Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 02:59 PM EST

PDB ID	:	3VUT
Title	:	Crystal structures of non-phosphorylated MAP2K4
Authors	:	Matsumoto, T.; Kinoshita, T.; Kirii, Y.; Tada, T.; Yamano, A.
Deposited on	:	2012-07-05
Resolution	:	3.50 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 (i) 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 (1)) were used in the production of this report:

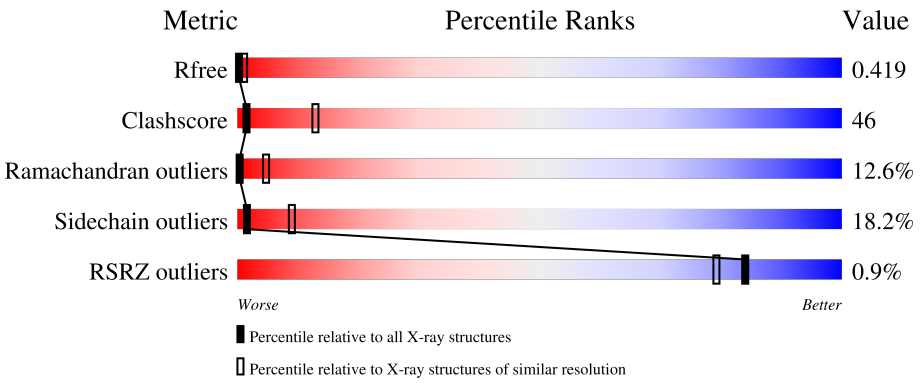
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	327	27% 24% 9% • 38%
1	B	327	% 30% 35% 12% • 20%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3457 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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	203	1563	1009	251	291	12	0	0	0
1	B	260	1894	1197	309	376	12	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

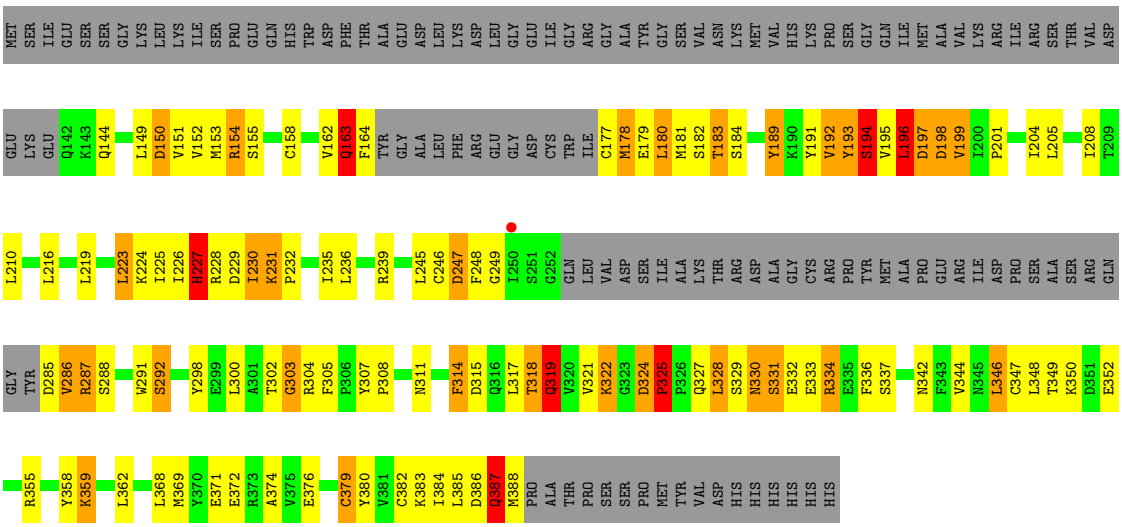
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	MET	-	expression tag	UNP P45985
A	400	HIS	-	expression tag	UNP P45985
A	401	HIS	-	expression tag	UNP P45985
A	402	HIS	-	expression tag	UNP P45985
A	403	HIS	-	expression tag	UNP P45985
A	404	HIS	-	expression tag	UNP P45985
A	405	HIS	-	expression tag	UNP P45985
B	79	MET	-	expression tag	UNP P45985
B	400	HIS	-	expression tag	UNP P45985
B	401	HIS	-	expression tag	UNP P45985
B	402	HIS	-	expression tag	UNP P45985
B	403	HIS	-	expression tag	UNP P45985
B	404	HIS	-	expression tag	UNP P45985
B	405	HIS	-	expression tag	UNP P45985

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.

