



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:45 am BST

PDB ID : 3TG1
Title : Crystal structure of p38alpha in complex with a MAPK docking partner
Authors : Zhang, Y.Y.; Wu, J.W.; Wang, Z.X.
Deposited on : 2011-08-17
Resolution : 2.71 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

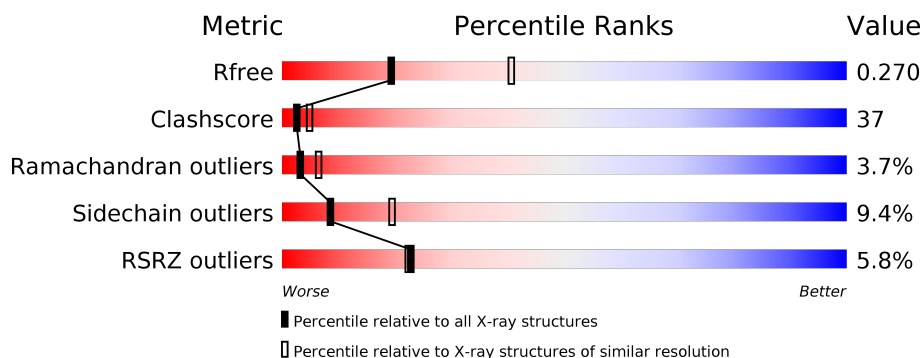
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	380	<div> <div>3%</div> <div> <div></div> <div>48%</div> <div>33%</div> <div>6%</div> <div>12%</div> </div> </div>
2	B	158	<div> <div>9%</div> <div> <div></div> <div>28%</div> <div>46%</div> <div>8%</div> <div>18%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3758 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 Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2699	1731	463	493	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P47811
A	-18	GLY	-	EXPRESSION TAG	UNP P47811
A	-17	SER	-	EXPRESSION TAG	UNP P47811
A	-16	SER	-	EXPRESSION TAG	UNP P47811
A	-15	HIS	-	EXPRESSION TAG	UNP P47811
A	-14	HIS	-	EXPRESSION TAG	UNP P47811
A	-13	HIS	-	EXPRESSION TAG	UNP P47811
A	-12	HIS	-	EXPRESSION TAG	UNP P47811
A	-11	HIS	-	EXPRESSION TAG	UNP P47811
A	-10	HIS	-	EXPRESSION TAG	UNP P47811
A	-9	SER	-	EXPRESSION TAG	UNP P47811
A	-8	SER	-	EXPRESSION TAG	UNP P47811
A	-7	GLY	-	EXPRESSION TAG	UNP P47811
A	-6	LEU	-	EXPRESSION TAG	UNP P47811
A	-5	VAL	-	EXPRESSION TAG	UNP P47811
A	-4	PRO	-	EXPRESSION TAG	UNP P47811
A	-3	ARG	-	EXPRESSION TAG	UNP P47811
A	-2	GLY	-	EXPRESSION TAG	UNP P47811
A	-1	SER	-	EXPRESSION TAG	UNP P47811
A	0	HIS	-	EXPRESSION TAG	UNP P47811

- Molecule 2 is a protein called Dual specificity protein phosphatase 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	130	Total	C	N	O	S	0	0	0
			1044	656	189	192	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	138	MET	-	EXPRESSION TAG	UNP Q9Y6W6
B	289	GLU	-	EXPRESSION TAG	UNP Q9Y6W6
B	290	HIS	-	EXPRESSION TAG	UNP Q9Y6W6
B	291	HIS	-	EXPRESSION TAG	UNP Q9Y6W6
B	292	HIS	-	EXPRESSION TAG	UNP Q9Y6W6
B	293	HIS	-	EXPRESSION TAG	UNP Q9Y6W6
B	294	HIS	-	EXPRESSION TAG	UNP Q9Y6W6
B	295	HIS	-	EXPRESSION TAG	UNP Q9Y6W6

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	4	Total O 4 4	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	72.43 Å 72.43 Å 226.14 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.21 – 2.71 36.21 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.5 (36.21-2.71) 98.5 (36.21-2.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.65 (at 2.72 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.216 , 0.260 0.230 , 0.270	Depositor DCC
R_{free} test set	854 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 82.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3758	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/2763	0.66	3/3750 (0.1%)
2	B	0.38	0/1060	0.54	0/1419
All	All	0.42	0/3823	0.63	3/5169 (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	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	15	LYS	CB-CA-C	-11.11	88.18	110.40
1	A	252	SER	CB-CA-C	7.01	123.43	110.10
1	A	15	LYS	N-CA-C	5.43	125.67	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	ASP	Peptide
1	A	228	HIS	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	2699	0	2692	178	0
2	B	1044	0	1078	100	0
3	A	11	0	0	1	0
3	B	4	0	0	1	0
All	All	3758	0	3770	275	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 37.

