



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2016 – 04:45 PM EDT

PDB ID : 5DOO
Title : The structure of PKMT2 from Rickettsia typhi
Authors : Noinaj, N.; Abeykoon, A.; He, Y.; Yang, D.C.; Buchanan, S.K.
Deposited on : 2015-09-11
Resolution : 3.13 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

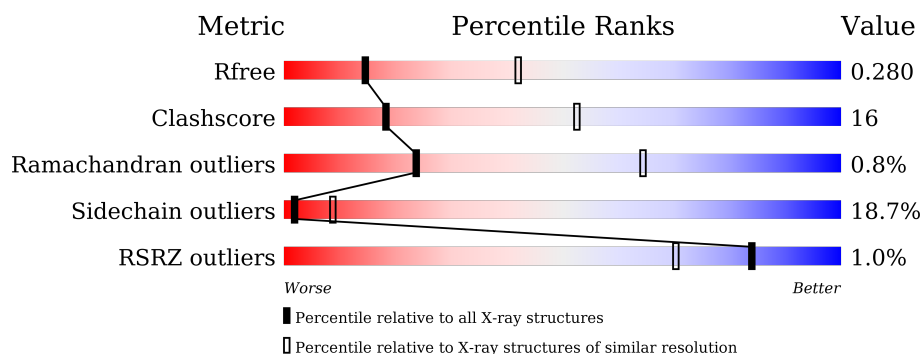
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	535	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>34%</div> <div>7%</div> <div>5%</div> </div> </div>
1	B	535	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>34%</div> <div>9%</div> <div>.</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8167 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4072	2638	660	760	14			
1	B	513	Total	C	N	O	S	0	0	0
			4093	2652	666	760	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q68XQ5
B	0	GLY	-	expression tag	UNP Q68XQ5

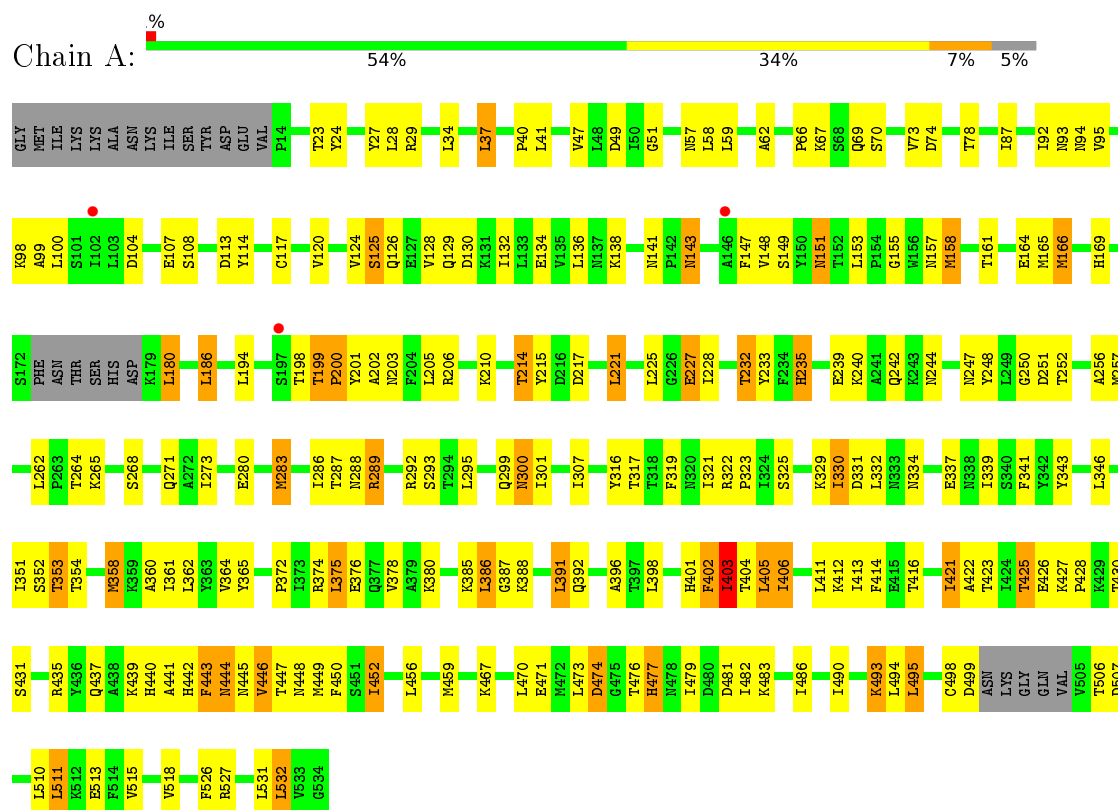
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