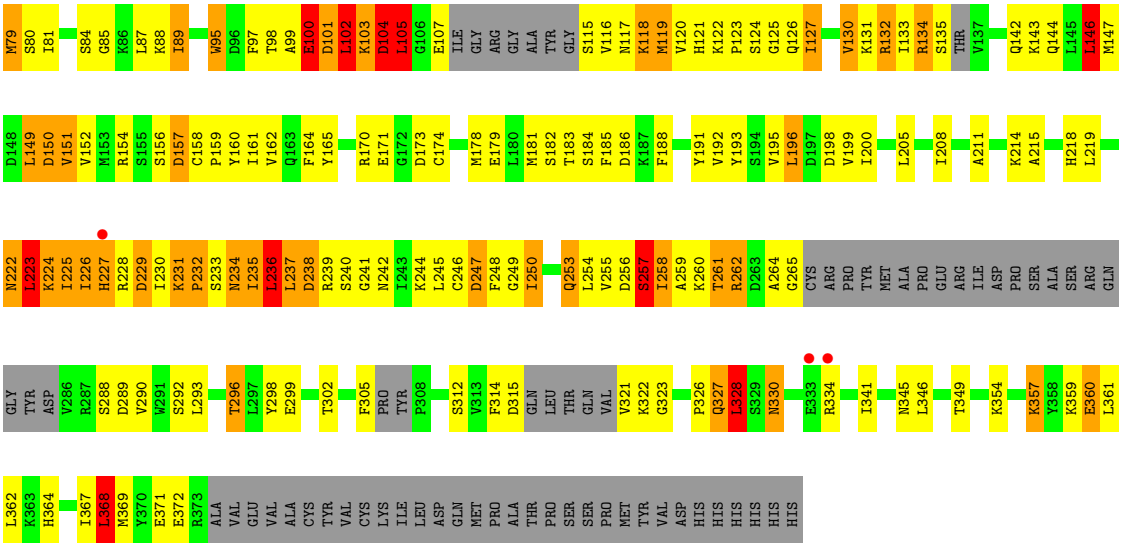
• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 4

Chain A: 27% 24% 9% • 38%



• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 4

Chain B: % 30% 35% 12% • 20%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.77Å 87.36Å 118.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 40.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-3.50) 98.3 (40.98-3.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.34 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.331 , 0.407 0.331 , 0.419	Depositor DCC
R_{free} test set	449 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	120.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 123.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	3457	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.54	0/1590	0.72	0/2153
1	B	0.59	1/1919 (0.1%)	0.92	10/2597 (0.4%)
All	All	0.57	1/3509 (0.0%)	0.84	10/4750 (0.2%)

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	B	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	TRP	CD2-CE2	5.56	1.48	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	257	SER	N-CA-C	-7.06	91.93	111.00
1	B	328	LEU	CA-CB-CG	6.84	131.03	115.30
1	B	146	LEU	CA-CB-CG	6.26	129.69	115.30
1	B	118	LYS	N-CA-C	-5.90	95.07	111.00
1	B	258	ILE	CB-CA-C	-5.75	100.11	111.60
1	B	236	LEU	CA-CB-CG	5.56	128.09	115.30
1	B	223	LEU	CA-CB-CG	-5.42	102.83	115.30
1	B	368	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	102	LEU	CA-CB-CG	5.18	127.22	115.30
1	B	104	ASP	N-CA-C	-5.05	97.35	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	100	GLU	Peptide
1	B	103	LYS	Peptide
1	B	105	LEU	Peptide
1	B	244	LYS	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	1563	0	1540	96	0
1	B	1894	0	1765	217	0
All	All	3457	0	3305	313	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 46.

