



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:22 PM UTC

PDB ID : 5B2K / pdb_00005b2k
Title : A crucial role of Cys218 in the stabilization of an unprecedented auto-inhibition form of MAP2K7
Authors : Sogabe, Y.; Hashimoto, T.; Matsumoto, T.; Kirii, Y.; Sawa, M.; Kinoshita, T.
Deposited on : 2016-01-19
Resolution : 2.75 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
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

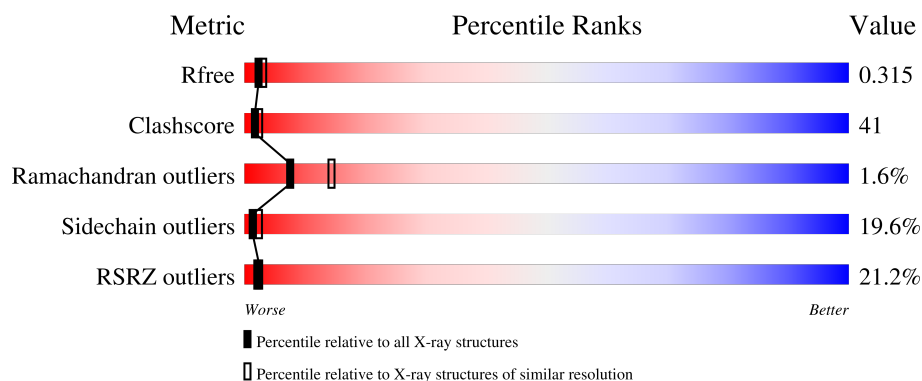
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	324	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2118 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 Dual specificity mitogen-activated protein kinase kinase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2106	1347	363	377	19	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	MET	-	initiating methionine	UNP O14733
A	436	HIS	-	expression tag	UNP O14733
A	437	HIS	-	expression tag	UNP O14733
A	438	HIS	-	expression tag	UNP O14733
A	439	HIS	-	expression tag	UNP O14733
A	440	HIS	-	expression tag	UNP O14733
A	441	HIS	-	expression tag	UNP O14733

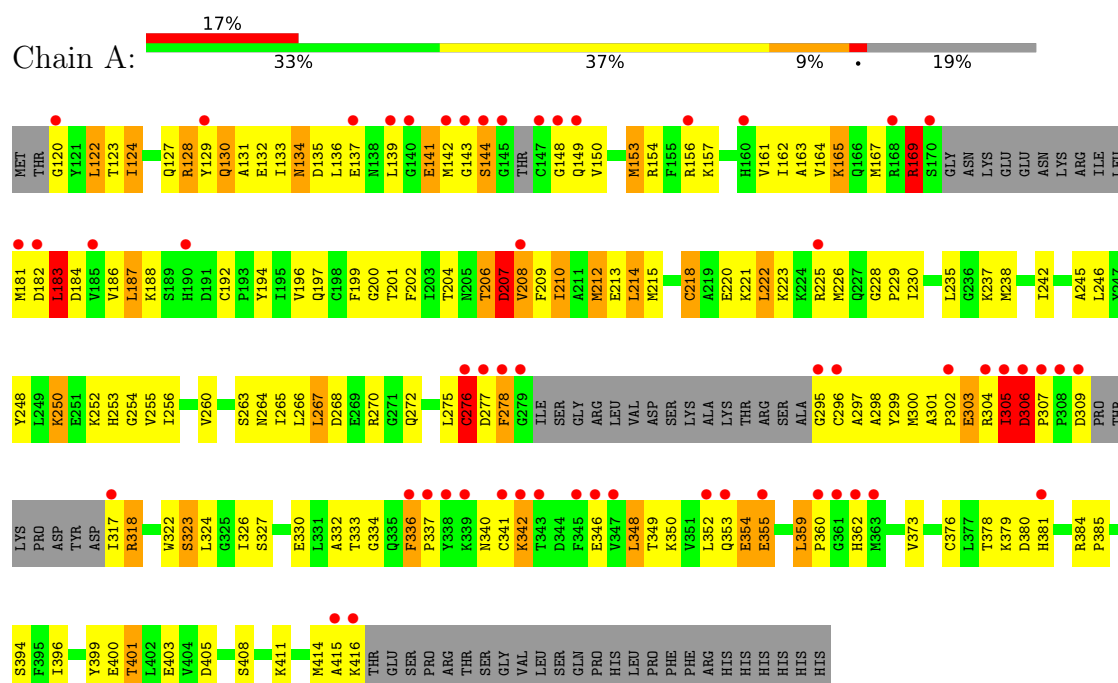
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		

