Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:27 PM GMT

PDB ID	:	3R2B
Title	:	MK2 kinase bound to Compound 5b
Authors	:	Oubrie, A.; van Zeeland, M.; Versteegh, J.
Deposited on	:	2011-03-14
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

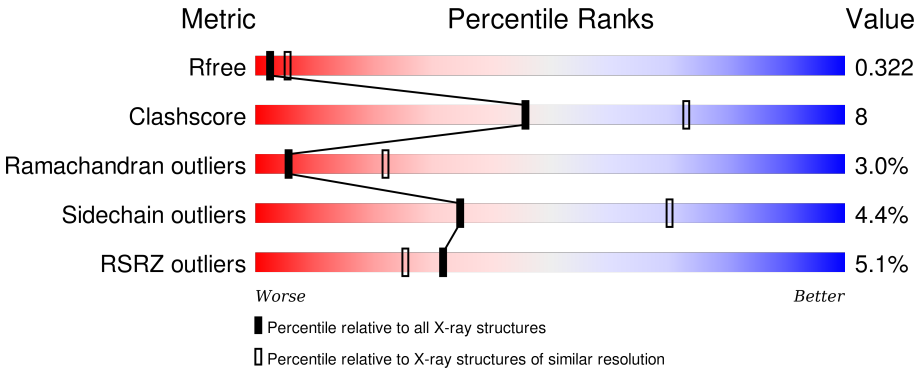
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	318	2% 67% 16% • 14%
1	B	318	3% 64% 19% • 14%
1	C	318	4% 69% 15% • 14%
1	D	318	3% 69% 14% • 14%
1	E	318	3% 66% 17% • 14%

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Mol	Chain	Length	Quality of chain
1	F	318	4% 68% 14% 14%
1	G	318	3% 68% 15% 14%
1	H	318	8% 69% 14% 14%
1	I	318	5% 68% 15% 14%
1	J	318	4% 69% 14% 14%
1	K	318	10% 67% 17% 14%
1	L	318	4% 65% 19% 14%

2 Entry composition (i)

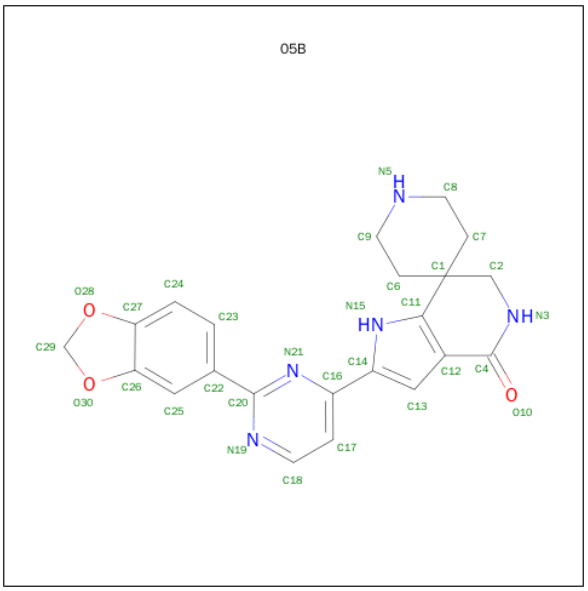
There are 2 unique types of molecules in this entry. The entry contains 26381 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	272	Total	C	N	O	S	0	0	0
			2194	1405	374	398	17			
1	B	272	Total	C	N	O	S	0	0	0
			2197	1405	376	399	17			
1	C	272	Total	C	N	O	S	0	0	0
			2197	1406	375	399	17			
1	D	272	Total	C	N	O	S	0	0	0
			2193	1404	374	398	17			
1	E	272	Total	C	N	O	S	0	0	0
			2198	1407	375	399	17			
1	F	272	Total	C	N	O	S	0	0	0
			2191	1402	374	398	17			
1	G	272	Total	C	N	O	S	0	0	0
			2191	1404	373	397	17			
1	H	272	Total	C	N	O	S	0	0	0
			2187	1400	373	397	17			
1	I	272	Total	C	N	O	S	0	0	0
			2181	1395	372	397	17			
1	J	272	Total	C	N	O	S	0	0	0
			2195	1405	375	398	17			
1	K	272	Total	C	N	O	S	0	0	0
			2196	1405	375	399	17			
1	L	272	Total	C	N	O	S	0	0	0
			2201	1410	375	399	17			

- Molecule 2 is 2'-[2-(1,3-BENZODIOXOL-5-YL)PYRIMIDIN-4-YL]-5',6'-DIHYDROSPIRO[PIPERIDINE-4,7'-PYRROLO[3,2-C]PYRIDIN]-4'(1'H)-ONE (three-letter code: 05B) (formula: $C_{22}H_{21}N_5O_3$).



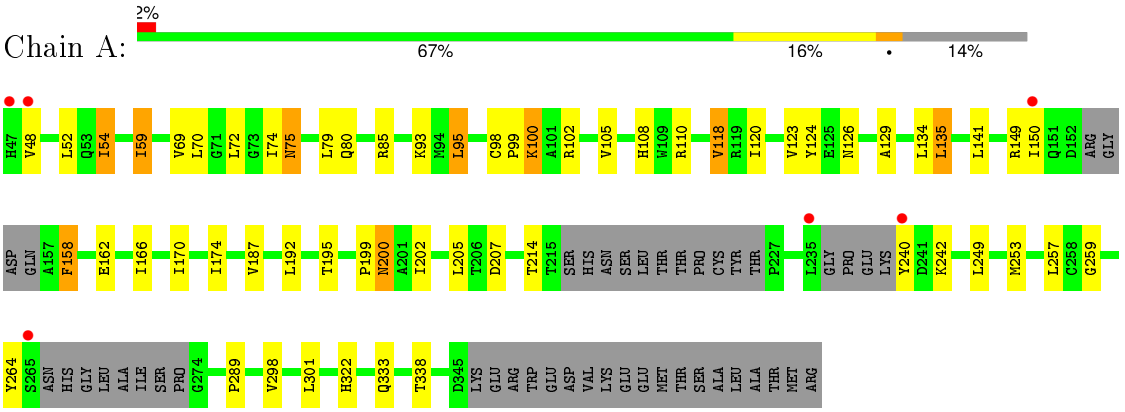
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	22	5	3		
2	B	1	Total	C	N	O	0	0
			30	22	5	3		

3 Residue-property plots (i)

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

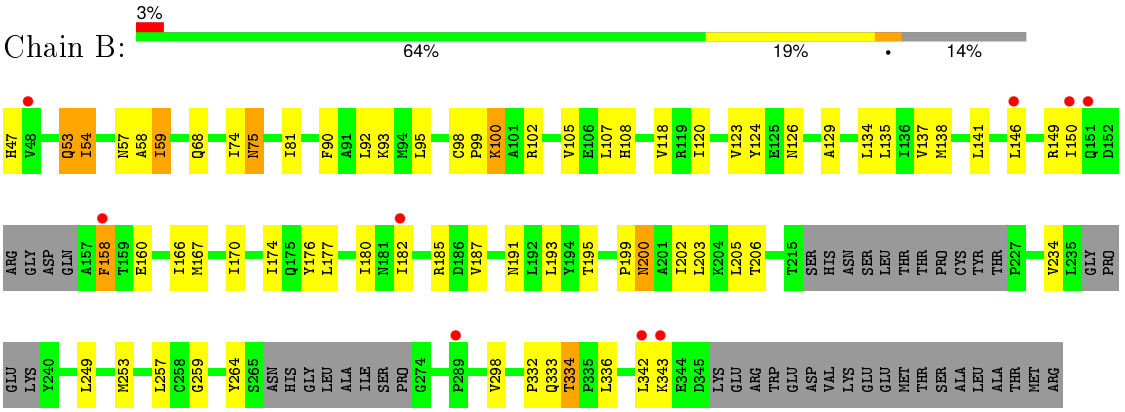
- Molecule 1: MAP kinase-activated protein kinase 2

Chain A:



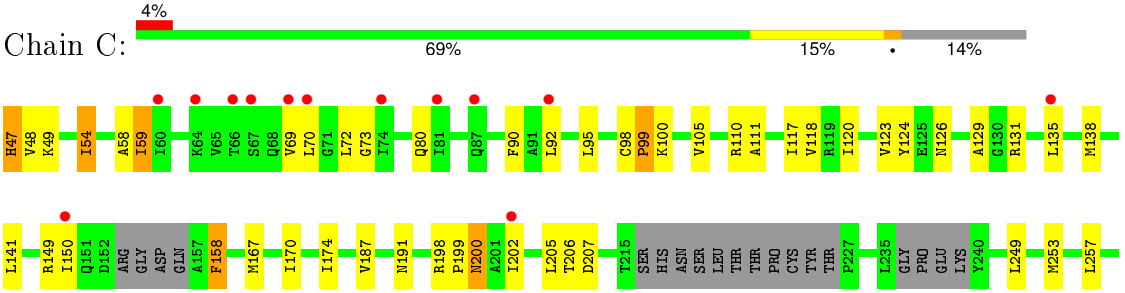
- Molecule 1: MAP kinase-activated protein kinase 2

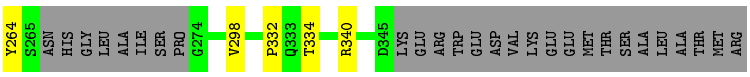
Chain B:



