



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:27 am BST

PDB ID : 5B2K
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

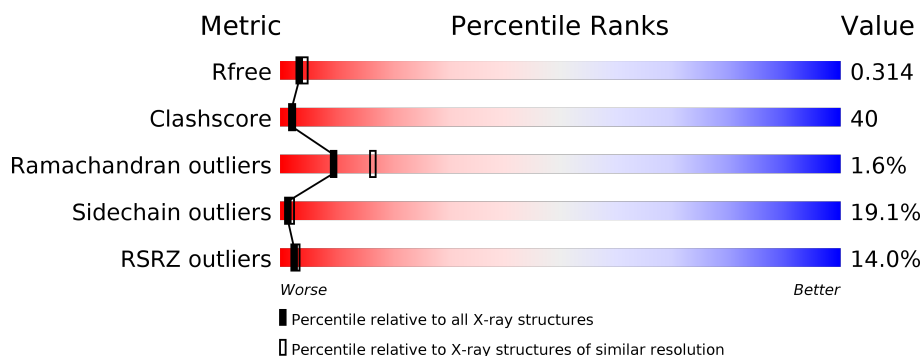
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 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

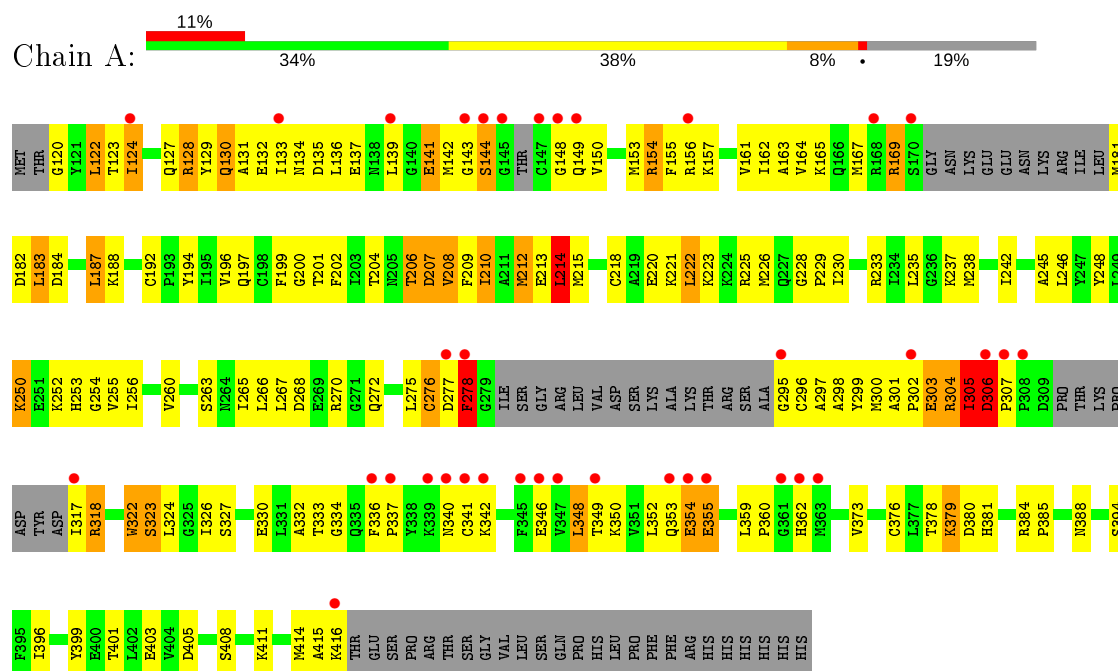
- Molecule 2 is water.

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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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	71.39 Å 71.39 Å 262.00 Å 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 2.77 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.270 , 0.328 0.264 , 0.314	Depositor DCC
R_{free} test set	460 reflections (4.70%)	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 , 60.6	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.72	1/2147 (0.0%)	0.86	3/2882 (0.1%)

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	322	TRP	CD2-CE2	6.33	1.49	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	ARG	N-CA-C	-5.88	95.11	111.00
1	A	214	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	306	ASP	C-N-CD	5.30	139.53	128.40

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 ⓘ

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	171	0
2	A	12	0	0	0	0
All	All	2118	0	2133	171	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 40.