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: Dual specificity mitogen-activated protein kinase kinase 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	71.39Å 71.39Å 262.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.96 – 2.75 44.96 – 2.75	Depositor EDS
% Data completeness (in resolution range)	88.4 (44.96-2.75) 88.4 (44.96-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.270 , 0.328 0.264 , 0.315	Depositor DCC
R_{free} test set	460 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	2118	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 4.11% 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

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	0.94	1/2147 (0.0%)	1.21	16/2882 (0.6%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	ASP	C-N	5.02	1.39	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	ARG	N-CA-C	-14.34	95.11	112.89
1	A	183	LEU	N-CA-C	-10.38	100.56	113.02
1	A	207	ASP	CA-C-N	6.42	133.26	121.70
1	A	207	ASP	C-N-CA	6.42	133.26	121.70
1	A	401	THR	N-CA-C	6.12	117.95	111.28
1	A	336	PHE	CA-C-N	6.05	127.41	119.84
1	A	336	PHE	C-N-CA	6.05	127.41	119.84
1	A	306	ASP	CA-C-N	-5.79	114.42	120.38
1	A	306	ASP	C-N-CA	-5.79	114.42	120.38
1	A	218	CYS	N-CA-CB	-5.70	102.57	110.38
1	A	276	CYS	CA-C-N	5.50	132.87	123.03
1	A	276	CYS	C-N-CA	5.50	132.87	123.03
1	A	400	GLU	CA-C-N	5.36	127.46	120.28
1	A	400	GLU	C-N-CA	5.36	127.46	120.28
1	A	169	ARG	N-CA-C	5.20	118.41	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASN	N-CA-C	5.02	119.13	113.15

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	CYS	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	2106	0	2133	173	0
2	A	12	0	0	0	0
All	All	2118	0	2133	173	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 41.