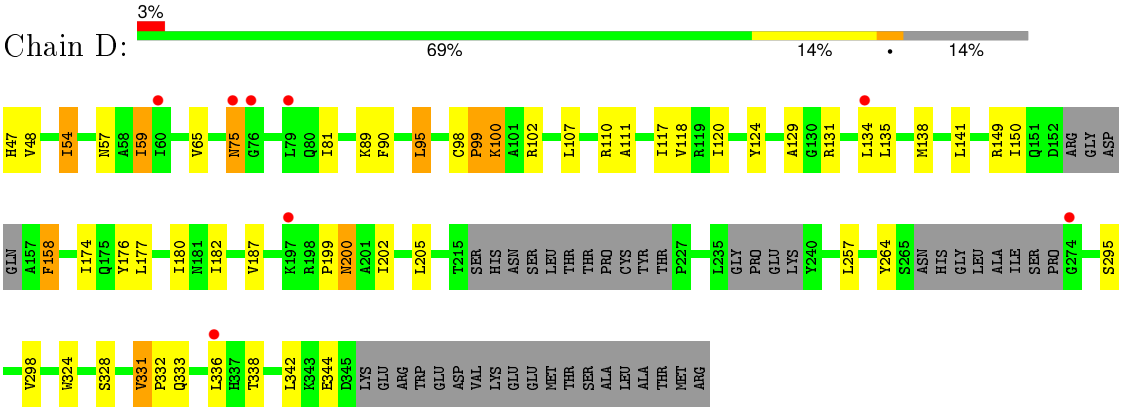
- Molecule 1: MAP kinase-activated protein kinase 2

Chain C:

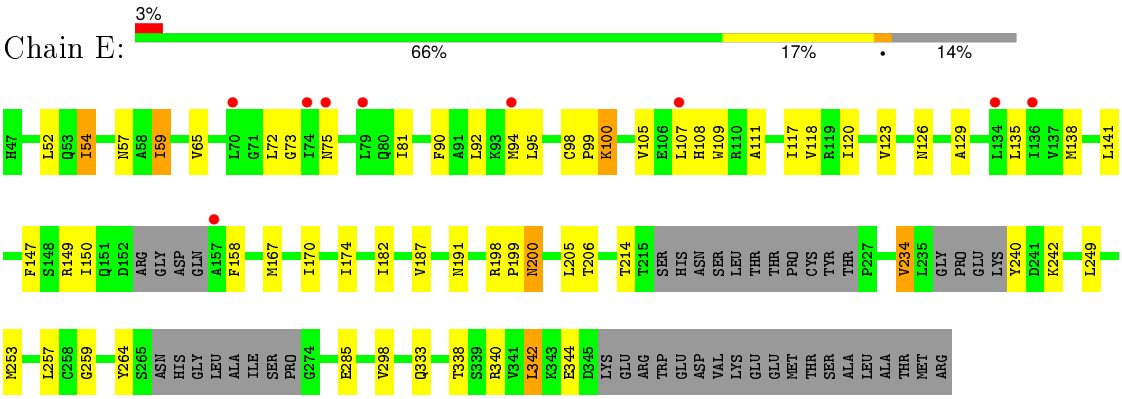




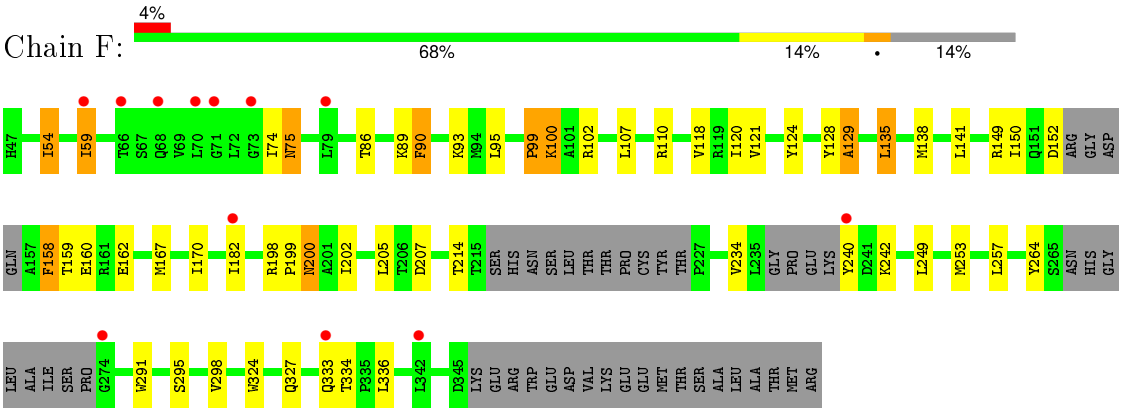
• Molecule 1: MAP kinase-activated protein kinase 2



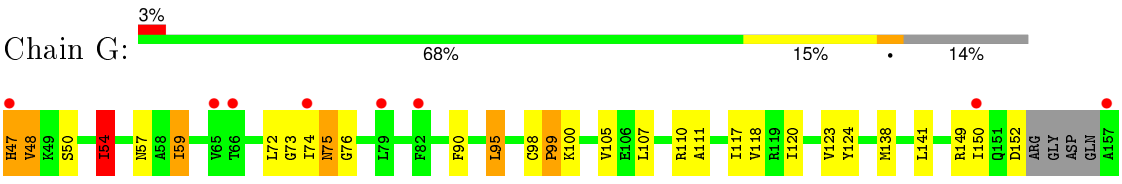
• Molecule 1: MAP kinase-activated protein kinase 2

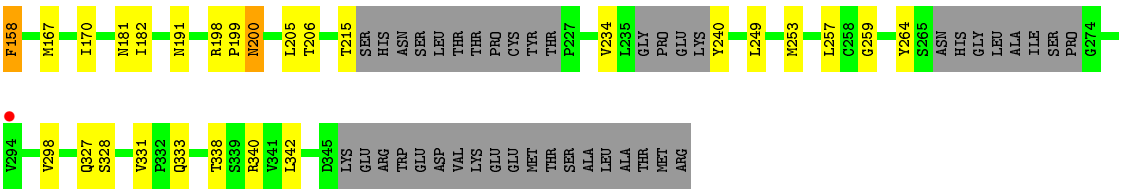


• Molecule 1: MAP kinase-activated protein kinase 2

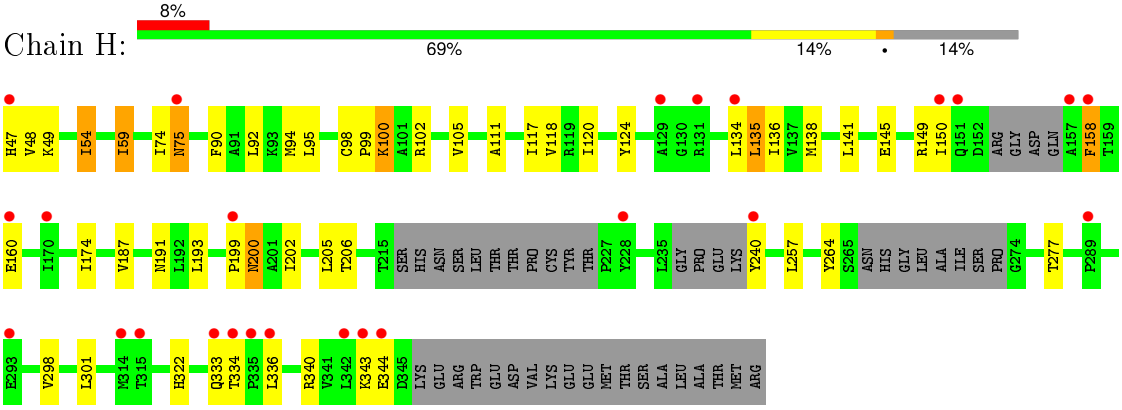


• Molecule 1: MAP kinase-activated protein kinase 2

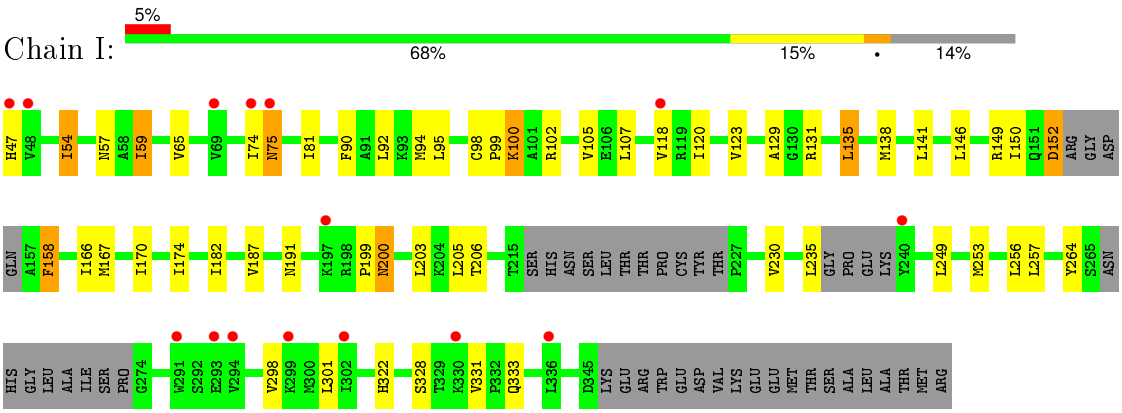




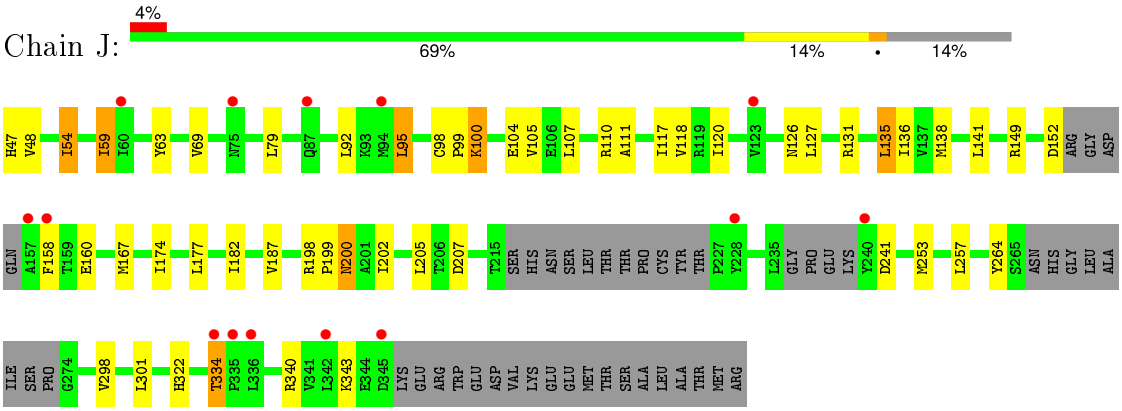
• Molecule 1: MAP kinase-activated protein kinase 2