All (275) 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:250:ILE:HG13	1:A:251:SER:N	1.17	1.16
2:B:160:THR:O	2:B:161:LYS:HG3	1.47	1.15
1:A:250:ILE:CG1	1:A:251:SER:N	2.11	1.09
2:B:220:GLU:HG3	2:B:224:SER:HA	1.26	1.09
1:A:228:HIS:HA	1:A:231:GLN:HB2	1.35	1.03
1:A:228:HIS:HA	1:A:231:GLN:CB	1.91	1.00
1:A:246:LEU:HD11	1:A:292:ASP:HB2	1.42	1.00
2:B:261:ARG:HB2	2:B:261:ARG:HH11	1.23	0.98
2:B:150:ILE:HD11	2:B:267:LEU:HD13	1.43	0.98
1:A:169:PHE:N	1:A:169:PHE:CD2	2.30	0.95
1:A:195:LEU:HB3	1:A:197:TRP:HE1	1.29	0.95
1:A:57:ARG:HD2	1:A:60:GLN:HB3	1.49	0.94
1:A:197:TRP:HE3	1:A:199:HIS:HE2	1.16	0.93
1:A:195:LEU:HB3	1:A:197:TRP:NE1	1.84	0.91
2:B:148:LYS:HB3	2:B:149:ILE:HD12	1.51	0.90
1:A:250:ILE:CG1	1:A:251:SER:H	1.78	0.89
1:A:49:ARG:HG3	1:A:49:ARG:HH11	1.32	0.89
1:A:169:PHE:N	1:A:169:PHE:HD2	1.69	0.89
1:A:247:LEU:HD12	1:A:248:LYS:N	1.87	0.89
2:B:261:ARG:HB2	2:B:261:ARG:NH1	1.88	0.89
1:A:227:ASP:O	1:A:228:HIS:CG	2.30	0.84
1:A:249:LYS:HE2	1:A:292:ASP:OD1	1.80	0.82
1:A:250:ILE:HG13	1:A:251:SER:H	1.00	0.81
1:A:57:ARG:N	1:A:58:PRO:HD3	1.96	0.79
2:B:160:THR:O	2:B:161:LYS:CG	2.28	0.78
2:B:276:PHE:O	2:B:280:HIS:HB2	1.84	0.78
2:B:220:GLU:HG3	2:B:224:SER:CA	2.12	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:HG2	1:A:19:GLU:HG2	1.69	0.75
1:A:109:MET:HG2	1:A:157:ALA:HB1	1.67	0.75
2:B:155:LEU:O	2:B:159:MET:HG3	1.86	0.74
1:A:278:ASN:HD22	1:A:279:PRO:N	1.85	0.74
1:A:7:THR:O	1:A:22:GLU:HG3	1.88	0.74
1:A:278:ASN:C	1:A:278:ASN:HD22	1.89	0.74
1:A:45:LYS:HG2	1:A:45:LYS:O	1.88	0.74
1:A:148:HIS:HD2	1:A:150:ASP:H	1.36	0.73
1:A:247:LEU:O	1:A:250:ILE:CG2	2.36	0.73
1:A:226:THR:O	1:A:227:ASP:OD2	2.06	0.72
1:A:49:ARG:HG3	1:A:49:ARG:NH1	2.02	0.72
2:B:181:MET:O	2:B:185:LYS:HG3	1.89	0.71
2:B:225:PHE:HA	2:B:228:ILE:HD12	1.72	0.71
1:A:248:LYS:HA	1:A:256:ARG:HH12	1.55	0.71
1:A:310:GLN:H	1:A:310:GLN:CD	1.94	0.70
1:A:127:VAL:HG11	1:A:217:LEU:HD13	1.72	0.70
1:A:249:LYS:HE2	1:A:292:ASP:CG	2.10	0.70
2:B:264:LYS:HD3	2:B:265:GLU:N	2.08	0.69
2:B:229:PHE:CE2	2:B:264:LYS:HG2	2.27	0.69
2:B:227:ARG:HH11	2:B:231:LYS:NZ	1.92	0.68