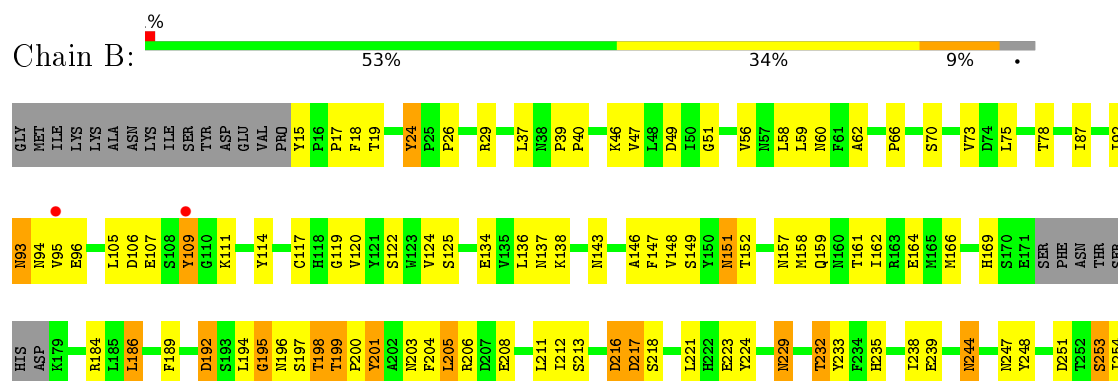
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: protein lysine methyltransferase 2



- Molecule 1: protein lysine methyltransferase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.72Å 90.53Å 106.20Å 90.00° 114.17° 90.00°	Depositor
Resolution (Å)	48.45 – 3.13 48.45 – 3.13	Depositor EDS
% Data completeness (in resolution range)	96.4 (48.45-3.13) 96.2 (48.45-3.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.280 0.231 , 0.280	Depositor DCC
R_{free} test set	1243 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8167	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: CA

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	0.31	0/4162	0.55	2/5646 (0.0%)
1	B	0.31	0/4184	0.56	0/5675
All	All	0.31	0/8346	0.55	2/11321 (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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	200	PRO	C-N-CA	8.58	143.15	121.70
1	A	386	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	GLU	Peptide
1	B	195	GLY	Peptide
1	B	507	ASP	Peptide

