



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:44 PM EDT

PDB ID : 3R2B / pdb_00003r2b
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

<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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

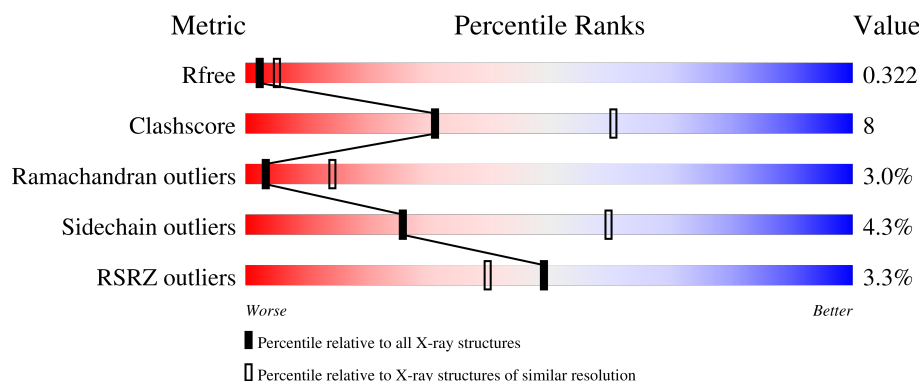
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	318	3% 66% 16% • 14%
1	B	318	2% 63% 20% • 14%
1	C	318	3% 69% 14% • 14%
1	D	318	3% 69% 14% • 14%
1	E	318	3% 67% 17% • 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	318	4% 67% 15% 14%
1	G	318	3% 68% 15% 14%
1	H	318	% 69% 14% 14%
1	I	318	4% 67% 16% 14%
1	J	318	4% 69% 14% 14%
1	K	318	2% 67% 16% 14%
1	L	318	3% 65% 18% 14%

2 Entry composition

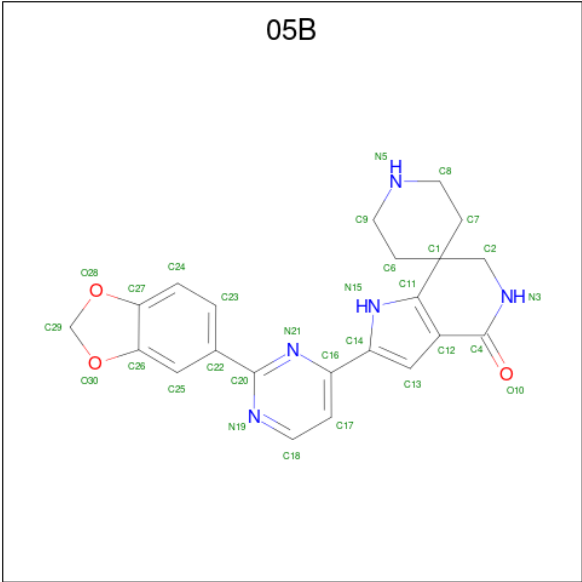
There are 2 unique types of molecules in this entry. The entry contains 26381 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 05B) (formula: C₂₂H₂₁N₅O₃).

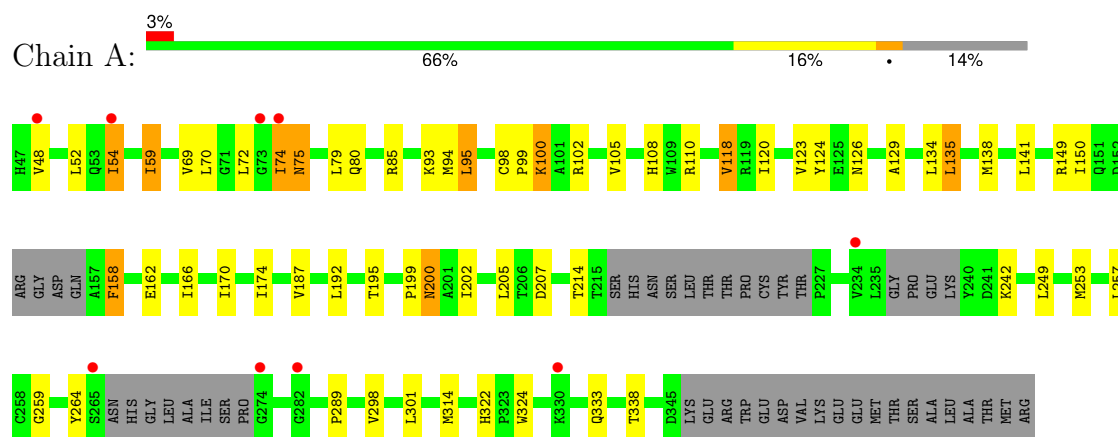


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	22	5	3		
2	B	1	Total	C	N	O	0	0
			30	22	5	3		

