Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 01:55 PM EDT

PDB ID	:	5DO0
Title	:	The structure of PKMT1 from Rickettsia prowazekii
Authors	:	Noinaj, N.; Abeykoon, A.; He, Y.; Yang, D.C.; Buchanan, S.K.
Deposited on	:	2015-09-10
Resolution	:	2.60 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 (i) 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 (1)) were used in the production of this report:

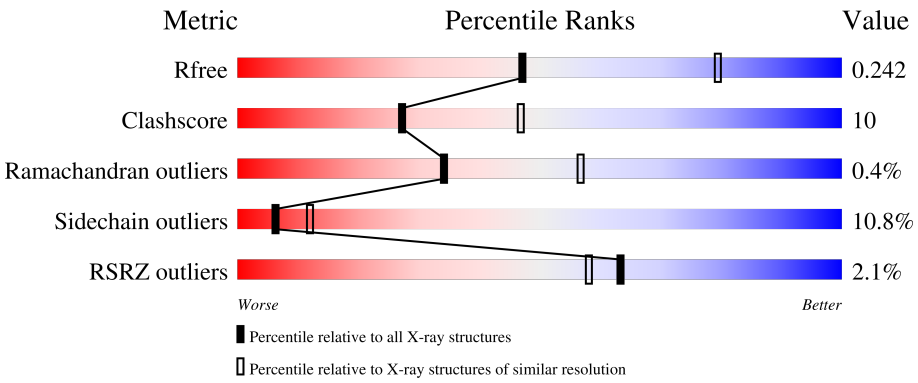
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	554	3% 65% 22% • 9%
1	B	554	% 69% 20% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8345 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 protein lysine methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	511	4046	2573	695	758	20	0	0	0
1	A	505	3966	2531	679	736	20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP O05979
A	0	GLY	-	expression tag	UNP O05979

- Molecule 2 is water.

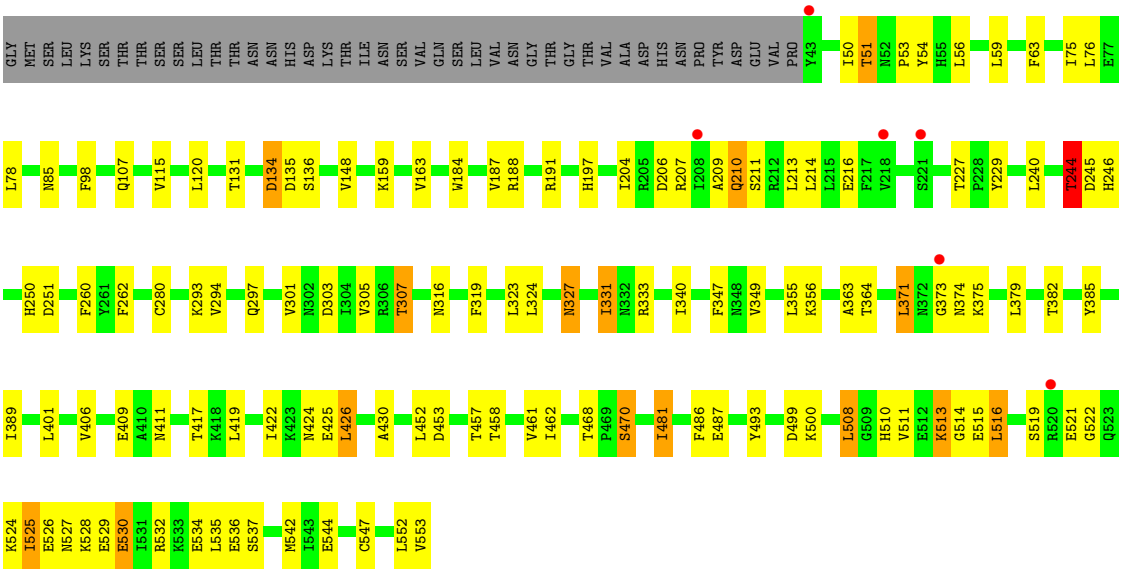
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	B	197	197	197	0	0
2	A	136	136	136	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

