



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2016 – 01:42 PM EDT

PDB ID : 5B2M
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 : 3.06 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-20027257
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-20027257

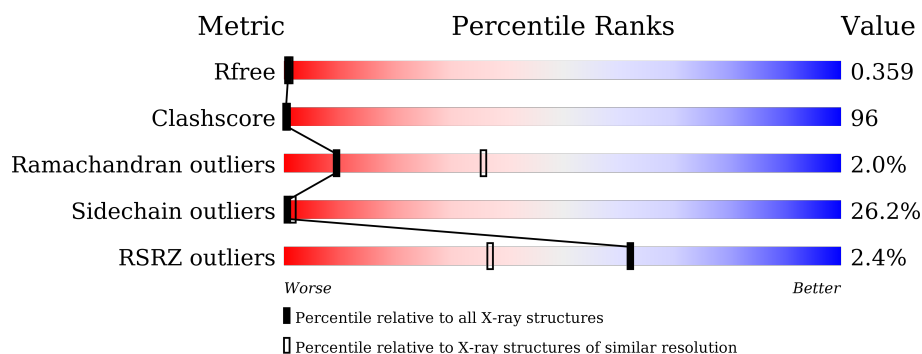
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	324	<div> <div>2%</div> <div>23% 37% 16% 21%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2041 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
1	A	255	Total	C	N	O	S	0	0	0
			2031	1300	352	362	17			

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

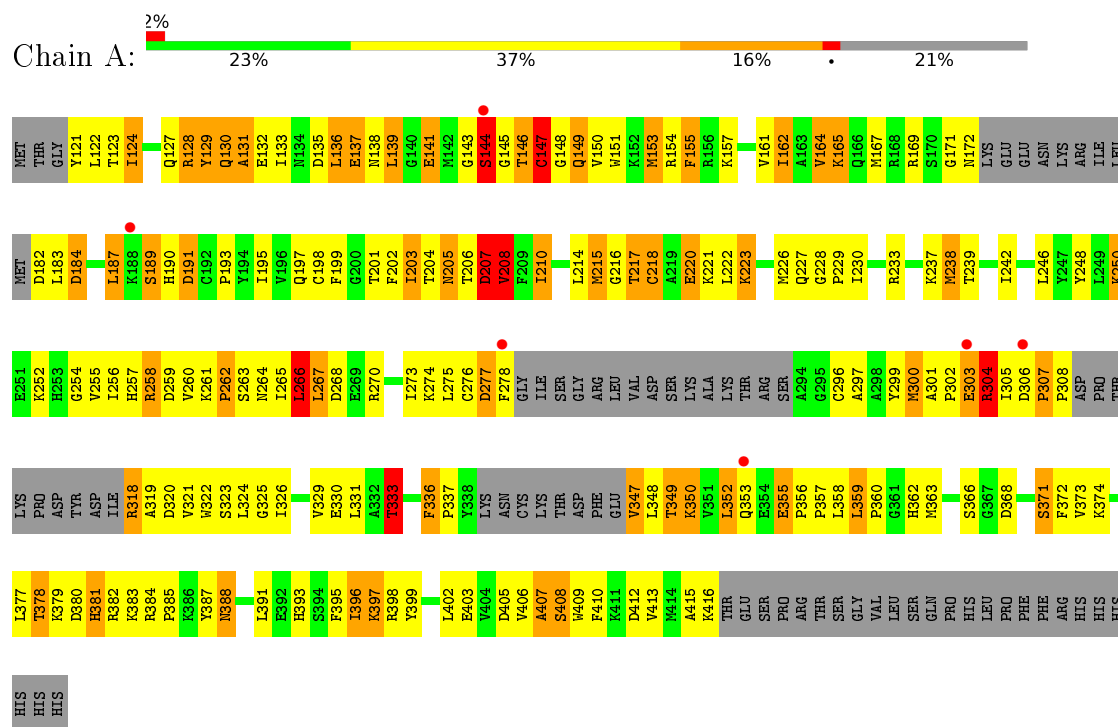
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		

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 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: 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	71.60 Å 71.60 Å 264.44 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.92 – 3.06 35.92 – 3.06	Depositor EDS
% Data completeness (in resolution range)	83.6 (35.92-3.06) 83.7 (35.92-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 3.06 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.288 , 0.364 0.284 , 0.359	Depositor DCC
R_{free} test set	337 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	2041	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.16	2/2071 (0.1%)	1.12	19/2783 (0.7%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	THR	C-N	8.44	1.53	1.34
1	A	145	GLY	C-N	-5.33	1.21	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	PRO	C-N-CD	-14.86	87.92	120.60
1	A	146	THR	O-C-N	-12.28	103.05	122.70
1	A	146	THR	CA-C-N	8.39	135.66	117.20
1	A	217	THR	N-CA-CB	-7.71	95.66	110.30
1	A	144	SER	O-C-N	-7.18	111.00	123.20
1	A	147	CYS	N-CA-C	7.13	130.24	111.00
1	A	349	THR	CB-CA-C	-6.86	93.07	111.60
1	A	146	THR	C-N-CA	6.72	138.51	121.70
1	A	145	GLY	O-C-N	6.69	133.40	122.70
1	A	147	CYS	CB-CA-C	-6.52	97.36	110.40
1	A	266	LEU	CB-CG-CD1	-6.18	100.50	111.00
1	A	208	VAL	N-CA-C	6.08	127.42	111.00
1	A	144	SER	CA-C-N	6.01	128.23	116.20
1	A	350	LYS	N-CA-C	-5.94	94.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	GLY	CA-C-N	-5.47	105.15	117.20
1	A	407	ALA	O-C-N	-5.46	113.96	122.70
1	A	333	THR	CB-CA-C	-5.46	96.86	111.60
1	A	303	GLU	N-CA-C	-5.41	96.40	111.00
1	A	408	SER	O-C-N	-5.26	114.28	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	ASP	Peptide
1	A	304	ARG	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	2031	0	2060	394	1
2	A	10	0	0	1	0
All	All	2041	0	2060	394	1

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 96.

