



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:59 AM GMT

PDB ID : 2OZA  
Title : Structure of p38alpha complex  
Authors : White, A.; Pargellis, C.A.; Studts, J.M.; Werneburg, B.G.; Farmer II, B.T.  
Deposited on : 2007-02-25  
Resolution : 2.70 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

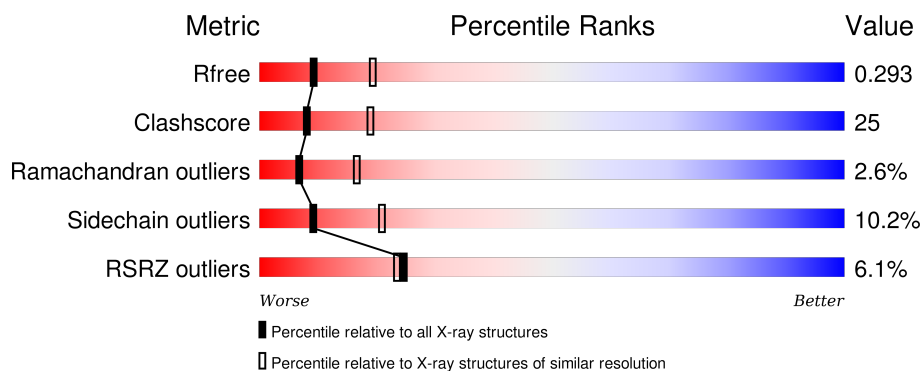
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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	356	 6% 48% 40% 5% 7%
2	B	366	 5% 49% 38% 5% 7%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5500 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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2703	1720	468	496	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLY	-	INSERTION	UNP P49137
A	46	SER	-	INSERTION	UNP P49137

- Molecule 2 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	340	Total	C	N	O	S	0	0	0
			2737	1759	466	500	12			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	MET	-	INSERTION	UNP P47811
B	-4	ALA	-	INSERTION	UNP P47811
B	-3	HIS	-	INSERTION	UNP P47811
B	-2	HIS	-	INSERTION	UNP P47811
B	-1	HIS	-	INSERTION	UNP P47811
B	0	HIS	-	INSERTION	UNP P47811
B	1	HIS	-	INSERTION	UNP P47811

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		

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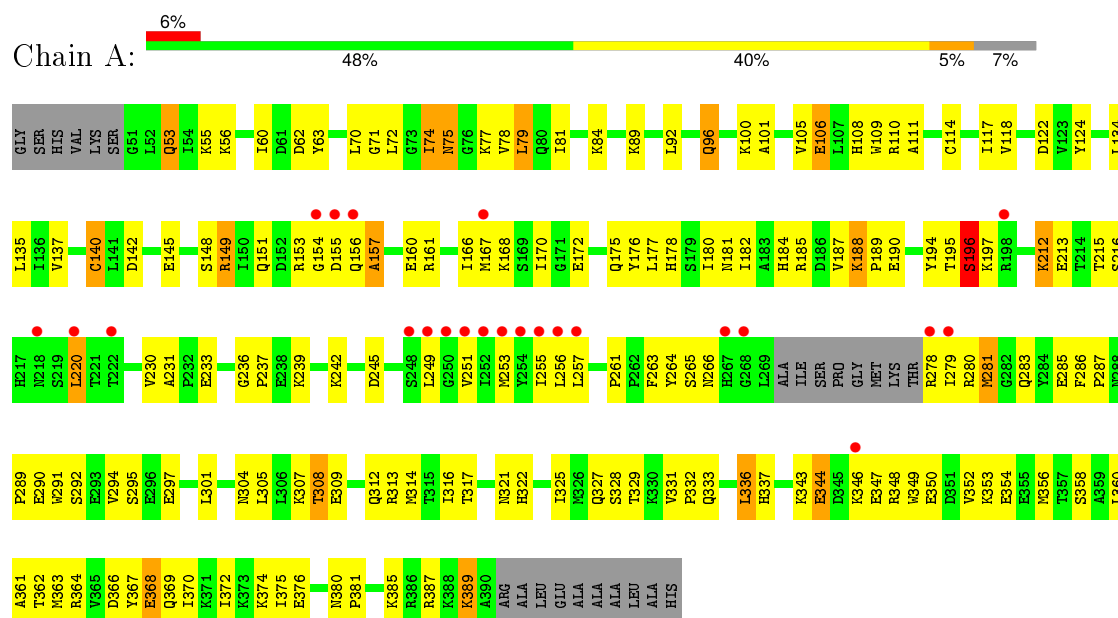
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	28	Total	O	0	0
			28	28		