• Molecule 1: MAP kinase-activated protein kinase 2

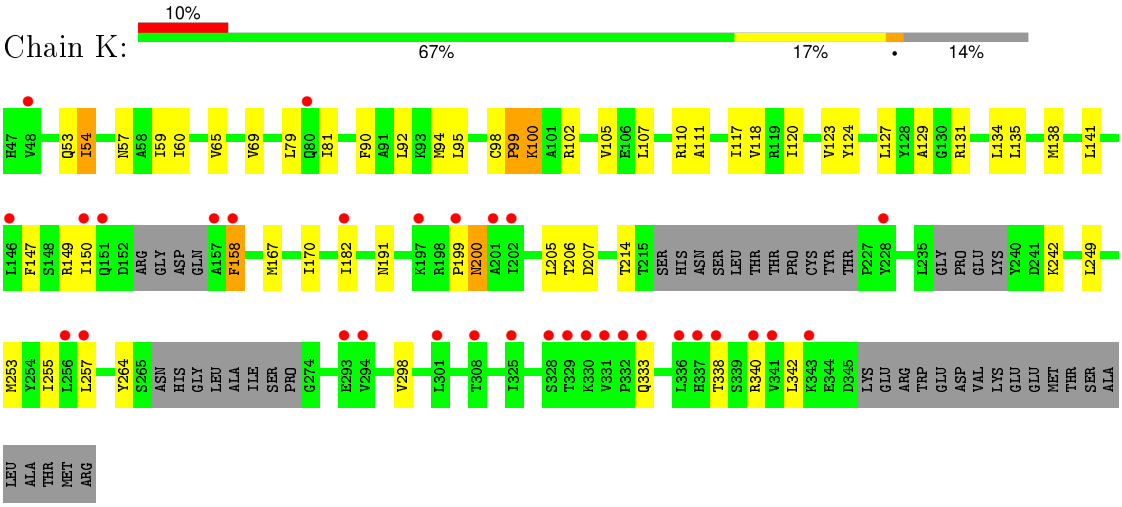


• Molecule 1: MAP kinase-activated protein kinase 2



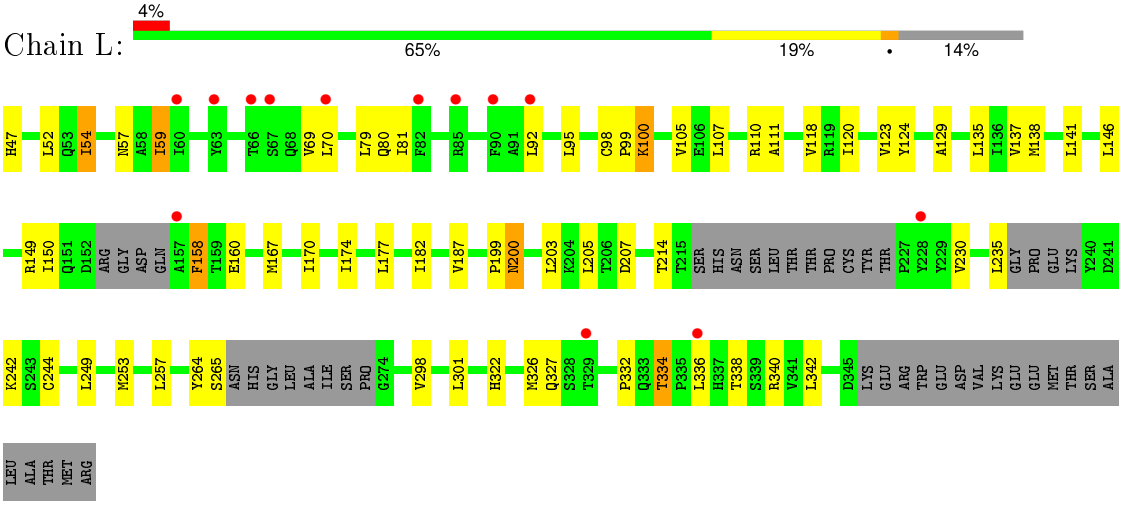
• Molecule 1: MAP kinase-activated protein kinase 2

Chain K:



• Molecule 1: MAP kinase-activated protein kinase 2

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	139.80Å 180.25Å 217.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.97 – 2.90 51.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	61.3 (51.97-2.90) 61.3 (51.97-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.4.0078	Depositor
R, R_{free}	0.277 , 0.316 0.282 , 0.322	Depositor DCC
R_{free} test set	3743 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	91.0	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 74643 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	26381	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 05B

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	0.33	0/2239	0.51	0/3020
1	B	0.31	0/2242	0.50	0/3022
1	C	0.33	0/2242	0.49	0/3024
1	D	0.33	0/2238	0.50	0/3018
1	E	0.31	0/2243	0.50	0/3025
1	F	0.33	0/2236	0.51	0/3016
1	G	0.31	0/2236	0.48	0/3016
1	H	0.30	0/2232	0.48	0/3011
1	I	0.31	0/2226	0.48	0/3004
1	J	0.31	0/2240	0.51	0/3020
1	K	0.30	0/2241	0.48	0/3022
1	L	0.31	0/2246	0.49	0/3029
All	All	0.31	0/26861	0.49	0/36227

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2194	0	2203	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2197	0	2204	45	0
1	C	2197	0	2207	35	0
1	D	2193	0	2198	32	0
1	E	2198	0	2209	33	0
1	F	2191	0	2194	32	0
1	G	2191	0	2199	38	0
1	H	2187	0	2188	26	0
1	I	2181	0	2170	31	0
1	J	2195	0	2205	33	0
1	K	2196	0	2202	35	0
1	L	2201	0	2218	39	0
2	A	30	0	21	1	0
2	B	30	0	21	1	0
All	All	26381	0	26439	405	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 8.

