



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:38 PM UTC

PDB ID : 2OZA / pdb_00002oza
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

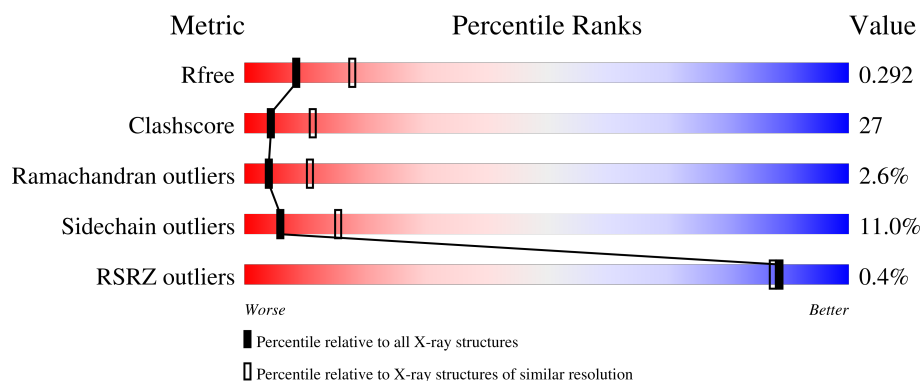
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	356	44% 42% 7% 7%
2	B	366	47% 39% 6% 7%

2 Entry composition

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		

Continued on next page...

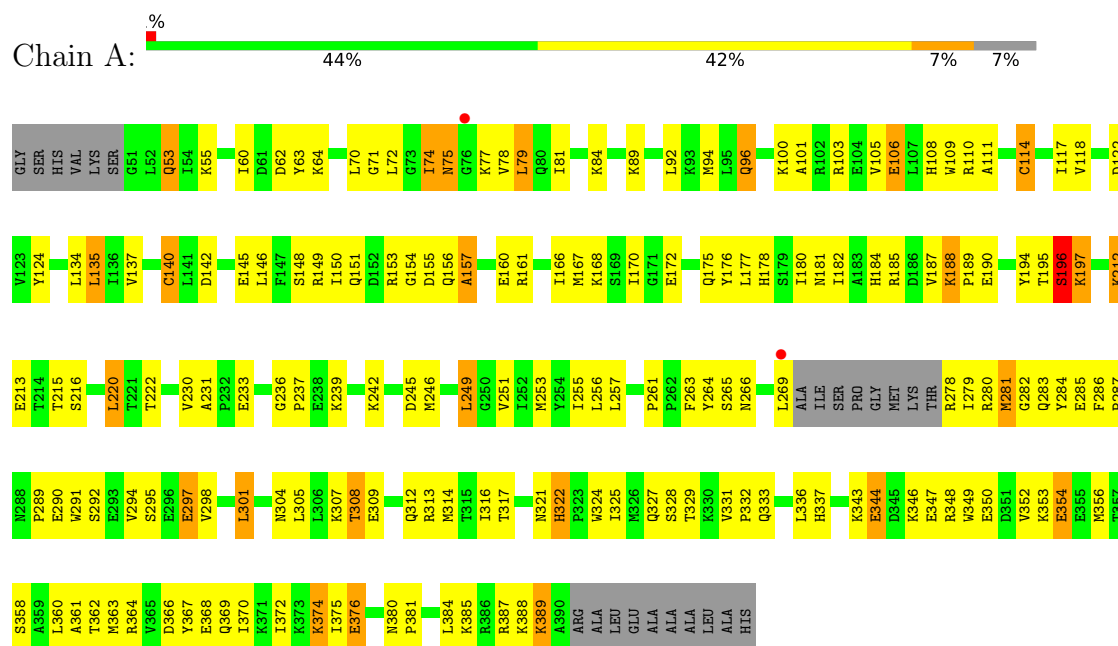
Continued from previous page...