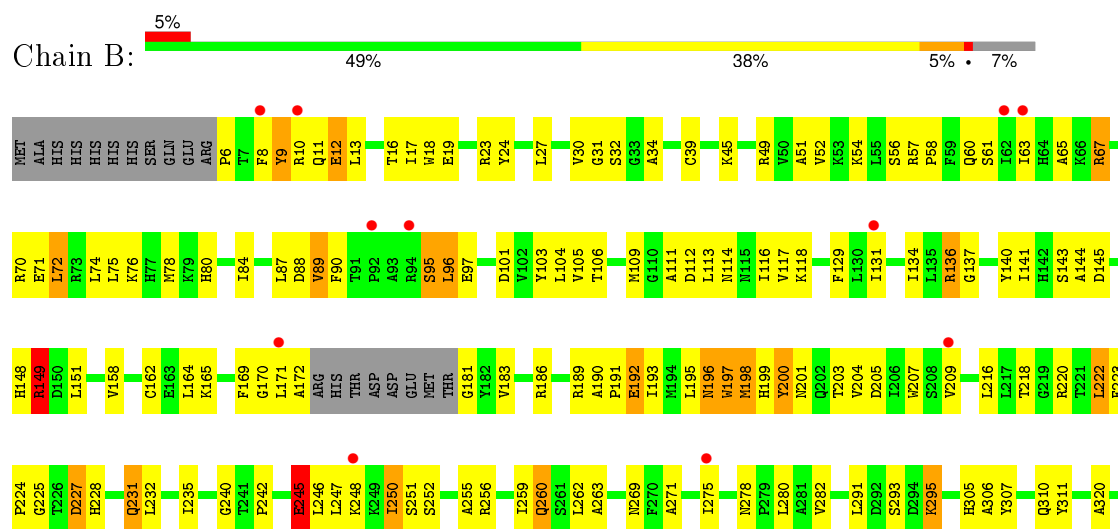
### 3 Residue-property plots

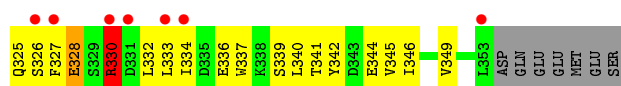
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: MAP kinase-activated protein kinase 2



#### • Molecule 2: Mitogen-activated protein kinase 14





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.31Å 83.31Å 231.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.80 – 2.70 26.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (26.80-2.70) 97.9 (26.80-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.72Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.239 , 0.296 0.236 , 0.293	Depositor DCC
$R_{free}$ test set	1110 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.2	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 22770 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5500	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.41	0/2759	0.58	0/3722
2	B	0.38	0/2802	0.57	0/3804
All	All	0.39	0/5561	0.57	0/7526

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
2	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	199	HIS	Peptide
2	B	6	PRO	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	2703	0	2741	127	0
2	B	2737	0	2735	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	32	0	0	2	0
3	B	28	0	0	1	0
All	All	5500	0	5476	268	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 25.