2:B:241:ASN:O	2:B:243:PRO:HD3	1.93	0.68
1:A:341:THR:O	1:A:345:VAL:HG23	1.93	0.68
2:B:274:SER:O	2:B:277:LYS:HG2	1.94	0.68
1:A:332:LEU:HB3	1:A:336:GLU:CD	2.15	0.68
1:A:193:ILE:HG23	1:A:204:VAL:HG21	1.75	0.68
1:A:197:TRP:HE3	1:A:199:HIS:NE2	1.89	0.68
1:A:230:ASP:HA	1:A:233:LYS:HD3	1.74	0.68
1:A:228:HIS:HA	1:A:231:GLN:HB3	1.76	0.68
1:A:232:LEU:HD21	1:A:259:ILE:HD11	1.74	0.67
1:A:198:MET:HG2	1:A:198:MET:O	1.94	0.67
1:A:133:GLN:HE22	1:A:163:GLU:HA	1.60	0.66
1:A:247:LEU:O	1:A:250:ILE:HG23	1.96	0.65
1:A:195:LEU:HD22	1:A:197:TRP:HE1	1.62	0.65
1:A:46:THR:HG23	1:A:48:HIS:H	1.61	0.64
1:A:43:ASP:HB3	1:A:46:THR:HG22	1.80	0.64
1:A:190:ALA:HB3	1:A:204:VAL:HG22	1.79	0.64
1:A:269:ASN:OD1	1:A:271:ALA:HB3	1.98	0.64
2:B:172:PRO:N	2:B:231:LYS:HD3	2.13	0.64
1:A:249:LYS:CE	1:A:292:ASP:OD2	2.46	0.63
2:B:229:PHE:CZ	2:B:264:LYS:HG2	2.34	0.63
2:B:172:PRO:CA	2:B:231:LYS:HD3	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:THR:HG21	1:A:99:PHE:HD1	1.64	0.62
2:B:219:ARG:HH11	2:B:219:ARG:HG3	1.64	0.62
2:B:275:SER:O	2:B:278:GLN:HG2	1.99	0.62
2:B:226:LYS:O	2:B:227:ARG:HB3	2.00	0.62
1:A:311:TYR:O	2:B:204:ARG:NH1	2.34	0.61
2:B:181:MET:HE2	2:B:181:MET:HA	1.83	0.60
2:B:148:LYS:HB3	2:B:149:ILE:CD1	2.29	0.60
2:B:227:ARG:H	2:B:230:SER:HB2	1.66	0.60
1:A:246:LEU:O	1:A:249:LYS:HB2	2.02	0.60
1:A:250:ILE:HG13	1:A:251:SER:CA	2.25	0.60
1:A:135:LEU:HB3	1:A:303:LEU:HD13	1.84	0.60
2:B:258:SER:O	2:B:262:GLU:HG3	2.02	0.60
2:B:225:PHE:CE2	2:B:229:PHE:HB2	2.36	0.60
1:A:278:ASN:ND2	1:A:280:LEU:H	2.00	0.59
2:B:150:ILE:HG22	2:B:151:TYR:N	2.17	0.59
2:B:212:VAL:HG12	2:B:258:SER:OG	2.02	0.59
1:A:189:ARG:NH2	1:A:193:ILE:HD12	2.17	0.59
1:A:191:PRO:O	1:A:194:MET:HB3	2.01	0.59
1:A:195:LEU:O	1:A:195:LEU:HD23	2.02	0.59
1:A:197:TRP:HB2	1:A:199:HIS:CD2	2.38	0.59
1:A:331:ASP:O	1:A:332:LEU:HD23	2.02	0.58
2:B:181:MET:CE	2:B:184:ASN:HD22	2.16	0.58
2:B:203:ARG:HG3	2:B:207:GLN:HE22	1.68	0.58
1:A:201:ASN:OD1	1:A:203:THR:HG22	2.04	0.58
1:A:186:ARG:HD3	1:A:228:HIS:HB3	1.85	0.58
2:B:278:GLN:NE2	2:B:278:GLN:HA	2.19	0.58