All (171) 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:300:MET:HE3	1:A:305:ILE:HG12	1.45	0.99
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:123:THR:HG22	1:A:128:ARG:HB2	1.49	0.91
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:148:GLY:HA3	1:A:149:GLN:C	1.97	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:144:SER:HB3	1:A:221:LYS:HG3	1.66	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:148:GLY:CA	1:A:149:GLN:C	2.57	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:A:169:ARG:HH11	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: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:201:THR:C	1:A:202:PHE:HD1	2.02	0.61
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:300:MET:HE3	1:A:305:ILE:CG1	2.26	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:HG13	1:A:208:VAL:O	2.00	0.59
1:A:141:GLU:C	1:A:142:MET:HG3	2.22	0.59
1:A:298:ALA:HB1	1:A:336:PHE:CZ	2.31	0.59
1:A:153:MET:HE3	1:A:164:VAL:HG21	1.86	0.57
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
1:A:303:GLU:O	1:A:304:ARG:CB	2.55	0.55
1:A:183:LEU:N	1:A:183:LEU:HD23	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:133:ILE:HD11	1:A:153:MET:HE3	1.90	0.54
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:255:VAL:C	1:A:256:ILE:HD12	2.28	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLN:HG3	1:A:130:GLN:O	2.10	0.52
1:A:201:THR:C	1:A:202:PHE:CD1	2.83	0.51
1:A:207:ASP:N	1:A:207:ASP:OD1	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:277:ASP:O	1:A:277:ASP:OD1	2.29	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:326:ILE:HG23	1:A:337:PRO:HG3	1.94	0.49
1:A:237:LYS:HE2	1:A:399:TYR:O	2.12	0.49
1:A:268:ASP:OD1	1:A:268:ASP:C	2.51	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:133:ILE:HD11	1:A:153:MET:CE	2.44	0.47
1:A:340:ASN:O	1:A:350:LYS:NZ	2.48	0.47
1:A:235:LEU:HD11	1:A:332:ALA:HA	1.96	0.47
1:A:355:GLU:OE1	1:A:355:GLU:HA	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
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:360:PRO:C	1:A:362:HIS:H	2.19	0.45
1:A:183:LEU:O	1:A:184:ASP:C	2.51	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:277:ASP:C	1:A:277:ASP:OD1	2.54	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:248:TYR:C	1:A:248:TYR:CD1	2.92	0.42
1:A:342:LYS:HD3	1:A:342:LYS:HA	1.38	0.42
1:A:169:ARG:HD3	1:A:206:THR:C	2.40	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:N	1:A:183:LEU:CD2	2.73	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: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:154:ARG:HG3	1:A:155:PHE:N	2.34	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:348:LEU:HA	1:A:348:LEU:HD22	1.86	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	254/324 (78%)	223 (88%)	27 (11%)	4 (2%)	9 16

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%)	186 (81%)	44 (19%)	1 2

All (44) 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	141	GLU
1	A	144	SER
1	A	154	ARG
1	A	157	LYS
1	A	169	ARG
1	A	183	LEU
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	233	ARG
1	A	246	LEU
1	A	250	LYS
1	A	252	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	267	LEU
1	A	275	LEU
1	A	278	PHE
1	A	303	GLU
1	A	304	ARG
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	348	LEU
1	A	352	LEU
1	A	354	GLU
1	A	355	GLU
1	A	379	LYS
1	A	388	ASN
1	A	394	SER
1	A	396	ILE
1	A	401	THR
1	A	403	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.75	37 (14%) 2 3	11, 40, 88, 115	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	CYS	8.6
1	A	308	PRO	8.5
1	A	144	SER	6.5
1	A	346	GLU	5.0
1	A	295	GLY	4.4
1	A	340	ASN	4.3
1	A	307	PRO	4.2
1	A	149	GLN	3.7
1	A	302	PRO	3.6
1	A	362	HIS	3.5
1	A	363	MET	3.1
1	A	317	ILE	3.0
1	A	143	GLY	3.0
1	A	345	PHE	3.0
1	A	168	ARG	2.9
1	A	148	GLY	2.8
1	A	353	GLN	2.7
1	A	337	PRO	2.7
1	A	339	LYS	2.7
1	A	278	PHE	2.7
1	A	336	PHE	2.7
1	A	145	GLY	2.7
1	A	347	VAL	2.5
1	A	361	GLY	2.4
1	A	306	ASP	2.4
1	A	156	ARG	2.3
1	A	342	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	147	CYS	2.3
1	A	354	GLU	2.3
1	A	277	ASP	2.2
1	A	139	LEU	2.2
1	A	416	LYS	2.2
1	A	355	GLU	2.2
1	A	349	THR	2.1
1	A	124	ILE	2.1
1	A	133	ILE	2.1
1	A	170	SER	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 carbohydrates 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.