All (173) 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:298:ALA:CB	1:A:336:PHE:HZ	1.42	1.32
1:A:298:ALA:CB	1:A:336:PHE:CZ	2.31	1.12
1:A:306:ASP:HB3	1:A:307:PRO:HD3	1.26	1.08
1:A:298:ALA:HB3	1:A:336:PHE:HZ	1.18	1.07
1:A:218:CYS:SG	1:A:263:SER:HA	1.94	1.07
1:A:207:ASP:HA	1:A:208:VAL:HG12	1.31	1.06
1:A:153:MET:HG3	1:A:164:VAL:CG2	1.87	1.04
1:A:405:ASP:OD2	1:A:408:SER:HB2	1.58	1.03
1:A:153:MET:HG3	1:A:164:VAL:HG23	1.47	0.96
1:A:306:ASP:HB3	1:A:307:PRO:CD	1.96	0.95
1:A:298:ALA:HB3	1:A:336:PHE:CZ	2.00	0.94
1:A:300:MET:HE3	1:A:305:ILE:HG12	1.52	0.91
1:A:123:THR:HG22	1:A:128:ARG:HB2	1.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLY:HA3	1:A:150:VAL:N	1.88	0.88
1:A:187:LEU:HD11	1:A:200:GLY:HA2	1.57	0.87
1:A:416:LYS:HE2	1:A:416:LYS:HA	1.57	0.86
1:A:297:ALA:O	1:A:300:MET:HB2	1.75	0.85
1:A:300:MET:CE	1:A:305:ILE:HG12	2.06	0.85
1:A:148:GLY:HA3	1:A:149:GLN:C	1.97	0.83
1:A:207:ASP:CA	1:A:208:VAL:HG12	2.09	0.82
1:A:342:LYS:HB2	1:A:346:GLU:HG3	1.60	0.82
1:A:299:TYR:OH	1:A:330:GLU:OE1	1.97	0.81
1:A:144:SER:CB	1:A:221:LYS:HG3	2.11	0.80
1:A:153:MET:HG3	1:A:164:VAL:HG21	1.61	0.79
1:A:167:MET:O	1:A:208:VAL:CG1	2.30	0.79
1:A:415:ALA:O	1:A:416:LYS:HG2	1.81	0.79
1:A:197:GLN:HG2	1:A:213:GLU:OE2	1.83	0.79
1:A:201:THR:O	1:A:202:PHE:HD1	1.65	0.79
1:A:354:GLU:O	1:A:379:LYS:NZ	2.17	0.78
1:A:384:ARG:HG3	1:A:385:PRO:HD2	1.66	0.78
1:A:183:LEU:HD21	1:A:201:THR:HG21	1.65	0.76
1:A:322:TRP:HE3	1:A:384:ARG:NH1	1.83	0.76
1:A:336:PHE:CD1	1:A:337:PRO:HD2	2.20	0.76
1:A:300:MET:HE1	1:A:304:ARG:O	1.85	0.76
1:A:144:SER:HB3	1:A:221:LYS:HG3	1.66	0.74
1:A:148:GLY:CA	1:A:149:GLN:C	2.57	0.74
1:A:127:GLN:HB3	1:A:129:TYR:CZ	2.22	0.74
1:A:303:GLU:OE2	1:A:384:ARG:NH2	2.20	0.74
1:A:137:GLU:OE2	1:A:139:LEU:HD11	1.88	0.73
1:A:142:MET:HB3	1:A:143:GLY:CA	2.18	0.73
1:A:342:LYS:HB2	1:A:346:GLU:CG	2.19	0.73
1:A:305:ILE:HD13	1:A:348:LEU:HD11	1.70	0.72
1:A:298:ALA:HB2	1:A:336:PHE:CZ	2.25	0.72
1:A:148:GLY:HA2	1:A:150:VAL:HG23	1.72	0.71
1:A:298:ALA:HB1	1:A:336:PHE:HZ	1.48	0.71
1:A:142:MET:CB	1:A:143:GLY:CA	2.68	0.70
1:A:169:ARG:HG2	1:A:169:ARG:HH11	1.57	0.70
1:A:350:LYS:HA	1:A:353:GLN:HB3	1.73	0.70
1:A:349:THR:O	1:A:353:GLN:N	2.24	0.69
1:A:135:ASP:O	1:A:156:ARG:NH1	2.24	0.69
1:A:183:LEU:H	1:A:183:LEU:CD2	2.06	0.69
1:A:142:MET:HB3	1:A:143:GLY:HA3	1.75	0.69
1:A:183:LEU:H	1:A:183:LEU:HD23	1.58	0.68
1:A:202:PHE:HB2	1:A:209:PHE:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:PRO:HB2	1:A:332:ALA:O	1.94	0.68
1:A:127:GLN:HB3	1:A:129:TYR:OH	1.94	0.68
1:A:201:THR:C	1:A:202:PHE:HD1	2.02	0.68