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	4072	0	4044	123	0
1	B	4093	0	4066	133	0
2	A	2	0	0	0	0
All	All	8167	0	8110	254	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 (254) 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:452:ILE:O	1:A:459:MET:HA	1.64	0.96
1:A:227:GLU:HB3	1:A:228:ILE:HA	1.61	0.83
1:A:217:ASP:O	1:A:221:LEU:HB2	1.78	0.82
1:A:435:ARG:NH1	1:A:473:LEU:O	2.15	0.80
1:B:396:ALA:O	1:B:400:GLN:HB2	1.81	0.80
1:B:137:ASN:ND2	1:B:244:ASN:O	2.18	0.76
1:B:271:GLN:OE1	1:B:305:ARG:NH2	2.19	0.76
1:B:474:ASP:N	1:B:474:ASP:OD1	2.18	0.75
1:B:184:ARG:NH2	1:B:213:SER:O	2.20	0.75
1:A:199:THR:OG1	1:A:203:ASN:ND2	2.18	0.75
1:A:194:LEU:HD22	1:A:202:ALA:HB1	1.69	0.74
1:B:194:LEU:HD11	1:B:205:LEU:HD13	1.71	0.73
1:B:442:HIS:HE1	1:B:451:SER:HB2	1.55	0.72
1:A:256:ALA:HB1	1:A:289:ARG:HH12	1.56	0.71
1:B:93:ASN:N	1:B:93:ASN:OD1	2.24	0.71
1:A:194:LEU:HD21	1:B:286:ILE:HG22	1.73	0.70
1:B:406:ILE:HG22	1:B:411:LEU:HB3	1.72	0.70
1:A:180:LEU:HD12	1:A:221:LEU:HG	1.75	0.69
1:A:300:ASN:N	1:A:300:ASN:OD1	2.25	0.69
1:A:446:VAL:N	1:A:447:THR:HA	2.09	0.68
1:A:428:PRO:HB2	1:A:473:LEU:HD22	1.76	0.68
1:A:493:LYS:HA	1:A:494:LEU:HB2	1.74	0.68
1:A:49:ASP:HB2	1:A:58:LEU:HD21	1.75	0.68
1:B:235:HIS:O	1:B:239:GLU:HB2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:HB3	1:A:240:LYS:HE2	1.76	0.67
1:B:159:GLN:HE22	1:B:212:ILE:HD11	1.60	0.67
1:A:143:ASN:N	1:A:143:ASN:OD1	2.28	0.67
1:A:29:ARG:NH1	1:A:40:PRO:O	2.28	0.66
1:B:380:LYS:HG2	1:B:391:LEU:HD11	1.78	0.66
1:B:229:ASN:HD22	1:B:229:ASN:H	1.44	0.65
1:B:300:ASN:OD1	1:B:300:ASN:N	2.27	0.64
1:B:442:HIS:CE1	1:B:451:SER:HB2	2.32	0.63
1:B:283:MET:O	1:B:287:THR:OG1	2.17	0.62
1:B:435:ARG:NH1	1:B:473:LEU:O	2.31	0.62
1:A:59:LEU:HD22	1:A:92:ILE:HD12	1.81	0.62
1:B:280:GLU:OE1	1:B:292:ARG:NH1	2.30	0.62
1:A:364:VAL:HG12	1:A:385:LYS:HE3	1.82	0.62
1:B:169:HIS:HB2	1:B:186:LEU:HD23	1.81	0.62
1:B:499:ASP:HB3	1:B:504:VAL:HG21	1.81	0.62
1:A:403:ILE:O	1:A:404:THR:HG22	1.99	0.61
1:A:40:PRO:HG2	1:A:113:ASP:HB3	1.81	0.61
1:A:398:LEU:HA	1:A:402:PHE:HB2	1.81	0.61
1:B:199:THR:OG1	1:B:199:THR:O	2.16	0.61
1:B:317:THR:HG21	1:B:375:LEU:HD13	1.80	0.61
1:B:152:THR:OG1	1:B:289:ARG:O	2.19	0.60
1:B:275:ASP:O	1:B:279:THR:OG1	2.20	0.60
1:A:445:ASN:C	1:A:447:THR:HA	2.22	0.60
1:B:62:ALA:HB1	1:B:94:ASN:HB2	1.83	0.59
1:B:49:ASP:HB2	1:B:58:LEU:HD21	1.84	0.59
1:B:238:ILE:HD12	1:B:248:TYR:HB2	1.85	0.59
1:A:232:THR:OG1	1:A:233:TYR:N	2.36	0.59
1:B:47:VAL:HG12	1:B:114:TYR:HB2	1.85	0.58
1:B:151:ASN:OD1	1:B:151:ASN:N	2.36	0.58
1:B:195:GLY:O	1:B:197:SER:N	2.35	0.58
1:A:117:CYS:O	1:A:148:VAL:HA	2.04	0.58
1:B:493:LYS:HA	1:B:494:LEU:HB2	1.85	0.58
1:A:392:GLN:O	1:A:396:ALA:HB2	2.04	0.57
1:A:479:ILE:HG12	1:A:483:LYS:HE3	1.85	0.57
1:A:227:GLU:HB3	1:A:228:ILE:CA	2.33	0.57
1:B:29:ARG:NH1	1:B:40:PRO:O	2.37	0.57
1:B:392:GLN:HA	1:B:395:LEU:HG	1.85	0.57
1:A:283:MET:O	1:A:287:THR:OG1	2.18	0.57
1:B:17:PRO:O	1:B:18:PHE:HD1	1.87	0.57