All (313) 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:B:219:LEU:O	1:B:222:ASN:O	1.54	1.25
1:B:115:SER:O	1:B:131:LYS:O	1.53	1.24
1:B:133:ILE:CB	1:B:174:CYS:O	1.87	1.22
1:B:223:LEU:HG	1:B:224:LYS:CB	1.69	1.20
1:B:256:ASP:OD2	1:B:261:THR:HG23	1.47	1.13
1:B:98:THR:HB	1:B:100:GLU:HG2	1.20	1.12
1:A:154:ARG:HG2	1:A:154:ARG:HH11	0.99	1.11
1:B:85:GLY:HA2	1:B:126:GLN:HE22	1.13	1.10
1:B:102:LEU:HD12	1:B:103:LYS:O	1.52	1.10
1:B:234:ASN:HA	1:B:235:ILE:CB	1.89	1.03
1:B:85:GLY:HA2	1:B:126:GLN:NE2	1.73	1.03
1:B:314:PHE:CE1	1:B:315:ASP:CG	2.37	0.98
1:B:225:ILE:HD11	1:B:228:ARG:CB	1.94	0.97
1:B:133:ILE:CB	1:B:174:CYS:HB3	1.96	0.95
1:B:223:LEU:CG	1:B:224:LYS:CB	2.44	0.95
1:A:154:ARG:HG2	1:A:154:ARG:NH1	1.75	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LEU:O	1:B:349:THR:OG1	1.86	0.93
1:A:314:PHE:HA	1:A:317:LEU:HB2	1.49	0.92
1:B:314:PHE:CE1	1:B:315:ASP:OD2	2.22	0.92
1:B:222:ASN:N	1:B:222:ASN:HD22	1.68	0.91
1:B:98:THR:CB	1:B:100:GLU:HG2	2.00	0.91
1:A:286:VAL:HG22	1:A:287:ARG:N	1.86	0.91
1:B:248:PHE:N	1:B:249:GLY:HA3	1.86	0.90
1:B:223:LEU:CB	1:B:224:LYS:CB	2.50	0.90
1:A:150:ASP:H	1:A:154:ARG:NH2	1.68	0.90
1:B:228:ARG:HA	1:B:229:ASP:HB2	1.53	0.89
1:A:286:VAL:O	1:A:288:SER:N	2.05	0.89
1:A:154:ARG:HH11	1:A:154:ARG:CG	1.85	0.89
1:B:223:LEU:HB3	1:B:224:LYS:CB	2.02	0.89
1:A:164:PHE:CB	1:A:177:CYS:N	2.37	0.87
1:A:314:PHE:O	1:A:318:THR:HG22	1.75	0.86
1:B:254:LEU:C	1:B:257:SER:OG	2.14	0.86
1:B:254:LEU:O	1:B:257:SER:OG	1.90	0.86
1:A:178:MET:HG3	1:A:179:GLU:H	1.40	0.86
1:B:224:LYS:O	1:B:225:ILE:HG23	1.75	0.84
1:B:232:PRO:CB	1:B:233:SER:HA	2.08	0.84
1:B:256:ASP:HB3	1:B:260:LYS:HA	1.59	0.83
1:B:154:ARG:O	1:B:218:HIS:HE1	1.59	0.83
1:A:321:VAL:HA	1:A:350:LYS:HZ1	1.43	0.83
1:B:225:ILE:CD1	1:B:228:ARG:CB	2.56	0.83
1:B:98:THR:HB	1:B:100:GLU:CG	2.05	0.83
1:B:133:ILE:CB	1:B:174:CYS:CB	2.57	0.82
1:A:321:VAL:HA	1:A:350:LYS:NZ	1.96	0.81
1:B:104:ASP:O	1:B:105:LEU:CB	2.29	0.81
1:A:191:TYR:O	1:A:196:LEU:HD13	1.79	0.81
1:B:102:LEU:O	1:B:119:MET:HG2	1.79	0.81
1:A:383:LYS:O	1:A:387:GLN:NE2	2.14	0.81
1:B:314:PHE:HE1	1:B:315:ASP:OD2	1.60	0.80
1:B:225:ILE:HD11	1:B:228:ARG:N	1.96	0.80
1:A:230:ILE:HG22	1:A:292:SER:HB2	1.64	0.79
1:A:342:ASN:O	1:A:346:LEU:HD21	1.83	0.78
1:B:232:PRO:HB2	1:B:233:SER:HA	1.65	0.78
1:B:231:LYS:HA	1:B:232:PRO:C	2.03	0.78
1:B:228:ARG:CB	1:B:229:ASP:HB3	2.14	0.78
1:B:219:LEU:O	1:B:223:LEU:CD1	2.32	0.77
1:B:107:GLU:HA	1:B:116:VAL:CG2	2.14	0.77
1:B:222:ASN:N	1:B:222:ASN:ND2	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:HIS:C	1:B:123:PRO:HD2	2.06	0.76
1:A:181:MET:HG3	1:A:236:LEU:HB3	1.68	0.76
1:B:100:GLU:HA	1:B:100:GLU:OE1	1.86	0.76
1:A:246:CYS:SG	1:A:247:ASP:N	2.59	0.75
1:B:143:LYS:HG3	1:B:254:LEU:HD21	1.67	0.75
1:A:151:VAL:C	1:A:154:ARG:HH12	1.89	0.74
1:B:100:GLU:OE1	1:B:100:GLU:CA	2.35	0.74
1:B:255:VAL:C	1:B:257:SER:OG	2.24	0.74
1:B:260:LYS:O	1:B:261:THR:HG22	1.88	0.74
1:A:286:VAL:CG2	1:A:287:ARG:N	2.52	0.73
1:B:255:VAL:O	1:B:256:ASP:O	2.06	0.73
1:B:256:ASP:OD2	1:B:260:LYS:C	2.27	0.73
1:B:256:ASP:CG	1:B:259:ALA:O	2.27	0.73
1:B:192:VAL:HB	1:B:198:ASP:HA	1.70	0.72
1:B:256:ASP:CB	1:B:260:LYS:HA	2.19	0.71
1:B:228:ARG:HA	1:B:229:ASP:CB	2.19	0.71
1:B:256:ASP:OD2	1:B:260:LYS:HA	1.91	0.71
1:B:255:VAL:O	1:B:256:ASP:C	2.29	0.71
1:B:181:MET:SD	1:B:237:LEU:HG	2.30	0.71
1:B:165:TYR:HE2	1:B:178:MET:O	1.73	0.70
1:B:330:ASN:HB3	1:B:334:ARG:HG2	1.72	0.70