All (268) 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)
2:B:136:ARG:HG2	2:B:136:ARG:HH11	0.97	1.09
2:B:16:THR:HG22	2:B:17:ILE:H	1.24	1.01
2:B:136:ARG:HG2	2:B:136:ARG:NH1	1.75	0.96
2:B:16:THR:HG21	2:B:54:LYS:HE2	1.46	0.94
1:A:154:GLY:N	1:A:155:ASP:HA	1.89	0.87
2:B:169:PHE:O	2:B:171:LEU:N	2.08	0.85
2:B:57:ARG:HB3	2:B:60:GLN:HG3	1.58	0.85
2:B:195:LEU:HB2	2:B:197:TRP:HE1	1.41	0.84
1:A:92:LEU:HD11	1:A:135:LEU:HB3	1.60	0.82
1:A:142:ASP:HB2	1:A:196:SER:HA	1.63	0.79
2:B:189:ARG:HB3	2:B:193:ILE:HD11	1.64	0.79
2:B:195:LEU:HB2	2:B:197:TRP:NE1	1.97	0.78
2:B:136:ARG:CG	2:B:136:ARG:HH11	1.89	0.78
2:B:16:THR:HG21	2:B:54:LYS:CE	2.12	0.77
2:B:245:GLU:HG3	2:B:246:LEU:N	1.98	0.76
2:B:342:TYR:CE1	2:B:346:ILE:HD11	2.21	0.75
1:A:145:GLU:HB3	3:A:532:HOH:O	1.86	0.73
2:B:242:PRO:HG2	2:B:259:ILE:HD13	1.70	0.73
1:A:281:MET:HG2	1:A:281:MET:O	1.90	0.72
1:A:100:LYS:HE2	1:A:368:GLU:HG2	1.73	0.71
2:B:71:GLU:O	2:B:75:LEU:HD13	1.92	0.70
1:A:70:LEU:HB2	1:A:78:VAL:HG23	1.74	0.70
1:A:354:GLU:HG2	2:B:34:ALA:O	1.93	0.68
2:B:137:GLY:O	2:B:141:ILE:HG13	1.93	0.68
1:A:153:ARG:HB3	1:A:155:ASP:HA	1.75	0.67
2:B:143:SER:C	2:B:145:ASP:H	1.95	0.67
1:A:101:ALA:O	1:A:105:VAL:HG23	1.95	0.67
2:B:112:ASP:OD1	2:B:114:ASN:HB3	1.94	0.66
1:A:63:TYR:HE2	1:A:124:TYR:HH	1.41	0.66
2:B:30:VAL:HG12	2:B:31:GLY:N	2.11	0.66
2:B:259:ILE:O	2:B:262:LEU:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:ILE:HD13	2:B:134:ILE:HD12	1.78	0.65
2:B:16:THR:CG2	2:B:17:ILE:H	2.02	0.64
2:B:332:LEU:HB3	2:B:336:GLU:HG3	1.79	0.64
2:B:16:THR:HG22	2:B:17:ILE:N	2.05	0.63
1:A:344:GLU:HB3	1:A:348:ARG:HH22	1.62	0.63
1:A:257:LEU:HA	1:A:336:LEU:HD22	1.80	0.63
2:B:54:LYS:HD2	2:B:103:TYR:CZ	2.34	0.62
2:B:51:ALA:HB3	2:B:106:THR:HG23	1.81	0.62
2:B:278:ASN:HD22	2:B:307:TYR:HE1	1.46	0.62
2:B:295:LYS:O	2:B:295:LYS:HG2	2.00	0.62
1:A:304:ASN:HA	1:A:307:LYS:HE3	1.82	0.61
2:B:275:ILE:HA	3:B:517:HOH:O	1.99	0.61
1:A:349:TRP:NE1	1:A:353:LYS:HD2	2.15	0.61
1:A:266:ASN:HD22	2:B:181:GLY:N	1.98	0.61
2:B:57:ARG:N	2:B:58:PRO:HD3	2.14	0.61
2:B:195:LEU:HD11	2:B:232:LEU:HD22	1.82	0.61
2:B:332:LEU:HB3	2:B:336:GLU:CB	2.31	0.60
2:B:84:ILE:HD11	2:B:106:THR:OG1	2.00	0.60
1:A:231:ALA:HB3	2:B:220:ARG:NH2	2.16	0.60
1:A:77:LYS:O	1:A:77:LYS:HG3	2.01	0.60
1:A:366:ASP:HB3	1:A:369:GLN:HG3	1.83	0.60
1:A:195:THR:O	1:A:196:SER:HB3	2.01	0.59
1:A:279:ILE:O	1:A:280:ARG:HD3	2.01	0.59
1:A:349:TRP:CD1	1:A:353:LYS:HD2	2.36	0.59
2:B:247:LEU:HD23	2:B:247:LEU:O	2.02	0.59
1:A:280:ARG:HG3	1:A:348:ARG:NH1	2.17	0.59
1:A:55:LYS:NZ	1:A:122:ASP:OD1	2.34	0.59
2:B:70:ARG:HH11	2:B:172:ALA:C	2.06	0.58
2:B:80:HIS:CE1	2:B:136:ARG:NH1	2.71	0.58
1:A:370:ILE:HG13	2:B:111:ALA:HB2	1.85	0.58
1:A:161:ARG:HH21	1:A:333:GLN:HB2	1.69	0.58
2:B:252:SER:O	2:B:256:ARG:HG3	2.04	0.58
1:A:361:ALA:HB2	2:B:32:SER:HB3	1.86	0.57
2:B:95:SER:HA	2:B:342:TYR:OH	2.04	0.57
1:A:160:GLU:HA	1:A:336:LEU:HD11	1.87	0.57
1:A:278:ARG:O	1:A:278:ARG:HG2	2.05	0.57