2:B:172:PRO:N	2:B:231:LYS:HZ3	2.00	0.58
1:A:298:THR:OG1	1:A:301:GLN:HG3	2.04	0.58
2:B:197:ALA:HB2	2:B:251:PRO:HG3	1.85	0.58
1:A:195:LEU:CD2	1:A:197:TRP:HE1	2.16	0.57
2:B:181:MET:HE1	2:B:184:ASN:HD22	1.66	0.57
2:B:271:GLY:HA3	2:B:275:SER:OG	2.04	0.57
1:A:193:ILE:CG2	1:A:204:VAL:HG21	2.35	0.57
1:A:23:ARG:HD3	1:A:45:LYS:HB3	1.86	0.57
1:A:10:ARG:HH21	1:A:17:ILE:HD13	1.68	0.57
1:A:10:ARG:NH2	1:A:17:ILE:HD13	2.18	0.57
1:A:115:ASN:HA	1:A:118:LYS:HE3	1.86	0.57
1:A:247:LEU:O	1:A:256:ARG:NH1	2.37	0.57
2:B:150:ILE:HG22	2:B:151:TYR:H	1.69	0.57
1:A:195:LEU:HD13	1:A:255:ALA:HB2	1.86	0.56
1:A:91:THR:HG21	1:A:99:PHE:CD1	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASN:C	1:A:278:ASN:ND2	2.58	0.56
1:A:91:THR:HG22	1:A:93:ALA:H	1.70	0.56
1:A:195:LEU:O	1:A:196:ASN:HB2	2.06	0.56
1:A:195:LEU:CB	1:A:197:TRP:HE1	2.10	0.56
1:A:109:MET:HE2	1:A:159:ASN:HB3	1.87	0.56
2:B:183:TYR:O	2:B:187:HIS:HD2	1.89	0.55
1:A:147:ILE:HD12	1:A:147:ILE:N	2.21	0.55
1:A:112:ASP:OD1	1:A:114:ASN:N	2.32	0.55
2:B:212:VAL:HG22	2:B:213:LEU:N	2.21	0.55
2:B:219:ARG:HG3	2:B:219:ARG:NH1	2.19	0.55
2:B:150:ILE:CD1	2:B:267:LEU:HD13	2.28	0.55
1:A:109:MET:HG2	1:A:157:ALA:CB	2.36	0.55
2:B:229:PHE:HE2	2:B:264:LYS:HE2	1.72	0.54
1:A:243:GLY:O	1:A:247:LEU:HD23	2.07	0.54
2:B:203:ARG:HG3	2:B:207:GLN:NE2	2.22	0.54
1:A:310:GLN:CD	1:A:310:GLN:N	2.60	0.54
1:A:122:LEU:CD2	2:B:181:MET:HE3	2.38	0.54
1:A:278:ASN:O	1:A:281:ALA:HB3	2.06	0.54
1:A:249:LYS:CE	1:A:292:ASP:CG	2.76	0.53
1:A:228:HIS:CD2	1:A:229:ILE:N	2.75	0.53
1:A:46:THR:CG2	1:A:48:HIS:H	2.21	0.53
1:A:67:ARG:HD3	1:A:67:ARG:C	2.29	0.53
2:B:205:LEU:C	2:B:207:GLN:H	2.12	0.53
1:A:186:ARG:CD	1:A:228:HIS:HB3	2.38	0.53
2:B:241:ASN:C	2:B:243:PRO:HD3	2.29	0.53
1:A:74:LEU:HD11	1:A:146:ILE:HD13	1.90	0.53
1:A:250:ILE:HD11	1:A:251:SER:O	2.08	0.53
1:A:127:VAL:HG11	1:A:217:LEU:CD1	2.39	0.53
1:A:164:LEU:HD23	1:A:164:LEU:C	2.30	0.53
1:A:269:ASN:HB3	1:A:272:ASN:HD22	1.74	0.53
2:B:154:ASP:HA	2:B:157:LYS:HE2	1.90	0.52
2:B:212:VAL:HG13	2:B:213:LEU:H	1.74	0.52
2:B:152:PRO:HD3	2:B:270:LYS:HG3	1.92	0.52