1:A:295:GLY:HA2	1:A:296:CYS:HB3	1.76	0.67
1:A:336:PHE:CG	1:A:337:PRO:HD2	2.29	0.67
1:A:222:LEU:O	1:A:226:MET:HG2	1.94	0.67
1:A:148:GLY:HA3	1:A:150:VAL:H	1.58	0.66
1:A:132:GLU:HB2	1:A:135:ASP:OD2	1.95	0.65
1:A:242:ILE:HD11	1:A:265:ILE:HG12	1.77	0.65
1:A:276:CYS:HB2	1:A:277:ASP:HB3	1.79	0.65
1:A:169:ARG:NE	1:A:204:THR:O	2.26	0.65
1:A:416:LYS:HA	1:A:416:LYS:CE	2.26	0.65
1:A:303:GLU:O	1:A:304:ARG:HB3	1.97	0.64
1:A:196:VAL:CG1	1:A:276:CYS:HB3	2.27	0.64
1:A:260:VAL:HB	1:A:323:SER:HB2	1.78	0.64
1:A:277:ASP:O	1:A:278:PHE:CB	2.45	0.64
1:A:169:ARG:HH11	1:A:169:ARG:CG	2.11	0.64
1:A:268:ASP:OD2	1:A:272:GLN:HB2	1.98	0.64
1:A:223:LYS:HE3	1:A:330:GLU:HG2	1.80	0.64
1:A:141:GLU:C	1:A:142:MET:HG3	2.22	0.64
1:A:238:MET:O	1:A:242:ILE:HG12	1.98	0.64
1:A:305:ILE:HD13	1:A:348:LEU:CD1	2.28	0.62
1:A:132:GLU:O	1:A:135:ASP:HB2	1.99	0.62
1:A:167:MET:O	1:A:208:VAL:HG12	2.00	0.62
1:A:322:TRP:CE3	1:A:384:ARG:NH1	2.66	0.62
1:A:268:ASP:OD1	1:A:270:ARG:N	2.31	0.61
1:A:256:ILE:HG13	1:A:317:ILE:CG2	2.30	0.61
1:A:148:GLY:CA	1:A:150:VAL:N	2.64	0.61
1:A:229:PRO:CB	1:A:332:ALA:O	2.49	0.60
1:A:301:ALA:HB1	1:A:303:GLU:OE1	2.01	0.60
1:A:137:GLU:OE2	1:A:139:LEU:CD1	2.50	0.60
1:A:169:ARG:HG2	1:A:169:ARG:NH1	2.16	0.60
1:A:242:ILE:CD1	1:A:265:ILE:HG12	2.31	0.60
1:A:208:VAL:O	1:A:208:VAL:HG13	2.00	0.59
1:A:298:ALA:HB1	1:A:336:PHE:CZ	2.31	0.59
1:A:255:VAL:C	1:A:256:ILE:HD12	2.28	0.58
1:A:133:ILE:HD11	1:A:153:MET:HE3	1.85	0.58
1:A:201:THR:C	1:A:202:PHE:CD1	2.83	0.56
1:A:277:ASP:O	1:A:278:PHE:HB3	2.05	0.56
1:A:411:LYS:O	1:A:414:MET:HB2	2.05	0.56
1:A:142:MET:CB	1:A:143:GLY:HA3	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLU:O	1:A:304:ARG:CB	2.55	0.55
1:A:183:LEU:HD23	1:A:183:LEU:N	2.18	0.55
1:A:123:THR:CG2	1:A:128:ARG:HB2	2.29	0.55
1:A:349:THR:O	1:A:353:GLN:CB	2.55	0.55
1:A:184:ASP:O	1:A:188:LYS:HG2	2.08	0.54
1:A:301:ALA:CB	1:A:303:GLU:OE1	2.54	0.54
1:A:256:ILE:HD12	1:A:256:ILE:N	2.23	0.54
1:A:162:ILE:HG22	1:A:199:PHE:HE2	1.73	0.54
1:A:144:SER:HB2	1:A:221:LYS:HG3	1.89	0.53
1:A:268:ASP:OD1	1:A:268:ASP:C	2.51	0.53
1:A:153:MET:HE3	1:A:164:VAL:HG21	1.90	0.53
1:A:359:LEU:HD22	1:A:373:VAL:HG21	1.89	0.52
1:A:196:VAL:HG12	1:A:276:CYS:HB3	1.89	0.52
1:A:376:CYS:O	1:A:384:ARG:HD2	2.10	0.52
1:A:130:GLN:O	1:A:130:GLN:HG3	2.10	0.52
1:A:207:ASP:OD1	1:A:207:ASP:N	2.44	0.50
1:A:167:MET:O	1:A:207:ASP:HB3	2.11	0.50
1:A:230:ILE:HB	1:A:235:LEU:HD21	1.92	0.50
1:A:183:LEU:O	1:A:184:ASP:C	2.51	0.50
1:A:277:ASP:O	1:A:277:ASP:OD1	2.29	0.50
1:A:360:PRO:C	1:A:362:HIS:H	2.19	0.50
1:A:378:THR:HG22	1:A:380:ASP:O	2.12	0.50
1:A:123:THR:HG22	1:A:128:ARG:CB	2.32	0.49