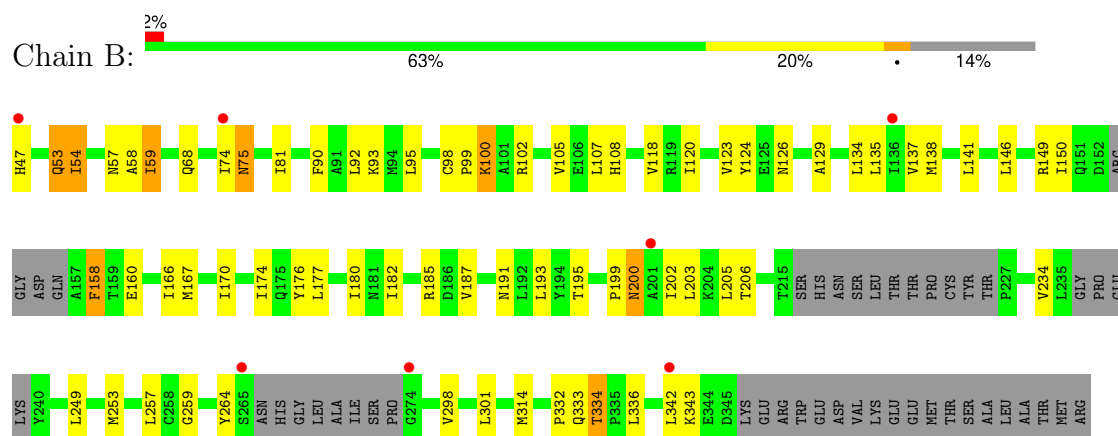
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

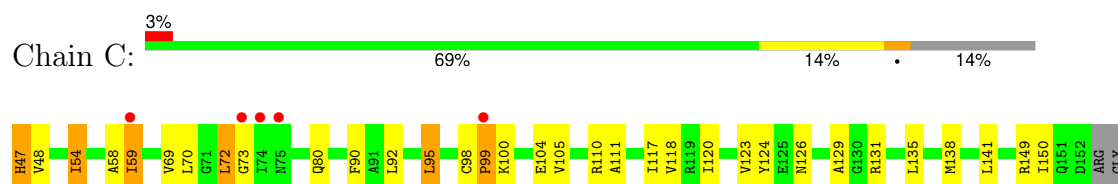
- Molecule 1: MAP kinase-activated protein kinase 2