1:A:57:ARG:N	1:A:58:PRO:CD	2.70	0.52
1:A:203:THR:HG21	1:A:293:SER:HB2	1.91	0.52
2:B:256:LEU:O	2:B:260:LYS:HG3	2.09	0.52
2:B:283:LEU:N	2:B:283:LEU:HD22	2.23	0.52
1:A:112:ASP:OD1	1:A:114:ASN:HB2	2.11	0.51
1:A:226:THR:O	1:A:227:ASP:CG	2.48	0.51
1:A:313:ASP:OD2	1:A:316:ASP:HB2	2.10	0.51
2:B:149:ILE:N	2:B:149:ILE:HD12	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LEU:HD11	1:A:107:HIS:NE2	2.26	0.51
2:B:203:ARG:CG	2:B:207:GLN:HE22	2.24	0.51
1:A:297:ILE:HG13	1:A:301:GLN:HE21	1.76	0.51
1:A:201:ASN:O	1:A:204:VAL:HB	2.11	0.50
2:B:264:LYS:HD3	2:B:265:GLU:H	1.75	0.50
1:A:8:PHE:CE2	1:A:21:PRO:HD3	2.46	0.50
2:B:150:ILE:HG12	2:B:267:LEU:HB3	1.92	0.50
1:A:228:HIS:O	1:A:231:GLN:HB3	2.12	0.49
1:A:229:ILE:HG23	1:A:258:TYR:OH	2.12	0.49
1:A:14:ASN:O	1:A:15:LYS:HB2	2.12	0.49
2:B:172:PRO:HA	2:B:231:LYS:HD3	1.93	0.49
1:A:195:LEU:HB3	1:A:197:TRP:CE2	2.44	0.49
1:A:190:ALA:HA	1:A:207:TRP:CD1	2.47	0.49
1:A:259:ILE:N	1:A:259:ILE:HD12	2.28	0.49
1:A:75:LEU:HB3	1:A:86:LEU:HD22	1.95	0.48
1:A:109:MET:CE	1:A:159:ASN:HB3	2.43	0.48
1:A:227:ASP:O	1:A:227:ASP:OD1	2.31	0.48
1:A:249:LYS:CE	1:A:292:ASP:OD1	2.55	0.48
2:B:225:PHE:O	2:B:228:ILE:HB	2.14	0.48
2:B:210:ILE:HG13	2:B:211:THR:H	1.79	0.48
1:A:96:LEU:HD11	1:A:339:SER:HA	1.96	0.48
2:B:248:PRO:HA	2:B:253:HIS:CD2	2.48	0.48
2:B:270:LYS:C	2:B:270:LYS:HD2	2.34	0.48
1:A:195:LEU:HD22	1:A:197:TRP:NE1	2.29	0.47
2:B:248:PRO:HA	2:B:253:HIS:CG	2.49	0.47
2:B:150:ILE:CG1	2:B:267:LEU:HB3	2.44	0.47
1:A:270:PHE:CD1	1:A:270:PHE:N	2.82	0.47
2:B:181:MET:CE	2:B:181:MET:HA	2.44	0.47
1:A:197:TRP:HB2	1:A:199:HIS:NE2	2.30	0.47
1:A:22:GLU:O	1:A:25:GLN:OE1	2.33	0.47
2:B:227:ARG:HH11	2:B:231:LYS:CE	2.28	0.47
1:A:227:ASP:O	1:A:228:HIS:ND1	2.48	0.46
2:B:233:ILE:HG13	2:B:264:LYS:HE3	1.97	0.46
1:A:57:ARG:HD2	1:A:60:GLN:CB	2.34	0.46
2:B:194:ILE:HD13	2:B:195:ASN:N	2.30	0.46
1:A:25:GLN:HB3	1:A:26:ASN:OD1	2.16	0.46
1:A:331:ASP:C	1:A:332:LEU:HD23	2.36	0.46
2:B:196:CYS:HA	2:B:201:SER:HB3	1.96	0.46
1:A:247:LEU:HD12	1:A:248:LYS:H	1.74	0.46
1:A:254:SER:O	1:A:255:ALA:C	2.54	0.46