1:A:27:TYR:HE2	1:A:252:THR:HB	1.68	0.57
1:B:322:ARG:HB2	1:B:342:TYR:HD2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LYS:O	1:A:244:ASN:ND2	2.37	0.56
1:B:328:ASN:N	1:B:328:ASN:OD1	2.27	0.56
1:B:507:ASP:HB3	1:B:508:PRO:HD3	1.87	0.56
1:B:147:PHE:CE1	1:B:293:SER:HB2	2.40	0.56
1:B:339:ILE:HD11	1:B:359:LYS:HG2	1.87	0.56
1:B:260:GLY:HA2	1:B:262:LEU:N	2.20	0.55
1:B:353:THR:HB	1:B:355:SER:N	2.22	0.55
1:A:27:TYR:OH	1:A:252:THR:O	2.20	0.55
1:B:487:ILE:HG12	1:B:515:VAL:HG21	1.88	0.55
1:A:448:ASN:HB3	1:A:449:MET:HE2	1.88	0.54
1:B:490:ILE:HD12	1:B:497:ALA:HB2	1.88	0.54
1:A:316:TYR:HB2	1:A:414:PHE:HB2	1.90	0.54
1:A:100:LEU:HD22	1:A:104:ASP:HB2	1.90	0.54
1:A:161:THR:O	1:A:165:MET:N	2.38	0.54
1:B:274:ASN:OD1	1:B:305:ARG:NH1	2.40	0.54
1:B:428:PRO:HB2	1:B:473:LEU:HD22	1.89	0.54
1:B:333:ASN:OD1	1:B:333:ASN:N	2.41	0.54
1:A:353:THR:HG22	1:A:354:THR:HB	1.89	0.53
1:A:421:ILE:HG23	1:A:423:THR:H	1.73	0.53
1:B:262:LEU:HD13	1:B:267:ALA:HB2	1.89	0.53
1:A:486:ILE:O	1:A:490:ILE:HG12	2.07	0.53
1:A:490:ILE:HD13	1:A:495:LEU:HB3	1.89	0.53
1:A:199:THR:O	1:A:199:THR:OG1	2.22	0.53
1:B:372:PRO:HG2	1:B:418:PRO:HD2	1.90	0.53
1:B:409:GLY:O	1:B:412:LYS:NZ	2.42	0.53
1:A:169:HIS:CD2	1:A:186:LEU:HD23	2.44	0.52
1:B:56:VAL:HA	1:B:59:LEU:HG	1.92	0.52
1:A:158:MET:O	1:A:161:THR:OG1	2.16	0.52
1:A:380:LYS:HG2	1:A:391:LEU:HD11	1.92	0.52
1:B:208:GLU:O	1:B:212:ILE:HG12	2.10	0.52
1:B:201:TYR:O	1:B:204:PHE:N	2.27	0.52
1:A:387:GLY:O	1:A:388:LYS:HD2	2.10	0.51
1:A:157:ASN:O	1:A:161:THR:HG23	2.10	0.51
1:A:28:LEU:HD22	1:A:295:LEU:HD21	1.91	0.51
1:B:313:LYS:HA	1:B:375:LEU:HB3	1.90	0.51
1:A:247:ASN:HB2	1:A:299:GLN:HB3	1.93	0.51
1:B:482:ILE:O	1:B:486:ILE:HG12	2.09	0.51
1:A:317:THR:HG21	1:A:375:LEU:HD22	1.92	0.51
1:B:316:TYR:O	1:B:413:ILE:HA	2.10	0.51
1:A:430:THR:HG21	1:A:470:LEU:HD11	1.93	0.50
1:B:73:VAL:HG21	1:B:105:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:THR:OG1	1:B:233:TYR:N	2.44	0.50
1:A:450:PHE:CE2	1:A:467:LYS:HD3	2.45	0.50
1:A:74:ASP:O	1:A:99:ALA:HA	2.11	0.50
1:A:280:GLU:OE1	1:A:292:ARG:NH2	2.31	0.50
1:A:62:ALA:O	1:A:94:ASN:ND2	2.41	0.50
1:B:147:PHE:HE1	1:B:293:SER:HB2	1.75	0.50
1:B:87:ILE:HG23	1:B:92:ILE:HB	1.94	0.50
1:A:403:ILE:HG22	1:A:404:THR:H	1.77	0.49
1:A:271:GLN:O	1:A:271:GLN:NE2	2.32	0.49
1:A:403:ILE:C	1:A:405:LEU:H	2.15	0.49
1:B:444:ASN:ND2	1:B:445:ASN:O	2.42	0.49
1:B:401:HIS:N	1:B:401:HIS:ND1	2.60	0.49
1:A:51:GLY:HA3	1:A:120:VAL:HG11	1.93	0.49
1:B:17:PRO:HD2	1:B:442:HIS:HD2	1.78	0.49
1:A:316:TYR:HB3	1:A:372:PRO:HB2	1.95	0.49
1:B:124:VAL:HG12	1:B:125:SER:H	1.78	0.49
1:A:206:ARG:O	1:A:210:LYS:HB2	2.13	0.48
1:A:467:LYS:O	1:A:471:GLU:HG3	2.13	0.48
1:B:157:ASN:O	1:B:161:THR:HG22	2.13	0.48
1:A:107:GLU:HG2	1:A:108:SER:H	1.79	0.48
1:B:314:ASP:O	1:B:374:ARG:NH1	2.46	0.48
1:A:422:ALA:O	1:A:527:ARG:NH1	2.34	0.48
1:B:24:TYR:CG	1:B:26:PRO:HD2	2.49	0.48
1:B:480:ASP:O	1:B:484:LYS:HB2	2.13	0.48
1:A:194:LEU:HD22	1:A:202:ALA:CB	2.42	0.48