All (405) 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:118:VAL:CG1	1:A:141:LEU:HD11	2.05	0.86
1:H:105:VAL:HG12	1:H:136:ILE:HD11	1.55	0.86
1:C:48:VAL:HG11	1:K:59:ILE:HD12	1.59	0.84
1:C:48:VAL:HG11	1:K:59:ILE:CD1	2.08	0.83
1:B:118:VAL:HG22	1:B:141:LEU:HD11	1.61	0.82
1:K:118:VAL:HG22	1:K:141:LEU:HD11	1.60	0.81
1:H:118:VAL:HG22	1:H:141:LEU:HD11	1.63	0.80
1:J:107:LEU:HD22	1:J:182:ILE:HD12	1.64	0.80
1:A:69:VAL:HG22	1:A:79:LEU:HD22	1.61	0.80
1:L:107:LEU:HD22	1:L:182:ILE:HD12	1.62	0.80
1:A:257:LEU:HD21	1:A:298:VAL:HG11	1.62	0.80
1:C:118:VAL:HG22	1:C:141:LEU:HD11	1.64	0.80
1:L:118:VAL:HG22	1:L:141:LEU:HD11	1.65	0.79
1:D:295:SER:OG	1:D:298:VAL:HG23	1.83	0.78
1:A:118:VAL:HG13	1:A:141:LEU:HD11	1.63	0.77
1:J:118:VAL:HG22	1:J:141:LEU:HD11	1.67	0.77
1:C:48:VAL:HG12	1:K:60:ILE:HG23	1.65	0.76
1:H:174:ILE:HD11	1:H:187:VAL:HG21	1.66	0.75
1:K:107:LEU:HD22	1:K:182:ILE:HD12	1.68	0.75
1:K:120:ILE:HG22	1:K:138:MET:HG2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:118:VAL:HG22	1:I:141:LEU:HD11	1.67	0.74
1:I:120:ILE:HG22	1:I:138:MET:HG2	1.70	0.74
1:F:118:VAL:HG22	1:F:141:LEU:HD11	1.70	0.74
1:E:107:LEU:HD22	1:E:182:ILE:CD1	2.18	0.73
1:C:118:VAL:CG2	1:C:141:LEU:HD11	2.19	0.72
1:D:118:VAL:HG22	1:D:141:LEU:HD11	1.72	0.72
1:J:257:LEU:HD21	1:J:298:VAL:HG11	1.71	0.72
1:F:107:LEU:HD22	1:F:182:ILE:CD1	2.20	0.71
1:C:332:PRO:HB2	1:C:334:THR:HG23	1.72	0.71
1:A:70:LEU:HD21	1:A:80:GLN:HB2	1.72	0.71
1:K:257:LEU:HD21	1:K:298:VAL:HG11	1.73	0.70
1:G:257:LEU:HD21	1:G:298:VAL:HG11	1.71	0.70
1:J:174:ILE:HD11	1:J:187:VAL:HG21	1.74	0.69
1:D:120:ILE:HG22	1:D:138:MET:HG2	1.75	0.68
1:B:170:ILE:HG22	1:B:249:LEU:HD21	1.74	0.68
1:A:170:ILE:HG22	1:A:249:LEU:HD21	1.77	0.67
1:J:107:LEU:HD22	1:J:182:ILE:CD1	2.24	0.67
1:I:107:LEU:HD22	1:I:182:ILE:CD1	2.25	0.67
1:K:105:VAL:HG21	1:K:123:VAL:HG11	1.78	0.66
1:D:107:LEU:HD22	1:D:182:ILE:HD12	1.77	0.66
1:H:111:ALA:HB1	1:H:117:ILE:HD13	1.76	0.66
1:D:111:ALA:HB1	1:D:117:ILE:HD13	1.78	0.66
1:C:111:ALA:HB1	1:C:117:ILE:HD13	1.76	0.66
1:B:54:ILE:O	1:B:54:ILE:HG23	1.96	0.66
1:L:69:VAL:HG22	1:L:79:LEU:CD2	2.27	0.65
1:B:53:GLN:O	1:B:54:ILE:HG22	1.97	0.65
1:G:54:ILE:O	1:G:54:ILE:HG23	1.97	0.65
1:C:48:VAL:CG1	1:K:60:ILE:HG23	2.27	0.65
1:B:107:LEU:HD22	1:B:182:ILE:CD1	2.27	0.64
1:G:118:VAL:HG22	1:G:141:LEU:HD11	1.77	0.64
1:I:257:LEU:HD21	1:I:298:VAL:HG11	1.80	0.64
1:D:107:LEU:HD22	1:D:182:ILE:CD1	2.28	0.64
1:A:257:LEU:HD21	1:A:298:VAL:CG1	2.27	0.63
1:L:118:VAL:HG11	1:L:138:MET:HE2	1.80	0.63
1:G:74:ILE:O	1:G:75:ASN:CB	2.47	0.63
1:E:118:VAL:HG22	1:E:141:LEU:HD11	1.81	0.63
1:B:120:ILE:HG22	1:B:138:MET:HG2	1.80	0.63
1:L:257:LEU:HD21	1:L:298:VAL:HG11	1.81	0.63
1:L:69:VAL:HG22	1:L:79:LEU:HD22	1.81	0.62
1:G:167:MET:HG3	1:G:253:MET:HE2	1.79	0.62
1:F:295:SER:OG	1:F:298:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:LEU:HD13	1:G:73:GLY:N	2.15	0.62
1:A:253:MET:HE3	1:A:301:LEU:HD23	1.81	0.62
1:C:167:MET:HG3	1:C:253:MET:HE2	1.82	0.61
1:G:111:ALA:HB1	1:G:117:ILE:HD13	1.80	0.61
1:H:257:LEU:HD21	1:H:298:VAL:HG11	1.81	0.61
1:K:107:LEU:HD22	1:K:182:ILE:CD1	2.30	0.61
1:H:191:ASN:O	1:H:206:THR:HG22	2.01	0.61
1:F:74:ILE:O	1:F:75:ASN:CB	2.50	0.60
1:L:118:VAL:HG11	1:L:138:MET:CE	2.31	0.60
1:F:214:THR:HG21	1:F:242:LYS:HG3	1.83	0.60
1:I:74:ILE:O	1:I:75:ASN:CB	2.48	0.60
1:I:174:ILE:HD11	1:I:187:VAL:HG21	1.83	0.60
1:C:118:VAL:HG23	1:C:205:LEU:O	2.02	0.60
1:D:118:VAL:HG23	1:D:205:LEU:O	2.02	0.60
1:B:93:LYS:HE2	1:B:95:LEU:HD11	1.85	0.59
1:E:191:ASN:O	1:E:206:THR:HG22	2.01	0.59
1:J:199:PRO:O	1:J:200:ASN:HB3	2.02	0.59
1:J:118:VAL:HG11	1:J:138:MET:CE	2.32	0.59
1:F:257:LEU:HD21	1:F:298:VAL:HG11	1.84	0.59
1:E:257:LEU:HD21	1:E:298:VAL:HG11	1.85	0.59
1:D:328:SER:O	1:D:331:VAL:HG13	2.02	0.59
1:H:120:ILE:HG22	1:H:138:MET:HG2	1.85	0.58
1:G:105:VAL:HG21	1:G:123:VAL:HG11	1.85	0.58
1:J:105:VAL:HG12	1:J:136:ILE:HD11	1.85	0.58
1:G:118:VAL:HG21	1:G:206:THR:HB	1.85	0.58
1:B:59:ILE:HD12	1:D:48:VAL:HG21	1.84	0.58
1:I:170:ILE:HG22	1:I:249:LEU:HD21	1.86	0.58
1:C:120:ILE:HG22	1:C:138:MET:HG2	1.83	0.58
1:D:102:ARG:NH1	1:D:134:LEU:HD21	2.19	0.58
1:A:59:ILE:HG23	1:A:124:TYR:CG	2.38	0.58
1:B:193:LEU:HD13	2:B:1000:05B:H25	1.86	0.58
1:B:234:VAL:O	1:B:234:VAL:HG12	2.03	0.57
1:B:257:LEU:HD21	1:B:298:VAL:HG11	1.84	0.57
1:F:54:ILE:HG23	1:F:54:ILE:O	2.04	0.57
1:I:199:PRO:O	1:I:200:ASN:HB3	2.05	0.57
1:L:214:THR:HG21	1:L:242:LYS:HG3	1.86	0.57
1:H:105:VAL:HG12	1:H:136:ILE:CD1	2.33	0.57
1:B:59:ILE:HG23	1:B:124:TYR:CG	2.40	0.57
1:H:118:VAL:HG23	1:H:205:LEU:O	2.04	0.57
1:B:107:LEU:HD22	1:B:182:ILE:HD11	1.87	0.57
1:E:105:VAL:HG21	1:E:123:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:NH1	1:A:134:LEU:HD11	2.20	0.57
1:C:48:VAL:HG11	1:K:59:ILE:HD11	1.86	0.56
1:B:177:LEU:HD22	1:B:182:ILE:HG21	1.87	0.56
1:C:48:VAL:HG12	1:K:60:ILE:CG2	2.35	0.56
1:D:331:VAL:HG23	1:D:332:PRO:HD2	1.87	0.56
1:D:98:CYS:O	1:D:100:LYS:N	2.38	0.56
1:I:191:ASN:O	1:I:206:THR:HG22	2.04	0.56
1:J:98:CYS:O	1:J:100:LYS:N	2.38	0.56
1:A:48:VAL:HG21	1:J:59:ILE:CD1	2.36	0.56
1:A:69:VAL:HG22	1:A:79:LEU:CD2	2.33	0.56
1:E:54:ILE:HG23	1:E:54:ILE:O	2.06	0.56
1:J:118:VAL:HG23	1:J:205:LEU:O	2.05	0.56
1:G:253:MET:O	1:G:257:LEU:HD13	2.05	0.55
1:C:170:ILE:HG22	1:C:249:LEU:HD21	1.88	0.55
1:E:170:ILE:HG22	1:E:249:LEU:HD21	1.88	0.55
1:H:74:ILE:O	1:H:75:ASN:CB	2.53	0.55
1:B:174:ILE:HD11	1:B:187:VAL:HG21	1.88	0.55
1:K:167:MET:HG3	1:K:253:MET:HE2	1.89	0.55
1:H:59:ILE:HG23	1:H:124:TYR:CG	2.41	0.55
1:B:59:ILE:CD1	1:D:48:VAL:HG21	2.37	0.55
1:I:118:VAL:HG23	1:I:205:LEU:O	2.06	0.55
1:E:118:VAL:HG23	1:E:205:LEU:O	2.06	0.55
1:B:150:ILE:HD12	1:B:158:PHE:CE1	2.42	0.55
1:G:107:LEU:HD22	1:G:182:ILE:CD1	2.37	0.55
1:E:147:PHE:HB3	1:E:342:LEU:HD21	1.89	0.55
1:A:74:ILE:O	1:A:75:ASN:CB	2.55	0.55
1:E:59:ILE:CD1	1:E:126:ASN:HD22	2.21	0.54
1:C:111:ALA:HB1	1:C:117:ILE:CD1	2.37	0.54
1:E:118:VAL:HG11	1:E:138:MET:HE2	1.88	0.54
1:A:48:VAL:HG21	1:J:59:ILE:HD12	1.90	0.54
1:J:167:MET:HG3	1:J:253:MET:HE2	1.89	0.54
1:J:118:VAL:HG11	1:J:138:MET:HE2	1.90	0.54
1:F:107:LEU:HD22	1:F:182:ILE:HD11	1.90	0.54
1:L:199:PRO:O	1:L:200:ASN:HB3	2.07	0.54
1:G:150:ILE:HD12	1:G:158:PHE:CE1	2.43	0.54
1:K:191:ASN:O	1:K:206:THR:HG22	2.08	0.54
1:L:301:LEU:HD13	1:L:322:HIS:CD2	2.42	0.54
1:E:94:MET:O	1:E:95:LEU:HD13	2.07	0.54
1:E:120:ILE:HG22	1:E:138:MET:HG2	1.89	0.54
1:G:120:ILE:HG22	1:G:138:MET:HG2	1.89	0.54
1:B:68:GLN:HG3	1:F:86:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:LEU:HD11	1:C:135:LEU:HB3	1.91	0.53
1:L:230:VAL:HG11	1:L:235:LEU:HD21	1.91	0.53
1:L:170:ILE:HG22	1:L:249:LEU:HD21	1.90	0.53
1:H:301:LEU:HD13	1:H:322:HIS:CD2	2.42	0.53
1:J:69:VAL:HG22	1:J:79:LEU:CD2	2.38	0.53
1:K:69:VAL:HG22	1:K:79:LEU:CD2	2.38	0.53
1:I:301:LEU:HD13	1:I:322:HIS:CD2	2.43	0.53
1:D:150:ILE:HD12	1:D:158:PHE:CE1	2.44	0.53
1:A:301:LEU:HD13	1:A:322:HIS:CD2	2.43	0.53
1:K:170:ILE:HG22	1:K:249:LEU:HD21	1.91	0.53
1:D:298:VAL:HG22	1:D:324:TRP:CD1	2.44	0.52
1:L:54:ILE:O	1:L:54:ILE:HG23	2.10	0.52
1:L:257:LEU:HA	1:L:336:LEU:HD13	1.91	0.52
1:L:98:CYS:O	1:L:100:LYS:N	2.43	0.52
1:B:160:GLU:HB2	1:B:334:THR:HG23	1.91	0.52
1:L:110:ARG:NH2	1:L:182:ILE:HD11	2.25	0.52
1:F:199:PRO:O	1:F:200:ASN:HB3	2.09	0.52
1:G:234:VAL:O	1:G:234:VAL:HG12	2.10	0.52
1:B:160:GLU:HA	1:B:336:LEU:HD11	1.93	0.51
1:L:92:LEU:HD11	1:L:135:LEU:HB3	1.92	0.51
1:A:150:ILE:HD12	1:A:158:PHE:CE1	2.45	0.51
1:L:167:MET:HG3	1:L:253:MET:HE2	1.90	0.51
1:G:111:ALA:HB1	1:G:117:ILE:CD1	2.41	0.51
1:G:48:VAL:HG21	1:I:59:ILE:HD12	1.92	0.51
1:D:257:LEU:HD21	1:D:298:VAL:HG11	1.92	0.51
1:J:301:LEU:HD13	1:J:322:HIS:CD2	2.46	0.51
1:F:167:MET:HE2	1:F:253:MET:HB2	1.93	0.51
1:C:191:ASN:O	1:C:206:THR:HG22	2.11	0.51
1:K:110:ARG:NH2	1:K:182:ILE:HD11	2.25	0.51
1:H:199:PRO:O	1:H:200:ASN:HB3	2.10	0.51
1:L:107:LEU:HD22	1:L:182:ILE:CD1	2.36	0.50
1:E:72:LEU:HD13	1:E:73:GLY:N	2.26	0.50
1:B:199:PRO:O	1:B:200:ASN:HB3	2.11	0.50
1:G:199:PRO:O	1:G:200:ASN:HB3	2.11	0.50
1:A:289:PRO:HB3	1:F:162:GLU:CD	2.32	0.50
1:D:59:ILE:HG23	1:D:124:TYR:CG	2.47	0.50
1:K:199:PRO:O	1:K:200:ASN:HB3	2.10	0.50
1:J:111:ALA:CB	1:J:177:LEU:HD21	2.41	0.50
1:D:111:ALA:HB1	1:D:117:ILE:CD1	2.39	0.50
1:I:166:ILE:HG21	1:I:256:LEU:HD11	1.93	0.50
1:K:92:LEU:HD11	1:K:135:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:54:ILE:HG23	1:K:54:ILE:O	2.12	0.50
1:E:174:ILE:HD11	1:E:187:VAL:HG21	1.93	0.50
1:C:150:ILE:HD12	1:C:158:PHE:CE1	2.47	0.49
1:J:110:ARG:NH2	1:J:182:ILE:HD11	2.27	0.49
1:E:167:MET:HG3	1:E:253:MET:HE2	1.95	0.49
1:L:146:LEU:HD13	1:L:203:LEU:HD22	1.95	0.49
1:A:105:VAL:HG21	1:A:123:VAL:HG11	1.94	0.49
1:K:59:ILE:HG23	1:K:124:TYR:CG	2.48	0.49
1:B:118:VAL:HG23	1:B:205:LEU:O	2.13	0.49
1:D:111:ALA:CB	1:D:177:LEU:HD21	2.43	0.49
1:I:92:LEU:HD11	1:I:135:LEU:HB3	1.95	0.49
1:A:174:ILE:HD11	1:A:187:VAL:HG21	1.95	0.49
1:C:199:PRO:O	1:C:200:ASN:HB3	2.13	0.49
1:F:90:PHE:CE2	1:F:121:VAL:HG11	2.47	0.49
1:H:92:LEU:HD11	1:H:135:LEU:HB3	1.95	0.49
1:D:257:LEU:HA	1:D:336:LEU:HD13	1.95	0.48
1:H:111:ALA:HB1	1:H:117:ILE:CD1	2.41	0.48
1:C:59:ILE:HG23	1:C:124:TYR:CG	2.48	0.48
1:I:94:MET:O	1:I:95:LEU:HD13	2.13	0.48
1:L:70:LEU:HD11	1:L:80:GLN:HB2	1.94	0.48
1:A:93:LYS:HE2	1:A:95:LEU:HD11	1.94	0.48
1:G:191:ASN:O	1:G:206:THR:HG22	2.13	0.48
1:B:105:VAL:HG21	1:B:123:VAL:HG11	1.95	0.48
1:G:59:ILE:HG23	1:G:124:TYR:CD1	2.48	0.48
1:L:120:ILE:HG22	1:L:138:MET:HG2	1.96	0.48