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

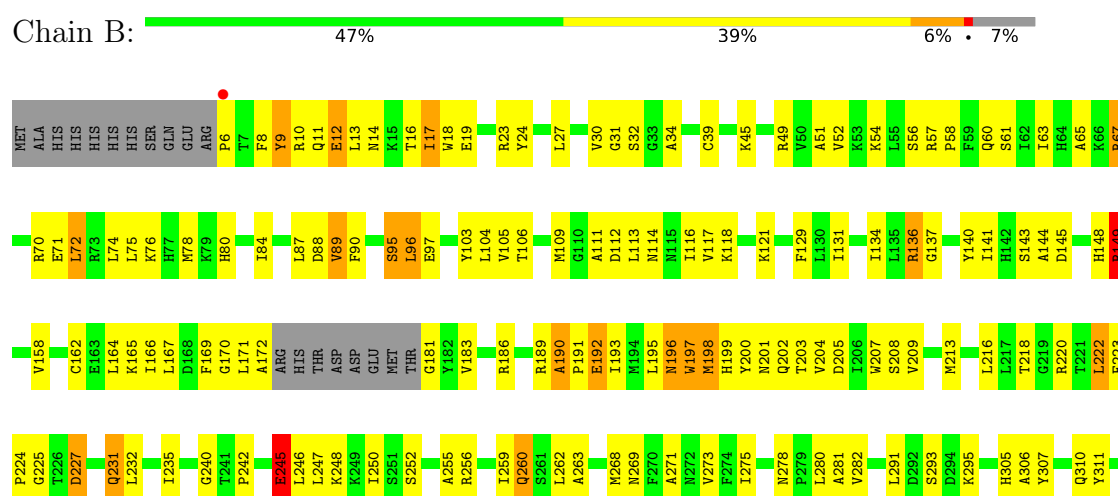
3 Residue-property plots [i](#)

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

• Molecule 1: 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, α , β , γ	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) 97.7 (26.80-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.72Å)	Xtriage
Refinement program	CNS, CNX	Depositor
R, R_{free}	0.239 , 0.296 0.237 , 0.292	Depositor DCC
R_{free} test set	1110 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	71.2	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5500	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.51	0/2759	0.91	7/3722 (0.2%)
2	B	0.48	0/2802	0.85	3/3804 (0.1%)
All	All	0.49	0/5561	0.88	10/7526 (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
2	B	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	HIS	CA-C-N	5.89	125.77	119.28
1	A	322	HIS	C-N-CA	5.89	125.77	119.28
1	A	374	LYS	N-CA-C	-5.84	102.40	110.35
1	A	222	THR	CA-C-N	5.67	125.64	120.03
1	A	222	THR	C-N-CA	5.67	125.64	120.03
2	B	190	ALA	CA-C-N	5.63	125.47	119.28
2	B	190	ALA	C-N-CA	5.63	125.47	119.28
1	A	114	CYS	CA-C-N	5.58	125.42	119.28
1	A	114	CYS	C-N-CA	5.58	125.42	119.28
2	B	202	GLN	N-CA-C	-5.17	106.80	113.01

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	199	HIS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	139	0
2	B	2737	0	2735	172	0
3	A	32	0	0	2	0
3	B	28	0	0	1	0
All	All	5500	0	5476	293	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 27.