1:A:146:ILE:HD11	1:A:323:TYR:CD2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:SER:HB3	1:A:255:ALA:HB3	1.98	0.46
1:A:185:THR:O	1:A:189:ARG:HG3	2.16	0.46
1:A:247:LEU:O	1:A:250:ILE:HG22	2.15	0.46
1:A:223:PHE:HZ	1:A:238:LEU:HD23	1.81	0.45
1:A:270:PHE:N	1:A:270:PHE:HD1	2.13	0.45
1:A:228:HIS:CD2	1:A:228:HIS:C	2.88	0.45
1:A:200:TYR:CD1	1:A:200:TYR:C	2.90	0.45
1:A:30:VAL:CG2	1:A:40:ALA:HB2	2.46	0.45
2:B:203:ARG:CG	2:B:207:GLN:NE2	2.79	0.45
2:B:218:CYS:O	2:B:219:ARG:HG3	2.16	0.45
1:A:251:SER:OG	1:A:252:SER:N	2.50	0.45
1:A:100:ASN:HD22	1:A:338:LYS:NZ	2.15	0.45
1:A:69:TYR:OH	1:A:73:ARG:HD2	2.17	0.45
2:B:217:SER:HA	2:B:228:ILE:HD13	1.99	0.45
1:A:195:LEU:O	1:A:196:ASN:CB	2.65	0.45
1:A:192:GLU:HA	1:A:197:TRP:CE3	2.52	0.45
1:A:133:GLN:NE2	1:A:164:LEU:H	2.15	0.45
2:B:227:ARG:NH1	2:B:231:LYS:HE3	2.32	0.45
1:A:255:ALA:O	1:A:259:ILE:HD13	2.17	0.44
1:A:120:GLN:HE21	2:B:185:LYS:HG2	1.83	0.44
1:A:249:LYS:NZ	1:A:292:ASP:OD2	2.49	0.44
1:A:45:LYS:CG	1:A:45:LYS:O	2.60	0.44
1:A:228:HIS:CA	1:A:231:GLN:HB2	2.26	0.44
2:B:185:LYS:O	2:B:186:SER:HB3	2.18	0.44
2:B:194:ILE:O	2:B:194:ILE:HG23	2.17	0.44
1:A:157:ALA:O	1:A:164:LEU:HA	2.17	0.44
2:B:207:GLN:C	2:B:209:LYS:H	2.21	0.44
1:A:269:ASN:HB3	1:A:272:ASN:ND2	2.32	0.44
2:B:252:LEU:HA	2:B:252:LEU:HD23	1.76	0.44
2:B:246:VAL:HG13	2:B:246:VAL:O	2.17	0.44
1:A:197:TRP:CD1	1:A:197:TRP:N	2.83	0.43
1:A:7:THR:HB	1:A:22:GLU:OE1	2.18	0.43
2:B:227:ARG:H	2:B:230:SER:CB	2.29	0.43
1:A:192:GLU:OE2	1:A:296:ARG:NH1	2.43	0.43
1:A:193:ILE:HG22	1:A:200:TYR:HB3	1.99	0.43
1:A:279:PRO:O	1:A:282:VAL:HG22	2.18	0.43
1:A:7:THR:HB	1:A:22:GLU:CD	2.38	0.43
1:A:191:PRO:HG3	1:A:235:ILE:HD13	1.99	0.43
1:A:193:ILE:HG22	1:A:200:TYR:CB	2.48	0.43
1:A:195:LEU:HD11	3:A:365:HOH:O	2.17	0.43
2:B:226:LYS:O	2:B:227:ARG:CB	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:HG2	1:A:186:ARG:O	2.17	0.43
1:A:227:ASP:C	1:A:228:HIS:CG	2.90	0.43
1:A:258:TYR:O	1:A:261:SER:HB3	2.19	0.43
2:B:211:THR:OG1	2:B:214:ASP:HB2	2.19	0.43
1:A:131:ILE:HD11	1:A:213:MET:HA	1.99	0.43
1:A:298:THR:H	1:A:301:GLN:NE2	2.16	0.43