1:E:52:LEU:HD11	1:E:123:VAL:HG23	1.96	0.48
1:B:176:TYR:CE2	1:B:180:ILE:HD13	2.49	0.48
1:J:160:GLU:HB2	1:J:334:THR:HG23	1.96	0.48
1:C:54:ILE:O	1:C:54:ILE:HG23	2.14	0.48
1:D:54:ILE:HG23	1:D:54:ILE:O	2.14	0.48
1:D:75:ASN:CB	1:D:95:LEU:HD12	2.44	0.48
1:K:338:THR:O	1:K:342:LEU:HD13	2.14	0.48
1:H:102:ARG:NH1	1:H:134:LEU:HD11	2.28	0.48
1:I:118:VAL:HG11	1:I:138:MET:HE2	1.96	0.47
1:B:160:GLU:CB	1:B:334:THR:HG23	2.44	0.47
1:I:98:CYS:O	1:I:100:LYS:N	2.47	0.47
1:B:191:ASN:O	1:B:206:THR:HG22	2.13	0.47
1:F:150:ILE:HD12	1:F:158:PHE:CE1	2.48	0.47
1:B:92:LEU:HD11	1:B:135:LEU:HB3	1.96	0.47
1:G:167:MET:HE3	1:G:249:LEU:HD22	1.95	0.47
1:A:259:GLY:HA2	1:A:338:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:54:ILE:HG23	1:I:54:ILE:O	2.14	0.47
1:B:146:LEU:HD11	1:B:166:ILE:HD13	1.95	0.47
1:J:120:ILE:HG22	1:J:138:MET:HG2	1.95	0.47
1:A:214:THR:HG21	1:A:242:LYS:HG3	1.96	0.47
1:G:48:VAL:HG21	1:I:59:ILE:CD1	2.44	0.47
1:E:59:ILE:HD11	1:E:126:ASN:HD22	1.79	0.47
1:F:159:THR:HG21	1:F:333:GLN:HE21	1.80	0.47
1:K:65:VAL:HA	1:K:81:ILE:HG22	1.97	0.47
1:A:59:ILE:HG23	1:A:124:TYR:CD2	2.50	0.47
1:L:81:ILE:HD11	1:L:137:VAL:HG13	1.97	0.47
1:H:98:CYS:O	1:H:100:LYS:N	2.48	0.47
1:J:92:LEU:HD11	1:J:135:LEU:HB3	1.97	0.47
1:J:54:ILE:O	1:J:54:ILE:HG23	2.15	0.47
1:C:70:LEU:HD11	1:C:80:GLN:HB2	1.97	0.47
1:H:257:LEU:HA	1:H:336:LEU:HD13	1.97	0.46
1:D:98:CYS:O	1:D:99:PRO:C	2.53	0.46
1:A:52:LEU:HD21	1:A:105:VAL:HG22	1.97	0.46
1:I:150:ILE:HD12	1:I:158:PHE:CE1	2.50	0.46
1:A:48:VAL:O	1:A:48:VAL:HG13	2.15	0.46
1:B:146:LEU:HD13	1:B:203:LEU:HD22	1.97	0.46
1:H:94:MET:O	1:H:95:LEU:HD13	2.16	0.46
1:C:253:MET:O	1:C:257:LEU:HD13	2.16	0.46
1:D:110:ARG:NH2	1:D:182:ILE:HD11	2.30	0.46
1:B:177:LEU:HD22	1:B:182:ILE:CG2	2.46	0.46
1:G:107:LEU:HD22	1:G:182:ILE:HD11	1.97	0.46
1:F:99:PRO:O	1:F:100:LYS:HB2	2.16	0.46
1:C:47:HIS:CD2	1:C:47:HIS:N	2.84	0.46
1:F:202:ILE:N	1:F:202:ILE:HD12	2.30	0.46
1:K:118:VAL:HG23	1:K:205:LEU:O	2.15	0.46
1:K:98:CYS:O	1:K:99:PRO:C	2.54	0.46
1:F:170:ILE:HG22	1:F:249:LEU:HD21	1.97	0.46
1:L:146:LEU:HD13	1:L:203:LEU:CD2	2.45	0.46
1:F:257:LEU:HD21	1:F:298:VAL:CG1	2.46	0.46
1:K:94:MET:O	1:K:95:LEU:HD13	2.16	0.46
1:F:234:VAL:O	1:F:234:VAL:HG12	2.16	0.46
1:F:59:ILE:CG1	1:F:135:LEU:HD23	2.46	0.46
1:F:59:ILE:HG23	1:F:124:TYR:CG	2.50	0.46
1:E:52:LEU:HD11	1:E:123:VAL:CG2	2.46	0.45
1:G:107:LEU:HD22	1:G:182:ILE:HD12	1.98	0.45
1:B:202:ILE:HD12	1:B:202:ILE:N	2.30	0.45
1:L:160:GLU:HB2	1:L:334:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:105:VAL:HG21	1:I:123:VAL:HG11	1.98	0.45
1:L:59:ILE:HG23	1:L:124:TYR:CD1	2.51	0.45
1:G:105:VAL:CG2	1:G:123:VAL:HG21	2.47	0.45
1:E:234:VAL:O	1:E:234:VAL:HG12	2.17	0.45
1:A:253:MET:CE	1:A:301:LEU:HD23	2.47	0.45
1:K:98:CYS:O	1:K:100:LYS:N	2.50	0.45
1:F:120:ILE:HG22	1:F:138:MET:HG2	1.99	0.45
1:B:81:ILE:HD11	1:B:137:VAL:HG13	1.98	0.45
1:C:105:VAL:HG21	1:C:123:VAL:HG11	1.97	0.45
1:D:65:VAL:HA	1:D:81:ILE:HG22	1.99	0.45
1:G:110:ARG:NH2	1:G:182:ILE:HD11	2.32	0.45
1:B:167:MET:HG3	1:B:253:MET:HE2	1.99	0.45
1:E:65:VAL:HA	1:E:81:ILE:HG22	1.98	0.45
1:E:107:LEU:HD22	1:E:182:ILE:HD12	1.96	0.45
1:G:72:LEU:HD22	1:G:76:GLY:O	2.17	0.45
1:I:107:LEU:HD22	1:I:182:ILE:HD12	1.99	0.44
1:E:199:PRO:O	1:E:200:ASN:HB3	2.17	0.44
1:F:93:LYS:HE2	1:F:95:LEU:HD11	1.99	0.44
1:F:298:VAL:HG22	1:F:324:TRP:CD1	2.52	0.44
1:K:111:ALA:HB1	1:K:117:ILE:CD1	2.47	0.44
1:E:150:ILE:HD12	1:E:158:PHE:CE1	2.52	0.44
1:C:98:CYS:O	1:C:99:PRO:C	2.55	0.44
1:A:118:VAL:HG22	1:A:205:LEU:O	2.18	0.44
1:K:214:THR:HG21	1:K:242:LYS:HG3	1.99	0.44
1:C:72:LEU:HD22	1:C:73:GLY:N	2.33	0.44
1:A:118:VAL:HG12	1:A:141:LEU:HD11	1.96	0.44
1:D:174:ILE:HD11	1:D:187:VAL:HG21	2.00	0.44
1:G:170:ILE:HG22	1:G:249:LEU:HD21	2.00	0.43
1:C:72:LEU:HD22	1:C:73:GLY:H	1.82	0.43
1:L:338:THR:O	1:L:342:LEU:HD23	2.18	0.43
1:G:98:CYS:O	1:G:99:PRO:C	2.56	0.43
1:D:199:PRO:O	1:D:200:ASN:CB	2.66	0.43
1:I:146:LEU:HD22	1:I:203:LEU:HD21	2.01	0.43
1:C:72:LEU:C	1:C:72:LEU:HD13	2.38	0.43
1:J:111:ALA:HB2	1:J:177:LEU:HD21	2.00	0.43
1:A:126:ASN:HB2	1:A:135:LEU:HD21	1.99	0.43
1:B:74:ILE:O	1:B:75:ASN:CB	2.67	0.43
1:J:59:ILE:CD1	1:J:126:ASN:HD22	2.31	0.43
1:I:102:ARG:HA	1:I:105:VAL:HG12	2.00	0.43
1:I:230:VAL:HG11	1:I:235:LEU:HD21	2.00	0.43
1:A:98:CYS:O	1:A:100:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:65:VAL:HA	1:I:81:ILE:HG22	2.00	0.43
1:A:70:LEU:N	1:A:70:LEU:HD22	2.34	0.43
1:I:59:ILE:HD12	1:I:59:ILE:H	1.83	0.43
1:D:338:THR:O	1:D:342:LEU:HD13	2.19	0.43
1:I:167:MET:HG3	1:I:253:MET:HE2	2.01	0.43
1:C:110:ARG:HD2	1:K:127:LEU:HD22	2.01	0.43
1:J:111:ALA:HB2	1:J:177:LEU:CD2	2.49	0.43
1:L:118:VAL:HG23	1:L:205:LEU:O	2.17	0.43
1:H:199:PRO:O	1:H:200:ASN:CB	2.67	0.43
1:G:54:ILE:O	1:G:54:ILE:CG2	2.67	0.43
1:B:54:ILE:CG2	1:B:54:ILE:O	2.64	0.42
1:G:75:ASN:CB	1:G:95:LEU:HD12	2.49	0.42
1:L:59:ILE:HD12	1:L:59:ILE:H	1.84	0.42
1:G:257:LEU:CD2	1:G:298:VAL:HG11	2.44	0.42
1:A:54:ILE:O	1:A:54:ILE:HG23	2.19	0.42
1:G:107:LEU:HD13	1:G:182:ILE:HD12	2.01	0.42
1:L:52:LEU:HD11	1:L:123:VAL:CG2	2.49	0.42
1:D:202:ILE:N	1:D:202:ILE:HD12	2.34	0.42
1:D:176:TYR:CE2	1:D:180:ILE:HD13	2.54	0.42
1:J:118:VAL:HG11	1:J:138:MET:HE3	2.00	0.42
1:K:147:PHE:CE1	1:K:255:ILE:HG22	2.54	0.42
1:C:58:ALA:HA	1:C:126:ASN:HD21	1.84	0.42
1:C:257:LEU:HD21	1:C:298:VAL:HG11	2.01	0.42
1:B:59:ILE:HD11	1:D:48:VAL:HG11	2.01	0.42
1:E:98:CYS:O	1:E:100:LYS:N	2.53	0.42
1:G:47:HIS:N	1:G:47:HIS:CD2	2.86	0.42
1:F:160:GLU:HA	1:F:336:LEU:HD11	2.01	0.42
1:L:174:ILE:HD11	1:L:187:VAL:HG21	2.02	0.42
1:F:107:LEU:HD22	1:F:182:ILE:HD12	1.98	0.42
1:L:160:GLU:CB	1:L:334:THR:HG23	2.48	0.42
1:E:92:LEU:HD11	1:E:135:LEU:HB3	2.00	0.42
1:A:59:ILE:HG23	1:A:124:TYR:CD1	2.55	0.42
1:J:59:ILE:HG22	1:J:63:TYR:HB2	2.02	0.42
1:A:162:GLU:O	1:A:166:ILE:HG12	2.19	0.42
1:K:102:ARG:NH1	1:K:134:LEU:HD11	2.34	0.42
1:A:118:VAL:CG1	1:A:141:LEU:CD1	2.88	0.42
1:G:259:GLY:HA2	1:G:338:THR:HG23	2.02	0.42
1:A:289:PRO:HB3	1:F:162:GLU:OE2	2.20	0.41
1:E:259:GLY:HA2	1:E:338:THR:HG23	2.02	0.41
1:A:70:LEU:HD21	1:A:80:GLN:CB	2.45	0.41
1:A:110:ARG:HD2	1:J:127:LEU:HD22	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:GLU:HA	1:H:193:LEU:HD23	2.02	0.41
1:L:301:LEU:HD22	1:L:322:HIS:CE1	2.54	0.41
1:L:326:MET:CE	1:L:327:GLN:HE22	2.34	0.41
1:I:328:SER:O	1:I:331:VAL:HG12	2.19	0.41
1:E:214:THR:HG21	1:E:242:LYS:HG3	2.01	0.41
1:F:110:ARG:NH2	1:F:182:ILE:HD11	2.34	0.41
1:D:111:ALA:HB2	1:D:177:LEU:HD21	2.03	0.41
1:E:108:HIS:CD2	1:E:120:ILE:HG23	2.55	0.41
1:B:58:ALA:HA	1:B:126:ASN:HD21	1.84	0.41
1:A:199:PRO:O	1:A:200:ASN:CB	2.68	0.41
1:A:195:THR:HG23	1:A:202:ILE:O	2.20	0.41
1:L:150:ILE:HD12	1:L:158:PHE:CE1	2.55	0.41
1:F:118:VAL:HG23	1:F:205:LEU:O	2.20	0.41
1:L:332:PRO:HB2	1:L:334:THR:HG22	2.02	0.41
1:K:111:ALA:HB1	1:K:117:ILE:HD12	2.02	0.41
1:L:105:VAL:HG21	1:L:123:VAL:HG11	2.02	0.41
1:H:160:GLU:HB2	1:H:334:THR:HG23	2.02	0.41
1:C:174:ILE:HD11	1:C:187:VAL:HG21	2.02	0.41
1:I:152:ASP:C	1:J:198:ARG:HG3	2.41	0.41
1:G:328:SER:O	1:G:331:VAL:HG12	2.20	0.41
1:E:52:LEU:HD13	1:E:109:TRP:CE3	2.56	0.41
1:L:199:PRO:O	1:L:200:ASN:CB	2.68	0.41
1:A:199:PRO:O	1:A:200:ASN:HB3	2.20	0.41
1:K:150:ILE:HD12	1:K:158:PHE:CE1	2.55	0.41
1:J:202:ILE:N	1:J:202:ILE:HD12	2.36	0.41
1:B:108:HIS:CD2	1:B:120:ILE:HG23	2.55	0.41
1:I:166:ILE:CG2	1:I:256:LEU:HD11	2.51	0.41
1:G:181:ASN:HD22	1:G:215:THR:CG2	2.33	0.41
1:A:108:HIS:CD2	1:A:120:ILE:HG23	2.55	0.41
1:G:118:VAL:HG23	1:G:205:LEU:O	2.21	0.41
1:J:95:LEU:HD21	1:J:104:GLU:OE2	2.20	0.41
1:A:192:LEU:HD21	1:A:205:LEU:HD13	2.02	0.41
1:K:118:VAL:CG2	1:K:141:LEU:HD11	2.41	0.41
1:B:332:PRO:HB2	1:B:334:THR:HG22	2.02	0.41
1:J:111:ALA:HB1	1:J:117:ILE:CD1	2.50	0.41
1:B:259:GLY:O	1:B:342:LEU:HD12	2.20	0.41
1:C:202:ILE:HD12	1:C:202:ILE:N	2.35	0.41
1:B:102:ARG:NH1	1:B:134:LEU:HD11	2.36	0.41
1:A:170:ILE:CG2	1:A:249:LEU:HD21	2.49	0.41
1:B:59:ILE:H	1:B:126:ASN:HD21	1.67	0.41
1:B:146:LEU:HD13	1:B:203:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:ILE:CG2	1:H:124:TYR:CD1	3.04	0.40
1:E:199:PRO:O	1:E:200:ASN:CB	2.69	0.40
1:B:98:CYS:O	1:B:100:LYS:N	2.55	0.40
1:F:257:LEU:HD23	1:F:291:TRP:CZ3	2.56	0.40
1:J:199:PRO:O	1:J:200:ASN:CB	2.69	0.40
1:E:59:ILE:HD12	1:E:59:ILE:H	1.86	0.40
1:G:59:ILE:HG23	1:G:124:TYR:CE1	2.57	0.40
1:H:150:ILE:HD12	1:H:158:PHE:CD1	2.56	0.40
1:H:54:ILE:O	1:H:54:ILE:HG23	2.21	0.40
1:B:195:THR:HG23	1:B:202:ILE:O	2.21	0.40
1:E:111:ALA:HB1	1:E:117:ILE:HD13	2.03	0.40
1:H:202:ILE:N	1:H:202:ILE:HD12	2.36	0.40
1:L:111:ALA:CB	1:L:177:LEU:HD21	2.51	0.40
1:A:70:LEU:HD12	2:A:1000:05B:C27	2.52	0.40
1:C:69:VAL:O	1:C:70:LEU:HD23	2.22	0.40
1:F:128:TYR:O	1:F:129:ALA:HB3	2.21	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	262/318 (82%)	235 (90%)	19 (7%)	8 (3%)	5 21
1	B	262/318 (82%)	237 (90%)	17 (6%)	8 (3%)	5 21
1	C	262/318 (82%)	238 (91%)	16 (6%)	8 (3%)	5 21
1	D	262/318 (82%)	238 (91%)	15 (6%)	9 (3%)	5 19
1	E	262/318 (82%)	239 (91%)	15 (6%)	8 (3%)	5 21
1	F	262/318 (82%)	240 (92%)	12 (5%)	10 (4%)	4 16
1	G	262/318 (82%)	240 (92%)	15 (6%)	7 (3%)	6 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	262/318 (82%)	239 (91%)	16 (6%)	7 (3%)	6 25
1	I	262/318 (82%)	239 (91%)	15 (6%)	8 (3%)	5 21
1	J	262/318 (82%)	243 (93%)	13 (5%)	6 (2%)	8 30
1	K	262/318 (82%)	242 (92%)	12 (5%)	8 (3%)	5 21
1	L	262/318 (82%)	237 (90%)	18 (7%)	7 (3%)	6 25
All	All	3144/3816 (82%)	2867 (91%)	183 (6%)	94 (3%)	5 22