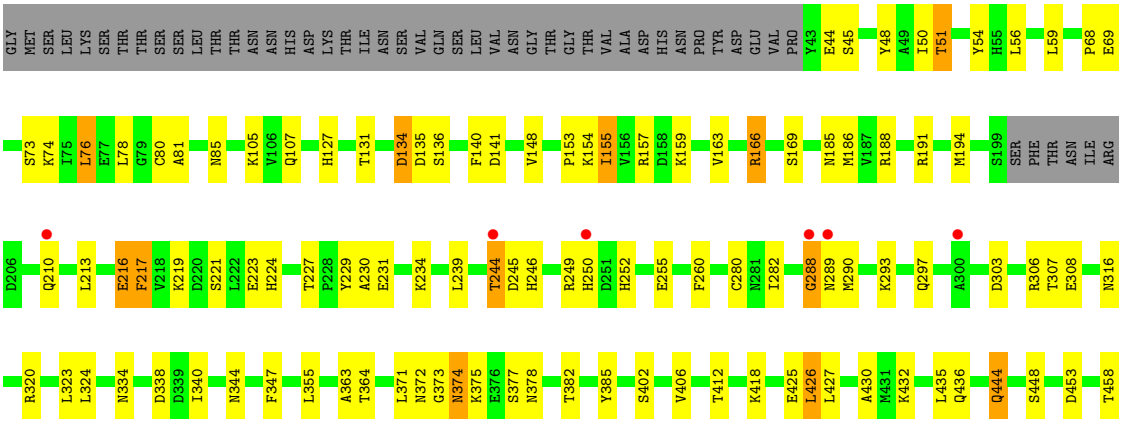
• Molecule 1: protein lysine methyltransferase 1

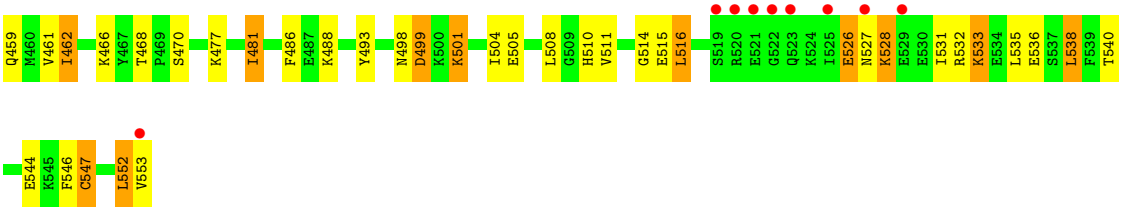
Chain B:



• Molecule 1: protein lysine methyltransferase 1

Chain A:




Q459
M460
V461
I462
K466
Y467
T468
P469
S470
K477
I481
F486
E487
K488
Y493
N498
D499
K500
K501
I504
E505
L508
G509
H510
V511
G514
E515
L516
S519
R520
E521
G522
Q523
K524
I525
E526
N527
K528
E529
E530
I531
R532
K533
E534
L535
E536
S537
L538
F539
T540
E544
K545
F546
C547
L552
V553

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.50Å 62.47Å 107.85Å 90.00° 100.78° 90.00°	Depositor
Resolution (Å)	48.38 – 2.60 48.38 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.38-2.60) 94.1 (48.38-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.58Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.243 0.213 , 0.242	Depositor DCC
R_{free} test set	2000 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8345	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.28	0/4048	0.52	1/5492 (0.0%)
1	B	0.29	0/4127	0.50	0/5593
All	All	0.28	0/8175	0.51	1/11085 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	288	GLY	N-CA-C	5.79	127.57	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	GLU	Peptide
1	A	244	THR	Peptide
1	A	260	PHE	Peptide
1	A	526	GLU	Peptide
1	B	244	THR	Peptide
1	B	260	PHE	Peptide

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	3966	0	3883	90	0
1	B	4046	0	3987	74	0
2	A	136	0	0	13	0
2	B	197	0	0	10	0
All	All	8345	0	7870	160	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 10.