1:A:120:GLY:CA	1:A:131:ALA:H	2.25	0.49
1:A:350:LYS:CA	1:A:353:GLN:HB3	2.41	0.49
1:A:256:ILE:HG13	1:A:317:ILE:HG22	1.94	0.49
1:A:237:LYS:HE2	1:A:399:TYR:O	2.12	0.49
1:A:326:ILE:HG23	1:A:337:PRO:HG3	1.94	0.49
1:A:277:ASP:OD1	1:A:277:ASP:C	2.54	0.48
1:A:142:MET:HB3	1:A:143:GLY:HA2	1.96	0.48
1:A:229:PRO:HB3	1:A:333:THR:O	2.13	0.48
1:A:201:THR:O	1:A:202:PHE:CD1	2.56	0.48
1:A:120:GLY:N	1:A:131:ALA:O	2.47	0.47
1:A:340:ASN:O	1:A:350:LYS:NZ	2.48	0.47
1:A:133:ILE:HD11	1:A:153:MET:CE	2.44	0.47
1:A:235:LEU:HD11	1:A:332:ALA:HA	1.96	0.47
1:A:248:TYR:CD1	1:A:248:TYR:C	2.92	0.47
1:A:169:ARG:HD3	1:A:206:THR:C	2.40	0.47
1:A:355:GLU:HA	1:A:355:GLU:OE1	2.15	0.47
1:A:378:THR:O	1:A:384:ARG:NH1	2.49	0.46
1:A:250:LYS:O	1:A:254:GLY:HA2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLY:HA2	1:A:296:CYS:CB	2.41	0.45
1:A:303:GLU:HG2	1:A:381:HIS:HB3	1.97	0.45
1:A:253:HIS:O	1:A:255:VAL:HG23	2.16	0.45
1:A:349:THR:O	1:A:353:GLN:HB3	2.17	0.45
1:A:187:LEU:CD1	1:A:200:GLY:HA2	2.39	0.45
1:A:162:ILE:CG2	1:A:199:PHE:CE2	3.00	0.45
1:A:192:CYS:HB2	1:A:248:TYR:CE2	2.51	0.45
1:A:405:ASP:OD2	1:A:408:SER:CB	2.47	0.45
1:A:133:ILE:HD12	1:A:136:LEU:HD12	1.99	0.44
1:A:215:MET:HG3	1:A:266:LEU:HD23	1.99	0.44
1:A:161:VAL:HG12	1:A:214:LEU:HD22	1.99	0.44
1:A:133:ILE:HG23	1:A:134:ASN:N	2.32	0.44
1:A:333:THR:OG1	1:A:334:GLY:N	2.50	0.44
1:A:303:GLU:OE2	1:A:381:HIS:CB	2.66	0.43
1:A:162:ILE:CG2	1:A:199:PHE:HE2	2.30	0.43
1:A:181:MET:HB3	1:A:182:ASP:H	1.65	0.43
1:A:122:LEU:HB3	1:A:124:ILE:HD11	2.01	0.43
1:A:192:CYS:HB2	1:A:248:TYR:CD2	2.53	0.43
1:A:194:TYR:HB2	1:A:245:ALA:HB2	2.00	0.43
1:A:153:MET:CG	1:A:164:VAL:HG23	2.34	0.42
1:A:342:LYS:HA	1:A:342:LYS:HD3	1.38	0.42
1:A:165:LYS:HB3	1:A:210:ILE:HG23	1.99	0.42
1:A:127:GLN:O	1:A:129:TYR:CE1	2.72	0.42
1:A:183:LEU:CD2	1:A:183:LEU:N	2.73	0.42
1:A:304:ARG:C	1:A:305:ILE:HG13	2.41	0.42
1:A:148:GLY:HA3	1:A:149:GLN:HA	1.65	0.42
1:A:163:ALA:HB3	1:A:212:MET:HG2	2.02	0.42
1:A:301:ALA:HB1	1:A:302:PRO:HD2	2.02	0.41
1:A:303:GLU:OE2	1:A:381:HIS:HB3	2.21	0.41
1:A:202:PHE:CD1	1:A:202:PHE:N	2.88	0.41
1:A:238:MET:HE2	1:A:267:LEU:HD21	2.01	0.41
1:A:229:PRO:HB3	1:A:332:ALA:O	2.20	0.41
1:A:148:GLY:CA	1:A:150:VAL:HG23	2.47	0.41
1:A:256:ILE:HG23	1:A:317:ILE:HG22	2.03	0.40
1:A:226:MET:O	1:A:228:GLY:N	2.48	0.40
1:A:307:PRO:C	1:A:309:ASP:H	2.30	0.40
1:A:348:LEU:HD22	1:A:348:LEU:HA	1.86	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	254/324 (78%)	223 (88%)	27 (11%)	4 (2%)	7	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	ASP
1	A	305	ILE
1	A	278	PHE
1	A	208	VAL