1:B:228:ARG:CA	1:B:229:ASP:CB	2.68	0.70
1:B:219:LEU:O	1:B:223:LEU:HD13	1.91	0.70
1:A:239:ARG:HG2	1:A:382:CYS:SG	2.32	0.70
1:A:154:ARG:NH1	1:A:154:ARG:H	1.90	0.70
1:B:122:LYS:N	1:B:123:PRO:CD	2.55	0.70
1:B:164:PHE:CE1	1:B:178:MET:SD	2.84	0.70
1:B:255:VAL:O	1:B:257:SER:OG	2.09	0.70
1:B:254:LEU:O	1:B:257:SER:CB	2.40	0.69
1:A:178:MET:HG3	1:A:179:GLU:N	2.06	0.69
1:B:183:THR:O	1:B:236:LEU:N	2.26	0.69
1:A:192:VAL:O	1:A:193:TYR:HB2	1.91	0.69
1:B:367:ILE:HD12	1:B:368:LEU:N	2.09	0.68
1:A:191:TYR:O	1:A:196:LEU:CD1	2.40	0.68
1:A:162:VAL:HG23	1:A:179:GLU:OE1	1.94	0.68
1:B:133:ILE:CB	1:B:174:CYS:C	2.60	0.68
1:B:122:LYS:N	1:B:123:PRO:HD2	2.09	0.67
1:B:364:HIS:O	1:B:367:ILE:HG13	1.95	0.67
1:B:107:GLU:HA	1:B:116:VAL:HG22	1.77	0.66
1:B:219:LEU:C	1:B:222:ASN:O	2.34	0.66
1:B:256:ASP:OD2	1:B:261:THR:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ILE:HG12	1:B:127:ILE:O	1.94	0.66
1:A:380:TYR:O	1:A:384:ILE:HG12	1.95	0.66
1:B:115:SER:O	1:B:131:LYS:C	2.32	0.66
1:B:234:ASN:CA	1:B:235:ILE:CB	2.68	0.66
1:B:120:VAL:CG2	1:B:127:ILE:HA	2.25	0.65
1:B:232:PRO:CG	1:B:233:SER:HA	2.27	0.65
1:A:321:VAL:O	1:A:322:LYS:HB2	1.97	0.65
1:B:157:ASP:HB2	1:B:218:HIS:NE2	2.12	0.64
1:A:328:LEU:HD11	1:A:336:PHE:HE2	1.61	0.64
1:A:385:LEU:O	1:A:388:MET:HG3	1.97	0.64
1:A:304:ARG:HD2	1:A:305:PHE:H	1.62	0.64
1:B:85:GLY:CA	1:B:126:GLN:NE2	2.56	0.63
1:B:258:ILE:HG22	1:B:258:ILE:O	1.99	0.63
1:A:307:TYR:OH	1:A:324:ASP:O	2.11	0.63
1:B:133:ILE:CB	1:B:174:CYS:CA	2.78	0.62
1:A:315:ASP:O	1:A:319:GLN:NE2	2.33	0.62
1:B:256:ASP:OD2	1:B:261:THR:CG2	2.37	0.62
1:B:225:ILE:HD11	1:B:228:ARG:CA	2.29	0.62
1:B:117:ASN:O	1:B:118:LYS:C	2.34	0.61
1:B:120:VAL:HG23	1:B:127:ILE:HA	1.81	0.61
1:B:361:LEU:O	1:B:367:ILE:HG12	2.00	0.61
1:B:314:PHE:CE1	1:B:315:ASP:OD1	2.54	0.61
1:B:256:ASP:CG	1:B:260:LYS:HA	2.22	0.60
1:A:344:VAL:HG12	1:A:348:LEU:HD11	1.83	0.60
1:B:193:TYR:H	1:B:196:LEU:HG	1.66	0.60
1:A:193:TYR:HA	1:A:198:ASP:HB3	1.83	0.60
1:B:160:TYR:HA	1:B:242:ASN:ND2	2.17	0.60
1:B:103:LYS:HA	1:B:119:MET:HG3	1.84	0.60
1:B:225:ILE:HG13	1:B:227:HIS:H	1.67	0.60
1:A:346:LEU:HD23	1:A:346:LEU:H	1.65	0.60
1:B:256:ASP:OD2	1:B:260:LYS:CA	2.50	0.59
1:B:134:ARG:O	1:B:135:SER:CB	2.51	0.59
1:B:248:PHE:N	1:B:249:GLY:CA	2.64	0.59
1:A:194:SER:OG	1:A:195:VAL:N	2.35	0.59
1:B:151:VAL:HG23	1:B:152:VAL:HG13	1.84	0.58
1:B:214:LYS:HE2	1:B:362:LEU:HD11	1.86	0.58
1:A:163:GLN:HA	1:A:178:MET:H	1.69	0.58
1:B:134:ARG:O	1:B:135:SER:HB2	2.04	0.58
1:B:232:PRO:HB2	1:B:233:SER:CA	2.31	0.58
1:B:368:LEU:HA	1:B:371:GLU:HB2	1.86	0.57
1:B:228:ARG:CB	1:B:229:ASP:CB	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:THR:O	1:B:262:ARG:CB	2.53	0.57
1:B:79:MET:SD	1:B:79:MET:N	2.78	0.57
1:B:85:GLY:CA	1:B:126:GLN:HE22	2.02	0.57
1:B:102:LEU:CD1	1:B:103:LYS:O	2.39	0.57
1:A:318:THR:O	1:A:321:VAL:N	2.38	0.56
1:B:321:VAL:O	1:B:323:GLY:N	2.38	0.56
1:A:154:ARG:NH1	1:A:154:ARG:N	2.53	0.56
1:B:232:PRO:HG2	1:B:233:SER:HA	1.87	0.56
1:B:260:LYS:C	1:B:261:THR:CG2	2.74	0.56
1:A:232:PRO:HB3	1:A:300:LEU:HD21	1.88	0.56
1:B:115:SER:HB2	1:B:132:ARG:CB	2.36	0.56
1:B:264:ALA:O	1:B:265:GLY:C	2.44	0.56
1:B:120:VAL:CG2	1:B:127:ILE:HG22	2.35	0.56
1:A:205:LEU:HA	1:A:208:ILE:HD12	1.88	0.55
1:B:165:TYR:CE2	1:B:178:MET:O	2.58	0.55
1:B:98:THR:CB	1:B:100:GLU:H	2.19	0.55
1:B:256:ASP:OD1	1:B:259:ALA:O	2.25	0.55
1:B:149:LEU:O	1:B:150:ASP:O	2.24	0.55
1:B:154:ARG:O	1:B:218:HIS:CE1	2.50	0.55