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	LYS
1	A	200	ASN
1	B	100	LYS
1	B	200	ASN
1	C	99	PRO
1	C	200	ASN
1	D	99	PRO
1	E	100	LYS
1	E	200	ASN
1	F	100	LYS
1	F	200	ASN
1	G	99	PRO
1	H	100	LYS
1	H	200	ASN
1	J	99	PRO
1	K	99	PRO
1	K	200	ASN
1	L	100	LYS
1	L	200	ASN
1	A	54	ILE
1	A	75	ASN
1	A	99	PRO
1	C	100	LYS
1	D	54	ILE
1	D	100	LYS
1	D	158	PHE
1	D	200	ASN
1	E	54	ILE
1	F	75	ASN
1	F	158	PHE

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Mol	Chain	Res	Type
1	G	75	ASN
1	G	158	PHE
1	G	200	ASN
1	H	54	ILE
1	H	75	ASN
1	H	99	PRO
1	I	54	ILE
1	I	75	ASN
1	I	99	PRO
1	I	100	LYS
1	I	200	ASN
1	J	100	LYS
1	J	200	ASN
1	K	54	ILE
1	K	100	LYS
1	L	54	ILE
1	L	99	PRO
1	A	158	PHE
1	B	99	PRO
1	B	129	ALA
1	C	54	ILE
1	C	158	PHE
1	C	207	ASP
1	D	129	ALA
1	E	75	ASN
1	E	99	PRO
1	F	90	PHE
1	G	100	LYS
1	K	90	PHE
1	L	158	PHE
1	A	129	ALA
1	A	207	ASP
1	B	75	ASN
1	B	90	PHE
1	D	89	LYS
1	F	54	ILE
1	F	129	ALA
1	I	90	PHE
1	I	129	ALA
1	I	158	PHE
1	J	54	ILE
1	K	158	PHE