All (394) 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:123:THR:C	1:A:124:ILE:HD13	1.29	1.45
1:A:169:ARG:HH22	1:A:203:ILE:CG1	1.30	1.39
1:A:190:HIS:HA	1:A:197:GLN:NE2	1.38	1.38
1:A:130:GLN:HA	1:A:131:ALA:CB	1.48	1.31
1:A:198:CYS:SG	1:A:210:ILE:CD1	2.19	1.30
1:A:182:ASP:CB	1:A:183:LEU:HB3	1.62	1.28
1:A:133:ILE:HB	1:A:202:PHE:CD2	1.69	1.26
1:A:183:LEU:O	1:A:187:LEU:HD11	1.25	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:VAL:O	1:A:333:THR:HG23	1.34	1.24
1:A:198:CYS:SG	1:A:210:ILE:HD11	1.76	1.23
1:A:138:ASN:C	1:A:139:LEU:HD13	1.57	1.23
1:A:182:ASP:CB	1:A:183:LEU:CB	2.20	1.20
1:A:132:GLU:O	1:A:135:ASP:HB2	1.40	1.20
1:A:148:GLY:H	1:A:149:GLN:CA	1.55	1.19
1:A:266:LEU:C	1:A:267:LEU:HD23	1.61	1.19
1:A:148:GLY:N	1:A:149:GLN:HA	1.52	1.18
1:A:184:ASP:C	1:A:187:LEU:HD13	1.61	1.17
1:A:124:ILE:HD13	1:A:124:ILE:N	1.50	1.17
1:A:182:ASP:HB2	1:A:183:LEU:CB	1.73	1.17
1:A:184:ASP:CA	1:A:187:LEU:HD13	1.78	1.13
1:A:169:ARG:NH2	1:A:203:ILE:CG1	2.13	1.11
1:A:130:GLN:CA	1:A:131:ALA:CB	2.23	1.10
1:A:182:ASP:CA	1:A:183:LEU:HB3	1.82	1.10
1:A:237:LYS:NZ	1:A:399:TYR:O	1.82	1.10
1:A:201:THR:O	1:A:202:PHE:HD1	1.35	1.10
1:A:162:ILE:CG2	1:A:199:PHE:HE2	1.65	1.09
1:A:123:THR:C	1:A:124:ILE:CD1	2.21	1.09
1:A:169:ARG:HH22	1:A:203:ILE:HG13	1.13	1.09
1:A:182:ASP:HB2	1:A:183:LEU:HB3	1.21	1.08
1:A:127:GLN:O	1:A:129:TYR:HE1	1.37	1.08
1:A:127:GLN:C	1:A:129:TYR:HE1	1.56	1.06
1:A:267:LEU:N	1:A:267:LEU:HD23	1.61	1.06
1:A:133:ILE:HD12	1:A:136:LEU:HD11	1.32	1.06
1:A:355:GLU:OE1	1:A:355:GLU:HA	1.45	1.05
1:A:133:ILE:HB	1:A:202:PHE:HD2	0.92	1.05
1:A:147:CYS:HB3	1:A:148:GLY:HA2	1.32	1.04
1:A:129:TYR:HD1	1:A:129:TYR:N	1.54	1.04
1:A:133:ILE:HD12	1:A:136:LEU:CD1	1.88	1.04
1:A:246:LEU:HD13	1:A:387:TYR:HE1	1.18	1.03
1:A:265:ILE:C	1:A:266:LEU:CD1	2.28	1.03
1:A:123:THR:CG2	1:A:128:ARG:HB2	1.89	1.03
1:A:147:CYS:HB3	1:A:148:GLY:CA	1.88	1.02
1:A:148:GLY:H	1:A:149:GLN:HA	0.86	1.02
1:A:277:ASP:CG	1:A:278:PHE:H	1.57	1.01
1:A:208:VAL:HG12	1:A:208:VAL:O	1.55	1.01
1:A:246:LEU:HD13	1:A:387:TYR:CE1	1.95	1.01
1:A:139:LEU:N	1:A:139:LEU:HD13	1.63	1.01
1:A:216:GLY:C	1:A:217:THR:HG23	1.77	1.01
1:A:266:LEU:C	1:A:267:LEU:CD2	2.28	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:HG22	1:A:128:ARG:HB2	1.43	1.01
1:A:184:ASP:O	1:A:187:LEU:HD13	1.61	1.01
1:A:359:LEU:HD12	1:A:360:PRO:HD2	1.39	1.01
1:A:169:ARG:HH22	1:A:203:ILE:HG12	1.26	1.00
1:A:130:GLN:CA	1:A:131:ALA:HB2	1.84	1.00
1:A:138:ASN:C	1:A:139:LEU:CD1	2.29	1.00
1:A:187:LEU:H	1:A:187:LEU:HD12	1.23	1.00
1:A:183:LEU:O	1:A:187:LEU:CD1	2.09	1.00
1:A:127:GLN:O	1:A:129:TYR:CE1	2.16	0.99
1:A:162:ILE:HG22	1:A:199:PHE:HE2	1.28	0.99