1:A:280:ARG:HG3	1:A:348:ARG:HH11	1.69	0.57
2:B:333:LEU:N	2:B:336:GLU:HG3	2.19	0.57
1:A:79:LEU:HD12	1:A:79:LEU:H	1.70	0.56
2:B:9:TYR:OH	2:B:24:TYR:O	2.21	0.56
2:B:220:ARG:HG3	2:B:220:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:SER:O	2:B:97:GLU:N	2.39	0.56
1:A:308:THR:HG21	2:B:224:PRO:HB2	1.86	0.55
1:A:100:LYS:HE2	1:A:368:GLU:CG	2.36	0.55
1:A:155:ASP:C	1:A:157:ALA:H	2.09	0.55
1:A:168:LYS:O	1:A:172:GLU:HG3	2.07	0.55
1:A:231:ALA:HB3	2:B:220:ARG:HH22	1.71	0.55
1:A:212:LYS:HE2	1:A:367:TYR:CE2	2.41	0.55
1:A:389:LYS:HG3	1:A:389:LYS:O	2.06	0.55
2:B:97:GLU:CD	2:B:97:GLU:H	2.10	0.54
2:B:195:LEU:HB2	2:B:197:TRP:CD1	2.42	0.54
2:B:10:ARG:NH1	2:B:10:ARG:HB2	2.23	0.54
2:B:84:ILE:O	2:B:84:ILE:HG23	2.06	0.54
2:B:220:ARG:HG3	2:B:220:ARG:HH11	1.73	0.54
2:B:222:LEU:HD13	2:B:223:PHE:CE2	2.42	0.54
2:B:252:SER:HB2	2:B:255:ALA:CB	2.38	0.54
1:A:189:PRO:HD3	1:A:356:MET:CE	2.38	0.54
2:B:191:PRO:HG3	2:B:235:ILE:CD1	2.38	0.53
1:A:285:GLU:O	1:A:287:PRO:HD3	2.08	0.53
2:B:223:PHE:O	2:B:231:GLN:NE2	2.42	0.53
1:A:230:VAL:HG21	2:B:218:THR:HG21	1.89	0.53
2:B:143:SER:C	2:B:145:ASP:N	2.62	0.53
2:B:305:HIS:ND1	2:B:306:ALA:N	2.57	0.53
1:A:286:PHE:HB3	1:A:291:TRP:HB3	1.91	0.53
2:B:325:GLN:HG3	2:B:328:GLU:HB2	1.90	0.52
1:A:344:GLU:HB3	1:A:348:ARG:NH2	2.24	0.52
1:A:63:TYR:HE2	1:A:124:TYR:OH	1.93	0.52
2:B:218:THR:HG22	2:B:220:ARG:H	1.74	0.52
1:A:178:HIS:CE1	1:A:242:LYS:HB3	2.44	0.52
2:B:332:LEU:HD22	2:B:336:GLU:HB3	1.91	0.52
1:A:79:LEU:N	1:A:79:LEU:HD12	2.23	0.52
2:B:192:GLU:HG2	2:B:198:MET:HE3	1.91	0.52
1:A:106:GLU:O	1:A:109:TRP:HB3	2.09	0.52
2:B:260:GLN:C	2:B:262:LEU:H	2.13	0.52
2:B:332:LEU:HB3	2:B:336:GLU:CG	2.40	0.51
2:B:205:ASP:O	2:B:209:VAL:HG23	2.10	0.51
1:A:184:HIS:O	1:A:185:ARG:HB2	2.10	0.51
2:B:325:GLN:O	2:B:327:PHE:N	2.43	0.51
1:A:289:PRO:HA	1:A:292:SER:OG	2.10	0.51
2:B:310:GLN:HB2	2:B:311:TYR:CD2	2.46	0.51
2:B:225:GLY:HA3	2:B:231:GLN:HG2	1.92	0.51
2:B:97:GLU:CD	2:B:97:GLU:N	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:VAL:CG1	2:B:31:GLY:N	2.73	0.51
1:A:189:PRO:HD3	1:A:356:MET:HE3	1.92	0.51
1:A:220:LEU:O	1:A:220:LEU:HG	2.10	0.51
1:A:114:CYS:HB2	1:A:176:TYR:CD1	2.46	0.51
2:B:201:ASN:HB3	2:B:203:THR:H	1.75	0.51
2:B:90:PHE:CE1	2:B:103:TYR:HB2	2.46	0.51
2:B:140:TYR:CZ	2:B:320:ALA:HB2	2.46	0.51
1:A:135:LEU:N	1:A:135:LEU:HD23	2.26	0.50
1:A:380:ASN:HB2	1:A:381:PRO:HD2	1.93	0.50
1:A:280:ARG:NH1	1:A:290:GLU:OE2	2.45	0.50
2:B:332:LEU:HB3	2:B:336:GLU:HB2	1.94	0.50
1:A:380:ASN:HB2	1:A:381:PRO:CD	2.42	0.50
2:B:164:LEU:HD23	2:B:165:LYS:N	2.27	0.50
2:B:80:HIS:CE1	2:B:136:ARG:HH12	2.30	0.49
2:B:195:LEU:CD1	2:B:232:LEU:HD22	2.43	0.49
2:B:18:TRP:CH2	2:B:39:CYS:SG	2.97	0.49
2:B:200:TYR:CD2	2:B:200:TYR:N	2.79	0.49
2:B:200:TYR:HB2	2:B:204:VAL:CG2	2.42	0.49
2:B:148:HIS:O	2:B:149:ARG:CB	2.61	0.49
2:B:337:TRP:CE3	2:B:340:LEU:HD12	2.47	0.49
2:B:131:ILE:CD1	2:B:134:ILE:HD12	2.41	0.49
2:B:245:GLU:O	2:B:248:LYS:HB2	2.13	0.48