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Mol	Chain	Res	Type
1	L	129	ALA
1	B	158	PHE
1	C	90	PHE
1	C	129	ALA
1	D	90	PHE
1	E	129	ALA
1	F	89	LYS
1	F	99	PRO
1	F	207	ASP
1	G	54	ILE
1	G	90	PHE
1	H	90	PHE
1	H	158	PHE
1	J	158	PHE
1	J	207	ASP
1	L	207	ASP
1	D	75	ASN
1	E	90	PHE
1	K	129	ALA
1	K	207	ASP
1	B	54	ILE
1	E	234	VAL

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	242/287 (84%)	232 (96%)	10 (4%)	37	73
1	B	242/287 (84%)	232 (96%)	10 (4%)	37	73
1	C	243/287 (85%)	234 (96%)	9 (4%)	41	77
1	D	241/287 (84%)	230 (95%)	11 (5%)	33	69
1	E	243/287 (85%)	232 (96%)	11 (4%)	34	70
1	F	241/287 (84%)	231 (96%)	10 (4%)	37	73
1	G	241/287 (84%)	225 (93%)	16 (7%)	21	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	240/287 (84%)	227 (95%)	13 (5%)	27 62
1	I	238/287 (83%)	229 (96%)	9 (4%)	40 76
1	J	242/287 (84%)	229 (95%)	13 (5%)	27 62
1	K	242/287 (84%)	235 (97%)	7 (3%)	50 83
1	L	244/287 (85%)	234 (96%)	10 (4%)	37 73
All	All	2899/3444 (84%)	2770 (96%)	129 (4%)	35 70

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	72	LEU
1	A	85	ARG
1	A	95	LEU
1	A	118	VAL
1	A	135	LEU
1	A	149	ARG
1	A	240	TYR
1	A	264	TYR
1	A	333	GLN
1	B	47	HIS
1	B	53	GLN
1	B	57	ASN
1	B	59	ILE
1	B	149	ARG
1	B	185	ARG
1	B	264	TYR
1	B	333	GLN
1	B	334	THR
1	B	343	LYS
1	C	47	HIS
1	C	49	LYS
1	C	59	ILE
1	C	95	LEU
1	C	131	ARG
1	C	149	ARG
1	C	198	ARG
1	C	264	TYR
1	C	340	ARG
1	D	47	HIS

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Mol	Chain	Res	Type
1	D	57	ASN
1	D	59	ILE
1	D	95	LEU
1	D	131	ARG
1	D	135	LEU
1	D	149	ARG
1	D	264	TYR
1	D	331	VAL
1	D	333	GLN
1	D	344	GLU
1	E	57	ASN
1	E	59	ILE
1	E	149	ARG
1	E	198	ARG
1	E	240	TYR
1	E	264	TYR
1	E	285	GLU
1	E	333	GLN
1	E	340	ARG
1	E	342	LEU
1	E	344	GLU
1	F	59	ILE
1	F	102	ARG
1	F	135	LEU
1	F	149	ARG
1	F	152	ASP
1	F	198	ARG
1	F	240	TYR
1	F	264	TYR
1	F	327	GLN
1	F	334	THR
1	G	47	HIS
1	G	48	VAL
1	G	50	SER
1	G	54	ILE
1	G	57	ASN
1	G	59	ILE
1	G	95	LEU
1	G	149	ARG
1	G	152	ASP
1	G	198	ARG
1	G	240	TYR

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Mol	Chain	Res	Type
1	G	264	TYR
1	G	327	GLN
1	G	333	GLN
1	G	340	ARG
1	G	342	LEU
1	H	47	HIS
1	H	48	VAL
1	H	49	LYS
1	H	59	ILE
1	H	135	LEU
1	H	149	ARG
1	H	240	TYR
1	H	264	TYR
1	H	277	THR
1	H	333	GLN
1	H	340	ARG
1	H	343	LYS
1	H	344	GLU
1	I	47	HIS
1	I	57	ASN
1	I	59	ILE
1	I	131	ARG
1	I	135	LEU
1	I	149	ARG
1	I	152	ASP
1	I	264	TYR
1	I	333	GLN
1	J	47	HIS
1	J	48	VAL
1	J	59	ILE
1	J	95	LEU
1	J	131	ARG
1	J	135	LEU
1	J	149	ARG
1	J	152	ASP
1	J	241	ASP
1	J	264	TYR
1	J	334	THR
1	J	340	ARG
1	J	343	LYS
1	K	53	GLN
1	K	57	ASN

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Mol	Chain	Res	Type
1	K	131	ARG
1	K	149	ARG
1	K	264	TYR
1	K	333	GLN
1	K	340	ARG
1	L	47	HIS
1	L	57	ASN
1	L	59	ILE
1	L	95	LEU
1	L	149	ARG
1	L	244	CYS
1	L	264	TYR
1	L	265	SER
1	L	334	THR
1	L	340	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	B	68	GLN
1	B	126	ASN
1	B	151	GLN
1	B	321	ASN
1	C	47	HIS
1	C	75	ASN
1	C	126	ASN
1	C	191	ASN
1	C	312	GLN
1	D	126	ASN
1	D	151	GLN
1	D	191	ASN
1	D	283	GLN
1	D	304	ASN
1	D	312	GLN
1	D	321	ASN
1	D	333	GLN
1	E	57	ASN
1	E	68	GLN
1	E	108	HIS
1	E	126	ASN
1	E	151	GLN