1:A:169:ARG:HG3	1:A:206:THR:O	1.63	0.98
1:A:162:ILE:HG21	1:A:199:PHE:CE2	1.98	0.98
1:A:128:ARG:C	1:A:129:TYR:HD1	1.68	0.97
1:A:190:HIS:CA	1:A:197:GLN:NE2	2.28	0.97
1:A:169:ARG:HH21	1:A:204:THR:N	1.63	0.97
1:A:265:ILE:O	1:A:266:LEU:HD12	1.65	0.96
1:A:303:GLU:HG3	1:A:381:HIS:HB3	1.45	0.96
1:A:162:ILE:CG2	1:A:199:PHE:CE2	2.48	0.96
1:A:190:HIS:CA	1:A:197:GLN:HE22	1.79	0.95
1:A:222:LEU:HD21	1:A:409:TRP:CH2	2.00	0.95
1:A:139:LEU:CD1	1:A:139:LEU:N	2.30	0.95
1:A:405:ASP:OD2	1:A:408:SER:HB2	1.67	0.95
1:A:143:GLY:O	1:A:144:SER:HB2	1.67	0.95
1:A:216:GLY:O	1:A:217:THR:CG2	2.15	0.95
1:A:266:LEU:N	1:A:266:LEU:CD1	2.30	0.94
1:A:222:LEU:HD21	1:A:409:TRP:HH2	1.30	0.94
1:A:169:ARG:NH2	1:A:203:ILE:HG12	1.79	0.94
1:A:123:THR:HG22	1:A:128:ARG:HA	1.48	0.93
1:A:299:TYR:OH	1:A:330:GLU:OE1	1.86	0.93
1:A:184:ASP:C	1:A:187:LEU:CD1	2.36	0.93
1:A:183:LEU:HD12	1:A:183:LEU:O	1.69	0.92
1:A:267:LEU:N	1:A:267:LEU:CD2	2.29	0.92
1:A:190:HIS:HA	1:A:197:GLN:HE22	1.18	0.92
1:A:265:ILE:C	1:A:266:LEU:HD13	1.89	0.92
1:A:129:TYR:CD1	1:A:129:TYR:N	2.30	0.91
1:A:368:ASP:OD2	1:A:395:PHE:HA	1.70	0.91
1:A:266:LEU:N	1:A:266:LEU:HD13	1.84	0.91
1:A:130:GLN:HA	1:A:131:ALA:HB2	0.92	0.91
1:A:169:ARG:HH21	1:A:204:THR:H	1.00	0.90
1:A:127:GLN:C	1:A:129:TYR:CE1	2.45	0.90
1:A:263:SER:OG	1:A:264:ASN:OD1	1.89	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:THR:HG22	1:A:349:THR:O	1.69	0.90
1:A:329:VAL:O	1:A:333:THR:CG2	2.19	0.90
1:A:130:GLN:CA	1:A:131:ALA:HB3	2.01	0.89
1:A:184:ASP:O	1:A:187:LEU:CD1	2.19	0.89
1:A:123:THR:HG22	1:A:128:ARG:CB	2.02	0.89
1:A:222:LEU:CD2	1:A:409:TRP:HH2	1.85	0.89
1:A:182:ASP:N	1:A:183:LEU:HB3	1.88	0.89
1:A:265:ILE:C	1:A:266:LEU:HD12	1.91	0.89
1:A:123:THR:HG22	1:A:128:ARG:CA	2.02	0.88
1:A:201:THR:C	1:A:202:PHE:HD1	1.75	0.88
1:A:169:ARG:NE	1:A:204:THR:O	2.07	0.88
1:A:155:PHE:CE1	1:A:157:LYS:HB2	2.08	0.88
1:A:182:ASP:CB	1:A:183:LEU:HB2	2.02	0.88
1:A:122:LEU:HD23	1:A:155:PHE:CE2	2.07	0.88
1:A:147:CYS:CB	1:A:148:GLY:HA2	2.01	0.87
1:A:183:LEU:CG	1:A:183:LEU:O	2.22	0.87
1:A:359:LEU:HD22	1:A:373:VAL:HG21	1.56	0.87
1:A:201:THR:O	1:A:202:PHE:CD1	2.24	0.86
1:A:378:THR:O	1:A:384:ARG:NH1	2.08	0.86
1:A:216:GLY:C	1:A:217:THR:CG2	2.43	0.86
1:A:128:ARG:C	1:A:129:TYR:CD1	2.49	0.86
1:A:183:LEU:O	1:A:183:LEU:CD1	2.22	0.86
1:A:193:PRO:O	1:A:274:LYS:HE2	1.76	0.85
1:A:246:LEU:CD1	1:A:387:TYR:HE1	1.90	0.85
1:A:155:PHE:CE1	1:A:157:LYS:CG	2.59	0.85
1:A:259:ASP:O	1:A:264:ASN:ND2	2.11	0.84
1:A:201:THR:C	1:A:202:PHE:CD1	2.51	0.84
1:A:133:ILE:CB	1:A:202:PHE:CD2	2.59	0.83
1:A:206:THR:OG1	1:A:207:ASP:OD1	1.96	0.83
1:A:302:PRO:HD2	1:A:303:GLU:H	1.43	0.83
1:A:130:GLN:CB	1:A:131:ALA:HB3	2.09	0.83