1:A:81:ILE:HD11	1:A:137:VAL:HG13	1.95	0.48
2:B:16:THR:HG21	2:B:54:LYS:NZ	2.28	0.48
2:B:18:TRP:CE3	2:B:27:LEU:HD13	2.48	0.48
2:B:190:ALA:HB2	2:B:207:TRP:CB	2.43	0.48
1:A:266:ASN:HB2	2:B:181:GLY:N	2.28	0.48
1:A:181:ASN:OD1	1:A:216:SER:HB3	2.14	0.48
2:B:191:PRO:HG3	2:B:235:ILE:HD13	1.95	0.48
2:B:252:SER:HB2	2:B:255:ALA:HB3	1.94	0.48
1:A:321:ASN:O	1:A:322:HIS:C	2.52	0.47
1:A:362:THR:O	2:B:118:LYS:NZ	2.47	0.47
2:B:61:SER:HA	2:B:334:ILE:HD11	1.95	0.47
1:A:358:SER:HB2	2:B:34:ALA:HB1	1.96	0.47
1:A:142:ASP:CB	1:A:196:SER:HA	2.38	0.47
2:B:271:ALA:HA	2:B:282:VAL:HG11	1.96	0.47
1:A:251:VAL:O	1:A:255:ILE:HG13	2.14	0.47
2:B:111:ALA:HB3	2:B:158:VAL:O	2.15	0.47
1:A:154:GLY:N	1:A:155:ASP:CA	2.68	0.47
2:B:190:ALA:O	2:B:193:ILE:HG12	2.15	0.47
1:A:105:VAL:HG21	1:A:134:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:SER:O	2:B:145:ASP:N	2.48	0.47
2:B:325:GLN:HG3	2:B:328:GLU:CG	2.45	0.47
1:A:74:ILE:HG22	1:A:75:ASN:N	2.30	0.47
1:A:53:GLN:HA	3:A:548:HOH:O	2.15	0.47
2:B:201:ASN:CB	2:B:203:THR:H	2.28	0.47
2:B:342:TYR:CZ	2:B:346:ILE:HD11	2.49	0.46
2:B:222:LEU:HD13	2:B:223:PHE:CZ	2.51	0.46
1:A:108:HIS:O	1:A:108:HIS:HD2	1.97	0.46
1:A:166:ILE:O	1:A:170:ILE:HG13	2.15	0.46
2:B:310:GLN:HB2	2:B:311:TYR:CE2	2.51	0.46
1:A:108:HIS:O	1:A:108:HIS:CD2	2.69	0.46
1:A:62:ASP:O	1:A:84:LYS:HG3	2.15	0.46
1:A:381:PRO:O	1:A:385:LYS:HG3	2.14	0.46
1:A:77:LYS:HB3	2:B:12:GLU:HG2	1.98	0.46
2:B:56:SER:O	2:B:57:ARG:C	2.54	0.46
2:B:262:LEU:HA	2:B:262:LEU:HD23	1.74	0.46
1:A:188:LYS:HB2	1:A:189:PRO:CD	2.46	0.46
1:A:180:ILE:HD11	1:A:182:ILE:HD12	1.97	0.46
1:A:309:GLU:HG2	1:A:312:GLN:HB2	1.97	0.46
2:B:333:LEU:H	2:B:336:GLU:HG3	1.82	0.45
2:B:280:LEU:HD23	2:B:280:LEU:HA	1.76	0.45
1:A:197:LYS:O	1:A:197:LYS:HG3	2.16	0.45
2:B:63:ILE:O	2:B:67:ARG:HB2	2.16	0.45
2:B:16:THR:CG2	2:B:54:LYS:NZ	2.80	0.45
1:A:160:GLU:CA	1:A:336:LEU:HD11	2.47	0.45
1:A:96:GLN:HB3	1:A:96:GLN:HE21	1.54	0.45
2:B:88:ASP:OD1	2:B:89:VAL:N	2.49	0.45
1:A:291:TRP:CZ3	1:A:294:VAL:HG11	2.52	0.44
2:B:11:GLN:HG2	2:B:13:LEU:HG	1.99	0.44
1:A:295:SER:OG	1:A:297:GLU:HG2	2.17	0.44
2:B:78:MET:HA	2:B:78:MET:HE2	1.98	0.44
2:B:216:LEU:HD23	2:B:216:LEU:N	2.31	0.44
2:B:96:LEU:N	2:B:342:TYR:CE2	2.86	0.44
2:B:333:LEU:HB2	2:B:336:GLU:HG2	2.00	0.44
1:A:389:LYS:HE3	1:A:389:LYS:HB2	1.69	0.44
2:B:201:ASN:HB2	2:B:203:THR:OG1	2.17	0.44
2:B:23:ARG:HH21	2:B:45:LYS:HB3	1.83	0.44
1:A:286:PHE:HB3	1:A:291:TRP:CB	2.47	0.44
1:A:360:LEU:O	1:A:364:ARG:HG2	2.18	0.44
2:B:195:LEU:CD1	2:B:197:TRP:HE1	2.30	0.44
1:A:167:MET:CE	1:A:253:MET:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:TRP:HB2	2:B:198:MET:H	1.46	0.43
1:A:361:ALA:CB	2:B:32:SER:HB3	2.48	0.43
1:A:290:GLU:N	1:A:290:GLU:OE1	2.36	0.43
1:A:118:VAL:HG13	1:A:118:VAL:O	2.18	0.43
2:B:65:ALA:HB1	2:B:337:TRP:HB2	1.99	0.43
2:B:349:VAL:O	2:B:349:VAL:CG2	2.66	0.43
1:A:372:ILE:HG13	2:B:116:ILE:HD13	2.01	0.43
1:A:327:GLN:O	1:A:331:VAL:HG23	2.19	0.43
1:A:347:GLU:O	1:A:350:GLU:HB2	2.18	0.43