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	230/285 (81%)	185 (80%)	45 (20%)	1	2

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

Mol	Chain	Res	Type
1	A	122	LEU
1	A	124	ILE
1	A	128	ARG
1	A	130	GLN
1	A	134	ASN
1	A	141	GLU
1	A	144	SER

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Mol	Chain	Res	Type
1	A	153	MET
1	A	154	ARG
1	A	157	LYS
1	A	165	LYS
1	A	169	ARG
1	A	183	LEU
1	A	186	VAL
1	A	187	LEU
1	A	206	THR
1	A	207	ASP
1	A	210	ILE
1	A	212	MET
1	A	214	LEU
1	A	220	GLU
1	A	222	LEU
1	A	225	ARG
1	A	246	LEU
1	A	250	LYS
1	A	252	LYS
1	A	267	LEU
1	A	275	LEU
1	A	303	GLU
1	A	305	ILE
1	A	318	ARG
1	A	323	SER
1	A	324	LEU
1	A	327	SER
1	A	341	CYS
1	A	342	LYS
1	A	348	LEU
1	A	352	LEU
1	A	354	GLU
1	A	355	GLU
1	A	359	LEU
1	A	394	SER
1	A	396	ILE
1	A	401	THR
1	A	403	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	190	HIS
1	A	227	GLN

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 oligosaccharides 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 ⓘ

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	264/324 (81%)	1.10	56 (21%) 2 2	11, 40, 88, 115	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	PRO	9.5
1	A	279	GLY	5.4
1	A	308	PRO	5.3
1	A	305	ILE	5.2
1	A	416	LYS	5.1
1	A	341	CYS	5.0
1	A	317	ILE	4.9
1	A	145	GLY	4.8
1	A	363	MET	4.8
1	A	277	ASP	4.6
1	A	362	HIS	4.4
1	A	140	GLY	4.3
1	A	278	PHE	4.1
1	A	182	ASP	4.0
1	A	181	MET	4.0
1	A	170	SER	4.0
1	A	139	LEU	3.9
1	A	345	PHE	3.9
1	A	346	GLU	3.8
1	A	144	SER	3.7
1	A	120	GLY	3.6
1	A	168	ARG	3.5
1	A	225	ARG	3.5
1	A	361	GLY	3.4
1	A	306	ASP	3.4
1	A	156	ARG	3.2
1	A	302	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	415	ALA	3.0
1	A	360	PRO	3.0
1	A	355	GLU	2.9
1	A	276	CYS	2.9
1	A	343	THR	2.9
1	A	339	LYS	2.9
1	A	185	VAL	2.9
1	A	137	GLU	2.8
1	A	295	GLY	2.8
1	A	353	GLN	2.7
1	A	208	VAL	2.7
1	A	337	PRO	2.7
1	A	352	LEU	2.7
1	A	336	PHE	2.7
1	A	143	GLY	2.6
1	A	149	GLN	2.6
1	A	381	HIS	2.6
1	A	296	CYS	2.6
1	A	309	ASP	2.5
1	A	342	LYS	2.5
1	A	129	TYR	2.5
1	A	148	GLY	2.5
1	A	142	MET	2.4
1	A	338	TYR	2.3
1	A	190	HIS	2.3
1	A	147	CYS	2.3
1	A	347	VAL	2.2
1	A	304	ARG	2.1
1	A	160	HIS	2.1

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.