All (293) 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:HH11	2:B:136:ARG:HG2	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:189:PRO:HD3	1:A:356:MET:HE3	1.53	0.88
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:HH11	2:B:136:ARG:CG	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:PRO:HG2	2:B:259:ILE:HD13	1.70	0.73
1:A:281:MET:O	1:A:281:MET:HG2	1.90	0.72
2:B:143:SER:C	2:B:145:ASP:H	1.95	0.71
1:A:253:MET:HE1	1:A:301:LEU:HD13	1.71	0.71
1:A:100:LYS:HE2	1:A:368:GLU:HG2	1.73	0.71
2:B:78:MET:HE2	2:B:78:MET:HA	1.72	0.70
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:167:MET:HE2	1:A:253:MET:HB2	1.73	0.69
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
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
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
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
1:A:79:LEU:HD11	1:A:94:MET:HE3	1.80	0.63
1:A:344:GLU:HB3	1:A:348:ARG:HH22	1.62	0.63
2:B:70:ARG:HH11	2:B:172:ALA:C	2.06	0.63
1:A:253:MET:HE1	1:A:301:LEU:CD1	2.29	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
1:A:231:ALA:HB3	2:B:220:ARG:NH2	2.16	0.60
2:B:84:ILE:HD11	2:B:106:THR:OG1	2.00	0.60
2:B:332:LEU:HB3	2:B:336:GLU:CB	2.31	0.60
1:A:77:LYS:HG3	1:A:77:LYS:O	2.01	0.60
1:A:366:ASP:HB3	1:A:369:GLN:HG3	1.83	0.60
1:A:155:ASP:C	1:A:157:ALA:H	2.09	0.60
1:A:195:THR:O	1:A:196:SER:HB3	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:O	1:A:280:ARG:HD3	2.01	0.59
2:B:97:GLU:CD	2:B:97:GLU:H	2.10	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:55:LYS:NZ	1:A:122:ASP:OD1	2.34	0.59
1:A:280:ARG:HG3	1:A:348:ARG:NH1	2.17	0.59
1:A:161:ARG:HH21	1:A:333:GLN:HB2	1.69	0.58
1:A:370:ILE:HG13	2:B:111:ALA:HB2	1.85	0.58
2:B:80:HIS:CE1	2:B:136:ARG:NH1	2.71	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
1:A:160:GLU:HA	1:A:336:LEU:HD11	1.87	0.57
2:B:95:SER:HA	2:B:342:TYR:OH	2.04	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:16:THR:HG22	2:B:17:ILE:N	2.05	0.56
2:B:143:SER:C	2:B:145:ASP:N	2.62	0.56
2:B:260:GLN:C	2:B:262:LEU:H	2.13	0.56
2:B:9:TYR:OH	2:B:24:TYR:O	2.21	0.56
2:B:220:ARG:NH1	2:B:220:ARG:HG3	2.20	0.56
2:B:95:SER:O	2:B:97:GLU:N	2.39	0.56
2:B:97:GLU:CD	2:B:97:GLU:N	2.64	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: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: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:285:GLU:O	1:A:287:PRO:HD3	2.08	0.53
2:B:191:PRO:HG3	2:B:235:ILE:CD1	2.38	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:305:HIS:ND1	2:B:306:ALA:N	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:HG23	1:A:281:MET:HE2	1.90	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:321:ASN:O	1:A:322:HIS:C	2.52	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
1:A:178:HIS:CE1	1:A:242:LYS:HB3	2.44	0.52
2:B:218:THR:HG22	2:B:220:ARG:H	1.74	0.52
1:A:79:LEU:HD12	1:A:79:LEU:N	2.23	0.52
2:B:332:LEU:HD22	2:B:336:GLU:HB3	1.91	0.52
1:A:106:GLU:O	1:A:109:TRP:HB3	2.09	0.52
1:A:184:HIS:O	1:A:185:ARG:HB2	2.10	0.51
2:B:205:ASP:O	2:B:209:VAL:HG23	2.10	0.51
2:B:332:LEU:HB3	2:B:336:GLU:CG	2.40	0.51
1:A:289:PRO:HA	1:A:292:SER:OG	2.10	0.51
2:B:325:GLN:O	2:B:327:PHE:N	2.43	0.51
2:B:192:GLU:HG2	2:B:198:MET:HE3	1.92	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