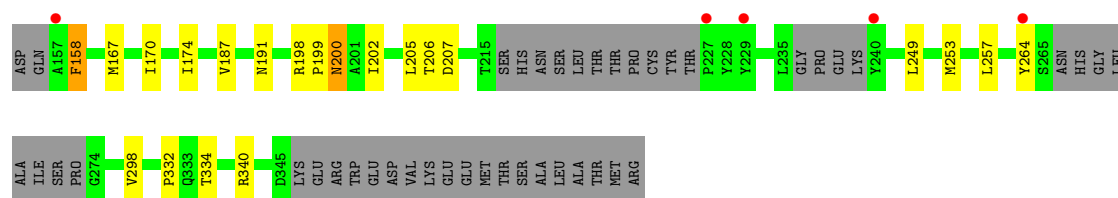


- Molecule 1: MAP kinase-activated protein kinase 2

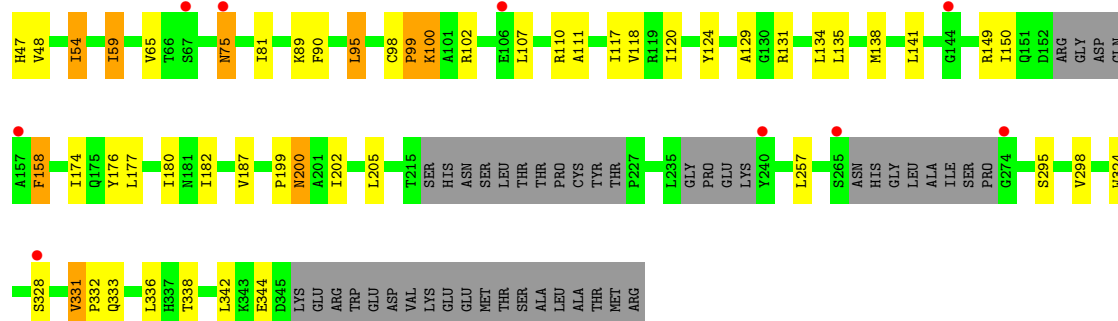


- Molecule 1: MAP kinase-activated protein kinase 2

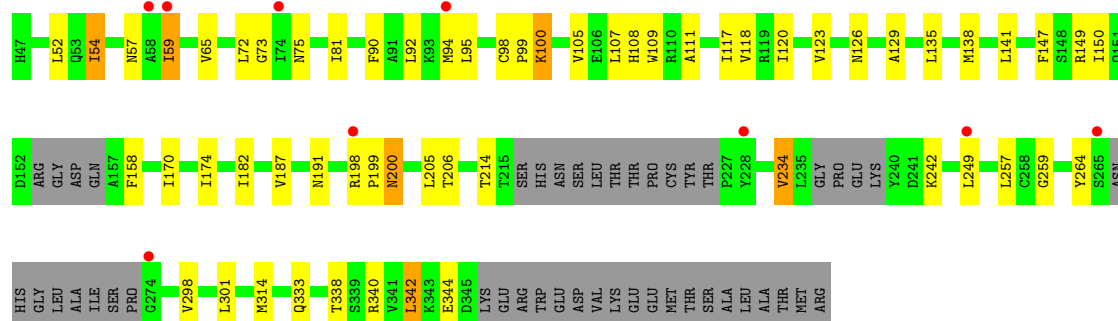




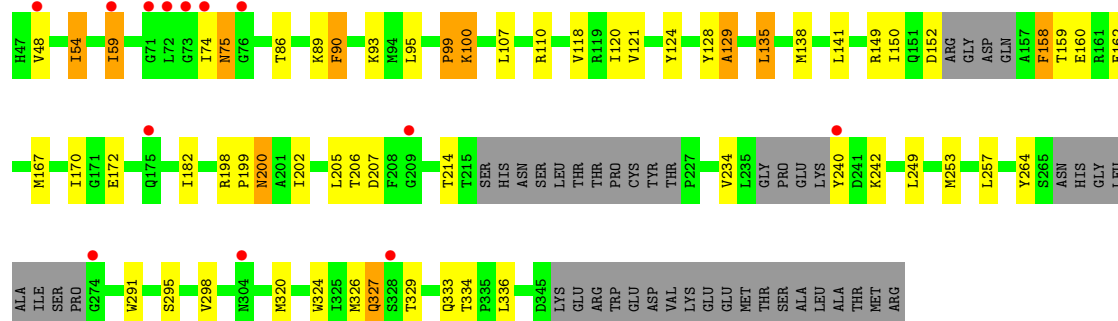
• Molecule 1: MAP kinase-activated protein kinase 2



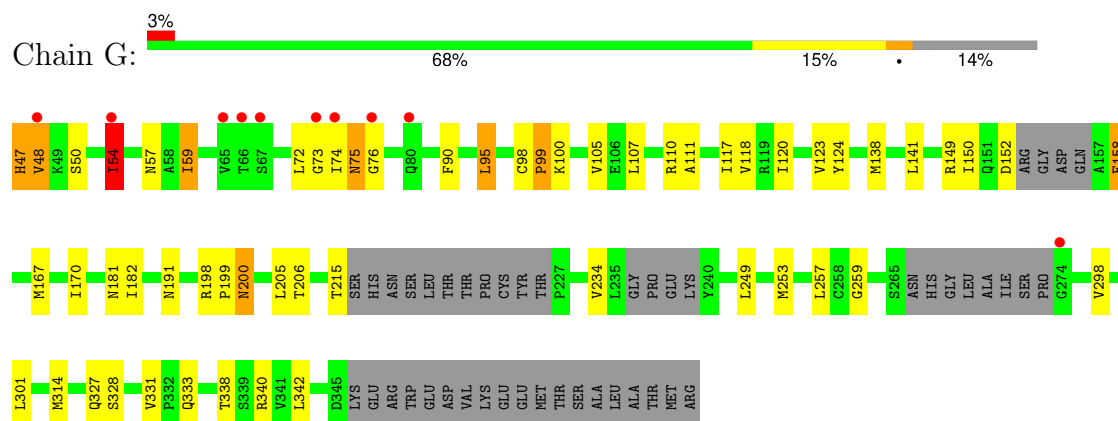
• Molecule 1: MAP kinase-activated protein kinase 2