1:A:130:GLN:HA	1:A:131:ALA:HB3	1.53	0.82
1:A:183:LEU:O	1:A:183:LEU:HG	1.78	0.81
1:A:184:ASP:HA	1:A:187:LEU:HD13	1.57	0.81
1:A:216:GLY:O	1:A:217:THR:HG23	1.78	0.81
1:A:127:GLN:HB3	1:A:129:TYR:OH	1.81	0.81
1:A:302:PRO:CD	1:A:303:GLU:H	1.94	0.80
1:A:182:ASP:HB2	1:A:183:LEU:HB2	1.63	0.80
1:A:208:VAL:CG1	1:A:208:VAL:O	2.30	0.80
1:A:198:CYS:SG	1:A:210:ILE:HD13	2.22	0.80
1:A:415:ALA:O	1:A:416:LYS:CG	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ILE:CD1	1:A:124:ILE:N	2.28	0.79
1:A:169:ARG:HH22	1:A:203:ILE:CB	1.94	0.79
1:A:355:GLU:OE1	1:A:355:GLU:CA	2.29	0.79
1:A:277:ASP:CG	1:A:278:PHE:N	2.31	0.78
1:A:123:THR:O	1:A:124:ILE:HD13	1.83	0.78
1:A:121:TYR:HA	1:A:129:TYR:O	1.83	0.78
1:A:223:LYS:HE3	1:A:331:LEU:HA	1.66	0.77
1:A:238:MET:HA	1:A:273:ILE:HD12	1.64	0.77
1:A:138:ASN:O	1:A:139:LEU:CD1	2.33	0.77
1:A:261:LYS:HD2	1:A:299:TYR:CE2	2.20	0.76
1:A:182:ASP:HB3	1:A:183:LEU:CB	2.14	0.76
1:A:246:LEU:CD1	1:A:387:TYR:CE1	2.66	0.75
1:A:155:PHE:HE1	1:A:157:LYS:CG	1.98	0.75
1:A:133:ILE:HA	1:A:202:PHE:HE2	1.50	0.75
1:A:303:GLU:O	1:A:304:ARG:HB2	1.87	0.75
1:A:306:ASP:HB3	1:A:307:PRO:HD3	1.69	0.75
1:A:250:LYS:O	1:A:254:GLY:HA2	1.87	0.74
1:A:155:PHE:CZ	1:A:157:LYS:HB2	2.21	0.74
1:A:301:ALA:HB1	1:A:302:PRO:HD2	1.68	0.74
1:A:151:TRP:HB3	1:A:153:MET:HE3	1.68	0.74
1:A:133:ILE:CD1	1:A:136:LEU:CD1	2.65	0.73
1:A:216:GLY:O	1:A:217:THR:HG22	1.86	0.73
1:A:138:ASN:O	1:A:139:LEU:HD12	1.88	0.73
1:A:297:ALA:HB1	1:A:300:MET:HG3	1.70	0.73
1:A:155:PHE:CE1	1:A:157:LYS:CB	2.71	0.73
1:A:397:LYS:CA	1:A:397:LYS:HE3	2.19	0.73
1:A:153:MET:SD	1:A:164:VAL:HG21	2.28	0.73
1:A:121:TYR:CD1	1:A:130:GLN:HB3	2.24	0.72
1:A:182:ASP:HB3	1:A:183:LEU:HB2	1.68	0.72
1:A:405:ASP:OD2	1:A:408:SER:CB	2.37	0.72
1:A:198:CYS:SG	1:A:210:ILE:HD12	2.27	0.72
1:A:368:ASP:OD2	1:A:395:PHE:CA	2.37	0.72
1:A:348:LEU:O	1:A:349:THR:HB	1.88	0.72
1:A:141:GLU:HB2	1:A:149:GLN:OE1	1.89	0.71
1:A:138:ASN:OD1	1:A:139:LEU:O	2.08	0.71
1:A:397:LYS:HA	1:A:397:LYS:HE3	1.69	0.71
1:A:206:THR:OG1	1:A:207:ASP:N	2.24	0.70
1:A:222:LEU:HD11	1:A:413:VAL:HG11	1.71	0.70
1:A:122:LEU:N	1:A:129:TYR:O	2.22	0.69
1:A:123:THR:HG21	1:A:128:ARG:HB2	1.75	0.69
1:A:184:ASP:CA	1:A:187:LEU:CD1	2.65	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:HIS:ND1	1:A:197:GLN:OE1	2.25	0.69
1:A:144:SER:O	1:A:221:LYS:HG3	1.92	0.69
1:A:143:GLY:O	1:A:144:SER:CB	2.38	0.69
1:A:189:SER:O	1:A:197:GLN:NE2	2.25	0.69
1:A:155:PHE:HE1	1:A:157:LYS:HG2	1.55	0.69
1:A:415:ALA:O	1:A:416:LYS:CB	2.41	0.69
1:A:301:ALA:O	1:A:303:GLU:O	2.11	0.68
1:A:169:ARG:NH2	1:A:203:ILE:HG13	1.90	0.68
1:A:162:ILE:HG22	1:A:199:PHE:CE2	2.20	0.68
1:A:260:VAL:HB	1:A:323:SER:HB2	1.76	0.68