All (160) 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:553:VAL:O	2:A:601:HOH:O	1.82	0.97
1:A:288:GLY:HA2	1:A:290:MET:H	1.34	0.92
1:A:514:GLY:HA2	1:A:515:GLU:HB2	1.58	0.83
1:A:282:ILE:HD11	1:A:435:LEU:HD23	1.64	0.80
1:A:501:LYS:HE2	1:A:501:LYS:H	1.47	0.80
1:A:249:ARG:HE	1:A:252:HIS:HB2	1.48	0.79
1:A:547:CYS:O	2:A:602:HOH:O	2.01	0.79
1:B:51:THR:HG21	1:B:85:ASN:HD21	1.49	0.76
1:B:527:ASN:HB3	1:B:530:GLU:HB2	1.68	0.76
1:A:51:THR:HG21	1:A:85:ASN:HD21	1.52	0.74
1:B:468:THR:HG22	1:B:470:SER:H	1.51	0.74
1:A:468:THR:HG22	1:A:470:SER:H	1.54	0.73
1:B:107:GLN:NE2	2:B:605:HOH:O	2.20	0.72
1:A:159:LYS:NZ	2:A:610:HOH:O	2.22	0.72
1:A:444:GLN:NE2	2:A:609:HOH:O	2.20	0.72
1:B:499:ASP:OD2	2:B:601:HOH:O	2.07	0.71
1:A:385:TYR:HB2	1:A:425:GLU:HG3	1.73	0.70
1:A:501:LYS:O	1:A:505:GLU:HB2	1.92	0.70
1:B:514:GLY:HA2	1:B:516:LEU:H	1.56	0.69
1:B:363:ALA:O	1:B:382:THR:OG1	2.11	0.69
1:B:511:VAL:HG12	1:B:516:LEU:HB3	1.76	0.68
1:B:500:LYS:NZ	1:B:536:GLU:OE1	2.27	0.68
1:A:166:ARG:NH1	2:A:612:HOH:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LEU:O	2:A:603:HOH:O	2.11	0.68
1:A:453:ASP:O	2:A:604:HOH:O	2.12	0.67
1:A:185:ASN:OD1	1:A:188:ARG:NH2	2.26	0.67
1:A:80:CYS:SG	1:A:81:ALA:N	2.68	0.66
1:B:514:GLY:N	1:B:515:GLU:HB2	2.11	0.66
1:A:493:TYR:OH	1:A:510:HIS:NE2	2.19	0.66
1:A:191:ARG:NH2	1:A:252:HIS:O	2.29	0.65
1:B:327:ASN:OD1	2:B:602:HOH:O	2.15	0.65
1:A:505:GLU:O	2:A:607:HOH:O	2.14	0.65
1:A:56:LEU:HD22	1:A:323:LEU:HD21	1.79	0.64
1:B:513:LYS:NZ	2:B:615:HOH:O	2.32	0.64
1:B:373:GLY:HA3	1:B:374:ASN:HB2	1.79	0.63
1:A:288:GLY:CA	1:A:290:MET:H	2.11	0.62
1:A:508:LEU:HA	1:A:511:VAL:HG12	1.80	0.61
1:B:115:VAL:HG13	1:B:120:LEU:HB2	1.80	0.61
1:B:493:TYR:OH	1:B:510:HIS:NE2	2.27	0.61
1:A:231:GLU:OE2	1:A:234:LYS:NZ	2.33	0.61
1:A:308:GLU:HB3	1:A:320:ARG:HH22	1.66	0.61
1:A:135:ASP:OD2	1:A:166:ARG:NH2	2.34	0.61
1:A:372:ASN:N	1:A:373:GLY:HA2	2.15	0.60
1:A:385:TYR:OH	2:A:605:HOH:O	2.12	0.60
1:A:303:ASP:HB3	1:A:306:ARG:HG2	1.84	0.60
1:A:504:ILE:HG23	1:A:535:LEU:HD13	1.84	0.59
1:B:385:TYR:HB2	1:B:425:GLU:HG3	1.83	0.59
1:A:288:GLY:HA2	1:A:290:MET:N	2.14	0.58
1:A:334:ASN:ND2	2:A:618:HOH:O	2.37	0.58
1:B:51:THR:HG21	1:B:85:ASN:ND2	2.19	0.57
1:A:526:GLU:O	1:A:528:LYS:N	2.27	0.57
1:A:374:ASN:N	1:A:374:ASN:OD1	2.38	0.56
1:B:206:ASP:O	1:B:210:GLN:HB2	2.05	0.56
1:A:303:ASP:O	1:A:307:THR:OG1	2.23	0.56
1:A:191:ARG:NH1	2:A:616:HOH:O	2.35	0.56