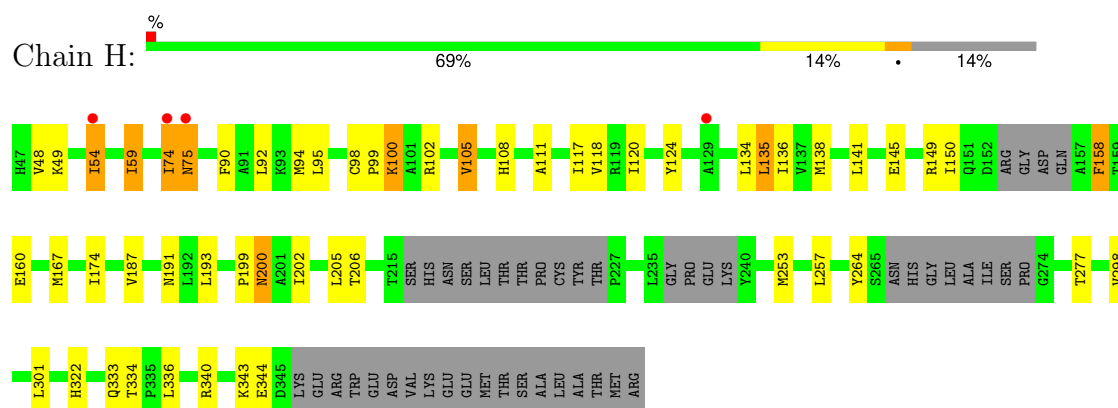
• Molecule 1: MAP kinase-activated protein kinase 2



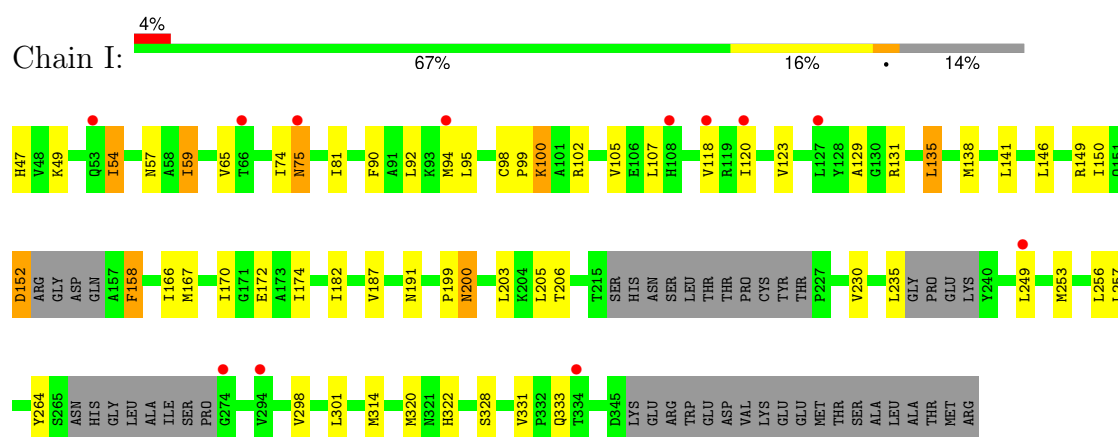
• Molecule 1: MAP kinase-activated protein kinase 2



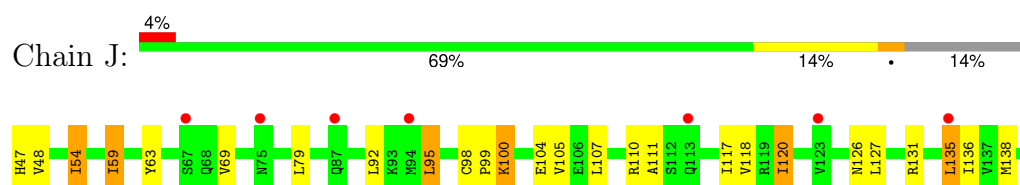
• Molecule 1: MAP kinase-activated protein kinase 2