1:A:133:ILE:HD12	1:A:136:LEU:HD12	1.76	0.68
1:A:123:THR:O	1:A:124:ILE:CD1	2.40	0.68
1:A:258:ARG:HA	1:A:320:ASP:OD1	1.94	0.67
1:A:169:ARG:HD2	1:A:205:ASN:O	1.95	0.67
1:A:261:LYS:HG3	1:A:299:TYR:CE2	2.28	0.67
1:A:155:PHE:CE1	1:A:157:LYS:HG2	2.29	0.67
1:A:218:CYS:SG	1:A:263:SER:HA	2.34	0.67
1:A:306:ASP:O	1:A:308:PRO:HD3	1.93	0.67
1:A:130:GLN:HB2	1:A:131:ALA:HB3	1.77	0.67
1:A:122:LEU:HD23	1:A:155:PHE:CD2	2.30	0.66
1:A:306:ASP:O	1:A:308:PRO:CD	2.43	0.66
1:A:368:ASP:OD2	1:A:398:ARG:NH2	2.28	0.66
1:A:302:PRO:CD	1:A:303:GLU:N	2.56	0.66
1:A:169:ARG:CZ	1:A:203:ILE:HG12	2.26	0.66
1:A:133:ILE:HB	1:A:202:PHE:CE2	2.29	0.65
1:A:205:ASN:OD1	1:A:205:ASN:N	2.30	0.65
1:A:356:PRO:HD3	1:A:379:LYS:HE3	1.77	0.65
1:A:146:THR:O	1:A:146:THR:HG22	1.95	0.65
1:A:169:ARG:NH2	1:A:204:THR:H	1.85	0.65
1:A:191:ASP:OD1	1:A:191:ASP:N	2.30	0.65
1:A:266:LEU:CA	1:A:267:LEU:HD23	2.26	0.65
1:A:167:MET:HE2	1:A:208:VAL:HG11	1.79	0.64
1:A:359:LEU:CD2	1:A:373:VAL:HG21	2.26	0.64
1:A:190:HIS:ND1	1:A:197:GLN:CD	2.52	0.63
1:A:187:LEU:H	1:A:187:LEU:CD1	2.00	0.63
1:A:222:LEU:CD2	1:A:409:TRP:CH2	2.70	0.63
1:A:301:ALA:HB1	1:A:302:PRO:CD	2.27	0.62
1:A:348:LEU:HD12	1:A:348:LEU:N	2.15	0.62
1:A:248:TYR:O	1:A:252:LYS:HB2	1.98	0.62
1:A:368:ASP:CB	1:A:398:ARG:HH21	2.12	0.62
1:A:123:THR:CA	1:A:124:ILE:HD13	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:HIS:HE2	1:A:277:ASP:H	1.46	0.62
1:A:266:LEU:C	1:A:267:LEU:HD22	2.19	0.61
1:A:169:ARG:NH2	1:A:204:THR:N	2.44	0.61
1:A:133:ILE:CD1	1:A:136:LEU:HD12	2.31	0.61
1:A:169:ARG:CZ	1:A:208:VAL:HG23	2.31	0.61
1:A:169:ARG:NH2	1:A:203:ILE:CA	2.64	0.61
1:A:415:ALA:O	1:A:416:LYS:HG2	2.00	0.60
1:A:146:THR:O	1:A:147:CYS:HB2	2.01	0.60
1:A:127:GLN:HB3	1:A:129:TYR:CZ	2.37	0.60
1:A:257:HIS:HE1	1:A:259:ASP:O	1.85	0.59
1:A:347:VAL:HB	1:A:348:LEU:HD12	1.83	0.59
1:A:318:ARG:NH2	1:A:382:ARG:O	2.35	0.59
1:A:222:LEU:HD23	1:A:230:ILE:CD1	2.32	0.59
1:A:302:PRO:HD2	1:A:303:GLU:N	2.15	0.59
1:A:133:ILE:CA	1:A:202:PHE:CE2	2.86	0.58
1:A:368:ASP:CG	1:A:398:ARG:HH21	2.07	0.58
1:A:266:LEU:O	1:A:267:LEU:HD22	2.04	0.58
1:A:306:ASP:C	1:A:308:PRO:HD3	2.23	0.58
1:A:349:THR:O	1:A:349:THR:CG2	2.42	0.58
1:A:368:ASP:HB2	1:A:398:ARG:NH2	2.17	0.58
1:A:147:CYS:CB	1:A:148:GLY:CA	2.67	0.58
1:A:121:TYR:HD1	1:A:130:GLN:HB3	1.69	0.58
1:A:133:ILE:CB	1:A:202:PHE:CE2	2.87	0.58
1:A:320:ASP:O	1:A:323:SER:N	2.37	0.58
1:A:239:THR:HG21	1:A:372:PHE:CE2	2.39	0.58
1:A:128:ARG:CA	1:A:129:TYR:HD1	2.15	0.57
1:A:257:HIS:HE2	1:A:277:ASP:N	2.02	0.57
1:A:187:LEU:N	1:A:187:LEU:HD12	2.07	0.57
1:A:133:ILE:CA	1:A:202:PHE:HE2	2.18	0.57
1:A:263:SER:OG	1:A:264:ASN:N	2.37	0.57
1:A:122:LEU:HG	1:A:124:ILE:HD11	1.87	0.57
1:A:190:HIS:N	1:A:197:GLN:HE22	2.03	0.57
