99	0.05	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.