2:B:8:PHE:N	2:B:8:PHE:CD1	2.86	0.43
1:A:215:THR:HG23	1:A:215:THR:O	2.18	0.43
2:B:344:GLU:OE1	2:B:344:GLU:HA	2.18	0.43
2:B:113:LEU:O	2:B:117:VAL:HG23	2.19	0.43
2:B:247:LEU:HD21	2:B:256:ARG:HB3	2.01	0.43
1:A:237:PRO:C	1:A:239:LYS:H	2.22	0.43
2:B:341:THR:O	2:B:345:VAL:HG23	2.19	0.43
1:A:167:MET:SD	1:A:256:LEU:HD12	2.59	0.43
1:A:89:LYS:HE2	1:A:140:CYS:SG	2.58	0.43
2:B:129:PHE:HD1	2:B:311:TYR:CE1	2.36	0.42
2:B:164:LEU:C	2:B:164:LEU:HD23	2.39	0.42
2:B:72:LEU:O	2:B:76:LYS:HG3	2.20	0.42
2:B:197:TRP:N	2:B:197:TRP:CD1	2.87	0.42
2:B:193:ILE:HG21	2:B:204:VAL:HG11	2.01	0.42
1:A:118:VAL:O	1:A:118:VAL:CG1	2.67	0.42
2:B:51:ALA:O	2:B:105:VAL:HA	2.20	0.42
1:A:233:GLU:OE2	2:B:220:ARG:HG2	2.19	0.42
2:B:10:ARG:CZ	2:B:10:ARG:HB2	2.50	0.42
2:B:109:MET:SD	2:B:165:LYS:HD2	2.59	0.42
1:A:305:LEU:O	1:A:313:ARG:CD	2.68	0.42
1:A:313:ARG:HG3	1:A:314:MET:N	2.35	0.42
1:A:290:GLU:HA	1:A:337:HIS:CD2	2.55	0.42
1:A:372:ILE:HD11	2:B:116:ILE:HD13	2.01	0.42
1:A:148:SER:O	1:A:151:GLN:HB3	2.19	0.42
2:B:8:PHE:O	2:B:9:TYR:HB3	2.20	0.42
2:B:280:LEU:CD2	2:B:306:ALA:HB3	2.49	0.42
2:B:18:TRP:CZ3	2:B:39:CYS:SG	3.12	0.42
2:B:30:VAL:CG1	2:B:31:GLY:H	2.32	0.42
2:B:330:ARG:C	2:B:330:ARG:HD2	2.40	0.42
1:A:325:ILE:O	1:A:328:SER:HB2	2.20	0.42
1:A:375:ILE:HG22	1:A:376:GLU:OE1	2.20	0.42
1:A:212:LYS:HE2	1:A:367:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLN:O	2:B:227:ASP:HB3	2.20	0.41
1:A:153:ARG:C	1:A:155:ASP:HA	2.40	0.41
1:A:230:VAL:HG13	1:A:230:VAL:O	2.20	0.41
1:A:187:VAL:HG23	1:A:245:ASP:OD1	2.21	0.41
2:B:90:PHE:C	2:B:90:PHE:CD1	2.94	0.41
2:B:232:LEU:O	2:B:232:LEU:HD12	2.20	0.41
2:B:260:GLN:C	2:B:262:LEU:N	2.74	0.41
2:B:252:SER:HB2	2:B:255:ALA:HB2	2.02	0.41
2:B:87:LEU:HD23	2:B:87:LEU:HA	1.78	0.41
2:B:325:GLN:HG3	2:B:328:GLU:CB	2.50	0.41
1:A:60:ILE:O	1:A:84:LYS:NZ	2.51	0.41
1:A:264:TYR:CD2	1:A:283:GLN:HG3	2.56	0.41
1:A:71:GLY:O	1:A:72:LEU:HD23	2.21	0.41
1:A:261:PRO:HB2	1:A:263:PHE:CD1	2.56	0.41
2:B:192:GLU:O	2:B:196:ASN:HA	2.21	0.41
2:B:222:LEU:HA	2:B:222:LEU:HD23	1.83	0.41
1:A:78:VAL:O	1:A:78:VAL:HG23	2.21	0.41
1:A:375:ILE:HG23	1:A:376:GLU:N	2.35	0.41
1:A:376:GLU:HA	1:A:387:ARG:HH22	1.86	0.41
2:B:52:VAL:HA	2:B:104:LEU:O	2.21	0.41
1:A:331:VAL:HA	1:A:332:PRO:HD2	1.88	0.40
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.81	0.40
2:B:250:ILE:CG2	2:B:251:SER:N	2.83	0.40
1:A:188:LYS:HB2	1:A:189:PRO:HD2	2.03	0.40
1:A:327:GLN:C	1:A:329:THR:H	2.24	0.40
1:A:155:ASP:C	1:A:157:ALA:N	2.75	0.40
1:A:261:PRO:HG3	1:A:352:VAL:HG22	2.03	0.40
1:A:111:ALA:HB1	1:A:117:ILE:HD13	2.03	0.40
2:B:201:ASN:HB3	2:B:203:THR:HG23	2.04	0.40
1:A:309:GLU:HB3	1:A:312:GLN:HE21	1.87	0.40
1:A:149:ARG:HG3	1:A:194:TYR:CD2	2.56	0.40
1:A:175:GLN:HA	1:A:316:ILE:HG12	2.03	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	328/356 (92%)	294 (90%)	29 (9%)	5 (2%)	13	32
2	B	336/366 (92%)	291 (87%)	33 (10%)	12 (4%)	4	9
All	All	664/722 (92%)	585 (88%)	62 (9%)	17 (3%)	7	16