1:A:339:ILE:O	1:A:352:SER:HA	2.14	0.47
1:A:343:TYR:O	1:A:346:LEU:HB2	2.14	0.47
1:A:59:LEU:HD21	1:A:87:ILE:HG12	1.95	0.47
1:B:375:LEU:HG	1:B:398:LEU:HD23	1.97	0.47
1:A:490:ILE:HG21	1:A:511:LEU:HD11	1.96	0.47
1:B:217:ASP:OD1	1:B:217:ASP:N	2.46	0.47
1:A:443:PHE:HD1	1:A:444:ASN:N	2.12	0.47
1:B:515:VAL:HA	1:B:518:VAL:HG22	1.96	0.47
1:A:428:PRO:O	1:A:473:LEU:HB3	2.14	0.47
1:B:326:PRO:O	1:B:330:ILE:HG22	2.15	0.47
1:A:147:PHE:CE2	1:A:252:THR:HG21	2.49	0.47
1:B:166:MET:HE1	1:B:224:TYR:HB3	1.97	0.47
1:B:435:ARG:NH1	1:B:474:ASP:HA	2.30	0.47
1:B:324:ILE:HD13	1:B:340:SER:H	1.79	0.47
1:A:334:ASN:OD1	1:A:337:GLU:N	2.47	0.47
1:B:486:ILE:O	1:B:490:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:HIS:CG	1:A:186:LEU:HD23	2.50	0.47
1:A:449:MET:HE3	1:A:449:MET:HB2	1.85	0.47
1:B:415:GLU:HA	1:B:416:THR:HA	1.75	0.47
1:A:235:HIS:C	1:A:235:HIS:CD2	2.88	0.46
1:A:317:THR:HA	1:A:412:LYS:O	2.15	0.46
1:B:51:GLY:HA3	1:B:120:VAL:HG11	1.97	0.46
1:B:322:ARG:HB2	1:B:342:TYR:HB2	1.95	0.46
1:B:353:THR:HB	1:B:354:THR:C	2.36	0.46
1:B:372:PRO:O	1:B:417:LYS:HE2	2.16	0.46
1:B:348:GLU:HA	1:B:349:PRO:HD3	1.80	0.46
1:B:506:THR:O	1:B:511:LEU:HG	2.16	0.46
1:A:23:THR:OG1	1:A:57:ASN:ND2	2.47	0.45
1:B:229:ASN:ND2	1:B:229:ASN:H	2.09	0.45
1:B:269:LYS:HE2	1:B:269:LYS:HB2	1.79	0.45
1:B:324:ILE:HD11	1:B:339:ILE:HG22	1.98	0.45
1:B:216:ASP:OD1	1:B:216:ASP:N	2.50	0.45
1:A:374:ARG:O	1:A:378:VAL:HG23	2.16	0.45
1:A:425:THR:C	1:A:427:LYS:H	2.19	0.45
1:B:17:PRO:C	1:B:18:PHE:HD1	2.19	0.45
1:A:515:VAL:HA	1:A:518:VAL:HG22	1.97	0.45
1:B:259:ILE:HD13	1:B:259:ILE:H	1.81	0.45
1:B:517:TYR:O	1:B:521:VAL:HG23	2.17	0.45
1:B:259:ILE:O	1:B:259:ILE:HG12	2.16	0.45
1:B:338:ASN:HA	1:B:353:THR:O	2.16	0.45
1:A:34:LEU:HD13	1:A:413:ILE:HD13	1.98	0.45
1:B:313:LYS:HB2	1:B:376:GLU:HB3	1.99	0.45
1:A:124:VAL:HG22	1:A:125:SER:H	1.81	0.45
1:A:147:PHE:HE2	1:A:252:THR:HG21	1.82	0.45
1:B:119:GLY:H	1:B:149:SER:HB2	1.82	0.45
1:B:339:ILE:HD11	1:B:359:LYS:HE2	1.99	0.45
1:A:73:VAL:HA	1:A:98:LYS:O	2.18	0.44
1:B:316:TYR:HA	1:B:374:ARG:HA	1.98	0.44
1:B:463:PRO:HD2	1:B:466:GLU:OE1	2.16	0.44
1:B:275:ASP:OD2	1:B:277:VAL:N	2.50	0.44
1:A:403:ILE:HA	1:A:406:ILE:HG23	2.00	0.44
1:B:260:GLY:HA2	1:B:261:ASN:C	2.38	0.44
1:B:136:LEU:HD23	1:B:146:ALA:HB1	2.00	0.44
1:A:165:MET:HG3	1:B:285:PHE:CD2	2.52	0.44
1:A:493:LYS:HB3	1:A:495:LEU:O	2.18	0.44
1:A:330:ILE:HD12	1:A:339:ILE:HD13	2.00	0.44
1:A:474:ASP:OD1	1:A:476:THR:OG1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:HA	1:A:94:ASN:HD21	1.83	0.43
1:B:361:ILE:HG21	1:B:402:PHE:CE2	2.52	0.43
1:A:227:GLU:CB	1:A:228:ILE:HA	2.37	0.43
1:A:361:ILE:HG21	1:A:398:LEU:HD11	1.99	0.43
1:A:430:THR:HG23	1:A:531:LEU:O	2.18	0.43
1:B:146:ALA:O	1:B:295:LEU:HA	2.19	0.43
1:B:508:PRO:C	1:B:510:LEU:H	2.22	0.43
1:A:442:HIS:O	1:A:450:PHE:HA	2.19	0.43
1:A:421:ILE:HA	1:A:421:ILE:HD13	1.87	0.43
1:B:189:PHE:HA	1:B:192:ASP:OD1	2.19	0.43
1:B:253:SER:HB2	1:B:256:ALA:HB2	2.00	0.43