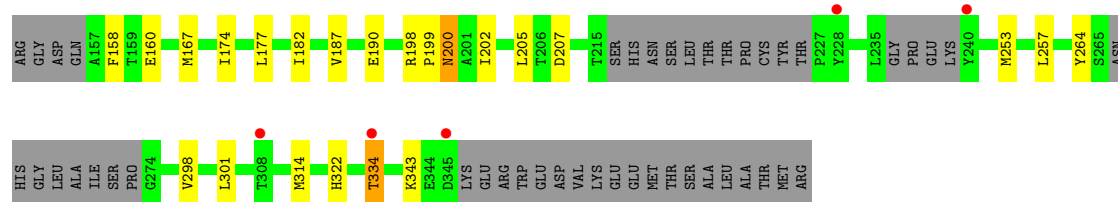


• Molecule 1: MAP kinase-activated protein kinase 2

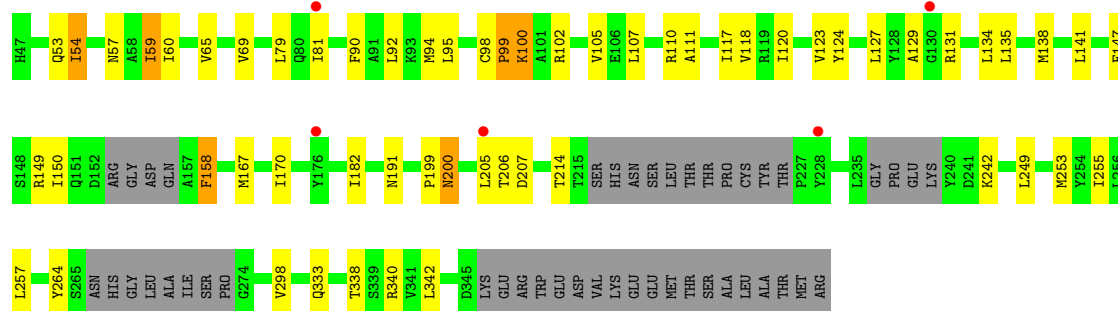


• Molecule 1: MAP kinase-activated protein kinase 2

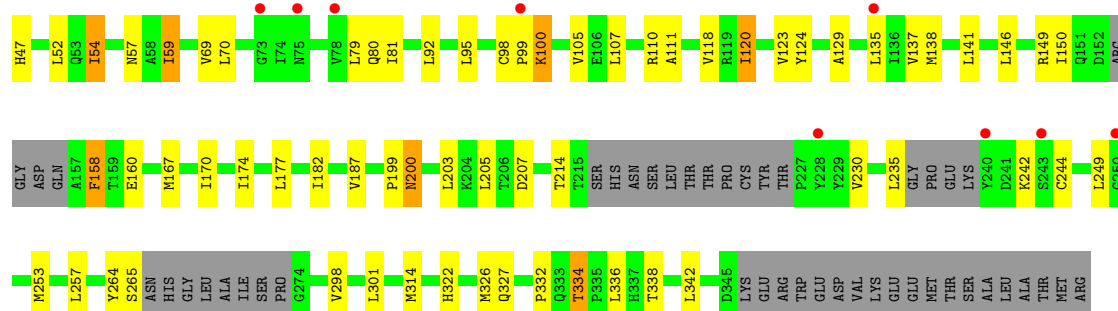




• Molecule 1: MAP kinase-activated protein kinase 2



• Molecule 1: MAP kinase-activated protein kinase 2



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	91.0	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.8	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	0.91	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.*

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](#)

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	0.45	0/2239	0.71	1/3020 (0.0%)
1	B	0.44	0/2242	0.70	0/3022
1	C	0.45	0/2242	0.69	0/3024
1	D	0.46	0/2238	0.70	0/3018
1	E	0.44	0/2243	0.69	0/3025
1	F	0.46	0/2236	0.69	0/3016
1	G	0.44	0/2236	0.69	0/3016
1	H	0.43	0/2232	0.70	1/3011 (0.0%)
1	I	0.44	0/2226	0.68	0/3004
1	J	0.43	0/2240	0.71	0/3020
1	K	0.43	0/2241	0.67	0/3022
1	L	0.44	0/2246	0.69	0/3029
All	All	0.44	0/26861	0.69	2/36227 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ILE	N-CA-C	5.81	112.43	106.21
1	H	74	ILE	N-CA-C	5.64	112.25	106.21

There are no chirality outliers.