1:B:182:SER:OG	1:B:237:LEU:HA	2.06	0.55
1:A:386:ASP:O	1:A:387:GLN:HB3	2.07	0.54
1:B:123:PRO:HG2	1:B:124:SER:H	1.72	0.54
1:B:182:SER:HB2	1:B:236:LEU:O	2.08	0.54
1:B:198:ASP:O	1:B:200:ILE:N	2.41	0.54
1:B:314:PHE:CD1	1:B:315:ASP:CG	2.81	0.54
1:B:185:PHE:HA	1:B:188:PHE:HB3	1.89	0.54
1:A:372:GLU:O	1:A:372:GLU:HG3	2.07	0.54
1:B:98:THR:OG1	1:B:100:GLU:HB2	2.08	0.54
1:B:158:CYS:SG	1:B:215:ALA:HA	2.47	0.54
1:B:150:ASP:O	1:B:152:VAL:N	2.41	0.54
1:B:238:ASP:CG	1:B:239:ARG:N	2.62	0.54
1:B:314:PHE:CD1	1:B:315:ASP:N	2.76	0.54
1:B:133:ILE:CA	1:B:174:CYS:O	2.56	0.53
1:B:205:LEU:HA	1:B:208:ILE:HD12	1.90	0.53
1:B:228:ARG:CA	1:B:229:ASP:HB2	2.29	0.53
1:B:253:GLN:O	1:B:257:SER:OG	2.26	0.53
1:A:223:LEU:O	1:A:225:ILE:N	2.42	0.53
1:B:254:LEU:O	1:B:257:SER:HB2	2.07	0.53
1:B:165:TYR:OH	1:B:179:GLU:HA	2.09	0.53
1:A:178:MET:CG	1:A:179:GLU:H	2.19	0.53
1:B:222:ASN:HD22	1:B:222:ASN:H	1.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:GLN:O	1:B:328:LEU:HD12	2.10	0.52
1:B:226:ILE:O	1:B:227:HIS:CB	2.58	0.52
1:B:100:GLU:OE1	1:B:100:GLU:N	2.42	0.52
1:A:177:CYS:O	1:A:178:MET:HB3	2.09	0.52
1:A:286:VAL:C	1:A:288:SER:N	2.58	0.52
1:B:80:SER:HB3	1:B:95:TRP:HA	1.92	0.51
1:A:197:ASP:OD1	1:A:199:VAL:HG22	2.10	0.51
1:A:210:LEU:HD11	1:A:371:GLU:HA	1.91	0.51
1:B:150:ASP:OD1	1:B:150:ASP:N	2.43	0.51
1:A:349:THR:O	1:A:355:ARG:NH1	2.39	0.51
1:B:232:PRO:CB	1:B:233:SER:CA	2.86	0.51
1:B:330:ASN:HD22	1:B:334:ARG:HA	1.75	0.51
1:A:319:GLN:N	1:A:319:GLN:CD	2.65	0.50
1:A:180:LEU:HD23	1:A:180:LEU:O	2.11	0.50
1:B:158:CYS:SG	1:B:161:ILE:HG13	2.52	0.50
1:B:184:SER:HA	1:B:235:ILE:N	2.26	0.49
1:A:226:ILE:HG21	1:A:285:ASP:O	2.12	0.49
1:A:302:THR:O	1:A:303:GLY:C	2.51	0.49
1:A:164:PHE:H	1:A:177:CYS:N	2.10	0.49
1:A:232:PRO:HA	1:A:235:ILE:HD12	1.93	0.49
1:A:330:ASN:HB2	1:A:334:ARG:HA	1.95	0.49
1:A:291:TRP:HA	1:A:347:CYS:O	2.12	0.49
1:B:120:VAL:CG2	1:B:127:ILE:CA	2.90	0.49
1:B:151:VAL:HG23	1:B:152:VAL:H	1.78	0.49
1:B:229:ASP:C	1:B:229:ASP:OD1	2.48	0.49
1:A:371:GLU:O	1:A:372:GLU:HB3	2.12	0.49
1:B:260:LYS:C	1:B:261:THR:HG22	2.32	0.49
1:A:198:ASP:OD1	1:A:198:ASP:N	2.45	0.48
1:B:142:GLN:O	1:B:146:LEU:HD22	2.14	0.48
1:A:152:VAL:N	1:A:154:ARG:HH12	2.12	0.48
1:B:185:PHE:CZ	1:B:236:LEU:HD23	2.48	0.48
1:B:237:LEU:HD12	1:B:239:ARG:O	2.14	0.48
1:A:286:VAL:O	1:A:287:ARG:C	2.51	0.47
1:A:386:ASP:N	1:A:387:GLN:HE22	2.11	0.47
1:B:298:TYR:O	1:B:302:THR:HG22	2.13	0.47
1:B:357:LYS:HB2	1:B:360:GLU:OE2	2.13	0.47
1:B:98:THR:CG2	1:B:100:GLU:HG2	2.44	0.47
1:B:121:HIS:O	1:B:125:GLY:N	2.41	0.47
1:B:84:SER:OG	1:B:89:ILE:HG13	2.15	0.47
1:B:124:SER:OG	1:B:125:GLY:N	2.48	0.47
1:B:120:VAL:HG22	1:B:127:ILE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ASP:O	1:B:292:SER:OG	2.30	0.47
1:A:325:PRO:HB2	1:A:327:GLN:HG2	1.97	0.47
1:B:120:VAL:HG13	1:B:121:HIS:N	2.29	0.47
1:B:360:GLU:CD	1:B:360:GLU:H	2.18	0.47
1:A:216:LEU:HD21	1:A:230:ILE:HD13	1.97	0.47
1:A:286:VAL:HG22	1:A:287:ARG:H	1.72	0.46
1:B:182:SER:H	1:B:237:LEU:HA	1.80	0.46
1:A:181:MET:HG3	1:A:236:LEU:CB	2.42	0.46
1:A:195:VAL:C	1:A:196:LEU:HG	2.36	0.46
1:B:116:VAL:HA	1:B:130:VAL:O	2.15	0.46
1:B:160:TYR:CD1	1:B:211:ALA:HA	2.50	0.46
1:B:299:GLU:HG3	1:B:305:PHE:HA	1.97	0.46
1:B:120:VAL:HG23	1:B:127:ILE:CA	2.43	0.46
1:B:170:ARG:N	1:B:173:ASP:O	2.48	0.46
1:A:162:VAL:N	1:A:179:GLU:OE1	2.48	0.46
1:A:164:PHE:N	1:A:177:CYS:N	2.65	0.46
1:A:342:ASN:C	1:A:346:LEU:HD21	2.36	0.46