1:B:443:PHE:HD2	1:B:450:PHE:CZ	2.37	0.43
1:A:153:LEU:N	1:A:232:THR:O	2.34	0.43
1:A:256:ALA:HB1	1:A:289:ARG:NH1	2.28	0.43
1:A:47:VAL:HA	1:A:114:TYR:O	2.18	0.43
1:B:532:LEU:HA	1:B:532:LEU:HD12	1.84	0.43
1:A:128:VAL:O	1:A:132:ILE:HG13	2.18	0.42
1:A:323:PRO:HA	1:A:341:PHE:CD1	2.54	0.42
1:A:474:ASP:OD1	1:A:474:ASP:N	2.47	0.42
1:B:29:ARG:HG3	1:B:39:PRO:HB2	2.00	0.42
1:B:437:GLN:O	1:B:441:ALA:HB2	2.18	0.42
1:B:235:HIS:O	1:B:239:GLU:CB	2.63	0.42
1:B:303:ILE:H	1:B:303:ILE:HD13	1.85	0.42
1:B:60:ASN:ND2	1:B:454:ASN:O	2.53	0.42
1:A:166:MET:H	1:A:166:MET:HG2	1.67	0.42
1:B:105:LEU:HA	1:B:109:TYR:OH	2.18	0.42
1:B:203:ASN:OD1	1:B:206:ARG:NH1	2.44	0.42
1:B:106:ASP:OD1	1:B:107:GLU:N	2.37	0.42
1:B:343:TYR:C	1:B:345:ASN:H	2.23	0.42
1:B:348:GLU:HG3	1:B:348:GLU:O	2.20	0.42
1:B:507:ASP:HB3	1:B:508:PRO:CD	2.50	0.42
1:A:62:ALA:HB1	1:A:94:ASN:HB2	2.02	0.42
1:B:364:VAL:O	1:B:368:ASN:ND2	2.32	0.42
1:A:134:GLU:HG2	1:A:138:LYS:HE2	2.02	0.42
1:A:358:MET:HA	1:A:361:ILE:HD12	2.01	0.42
1:B:284:ASP:CG	1:B:292:ARG:HH21	2.22	0.42
1:A:286:ILE:HG13	1:A:286:ILE:H	1.67	0.42
1:B:340:SER:HB3	1:B:349:PRO:HG2	2.02	0.42
1:A:330:ILE:HG12	1:A:331:ASP:N	2.34	0.41
1:B:398:LEU:HA	1:B:402:PHE:CD2	2.54	0.41
1:B:17:PRO:HD2	1:B:442:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:PRO:O	1:B:94:ASN:ND2	2.53	0.41
1:B:357:ILE:HG13	1:B:394:PHE:CE2	2.55	0.41
1:B:46:LYS:HE2	1:B:46:LYS:HB3	1.87	0.41
1:A:362:LEU:HA	1:A:362:LEU:HD23	1.89	0.41
1:B:158:MET:O	1:B:162:ILE:HG13	2.20	0.41
1:B:398:LEU:HG	1:B:402:PHE:CD2	2.55	0.41
1:A:58:LEU:HD22	1:A:70:SER:HB3	2.02	0.41
1:A:321:ILE:HG23	1:A:341:PHE:HB3	2.03	0.41
1:A:437:GLN:O	1:A:441:ALA:N	2.53	0.41
1:A:477:HIS:HB3	1:A:481:ASP:HB2	2.03	0.41
1:A:235:HIS:O	1:A:239:GLU:HB3	2.21	0.41
1:A:248:TYR:CZ	1:A:250:GLY:HA2	2.55	0.41
1:B:305:ARG:HG2	1:B:305:ARG:O	2.21	0.41
1:B:490:ILE:HA	1:B:495:LEU:O	2.21	0.41
1:A:360:ALA:O	1:A:364:VAL:HG13	2.21	0.41
1:A:482:ILE:O	1:A:486:ILE:HG12	2.21	0.41
1:B:117:CYS:O	1:B:148:VAL:HA	2.21	0.40
1:A:214:THR:HB	1:A:215:TYR:H	1.78	0.40
1:A:155:GLY:HA2	1:A:288:ASN:ND2	2.36	0.40
1:A:37:LEU:HG	1:A:301:ILE:HG21	2.03	0.40
1:A:126:GLN:OE1	1:A:129:GLN:NE2	2.54	0.40
1:A:151:ASN:OD1	1:A:151:ASN:N	2.55	0.40
1:A:526:PHE:HB3	1:A:532:LEU:HD13	2.02	0.40
1:B:134:GLU:O	1:B:138:LYS:HG3	2.20	0.40
1:A:41:LEU:HA	1:A:41:LEU:HD23	1.93	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	504/535 (94%)	455 (90%)	47 (9%)	2 (0%)	39 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	509/535 (95%)	458 (90%)	45 (9%)	6 (1%)	16	53
All	All	1013/1070 (95%)	913 (90%)	92 (9%)	8 (1%)	24	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	505	VAL
1	B	446	VAL
1	B	196	ASN
1	B	198	THR
1	B	200	PRO
1	B	415	GLU
1	A	200	PRO
1	A	403	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	447/484 (92%)	363 (81%)	84 (19%)	2	9
1	B	447/484 (92%)	364 (81%)	83 (19%)	2	9
All	All	894/968 (92%)	727 (81%)	167 (19%)	2	9