1:A:261:LYS:CG	1:A:262:PRO:HD2	2.34	0.57
1:A:169:ARG:NH1	1:A:208:VAL:HG23	2.19	0.57
1:A:133:ILE:CD1	1:A:136:LEU:HD11	2.19	0.57
1:A:368:ASP:OD1	1:A:395:PHE:N	2.38	0.57
1:A:122:LEU:CD2	1:A:155:PHE:CD2	2.87	0.57
1:A:131:ALA:HB3	2:A:503:HOH:O	2.03	0.57
1:A:384:ARG:HG3	1:A:385:PRO:HD2	1.87	0.57
1:A:222:LEU:CD1	1:A:413:VAL:HG11	2.34	0.57
1:A:303:GLU:CG	1:A:381:HIS:HB3	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:TRP:HB3	1:A:153:MET:CE	2.33	0.56
1:A:138:ASN:OD1	1:A:139:LEU:N	2.38	0.56
1:A:255:VAL:HG12	1:A:256:ILE:N	2.20	0.56
1:A:265:ILE:O	1:A:266:LEU:CD1	2.38	0.56
1:A:223:LYS:CE	1:A:331:LEU:HA	2.34	0.56
1:A:226:MET:O	1:A:227:GLN:HB2	2.05	0.56
1:A:261:LYS:HG3	1:A:262:PRO:HD2	1.86	0.56
1:A:270:ARG:O	1:A:407:ALA:HB2	2.06	0.56
1:A:303:GLU:O	1:A:304:ARG:CB	2.50	0.56
1:A:302:PRO:CG	1:A:303:GLU:H	2.19	0.56
1:A:256:ILE:O	1:A:256:ILE:HG22	2.06	0.55
1:A:255:VAL:CG2	1:A:278:PHE:CE2	2.53	0.55
1:A:391:LEU:O	1:A:396:ILE:HG21	2.06	0.55
1:A:348:LEU:N	1:A:348:LEU:CD1	2.70	0.55
1:A:202:PHE:N	1:A:202:PHE:CD1	2.65	0.55
1:A:319:ALA:O	1:A:322:TRP:N	2.39	0.55
1:A:162:ILE:HG21	1:A:199:PHE:CD2	2.42	0.54
1:A:381:HIS:CE1	1:A:382:ARG:HG2	2.42	0.54
1:A:238:MET:CA	1:A:273:ILE:HD12	2.34	0.54
1:A:155:PHE:CE1	1:A:157:LYS:HG3	2.43	0.54
1:A:393:HIS:O	1:A:397:LYS:HG2	2.08	0.53
1:A:169:ARG:NH1	1:A:203:ILE:HG12	2.24	0.53
1:A:151:TRP:CB	1:A:153:MET:CE	2.87	0.53
1:A:148:GLY:H	1:A:149:GLN:C	2.07	0.53
1:A:133:ILE:HA	1:A:202:PHE:CE2	2.36	0.53
1:A:261:LYS:HD2	1:A:299:TYR:HE2	1.71	0.53
1:A:395:PHE:CE1	1:A:399:TYR:CE2	2.97	0.53
1:A:242:ILE:HG22	1:A:242:ILE:O	2.07	0.52
1:A:169:ARG:HH22	1:A:203:ILE:CA	2.21	0.52
1:A:388:ASN:HA	1:A:391:LEU:HD12	1.90	0.52
1:A:410:PHE:C	1:A:412:ASP:N	2.59	0.52
1:A:189:SER:C	1:A:197:GLN:HE22	2.13	0.52
1:A:257:HIS:CE1	1:A:259:ASP:O	2.63	0.52
1:A:127:GLN:HB3	1:A:129:TYR:CE1	2.44	0.52
1:A:150:VAL:HG23	1:A:165:LYS:HD3	1.89	0.52
1:A:302:PRO:CG	1:A:303:GLU:N	2.74	0.51
1:A:239:THR:CG2	1:A:372:PHE:CE2	2.93	0.51
1:A:137:GLU:O	1:A:153:MET:HG2	2.11	0.51
1:A:261:LYS:CD	1:A:299:TYR:CE2	2.93	0.51
1:A:121:TYR:HE1	1:A:130:GLN:HG2	1.74	0.51
1:A:222:LEU:HD23	1:A:230:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ARG:NH2	1:A:203:ILE:CB	2.62	0.50
1:A:347:VAL:O	1:A:349:THR:OG1	2.17	0.50
1:A:412:ASP:OD1	1:A:412:ASP:O	2.30	0.50
1:A:190:HIS:HA	1:A:197:GLN:CD	2.24	0.50
1:A:206:THR:OG1	1:A:207:ASP:CG	2.50	0.50
1:A:303:GLU:OE1	1:A:307:PRO:HG2	2.12	0.50
1:A:214:LEU:O	1:A:215:MET:HG2	2.11	0.50
1:A:360:PRO:HB2	1:A:363:MET:HB2	1.94	0.50
1:A:169:ARG:NH2	1:A:203:ILE:HA	2.26	0.50
1:A:250:LYS:O	1:A:254:GLY:CA	2.57	0.50
1:A:381:HIS:CG	1:A:382:ARG:N	2.80	0.50