1:B:223:LEU:HA	1:B:223:LEU:HD12	1.21	0.46
1:B:326:PRO:O	1:B:328:LEU:N	2.42	0.46
1:A:286:VAL:C	1:A:288:SER:H	2.19	0.45
1:B:193:TYR:CB	1:B:198:ASP:CB	2.94	0.45
1:B:290:VAL:HA	1:B:293:LEU:HB3	1.97	0.45
1:A:298:TYR:HE1	1:A:328:LEU:HA	1.81	0.45
1:B:84:SER:OG	1:B:84:SER:O	2.32	0.45
1:B:156:SER:O	1:B:157:ASP:C	2.54	0.45
1:B:256:ASP:C	1:B:257:SER:OG	2.53	0.45
1:A:346:LEU:HD23	1:A:346:LEU:N	2.29	0.45
1:A:226:ILE:O	1:A:227:HIS:ND1	2.50	0.45
1:B:89:ILE:HG12	1:B:89:ILE:O	2.16	0.45
1:B:349:THR:HG21	1:B:354:LYS:O	2.17	0.45
1:B:185:PHE:O	1:B:186:ASP:C	2.55	0.45
1:B:226:ILE:HG21	1:B:264:ALA:O	2.16	0.45
1:A:178:MET:O	1:A:179:GLU:HB3	2.17	0.44
1:A:331:SER:O	1:A:332:GLU:HG2	2.17	0.44
1:A:229:ASP:O	1:A:248:PHE:HZ	2.00	0.44
1:A:329:SER:O	1:A:331:SER:N	2.51	0.44
1:B:123:PRO:HG2	1:B:124:SER:N	2.32	0.44
1:B:123:PRO:CG	1:B:124:SER:H	2.30	0.44
1:B:193:TYR:N	1:B:196:LEU:HG	2.32	0.44
1:B:219:LEU:O	1:B:223:LEU:HD12	2.13	0.44
1:A:376:GLU:HG3	1:A:379:CYS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ILE:HD11	1:B:228:ARG:H	1.79	0.44
1:A:319:GLN:NE2	1:A:319:GLN:N	2.66	0.44
1:A:321:VAL:HA	1:A:350:LYS:HZ3	1.81	0.44
1:B:81:ILE:HD12	1:B:97:PHE:CB	2.47	0.44
1:A:163:GLN:HE21	1:A:163:GLN:HB3	1.56	0.44
1:A:319:GLN:NE2	1:A:319:GLN:H	2.16	0.44
1:B:143:LYS:HG2	1:B:144:GLN:N	2.33	0.44
1:B:288:SER:O	1:B:289:ASP:C	2.55	0.43
1:A:230:ILE:CG2	1:A:292:SER:HB2	2.43	0.43
1:A:386:ASP:C	1:A:387:GLN:NE2	2.71	0.43
1:B:147:MET:SD	1:B:147:MET:C	2.97	0.43
1:B:226:ILE:O	1:B:226:ILE:HG12	2.12	0.43
1:A:195:VAL:H	1:A:196:LEU:HG	1.83	0.43
1:B:99:ALA:C	1:B:100:GLU:OE1	2.57	0.43
1:B:230:ILE:HD13	1:B:296:THR:OG1	2.19	0.43
1:A:150:ASP:HB3	1:A:163:GLN:HE22	1.83	0.43
1:B:130:VAL:O	1:B:130:VAL:CG2	2.66	0.43
1:B:326:PRO:C	1:B:328:LEU:H	2.20	0.43
1:B:143:LYS:HG3	1:B:254:LEU:CD2	2.45	0.43
1:B:341:ILE:HG12	1:B:345:ASN:HD21	1.84	0.43
1:B:79:MET:O	1:B:97:PHE:CB	2.67	0.43
1:B:237:LEU:HD13	1:B:238:ASP:OD2	2.19	0.43
1:A:227:HIS:HD2	1:A:248:PHE:CZ	2.37	0.42
1:B:123:PRO:CG	1:B:124:SER:N	2.83	0.42
1:B:181:MET:SD	1:B:237:LEU:CG	3.05	0.42
1:B:152:VAL:HB	1:B:164:PHE:HD2	1.84	0.42
1:A:183:THR:HG23	1:A:184:SER:O	2.20	0.42
1:A:189:TYR:O	1:A:193:TYR:HD2	2.03	0.42
1:B:214:LYS:HD3	1:B:362:LEU:HD21	2.02	0.42
1:A:358:TYR:O	1:A:362:LEU:HB2	2.19	0.42
1:B:158:CYS:HA	1:B:159:PRO:HD3	1.81	0.42
1:B:120:VAL:HG23	1:B:127:ILE:CB	2.50	0.41
1:B:247:ASP:HB2	1:B:250:ILE:HG22	2.01	0.41
1:A:219:LEU:O	1:A:223:LEU:O	2.38	0.41
1:B:149:LEU:HB3	1:B:150:ASP:H	1.58	0.41
1:A:231:LYS:O	1:A:235:ILE:HG13	2.20	0.41
1:B:151:VAL:HG23	1:B:152:VAL:N	2.36	0.41
1:B:158:CYS:HB2	1:B:218:HIS:CG	2.56	0.41
1:B:182:SER:CB	1:B:236:LEU:O	2.68	0.41
1:B:230:ILE:CG1	1:B:292:SER:HB2	2.50	0.41
1:B:224:LYS:O	1:B:225:ILE:CG2	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:CYS:SG	1:B:160:TYR:HB2	2.61	0.41
1:B:229:ASP:OD1	1:B:230:ILE:N	2.54	0.40
1:B:327:GLN:O	1:B:328:LEU:CD1	2.69	0.40
1:B:191:TYR:O	1:B:196:LEU:HD11	2.22	0.40
1:B:245:LEU:HA	1:B:245:LEU:HD12	1.80	0.40
1:B:253:GLN:O	1:B:257:SER:CB	2.70	0.40
1:A:201:PRO:HB2	1:A:204:ILE:H	1.86	0.40
1:B:131:LYS:O	1:B:132:ARG:CB	2.68	0.40
1:B:253:GLN:HE21	1:B:253:GLN:HB2	1.71	0.40
1:B:314:PHE:CG	1:B:315:ASP:N	2.89	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	197/327 (60%)	142 (72%)	26 (13%)	29 (15%)	0 3
1	B	248/327 (76%)	169 (68%)	52 (21%)	27 (11%)	0 6
All	All	445/654 (68%)	311 (70%)	78 (18%)	56 (13%)	0 5