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TYR
1	A	37	LEU
1	A	67	LYS
1	A	69	GLN
1	A	78	THR
1	A	93	ASN
1	A	95	VAL
1	A	125	SER

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Mol	Chain	Res	Type
1	A	136	LEU
1	A	141	ASN
1	A	143	ASN
1	A	149	SER
1	A	151	ASN
1	A	158	MET
1	A	164	GLU
1	A	166	MET
1	A	180	LEU
1	A	186	LEU
1	A	198	THR
1	A	199	THR
1	A	201	TYR
1	A	205	LEU
1	A	214	THR
1	A	221	LEU
1	A	225	LEU
1	A	232	THR
1	A	235	HIS
1	A	242	GLN
1	A	251	ASP
1	A	257	MET
1	A	262	LEU
1	A	264	THR
1	A	265	LYS
1	A	268	SER
1	A	273	ILE
1	A	283	MET
1	A	289	ARG
1	A	293	SER
1	A	300	ASN
1	A	307	ILE
1	A	319	PHE
1	A	322	ARG
1	A	325	SER
1	A	329	LYS
1	A	330	ILE
1	A	332	LEU
1	A	351	ILE
1	A	353	THR
1	A	358	MET
1	A	365	TYR

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Mol	Chain	Res	Type
1	A	375	LEU
1	A	376	GLU
1	A	386	LEU
1	A	391	LEU
1	A	401	HIS
1	A	402	PHE
1	A	403	ILE
1	A	405	LEU
1	A	406	ILE
1	A	411	LEU
1	A	416	THR
1	A	421	ILE
1	A	425	THR
1	A	426	GLU
1	A	431	SER
1	A	439	LYS
1	A	440	HIS
1	A	443	PHE
1	A	444	ASN
1	A	446	VAL
1	A	452	ILE
1	A	456	LEU
1	A	474	ASP
1	A	477	HIS
1	A	493	LYS
1	A	495	LEU
1	A	498	CYS
1	A	499	ASP
1	A	506	THR
1	A	507	ASP
1	A	510	LEU
1	A	511	LEU
1	A	513	GLU
1	A	532	LEU
1	B	15	TYR
1	B	19	THR
1	B	24	TYR
1	B	37	LEU
1	B	70	SER
1	B	75	LEU
1	B	78	THR
1	B	93	ASN