1:A:220:LEU:O	1:A:220:LEU:HG	2.10	0.51
2:B:30:VAL:CG1	2:B:31:GLY:N	2.73	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
2:B:56:SER:O	2:B:57:ARG:C	2.54	0.50
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
1:A:380:ASN:HB2	1:A:381:PRO:CD	2.42	0.50
2:B:332:LEU:HB3	2:B:336:GLU:HB2	1.94	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
1:A:253:MET:HE3	1:A:324:TRP:CZ3	2.46	0.49
2:B:18:TRP:CH2	2:B:39:CYS:SG	2.97	0.49
2:B:195:LEU:CD1	2:B:232:LEU:HD22	2.43	0.49
2:B:200:TYR:N	2:B:200:TYR:CD2	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:213:MET:HE3	2:B:281:ALA:HB1	1.94	0.49
2:B:268:MET:HE3	2:B:273:VAL:HG22	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:169:PHE:C	2:B:171:LEU:H	2.17	0.48
1:A:81:ILE:HD11	1:A:137:VAL:HG13	1.95	0.48
2:B:245:GLU:O	2:B:248:LYS:HB2	2.13	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
1:A:266:ASN:HB2	2:B:181:GLY:N	2.28	0.48
2:B:190:ALA:HB2	2:B:207:TRP:CB	2.43	0.48
1:A:181:ASN:OD1	1:A:216:SER:HB3	2.14	0.48
1:A:237:PRO:C	1:A:239:LYS:H	2.22	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: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:164:LEU:HD23	2:B:164:LEU:C	2.39	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:70:ARG:NH1	2:B:172:ALA:C	2.73	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
1:A:53:GLN:HA	3:A:548:HOH:O	2.15	0.47
1:A:74:ILE:HG22	1:A:75:ASN:N	2.30	0.47
1:A:253:MET:HE2	1:A:298:VAL:HG13	1.97	0.47
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
2:B:201:ASN:CB	2:B:203:THR:H	2.28	0.47
2:B:222:LEU:HD13	2:B:223:PHE:CZ	2.51	0.46
2:B:330:ARG:HD2	2:B:330:ARG:C	2.40	0.46
2:B:342:TYR:CZ	2:B:346:ILE:HD11	2.49	0.46
1:A:108:HIS:HD2	1:A:108:HIS:O	1.97	0.46
1:A:166:ILE:O	1:A:170:ILE:HG13	2.15	0.46
1:A:108:HIS:O	1:A:108:HIS:CD2	2.69	0.46
1:A:153:ARG:C	1:A:155:ASP:HA	2.40	0.46
2:B:310:GLN:HB2	2:B:311:TYR:CE2	2.51	0.46
1:A:62:ASP:O	1:A:84:LYS:HG3	2.15	0.46
2:B:90:PHE:CD1	2:B:90:PHE:C	2.94	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:260:GLN:C	2:B:262:LEU:N	2.74	0.46
1:A:180:ILE:HD11	1:A:182:ILE:HD12	1.97	0.46
1:A:188:LYS:HB2	1:A:189:PRO:CD	2.46	0.46
2:B:262:LEU:HD23	2:B:262:LEU:HA	1.74	0.46
1:A:309:GLU:HG2	1:A:312:GLN:HB2	1.97	0.46
2:B:280:LEU:HD23	2:B:280:LEU:HA	1.76	0.45
2:B:333:LEU:H	2:B:336:GLU:HG3	1.82	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
1:A:327:GLN:C	1:A:329:THR:H	2.24	0.45
1:A:96:GLN:HE21	1:A:96:GLN:HB3	1.54	0.45
1:A:160:GLU:CA	1:A:336:LEU:HD11	2.47	0.45
2:B:16:THR:CG2	2:B:54:LYS:NZ	2.80	0.45
2:B:88:ASP:OD1	2:B:89:VAL:N	2.49	0.45
2:B:325:GLN:CD	2:B:328:GLU:HG3	2.42	0.45
1:A:291:TRP:CZ3	1:A:294:VAL:HG11	2.52	0.44
1:A:295:SER:OG	1:A:297:GLU:HG2	2.17	0.44
2:B:11:GLN:HG2	2:B:13:LEU:HG	1.99	0.44
2:B:216:LEU:N	2:B:216:LEU:HD23	2.31	0.44
1:A:389:LYS:HE3	1:A:389:LYS:HB2	1.69	0.44
2:B:23:ARG:HH21	2:B:45:LYS:HB3	1.83	0.44
2:B:96:LEU:N	2:B:342:TYR:CE2	2.86	0.44
2:B:201:ASN:HB2	2:B:203:THR:OG1	2.17	0.44
2:B:333:LEU:HB2	2:B:336:GLU:HG2	2.00	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
1:A:150:ILE:O	1:A:151:GLN:C	2.61	0.44
2:B:195:LEU:CD1	2:B:197:TRP:HE1	2.30	0.44
2:B:197:TRP:HB2	2:B:198:MET:H	1.46	0.43
1:A:269:LEU:C	1:A:269:LEU:HD12	2.43	0.43
1:A:361:ALA:CB	2:B:32:SER:HB3	2.48	0.43