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Mol	Chain	Res	Type
1	E	191	ASN
1	E	283	GLN
1	F	126	ASN
1	F	151	GLN
1	F	184	HIS
1	F	312	GLN
1	F	327	GLN
1	F	333	GLN
1	G	47	HIS
1	G	57	ASN
1	G	126	ASN
1	G	151	GLN
1	G	191	ASN
1	G	327	GLN
1	G	333	GLN
1	H	126	ASN
1	H	191	ASN
1	H	312	GLN
1	H	327	GLN
1	H	333	GLN
1	I	57	ASN
1	I	126	ASN
1	I	151	GLN
1	I	184	HIS
1	I	191	ASN
1	I	312	GLN
1	I	321	ASN
1	I	333	GLN
1	J	126	ASN
1	J	151	GLN
1	J	191	ASN
1	J	312	GLN
1	J	327	GLN
1	K	53	GLN
1	K	57	ASN
1	K	151	GLN
1	K	184	HIS
1	K	191	ASN
1	K	312	GLN
1	K	333	GLN
1	L	57	ASN
1	L	126	ASN

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Mol	Chain	Res	Type
1	L	151	GLN
1	L	312	GLN
1	L	321	ASN
1	L	327	GLN
1	L	333	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	05B	A	1000	-	33,35,35	0.72	0	37,52,52	2.15	12 (32%)
2	05B	B	1000	-	33,35,35	0.74	1 (3%)	37,52,52	2.01	10 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	05B	A	1000	-	-	0/6/40/40	0/6/6/6
2	05B	B	1000	-	-	0/6/40/40	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	05B	C13-C14	-2.01	1.36	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1000	05B	N19-C20-N21	-4.92	120.88	125.37
2	B	1000	05B	N19-C20-N21	-4.55	121.21	125.37
2	B	1000	05B	C17-C18-N19	-3.58	119.81	123.90
2	A	1000	05B	C17-C18-N19	-3.38	120.04	123.90
2	A	1000	05B	O30-C29-O28	-2.96	103.12	108.12
2	B	1000	05B	O30-C29-O28	-2.57	103.77	108.12
2	A	1000	05B	C17-C16-N21	-2.22	118.94	122.01
2	B	1000	05B	C17-C16-N21	-2.20	118.98	122.01
2	B	1000	05B	O30-C26-C25	2.31	131.19	127.88
2	A	1000	05B	O28-C27-C24	2.35	131.71	127.96
2	B	1000	05B	O28-C27-C24	2.38	131.75	127.96
2	A	1000	05B	C9-N5-C8	2.48	118.55	110.33
2	A	1000	05B	C14-C16-N21	2.50	119.35	116.26
2	A	1000	05B	O30-C26-C25	2.57	131.57	127.88
2	B	1000	05B	C9-N5-C8	2.84	119.77	110.33
2	A	1000	05B	C12-C4-N3	3.05	117.66	115.81
2	B	1000	05B	C22-C20-N19	3.11	120.64	117.30
2	A	1000	05B	C22-C20-N19	3.34	120.90	117.30
2	B	1000	05B	C16-N21-C20	4.92	121.19	116.81
2	A	1000	05B	C18-N19-C20	5.08	120.79	115.93
2	B	1000	05B	C18-N19-C20	5.13	120.84	115.93
2	A	1000	05B	C16-N21-C20	5.17	121.42	116.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	05B	1	0
2	B	1000	05B	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	272/318 (85%)	0.37	6 (2%) 65 60	76, 86, 104, 117	0
1	B	272/318 (85%)	0.46	9 (3%) 50 42	83, 93, 109, 129	0
1	C	272/318 (85%)	0.49	13 (4%) 34 28	80, 95, 122, 131	0
1	D	272/318 (85%)	0.50	8 (2%) 55 49	78, 89, 106, 113	0
1	E	272/318 (85%)	0.43	9 (3%) 50 42	85, 96, 118, 129	0
1	F	272/318 (85%)	0.52	12 (4%) 38 32	76, 89, 105, 115	0
1	G	272/318 (85%)	0.51	9 (3%) 50 42	87, 102, 123, 132	0
1	H	272/318 (85%)	0.67	25 (9%) 11 7	93, 110, 137, 154	0
1	I	272/318 (85%)	0.60	15 (5%) 29 22	101, 112, 125, 141	0
1	J	272/318 (85%)	0.45	14 (5%) 32 25	83, 96, 112, 125	0
1	K	272/318 (85%)	0.80	32 (11%) 6 4	104, 113, 137, 144	0
1	L	272/318 (85%)	0.55	13 (4%) 34 28	90, 105, 126, 138	0
All	All	3264/3816 (85%)	0.53	165 (5%) 32 25	76, 99, 125, 154	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	157	ALA	6.6
1	I	75	ASN	5.3
1	K	328	SER	5.1
1	L	67	SER	4.6
1	L	66	THR	4.6
1	E	74	ILE	4.6
1	I	294	VAL	4.5
1	K	146	LEU	4.2
1	L	228	TYR	4.2
1	K	150	ILE	4.1
1	H	158	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	157	ALA	4.0
1	K	331	VAL	4.0
1	J	345	ASP	4.0
1	K	257	LEU	3.9
1	G	66	THR	3.8
1	H	334	THR	3.8
1	F	73	GLY	3.8
1	H	228	TYR	3.7
1	K	294	VAL	3.6
1	K	199	PRO	3.6
1	G	65	VAL	3.5
1	K	158	PHE	3.5
1	K	336	LEU	3.5
1	I	240	TYR	3.5
1	J	240	TYR	3.5
1	F	59	ILE	3.4
1	B	342	LEU	3.3
1	G	82	PHE	3.3
1	J	75	ASN	3.3
1	K	337	HIS	3.2
1	J	334	THR	3.2
1	C	87	GLN	3.2
1	K	329	THR	3.2
1	J	228	TYR	3.2
1	K	343	LYS	3.1
1	H	129	ALA	3.1
1	H	343	LYS	3.1
1	C	66	THR	3.0
1	H	336	LEU	3.0
1	J	157	ALA	3.0
1	K	330	LYS	3.0
1	I	74	ILE	3.0
1	K	228	TYR	2.9
1	K	202	ILE	2.9
1	B	146	LEU	2.9
1	A	240	TYR	2.9
1	L	70	LEU	2.9
1	C	70	LEU	2.8
1	I	330	LYS	2.8
1	F	79	LEU	2.8
1	H	289	PRO	2.8
1	G	150	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	182	ILE	2.8
1	K	325	ILE	2.8
1	L	82	PHE	2.8
1	K	341	VAL	2.8
1	I	336	LEU	2.7
1	B	289	PRO	2.7
1	H	150	ILE	2.7
1	J	158	PHE	2.7
1	H	151	GLN	2.7
1	J	94	MET	2.7
1	E	107	LEU	2.7
1	D	79	LEU	2.6
1	B	343	LYS	2.6
1	K	301	LEU	2.6
1	L	85	ARG	2.6
1	B	151	GLN	2.6
1	C	67	SER	2.6
1	L	90	PHE	2.6
1	F	274	GLY	2.6
1	D	134	LEU	2.6
1	L	92	LEU	2.6
1	C	81	ILE	2.6
1	F	66	THR	2.5
1	I	47	HIS	2.5
1	K	293	GLU	2.5
1	H	75	ASN	2.5
1	A	47	HIS	2.5
1	I	69	VAL	2.5
1	E	70	LEU	2.5
1	H	342	LEU	2.5
1	H	333	GLN	2.5
1	D	197	LYS	2.5
1	E	79	LEU	2.5
1	G	47	HIS	2.5
1	J	342	LEU	2.4
1	F	71	GLY	2.4
1	L	157	ALA	2.4
1	B	150	ILE	2.4
1	K	333	GLN	2.4
1	C	202	ILE	2.4
1	L	329	THR	2.4
1	I	197	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	201	ALA	2.4
1	H	293	GLU	2.4
1	J	335	PRO	2.4
1	G	294	VAL	2.4
1	G	79	LEU	2.3
1	F	68	GLN	2.3
1	E	157	ALA	2.3
1	D	274	GLY	2.3
1	B	48	VAL	2.3
1	C	135	LEU	2.3
1	F	70	LEU	2.3
1	H	47	HIS	2.3
1	K	338	THR	2.3
1	E	134	LEU	2.3
1	D	76	GLY	2.3
1	E	75	ASN	2.3
1	L	63	TYR	2.3
1	C	60	ILE	2.3
1	H	315	THR	2.3
1	I	48	VAL	2.3
1	D	60	ILE	2.3
1	A	265	SER	2.2
1	A	235	LEU	2.2
1	J	87	GLN	2.2
1	G	157	ALA	2.2
1	G	74	ILE	2.2
1	H	335	PRO	2.2
1	B	182	ILE	2.2
1	L	60	ILE	2.2
1	F	240	TYR	2.2
1	I	118	VAL	2.2
1	J	123	VAL	2.2
1	B	158	PHE	2.2
1	C	150	ILE	2.2
1	L	336	LEU	2.2
1	K	332	PRO	2.2
1	H	131	ARG	2.2
1	H	344	GLU	2.2
1	C	69	VAL	2.2
1	C	92	LEU	2.2
1	J	336	LEU	2.2
1	A	150	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	60	ILE	2.2
1	K	197	LYS	2.1
1	A	48	VAL	2.1
1	K	340	ARG	2.1
1	F	333	GLN	2.1
1	K	48	VAL	2.1
1	E	94	MET	2.1
1	K	256	LEU	2.1
1	I	293	GLU	2.1
1	H	314	MET	2.1
1	D	75	ASN	2.1
1	K	80	GLN	2.1
1	K	151	GLN	2.1
1	C	64	LYS	2.1
1	D	336	LEU	2.1
1	H	170	ILE	2.1
1	I	302	ILE	2.1
1	F	342	LEU	2.1
1	C	74	ILE	2.0
1	F	182	ILE	2.0
1	K	308	THR	2.0
1	H	240	TYR	2.0
1	H	199	PRO	2.0
1	E	136	ILE	2.0
1	I	299	LYS	2.0
1	I	291	TRP	2.0
1	H	134	LEU	2.0
1	H	160	GLU	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	05B	B	1000	30/30	0.91	0.28	0.93	85,86,91,91	0
2	05B	A	1000	30/30	0.93	0.21	-0.10	88,89,91,91	0

6.5 Other polymers (i)

There are no such residues in this entry.