1:B:56:LEU:HD22	1:B:323:LEU:HD21	1.87	0.55
1:B:487:GLU:HG2	1:B:542:MET:HG3	1.88	0.55
1:A:191:ARG:HA	1:A:194:MET:HE2	1.89	0.55
1:A:371:LEU:C	1:A:373:GLY:HA2	2.28	0.54
1:A:308:GLU:HB3	1:A:320:ARG:NH2	2.23	0.54
1:B:207:ARG:O	1:B:210:GLN:HB3	2.08	0.54
1:B:521:GLU:HG2	1:B:522:GLY:H	1.72	0.53
1:B:374:ASN:OD1	1:B:375:LYS:N	2.41	0.53
1:B:135:ASP:O	2:B:603:HOH:O	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ARG:HA	1:A:535:LEU:HD12	1.91	0.52
1:A:68:PRO:HG2	1:A:141:ASP:HB3	1.92	0.52
1:A:468:THR:O	1:A:488:LYS:NZ	2.32	0.52
1:B:349:VAL:HG12	1:B:371:LEU:HD12	1.92	0.52
1:B:514:GLY:HA2	1:B:516:LEU:N	2.22	0.51
1:A:81:ALA:HB1	1:A:107:GLN:HB3	1.92	0.51
1:A:216:GLU:OE1	1:A:219:LYS:NZ	2.42	0.51
1:A:426:LEU:HD22	1:A:430:ALA:HB2	1.92	0.51
1:B:401:LEU:HD23	1:B:406:VAL:HG22	1.92	0.51
1:B:210:GLN:O	1:B:213:LEU:N	2.42	0.51
1:B:426:LEU:O	1:B:430:ALA:HB2	2.11	0.50
1:A:45:SER:O	2:A:608:HOH:O	2.18	0.50
1:B:131:THR:HA	1:B:159:LYS:HG2	1.93	0.50
1:A:74:LYS:NZ	2:A:626:HOH:O	2.44	0.50
1:A:546:PHE:HB3	1:A:552:LEU:HD13	1.93	0.50
1:B:356:LYS:NZ	2:B:634:HOH:O	2.44	0.49
1:B:197:HIS:CD2	1:B:214:LEU:HB2	2.47	0.49
1:B:209:ALA:HA	1:B:210:GLN:C	2.33	0.49
1:B:532:ARG:O	1:B:536:GLU:HG2	2.12	0.49
1:B:530:GLU:OE1	2:B:604:HOH:O	2.19	0.49
1:B:197:HIS:HD2	1:B:214:LEU:HB2	1.78	0.48
1:B:244:THR:O	1:B:246:HIS:N	2.36	0.48
1:B:50:ILE:HG12	1:B:280:CYS:HB3	1.94	0.48
1:A:154:LYS:HD2	1:A:157:ARG:HH12	1.78	0.48
1:A:51:THR:HG21	1:A:85:ASN:ND2	2.27	0.47
1:A:210:GLN:HA	1:A:213:LEU:HG	1.95	0.47
1:A:402:SER:O	1:A:406:VAL:HG23	2.15	0.47
1:B:187:VAL:HG12	1:B:191:ARG:HD2	1.96	0.47
1:B:426:LEU:HD22	1:B:430:ALA:HB2	1.97	0.46
1:A:499:ASP:OD1	1:A:499:ASP:N	2.35	0.46
1:A:44:GLU:OE1	1:A:470:SER:OG	2.29	0.46
1:A:48:TYR:O	1:A:51:THR:HG22	2.15	0.46
1:A:134:ASP:HB3	1:A:136:SER:H	1.81	0.46
1:A:230:ALA:O	1:A:234:LYS:HB2	2.15	0.46
1:A:338:ASP:OD1	1:A:338:ASP:N	2.39	0.46
1:A:459:GLN:HA	1:A:462:ILE:HD11	1.98	0.45
1:B:519:SER:HA	1:B:524:LYS:HA	1.98	0.45
1:A:213:LEU:O	1:A:217:PHE:HB2	2.15	0.45
1:B:529:GLU:O	1:B:532:ARG:HG2	2.17	0.45
1:B:514:GLY:CA	1:B:516:LEU:H	2.28	0.45
1:A:131:THR:HA	1:A:159:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LYS:HE3	1:A:536:GLU:HG3	1.99	0.45
1:A:246:HIS:O	1:A:246:HIS:ND1	2.47	0.44
1:A:481:ILE:O	1:A:481:ILE:HG13	2.17	0.44
1:B:53:PRO:HG2	1:B:75:ILE:HD13	1.98	0.44
1:B:63:PHE:HB3	1:B:331:ILE:HD12	2.00	0.44
1:B:75:ILE:HD12	1:B:98:PHE:CE2	2.53	0.44