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	GLU
2	B	96	LEU
2	B	170	GLY
1	A	74	ILE
1	A	196	SER
2	B	330	ARG
2	B	149	ARG
2	B	198	MET
2	B	245	GLU
2	B	326	SER
2	B	9	TYR
2	B	144	ALA
2	B	263	ALA
2	B	328	GLU
1	A	157	ALA
2	B	240	GLY
1	A	236	GLY

### 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	301/317 (95%)	272 (90%)	29 (10%)	10	24
2	B	299/324 (92%)	267 (89%)	32 (11%)	8	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	600/641 (94%)	539 (90%)	61 (10%)	9 21

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	56	LYS
1	A	75	ASN
1	A	79	LEU
1	A	96	GLN
1	A	106	GLU
1	A	110	ARG
1	A	140	CYS
1	A	149	ARG
1	A	156	GLN
1	A	188	LYS
1	A	190	GLU
1	A	196	SER
1	A	212	LYS
1	A	213	GLU
1	A	220	LEU
1	A	249	LEU
1	A	265	SER
1	A	281	MET
1	A	301	LEU
1	A	308	THR
1	A	317	THR
1	A	336	LEU
1	A	343	LYS
1	A	346	LYS
1	A	363	MET
1	A	368	GLU
1	A	374	LYS
1	A	389	LYS
2	B	12	GLU
2	B	19	GLU
2	B	49	ARG
2	B	67	ARG
2	B	72	LEU
2	B	74	LEU
2	B	89	VAL
2	B	95	SER