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	MET
1	A	247	ASP
1	A	287	ARG
1	A	330	ASN
1	A	334	ARG
1	A	387	GLN
1	B	89	ILE
1	B	105	LEU

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Mol	Chain	Res	Type
1	B	150	ASP
1	B	151	VAL
1	B	227	HIS
1	B	229	ASP
1	B	231	LYS
1	B	232	PRO
1	B	235	ILE
1	B	322	LYS
1	A	150	ASP
1	A	155	SER
1	A	224	LYS
1	A	231	LYS
1	A	249	GLY
1	A	303	GLY
1	A	308	PRO
1	A	311	ASN
1	A	319	GLN
1	A	322	LYS
1	A	325	PRO
1	B	101	ASP
1	B	149	LEU
1	B	225	ILE
1	B	262	ARG
1	B	327	GLN
1	B	330	ASN
1	A	194	SER
1	A	196	LEU
1	A	227	HIS
1	A	228	ARG
1	A	328	LEU
1	A	374	ALA
1	B	87	LEU
1	B	134	ARG
1	B	157	ASP
1	B	224	LYS
1	A	197	ASP
1	A	359	LYS
1	B	240	SER
1	B	312	SER
1	B	357	LYS
1	A	163	GLN
1	A	193	TYR

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Mol	Chain	Res	Type
1	A	337	SER
1	B	104	ASP
1	B	132	ARG
1	B	199	VAL
1	A	199	VAL
1	B	241	GLY