1:B:373:GLY:HA3	1:B:374:ASN:CB	2.48	0.44
1:A:374:ASN:CG	1:A:375:LYS:H	2.21	0.44
1:B:204:ILE:HB	1:B:250:HIS:HE1	1.82	0.44
1:B:508:LEU:HA	1:B:511:VAL:HG22	1.99	0.44
1:B:457:THR:HG23	1:B:462:ILE:HG13	2.00	0.44
1:B:458:THR:HG22	1:B:553:VAL:HG23	1.99	0.44
1:B:134:ASP:HB3	1:B:136:SER:H	1.83	0.43
1:A:153:PRO:HB2	1:A:155:ILE:HD12	2.00	0.43
1:B:331:ILE:O	1:B:331:ILE:HG13	2.15	0.43
1:A:510:HIS:O	1:A:514:GLY:N	2.52	0.43
1:B:303:ASP:O	1:B:307:THR:OG1	2.37	0.43
1:B:527:ASN:ND2	2:B:639:HOH:O	2.52	0.43
1:A:250:HIS:O	1:A:250:HIS:ND1	2.52	0.43
1:A:531:ILE:HG22	1:A:532:ARG:N	2.34	0.43
1:B:486:PHE:HE1	1:B:535:LEU:HD22	1.83	0.42
1:A:76:LEU:HB2	1:A:140:PHE:CG	2.54	0.42
1:A:50:ILE:HG12	1:A:280:CYS:HB3	2.01	0.42
1:B:316:ASN:HB2	1:A:229:TYR:CE2	2.54	0.42
1:B:184:TRP:CZ3	1:B:188:ARG:HG3	2.55	0.42
1:B:294:VAL:HG11	1:A:221:SER:HB3	2.00	0.42
1:A:69:GLU:O	1:A:73:SER:HB3	2.19	0.42
1:A:385:TYR:HE1	1:A:418:LYS:HG2	1.84	0.42
1:B:210:GLN:HB3	1:B:211:SER:H	1.63	0.42
1:B:426:LEU:O	1:B:430:ALA:CB	2.68	0.42
1:A:219:LYS:HB3	1:A:219:LYS:HE2	1.68	0.42
1:A:486:PHE:CE2	1:A:538:LEU:HB3	2.54	0.42
1:B:316:ASN:HB2	1:A:229:TYR:CD2	2.55	0.42
1:B:481:ILE:O	1:B:481:ILE:HG13	2.18	0.42
1:B:524:LYS:HG2	1:B:525:ILE:N	2.35	0.42
1:A:477:LYS:HB3	1:A:477:LYS:HE2	1.87	0.42
1:B:159:LYS:O	1:B:163:VAL:HG13	2.19	0.42
1:A:514:GLY:CA	1:A:516:LEU:H	2.33	0.42
1:B:411:ASN:ND2	1:B:419:LEU:HB2	2.35	0.41
1:B:229:TYR:CE2	1:A:316:ASN:HB2	2.56	0.41
1:A:252:HIS:HA	1:A:255:GLU:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ILE:HD11	1:B:333:ARG:CZ	2.50	0.41
1:B:426:LEU:HD23	1:B:426:LEU:HA	1.83	0.41
1:A:363:ALA:O	1:A:382:THR:OG1	2.39	0.41
1:A:493:TYR:HB3	1:A:498:ASN:HD22	1.86	0.41
1:A:514:GLY:HA3	1:A:516:LEU:H	1.86	0.41
1:A:105:LYS:HB2	1:A:127:HIS:CE1	2.55	0.41
1:B:409:GLU:OE2	2:B:606:HOH:O	2.22	0.41
1:B:430:ALA:HB3	2:B:626:HOH:O	2.21	0.41
1:B:521:GLU:HG2	1:B:522:GLY:N	2.35	0.41
1:A:249:ARG:O	1:A:250:HIS:HB3	2.21	0.41
1:A:432:LYS:HE2	1:A:436:GLN:NE2	2.36	0.41
1:B:262:PHE:HE2	1:B:305:VAL:HA	1.86	0.40
1:B:389:ILE:HD11	1:B:422:ILE:HG23	2.04	0.40
1:A:344:ASN:ND2	1:A:444:GLN:O	2.46	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	501/554 (90%)	480 (96%)	18 (4%)	3 (1%)	25	47
1	B	509/554 (92%)	497 (98%)	11 (2%)	1 (0%)	47	71
All	All	1010/1108 (91%)	977 (97%)	29 (3%)	4 (0%)	34	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	ASN
1	A	527	ASN
1	B	245	ASP
1	A	289	ASN