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Mol	Chain	Res	Type
2	B	101	ASP
2	B	136	ARG
2	B	149	ARG
2	B	151	LEU
2	B	162	CYS
2	B	183	VAL
2	B	186	ARG
2	B	192	GLU
2	B	196	ASN
2	B	197	TRP
2	B	200	TYR
2	B	222	LEU
2	B	227	ASP
2	B	228	HIS
2	B	231	GLN
2	B	245	GLU
2	B	250	ILE
2	B	260	GLN
2	B	269	ASN
2	B	291	LEU
2	B	293	SER
2	B	295	LYS
2	B	330	ARG
2	B	339	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	288	ASN
1	A	312	GLN
1	A	337	HIS
2	B	26	ASN
2	B	60	GLN
2	B	201	ASN
2	B	202	GLN
2	B	228	HIS
2	B	231	GLN
2	B	257	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	332/356 (93%)	0.22	23 (6%)	20 18	39, 67, 101, 135	0
2	B	340/366 (92%)	0.20	18 (5%)	30 28	46, 71, 108, 140	0
All	All	672/722 (93%)	0.21	41 (6%)	25 23	39, 69, 107, 140	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	GLY	6.2
2	B	326	SER	4.6
2	B	62	ILE	4.1
2	B	330	ARG	3.8
1	A	220	LEU	3.7
2	B	327	PHE	3.6
1	A	278	ARG	3.5
2	B	10	ARG	3.5
1	A	268	GLY	3.4
2	B	331	ASP	3.4
1	A	250	GLY	3.3
1	A	155	ASP	3.3
2	B	248	LYS	3.3
1	A	267	HIS	3.2
2	B	94	ARG	3.2
2	B	353	LEU	3.1
1	A	218	ASN	3.0
1	A	252	ILE	2.9
1	A	279	ILE	2.9
1	A	253	MET	2.9
2	B	131	ILE	2.8
2	B	334	ILE	2.8
1	A	256	LEU	2.7
2	B	333	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	275	ILE	2.7
2	B	8	PHE	2.7
1	A	167	MET	2.6
1	A	222	THR	2.6
1	A	251	VAL	2.5
2	B	171	LEU	2.5
1	A	254	TYR	2.5
1	A	248	SER	2.4
1	A	346	LYS	2.3
2	B	63	ILE	2.2
2	B	92	PRO	2.2
1	A	249	LEU	2.1
1	A	255	ILE	2.1
2	B	209	VAL	2.1
1	A	257	LEU	2.1
1	A	198	ARG	2.0
1	A	156	GLN	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.