1:A:118:VAL:O	1:A:118:VAL:HG13	2.18	0.43
1:A:290:GLU:OE1	1:A:290:GLU:N	2.36	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
1:A:372:ILE:HG13	2:B:116:ILE:HD13	2.01	0.43
2:B:65:ALA:HB1	2:B:337:TRP:HB2	1.99	0.43
1:A:370:ILE:HD12	1:A:370:ILE:C	2.42	0.43
1:A:215:THR:HG23	1:A:215:THR:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:PHE:CD1	2:B:8:PHE:N	2.86	0.43
2:B:113:LEU:O	2:B:117:VAL:HG23	2.19	0.43
2:B:344:GLU:OE1	2:B:344:GLU:HA	2.18	0.43
2:B:247:LEU:HD21	2:B:256:ARG:HB3	2.01	0.43
2:B:341:THR:O	2:B:345:VAL:HG23	2.19	0.43
1:A:331:VAL:O	1:A:332:PRO:C	2.62	0.43
1:A:89:LYS:HE2	1:A:140:CYS:SG	2.58	0.43
1:A:167:MET:SD	1:A:256:LEU:HD12	2.59	0.43
2:B:337:TRP:C	2:B:339:SER:H	2.27	0.43
2:B:129:PHE:HD1	2:B:311:TYR:CE1	2.36	0.42
2:B:72:LEU:O	2:B:76:LYS:HG3	2.20	0.42
2:B:193:ILE:HG21	2:B:204:VAL:HG11	2.01	0.42
2:B:197:TRP:CD1	2:B:197:TRP:N	2.87	0.42
1:A:118:VAL:O	1:A:118:VAL:CG1	2.67	0.42
1:A:233:GLU:OE2	2:B:220:ARG:HG2	2.19	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
2:B:10:ARG:HB2	2:B:10:ARG:CZ	2.50	0.42
2:B:51:ALA:O	2:B:105:VAL:HA	2.20	0.42
2:B:109:MET:SD	2:B:165:LYS:HD2	2.59	0.42
2:B:268:MET:HE3	2:B:273:VAL:CG2	2.49	0.42
1:A:148:SER:O	1:A:151:GLN:HB3	2.19	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
2:B:8:PHE:O	2:B:9:TYR:HB3	2.20	0.42
2:B:166:ILE:C	2:B:167:LEU:HD12	2.45	0.42
2:B:280:LEU:CD2	2:B:306:ALA:HB3	2.49	0.42
2:B:325:GLN:O	2:B:326:SER:C	2.62	0.42
2:B:337:TRP:C	2:B:339:SER:N	2.77	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
2:B:30:VAL:CG1	2:B:31:GLY:H	2.32	0.42
1:A:155:ASP:C	1:A:157:ALA:N	2.75	0.41
1:A:212:LYS:HE2	1:A:367:TYR:CZ	2.55	0.41
1:A:283:GLN:O	2:B:227:ASP:HB3	2.20	0.41
1:A:230:VAL:O	1:A:230:VAL:HG13	2.20	0.41
2:B:14:ASN:C	2:B:16:THR:N	2.78	0.41
2:B:18:TRP:CZ3	2:B:39:CYS:SG	3.12	0.41
1:A:187:VAL:HG23	1:A:245:ASP:OD1	2.21	0.41
2:B:87:LEU:HD23	2:B:87:LEU:HA	1.78	0.41
2:B:232:LEU:HD12	2:B:232:LEU:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:SER:HB2	2:B:255:ALA:HB2	2.02	0.41
1:A:60:ILE:O	1:A:84:LYS:NZ	2.51	0.41
1:A:71:GLY:O	1:A:72:LEU:HD23	2.21	0.41
1:A:264:TYR:CD2	1:A:283:GLN:HG3	2.56	0.41
2:B:325:GLN:HG3	2:B:328:GLU:CB	2.50	0.41
1:A:261:PRO:HB2	1:A:263:PHE:CD1	2.56	0.41
1:A:327:GLN:C	1:A:329:THR:N	2.78	0.41
2:B:192:GLU:O	2:B:196:ASN:HA	2.21	0.41
2:B:222:LEU:HD23	2:B:222:LEU:HA	1.83	0.41
2:B:333:LEU:C	2:B:336:GLU:HG2	2.46	0.41
1:A:78:VAL:HG23	1:A:78:VAL:O	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
2:B:197:TRP:C	2:B:198:MET:O	2.63	0.41
2:B:349:VAL:O	2:B:349:VAL:CG2	2.66	0.41
1:A:177:LEU:HA	1:A:177:LEU:HD23	1.81	0.40
1:A:331:VAL:HA	1:A:332:PRO:HD2	1.88	0.40
1:A:188:LYS:HB2	1:A:189:PRO:HD2	2.03	0.40
1:A:111:ALA:HB1	1:A:117:ILE:HD13	2.03	0.40
1:A:261:PRO:HG3	1:A:352:VAL:HG22	2.03	0.40
1:A:264:TYR:OH	2:B:227:ASP:C	2.64	0.40
1:A:246:MET:HE1	1:A:249:LEU:HD23	2.02	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
1:A:282:GLY:C	1:A:284:TYR:N	2.80	0.40
1:A:309:GLU:HB3	1:A:312:GLN:HE21	1.87	0.40
2:B:113:LEU:O	2:B:114:ASN:C	2.63	0.40
2:B:201:ASN:HB3	2:B:203:THR:HG23	2.04	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%)	8	22
2	B	336/366 (92%)	291 (87%)	33 (10%)	12 (4%)	2	6
All	All	664/722 (92%)	585 (88%)	62 (9%)	17 (3%)	4	11