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	429/504 (85%)	382 (89%)	47 (11%)	6 11
1	B	443/504 (88%)	396 (89%)	47 (11%)	6 12
All	All	872/1008 (86%)	778 (89%)	94 (11%)	6 12

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	51	THR
1	B	54	TYR
1	B	59	LEU
1	B	76	LEU
1	B	78	LEU
1	B	134	ASP
1	B	148	VAL
1	B	210	GLN
1	B	216	GLU
1	B	227	THR
1	B	240	LEU
1	B	244	THR
1	B	251	ASP
1	B	293	LYS
1	B	297	GLN
1	B	301	VAL
1	B	307	THR
1	B	319	PHE
1	B	324	LEU
1	B	327	ASN
1	B	331	ILE
1	B	340	ILE
1	B	347	PHE
1	B	355	LEU
1	B	364	THR
1	B	371	LEU
1	B	379	LEU

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Mol	Chain	Res	Type
1	B	417	THR
1	B	424	ASN
1	B	426	LEU
1	B	452	LEU
1	B	453	ASP
1	B	461	VAL
1	B	470	SER
1	B	481	ILE
1	B	508	LEU
1	B	513	LYS
1	B	516	LEU
1	B	525	ILE
1	B	526	GLU
1	B	528	LYS
1	B	530	GLU
1	B	534	GLU
1	B	537	SER
1	B	544	GLU
1	B	547	CYS
1	B	552	LEU
1	A	51	THR
1	A	54	TYR
1	A	59	LEU
1	A	76	LEU
1	A	78	LEU
1	A	134	ASP
1	A	148	VAL
1	A	155	ILE
1	A	163	VAL
1	A	166	ARG
1	A	169	SER
1	A	186	MET
1	A	216	GLU
1	A	217	PHE
1	A	224	HIS
1	A	227	THR
1	A	239	LEU
1	A	244	THR
1	A	245	ASP
1	A	293	LYS
1	A	297	GLN
1	A	324	LEU

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Mol	Chain	Res	Type
1	A	340	ILE
1	A	347	PHE
1	A	355	LEU
1	A	364	THR
1	A	377	SER
1	A	378	ASN
1	A	412	THR
1	A	426	LEU
1	A	444	GLN
1	A	448	SER
1	A	458	THR
1	A	461	VAL
1	A	462	ILE
1	A	466	LYS
1	A	481	ILE
1	A	499	ASP
1	A	501	LYS
1	A	516	LEU
1	A	528	LYS
1	A	533	LYS
1	A	538	LEU
1	A	540	THR
1	A	544	GLU
1	A	547	CYS
1	A	552	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
1	A	478	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	505/554 (91%)	-0.01	15 (2%)	50	43	23, 45, 87, 124	0
1	B	511/554 (92%)	-0.14	6 (1%)	79	76	17, 38, 76, 91	0
All	All	1016/1108 (91%)	-0.07	21 (2%)	63	58	17, 41, 82, 124	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	523	GLN	8.5
1	A	522	GLY	4.8
1	B	373	GLY	4.2
1	A	525	ILE	3.7
1	A	527	ASN	3.4
1	A	519	SER	3.4
1	B	43	TYR	3.3
1	A	300	ALA	3.1
1	A	520	ARG	2.7
1	A	244	THR	2.5
1	B	221	SER	2.4
1	A	210	GLN	2.4
1	B	520	ARG	2.3
1	A	289	ASN	2.3
1	A	250	HIS	2.3
1	A	553	VAL	2.2
1	A	521	GLU	2.2
1	A	288	GLY	2.2
1	B	208	ILE	2.1
1	B	218	VAL	2.1
1	A	529	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.