5.3.2 Protein sidechains (i)

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	172/296 (58%)	138 (80%)	34 (20%)	1 7
1	B	196/296 (66%)	163 (83%)	33 (17%)	2 12
All	All	368/592 (62%)	301 (82%)	67 (18%)	1 9

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	149	LEU
1	A	153	MET
1	A	154	ARG
1	A	158	CYS
1	A	163	GLN
1	A	180	LEU
1	A	182	SER
1	A	183	THR
1	A	189	TYR
1	A	192	VAL
1	A	194	SER
1	A	196	LEU
1	A	198	ASP
1	A	223	LEU
1	A	227	HIS
1	A	230	ILE

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Mol	Chain	Res	Type
1	A	245	LEU
1	A	286	VAL
1	A	292	SER
1	A	314	PHE
1	A	318	THR
1	A	319	GLN
1	A	324	ASP
1	A	325	PRO
1	A	331	SER
1	A	333	GLU
1	A	346	LEU
1	A	352	GLU
1	A	359	LYS
1	A	368	LEU
1	A	369	MET
1	A	379	CYS
1	A	387	GLN
1	B	79	MET
1	B	88	LYS
1	B	100	GLU
1	B	101	ASP
1	B	102	LEU
1	B	119	MET
1	B	127	ILE
1	B	130	VAL
1	B	146	LEU
1	B	162	VAL
1	B	171	GLU
1	B	195	VAL
1	B	196	LEU
1	B	222	ASN
1	B	223	LEU
1	B	226	ILE
1	B	234	ASN
1	B	236	LEU
1	B	237	LEU
1	B	238	ASP
1	B	246	CYS
1	B	247	ASP
1	B	250	ILE
1	B	253	GLN
1	B	257	SER

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Mol	Chain	Res	Type
1	B	261	THR
1	B	296	THR
1	B	328	LEU
1	B	359	LYS
1	B	360	GLU
1	B	368	LEU
1	B	369	MET
1	B	372	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	B	126	GLN
1	B	218	HIS
1	B	222	ASN
1	B	242	ASN
1	B	253	GLN
1	B	345	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 monosaccharides 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	203/327 (62%)	-0.28	1 (0%)	91	88	64, 98, 143, 166	0
1	B	260/327 (79%)	-0.19	3 (1%)	79	73	58, 99, 134, 171	0
All	All	463/654 (70%)	-0.23	4 (0%)	84	79	58, 99, 137, 171	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	ILE	3.3
1	B	333	GLU	3.0
1	B	227	HIS	2.5
1	B	334	ARG	2.3

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 monosaccharides 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.