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%)	266 (88%)	35 (12%)	5	13
2	B	299/324 (92%)	268 (90%)	31 (10%)	7	17
All	All	600/641 (94%)	534 (89%)	66 (11%)	6	15

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	64	LYS
1	A	75	ASN
1	A	79	LEU
1	A	96	GLN
1	A	103	ARG
1	A	106	GLU
1	A	110	ARG
1	A	135	LEU
1	A	140	CYS
1	A	146	LEU
1	A	156	GLN
1	A	188	LYS
1	A	190	GLU
1	A	196	SER
1	A	197	LYS
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	297	GLU
1	A	301	LEU
1	A	308	THR
1	A	317	THR
1	A	343	LYS
1	A	346	LYS
1	A	354	GLU
1	A	363	MET
1	A	374	LYS
1	A	376	GLU
1	A	384	LEU
1	A	388	LYS
1	A	389	LYS
2	B	12	GLU
2	B	17	ILE
2	B	19	GLU
2	B	49	ARG
2	B	67	ARG
2	B	72	LEU
2	B	74	LEU
2	B	89	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	95	SER
2	B	121	LYS
2	B	136	ARG
2	B	149	ARG
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	208	SER
2	B	222	LEU
2	B	227	ASP
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	330	ARG
2	B	339	SER
2	B	349	VAL

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

Mol	Chain	Res	Type
1	A	217	HIS
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	142	HIS
2	B	202	GLN
2	B	228	HIS
2	B	231	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	332/356 (93%)	-0.18	2 (0%) 85 85	39, 67, 101, 135	0
2	B	340/366 (92%)	-0.15	1 (0%) 90 89	46, 71, 108, 140	0
All	All	672/722 (93%)	-0.16	3 (0%) 88 87	39, 69, 106, 140	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	LEU	3.4
1	A	76	GLY	2.7
2	B	6	PRO	2.5

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 oligosaccharides 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.