1:A:351:PRO:HA	1:A:352:PRO:HD3	1.55	0.43
2:B:156:ALA:O	2:B:159:MET:HB2	2.19	0.43
1:A:191:PRO:HD3	1:A:207:TRP:CE2	2.54	0.42
1:A:91:THR:HG22	1:A:93:ALA:N	2.33	0.42
2:B:273:LEU:HD23	3:B:15:HOH:O	2.19	0.42
1:A:278:ASN:HD22	1:A:279:PRO:CD	2.32	0.42
2:B:194:ILE:HD12	2:B:196:CYS:HB3	2.00	0.42
2:B:208:GLY:O	2:B:209:LYS:C	2.58	0.42
1:A:113:LEU:HB2	1:A:156:LEU:HB2	2.01	0.42
1:A:131:ILE:HD13	1:A:213:MET:HG3	2.02	0.42
1:A:196:ASN:C	1:A:197:TRP:CD1	2.93	0.42
2:B:188:ILE:O	2:B:189:GLN:C	2.57	0.42
2:B:229:PHE:CE2	2:B:264:LYS:HE2	2.54	0.42
1:A:321:ASP:OD1	1:A:321:ASP:N	2.52	0.42
1:A:228:HIS:CA	1:A:231:GLN:HB3	2.47	0.42
1:A:244:ALA:O	1:A:247:LEU:HD11	2.19	0.42
2:B:218:CYS:HB2	2:B:219:ARG:HH12	1.85	0.42
1:A:259:ILE:N	1:A:259:ILE:CD1	2.82	0.42
1:A:99:PHE:O	1:A:100:ASN:HB2	2.20	0.41
1:A:152:LYS:HG2	1:A:155:ASN:HD22	1.86	0.41
2:B:160:THR:C	2:B:161:LYS:HG3	2.29	0.41
2:B:210:ILE:HG13	2:B:211:THR:N	2.34	0.41
1:A:203:THR:CG2	1:A:293:SER:HB2	2.50	0.41
1:A:35:TYR:N	1:A:35:TYR:CD1	2.87	0.41
2:B:207:GLN:HB3	2:B:209:LYS:HD3	2.02	0.41
1:A:192:GLU:HA	1:A:197:TRP:CZ3	2.55	0.41
1:A:228:HIS:CA	1:A:231:GLN:CB	2.81	0.41
2:B:264:LYS:O	2:B:266:PRO:HD3	2.19	0.41
2:B:212:VAL:HG12	2:B:258:SER:CB	2.50	0.41
2:B:215:LEU:C	2:B:217:SER:H	2.23	0.41
2:B:172:PRO:HA	2:B:231:LYS:HB3	2.02	0.41
1:A:191:PRO:O	1:A:194:MET:CB	2.66	0.41
2:B:256:LEU:HD21	2:B:268:VAL:HG21	2.03	0.41
2:B:193:HIS:CG	2:B:194:ILE:N	2.88	0.41
2:B:215:LEU:O	2:B:217:SER:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:PRO:O	2:B:255:VAL:HG23	2.21	0.40
1:A:50:VAL:HA	1:A:108:LEU:H	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	330/380 (87%)	288 (87%)	34 (10%)	8 (2%)	6	13
2	B	126/158 (80%)	91 (72%)	26 (21%)	9 (7%)	1	1
All	All	456/538 (85%)	379 (83%)	60 (13%)	17 (4%)	3	6

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	THR
1	A	100	ASN
1	A	15	LYS
1	A	168	ASP
1	A	196	ASN
2	B	216	ILE
2	B	225	PHE
2	B	276	PHE
1	A	242	PRO
2	B	203	ARG
2	B	204	ARG
1	A	228	HIS
2	B	221	GLY
2	B	228	ILE
2	B	239	ASN
2	B	208	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	6	PRO