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Mol	Chain	Res	Type
1	B	95	VAL
1	B	96	GLU
1	B	109	TYR
1	B	111	LYS
1	B	122	SER
1	B	143	ASN
1	B	151	ASN
1	B	164	GLU
1	B	186	LEU
1	B	192	ASP
1	B	198	THR
1	B	199	THR
1	B	201	TYR
1	B	205	LEU
1	B	211	LEU
1	B	216	ASP
1	B	217	ASP
1	B	218	SER
1	B	221	LEU
1	B	223	GLU
1	B	229	ASN
1	B	232	THR
1	B	244	ASN
1	B	247	ASN
1	B	251	ASP
1	B	253	SER
1	B	254	ILE
1	B	257	MET
1	B	259	ILE
1	B	262	LEU
1	B	264	THR
1	B	265	LYS
1	B	279	THR
1	B	286	ILE
1	B	292	ARG
1	B	300	ASN
1	B	303	ILE
1	B	306	LYS
1	B	310	ASP
1	B	319	PHE
1	B	321	ILE
1	B	328	ASN

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Mol	Chain	Res	Type
1	B	331	ASP
1	B	332	LEU
1	B	333	ASN
1	B	339	ILE
1	B	346	LEU
1	B	348	GLU
1	B	350	PHE
1	B	353	THR
1	B	391	LEU
1	B	400	GLN
1	B	401	HIS
1	B	402	PHE
1	B	405	LEU
1	B	411	LEU
1	B	416	THR
1	B	425	THR
1	B	442	HIS
1	B	446	VAL
1	B	456	LEU
1	B	467	LYS
1	B	470	LEU
1	B	474	ASP
1	B	485	SER
1	B	493	LYS
1	B	494	LEU
1	B	495	LEU
1	B	506	THR
1	B	508	PRO
1	B	509	LYS
1	B	510	LEU
1	B	511	LEU
1	B	513	GLU
1	B	532	LEU

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

Mol	Chain	Res	Type
1	A	129	GLN
1	B	196	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	510/535 (95%)	-0.05	3 (0%) 90 81	35, 70, 113, 176	0
1	B	513/535 (95%)	0.02	7 (1%) 78 61	41, 79, 133, 185	0
All	All	1023/1070 (95%)	-0.01	10 (0%) 84 70	35, 74, 126, 185	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	SER	3.4
1	B	331	ASP	2.9
1	B	534	GLY	2.8
1	B	109	TYR	2.6
1	B	446	VAL	2.5
1	A	146	ALA	2.4
1	B	470	LEU	2.4
1	B	402	PHE	2.2
1	B	95	VAL	2.0
1	A	102	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	A	602	1/1	0.96	0.12	-1.92	87,87,87,87	0
2	CA	A	601	1/1	0.92	0.21	-	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.