1:A:128:ARG:CA	1:A:129:TYR:CD1	2.95	0.49
1:A:148:GLY:N	1:A:149:GLN:CA	2.25	0.49
1:A:368:ASP:CB	1:A:398:ARG:NH2	2.75	0.49
1:A:246:LEU:HB3	1:A:387:TYR:CZ	2.48	0.49
1:A:226:MET:C	1:A:228:GLY:H	2.15	0.48
1:A:133:ILE:HD13	1:A:202:PHE:CE2	2.48	0.48
1:A:167:MET:HE2	1:A:208:VAL:CG1	2.43	0.48
1:A:222:LEU:HD23	1:A:230:ILE:HD11	1.95	0.48
1:A:306:ASP:HB3	1:A:307:PRO:CD	2.42	0.48
1:A:352:LEU:O	1:A:352:LEU:CD2	2.62	0.48
1:A:133:ILE:CD1	1:A:202:PHE:CE2	2.96	0.48
1:A:319:ALA:O	1:A:322:TRP:HB3	2.14	0.48
1:A:409:TRP:O	1:A:413:VAL:N	2.30	0.47
1:A:150:VAL:CG2	1:A:165:LYS:HD3	2.45	0.47
1:A:306:ASP:O	1:A:308:PRO:HD2	2.13	0.47
1:A:413:VAL:O	1:A:413:VAL:HG12	2.13	0.47
1:A:133:ILE:HD11	1:A:164:VAL:HG11	1.96	0.47
1:A:371:SER:HB3	1:A:393:HIS:HE2	1.80	0.47
1:A:184:ASP:HA	1:A:187:LEU:CD1	2.37	0.47
1:A:261:LYS:HG3	1:A:299:TYR:CZ	2.49	0.47
1:A:297:ALA:O	1:A:300:MET:HG3	2.15	0.47
1:A:347:VAL:HB	1:A:348:LEU:CD1	2.45	0.47
1:A:413:VAL:O	1:A:413:VAL:CG1	2.63	0.47
1:A:380:ASP:OD1	1:A:380:ASP:C	2.54	0.46
1:A:148:GLY:H	1:A:150:VAL:N	2.12	0.46
1:A:325:GLY:O	1:A:329:VAL:HG23	2.16	0.46
1:A:268:ASP:O	1:A:410:PHE:CD2	2.68	0.46
1:A:189:SER:HB3	1:A:248:TYR:CE2	2.50	0.46
1:A:256:ILE:CG2	1:A:258:ARG:HD3	2.45	0.46
1:A:368:ASP:OD2	1:A:395:PHE:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LEU:HD13	1:A:374:LYS:HB2	1.98	0.46
1:A:184:ASP:O	1:A:187:LEU:HB2	2.16	0.46
1:A:352:LEU:HD22	1:A:352:LEU:O	2.16	0.46
1:A:146:THR:O	1:A:146:THR:CG2	2.61	0.46
1:A:415:ALA:O	1:A:416:LYS:HB2	2.16	0.46
1:A:171:GLY:HA2	1:A:172:ASN:HA	1.63	0.45
1:A:190:HIS:O	1:A:190:HIS:CG	2.68	0.45
1:A:307:PRO:N	1:A:308:PRO:HD3	2.25	0.45
1:A:320:ASP:O	1:A:321:VAL:C	2.52	0.45
1:A:381:HIS:HA	1:A:384:ARG:CZ	2.46	0.45
1:A:368:ASP:CG	1:A:395:PHE:CA	2.85	0.45
1:A:321:VAL:O	1:A:322:TRP:C	2.49	0.45
1:A:261:LYS:CG	1:A:299:TYR:CE2	2.98	0.45
1:A:381:HIS:O	1:A:384:ARG:CB	2.64	0.44
1:A:336:PHE:CB	1:A:337:PRO:CD	2.95	0.44
1:A:220:GLU:HB2	1:A:262:PRO:HB2	2.00	0.44
1:A:226:MET:C	1:A:228:GLY:N	2.71	0.44
1:A:348:LEU:O	1:A:349:THR:CB	2.57	0.44
1:A:127:GLN:CB	1:A:129:TYR:CE1	3.01	0.44
1:A:242:ILE:O	1:A:242:ILE:CG2	2.61	0.44
1:A:121:TYR:CE1	1:A:130:GLN:HB3	2.52	0.43
1:A:402:LEU:HD12	1:A:403:GLU:H	1.83	0.43
1:A:121:TYR:CA	1:A:129:TYR:O	2.61	0.43
1:A:261:LYS:HD2	1:A:299:TYR:CD2	2.53	0.43
1:A:183:LEU:C	1:A:187:LEU:CD1	2.85	0.43
1:A:204:THR:OG1	1:A:207:ASP:O	2.06	0.43
1:A:301:ALA:C	1:A:303:GLU:O	2.56	0.43
1:A:184:ASP:O	1:A:187:LEU:HD12	2.13	0.43
1:A:357:PRO:HG2	1:A:357:PRO:O	2.19	0.43
1:A:255:VAL:CG1	1:A:256:ILE:N	2.82	0.42
1:A:412:ASP:C	1:A:412:ASP:OD1	2.56	0.42
1:A:322:TRP:O	1:A:325:GLY:N	2.51	0.42
1:A:169:ARG:HH12	1:A:203:ILE:CG1	2.33	0.42