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	296/336 (88%)	267 (90%)	29 (10%)	8	18
2	B	121/146 (83%)	111 (92%)	10 (8%)	11	25
All	All	417/482 (86%)	378 (91%)	39 (9%)	8	19

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	38	VAL
1	A	46	THR
1	A	49	ARG
1	A	55	LEU
1	A	67	ARG
1	A	94	ARG
1	A	101	ASP
1	A	109	MET
1	A	112	ASP
1	A	120	GLN
1	A	130	LEU
1	A	135	LEU
1	A	169	PHE
1	A	185	THR
1	A	199	HIS
1	A	204	VAL
1	A	216	LEU
1	A	217	LEU
1	A	227	ASP
1	A	248	LYS
1	A	249	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	250	ILE
1	A	262	LEU
1	A	264	GLN
1	A	278	ASN
1	A	303	LEU
1	A	321	ASP
1	A	343	ASP
2	B	182	GLU
2	B	192	VAL
2	B	194	ILE
2	B	195	ASN
2	B	212	VAL
2	B	214	ASP
2	B	225	PHE
2	B	229	PHE
2	B	241	ASN
2	B	270	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	100	ASN
1	A	120	GLN
1	A	128	GLN
1	A	133	GLN
1	A	148	HIS
1	A	155	ASN
1	A	202	GLN
1	A	228	HIS
1	A	272	ASN
1	A	278	ASN
1	A	301	GLN
1	A	310	GLN
2	B	184	ASN
2	B	187	HIS
2	B	193	HIS
2	B	195	ASN
2	B	206	GLN
2	B	207	GLN
2	B	241	ASN
2	B	253	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	278	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 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 ⓘ

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	334/380 (87%)	0.11	12 (3%) 42 42	38, 78, 131, 160	0
2	B	130/158 (82%)	0.55	15 (11%) 4 4	55, 95, 186, 234	0
All	All	464/538 (86%)	0.23	27 (5%) 23 22	38, 82, 139, 234	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	224	SER	6.9
2	B	220	GLU	6.1
2	B	230	SER	5.5
2	B	221	GLY	5.4
2	B	287	SER	5.1
2	B	223	ASP	4.9
2	B	228	ILE	4.4
2	B	222	LYS	4.2
1	A	246	LEU	3.8
1	A	243	GLY	3.4
2	B	161	LYS	3.2
2	B	283	LEU	3.2
1	A	195	LEU	3.1
2	B	227	ARG	3.1
1	A	35	TYR	3.0
1	A	198	MET	2.9
2	B	225	PHE	2.7
1	A	329	SER	2.6
2	B	226	LYS	2.6
1	A	245	GLU	2.5
1	A	227	ASP	2.5
1	A	331	ASP	2.3
1	A	327	PHE	2.2
1	A	244	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	219	ARG	2.2
1	A	334	ILE	2.1
2	B	155	LEU	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.