1:A:169:ARG:HH12	1:A:203:ILE:HG12	1.83	0.42
1:A:349:THR:O	1:A:353:GLN:HB2	2.20	0.42
1:A:150:VAL:HG22	1:A:165:LYS:HB2	2.01	0.42
1:A:322:TRP:CZ3	1:A:377:LEU:O	2.73	0.42
1:A:223:LYS:HZ1	1:A:229:PRO:HA	1.85	0.42
1:A:362:HIS:CG	1:A:362:HIS:O	2.70	0.42
1:A:307:PRO:HA	1:A:308:PRO:HD2	1.82	0.42
1:A:203:ILE:O	1:A:203:ILE:HG22	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ARG:CZ	1:A:203:ILE:CG1	2.87	0.41
1:A:246:LEU:HB3	1:A:387:TYR:CE1	2.54	0.41
1:A:218:CYS:SG	1:A:263:SER:O	2.78	0.41
1:A:151:TRP:CB	1:A:153:MET:HE1	2.50	0.41
1:A:348:LEU:C	1:A:350:LYS:H	2.23	0.41
1:A:260:VAL:HB	1:A:323:SER:CB	2.49	0.41
1:A:266:LEU:O	1:A:267:LEU:CD2	2.57	0.41
1:A:381:HIS:C	1:A:381:HIS:ND1	2.73	0.41
1:A:391:LEU:O	1:A:396:ILE:CG2	2.67	0.41
1:A:136:LEU:HG	1:A:136:LEU:H	1.54	0.41
1:A:406:VAL:O	1:A:409:TRP:HB3	2.20	0.41
1:A:189:SER:HB3	1:A:248:TYR:HE2	1.86	0.40
1:A:161:VAL:O	1:A:162:ILE:HG23	2.21	0.40
1:A:242:ILE:O	1:A:246:LEU:HG	2.21	0.40
1:A:406:VAL:HG12	1:A:407:ALA:N	2.34	0.40
1:A:256:ILE:HG21	1:A:258:ARG:CD	2.51	0.40
1:A:302:PRO:C	1:A:303:GLU:O	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ASN:ND2	1:A:388:ASN:ND2[10_444]	1.44	0.76

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	245/324 (76%)	220 (90%)	20 (8%)	5 (2%)	9	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	ALA
1	A	147	CYS
1	A	144	SER
1	A	277	ASP
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	221/285 (78%)	163 (74%)	58 (26%)	0 1

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ILE
1	A	128	ARG
1	A	129	TYR
1	A	130	GLN
1	A	136	LEU
1	A	137	GLU
1	A	139	LEU
1	A	141	GLU
1	A	149	GLN
1	A	153	MET
1	A	154	ARG
1	A	155	PHE
1	A	162	ILE
1	A	164	VAL
1	A	165	LYS
1	A	184	ASP
1	A	187	LEU
1	A	189	SER
1	A	191	ASP
1	A	195	ILE
1	A	203	ILE
1	A	205	ASN

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Mol	Chain	Res	Type
1	A	207	ASP
1	A	210	ILE
1	A	215	MET
1	A	218	CYS
1	A	220	GLU
1	A	223	LYS
1	A	233	ARG
1	A	238	MET
1	A	250	LYS
1	A	258	ARG
1	A	262	PRO
1	A	266	LEU
1	A	267	LEU
1	A	275	LEU
1	A	276	CYS
1	A	296	CYS
1	A	300	MET
1	A	304	ARG
1	A	305	ILE
1	A	318	ARG
1	A	324	LEU
1	A	326	ILE
1	A	333	THR
1	A	336	PHE
1	A	347	VAL
1	A	352	LEU
1	A	355	GLU
1	A	359	LEU
1	A	366	SER
1	A	371	SER
1	A	378	THR
1	A	381	HIS
1	A	383	LYS
1	A	388	ASN
1	A	396	ILE
1	A	397	LYS

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 [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	255/324 (78%)	-0.03	6 (2%) 62 37	24, 63, 109, 137	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	GLN	2.7
1	A	306	ASP	2.7
1	A	278	PHE	2.7
1	A	144	SER	2.3
1	A	303	GLU	2.1
1	A	188	LYS	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.