There are no planarity outliers.

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	2194	0	2203	48	0
1	B	2197	0	2204	49	0
1	C	2197	0	2207	37	0
1	D	2193	0	2198	33	0
1	E	2198	0	2209	34	0
1	F	2191	0	2194	36	0
1	G	2191	0	2199	40	0
1	H	2187	0	2188	28	0
1	I	2181	0	2170	34	0
1	J	2195	0	2205	34	0
1	K	2196	0	2202	35	0
1	L	2201	0	2218	42	0
2	A	30	0	21	1	0
2	B	30	0	21	1	0
All	All	26381	0	26439	431	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 (431) 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:L:118:VAL:HG11	1:L:138:MET:HE2	1.43	1.00
1:A:253:MET:HE1	1:A:301:LEU:HD23	1.54	0.87
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:I:118:VAL:HG11	1:I:138:MET:HE2	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:L:326:MET:HE3	1:L:327:GLN:HE22	1.46	0.80
1:C:118:VAL:HG22	1:C:141:LEU:HD11	1.64	0.80
1:I:167:MET:HE2	1:I:253:MET:HE3	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:118:VAL:HG22	1:I:141:LEU:HD11	1.67	0.74
1:F:118:VAL:HG11	1:F:138:MET:HE2	1.70	0.74
1:I:120:ILE:HG22	1:I:138:MET:HG2	1.70	0.74
1:A:253:MET:HE3	1:A:324:TRP:CZ3	2.22	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:E:118:VAL:HG11	1:E:138:MET:HE2	1.71	0.73
1:C:118:VAL:CG2	1:C:141:LEU:HD11	2.19	0.72
1:G:167:MET:HE2	1:G:253:MET:HE3	1.71	0.72
1:D:118:VAL:HG22	1:D:141:LEU:HD11	1.72	0.72
1:H:167:MET:HE2	1:H:253:MET:HE3	1.70	0.72
1:J:257:LEU:HD21	1:J:298:VAL:HG11	1.71	0.72
1:K:167:MET:HE2	1:K:253:MET:HE3	1.72	0.72
1:F:107:LEU:HD22	1:F:182:ILE:CD1	2.20	0.71
1:D:118:VAL:HG11	1:D:138:MET:HE2	1.73	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:118:VAL:HG11	1:G:138:MET:HE2	1.71	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:L:301:LEU:HD12	1:L:314:MET:HE1	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:I:107:LEU:HD22	1:I:182:ILE:CD1	2.25	0.67
1:J:107:LEU:HD22	1:J:182:ILE:CD1	2.24	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:C:111:ALA:HB1	1:C:117:ILE:HD13	1.76	0.66
1:D:111:ALA:HB1	1:D:117:ILE:HD13	1.78	0.66
1:L:69:VAL:HG22	1:L:79:LEU:CD2	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:GLN:O	1:B:54:ILE:HG22	1.97	0.65
1:C:48:VAL:CG1	1:K:60:ILE:HG23	2.27	0.65
1:B:54:ILE:HG23	1:B:54:ILE:O	1.96	0.64
1:B:107:LEU:HD22	1:B:182:ILE:CD1	2.27	0.64
1:L:301:LEU:CD1	1:L:314:MET:HE1	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:G:54:ILE:HG23	1:G:54:ILE:O	1.97	0.64
1:E:118:VAL:CG1	1:E:138:MET:HE2	2.28	0.64
1:A:257:LEU:HD21	1:A:298:VAL:CG1	2.27	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:F:167:MET:HE2	1:F:253:MET:HE3	1.80	0.62
1:F:295:SER:OG	1:F:298:VAL:HG23	2.00	0.62
1:G:72:LEU:HD13	1:G:73:GLY:N	2.15	0.62
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:A:301:LEU:HD12	1:A:314:MET:HE1	1.81	0.61
1:H:191:ASN:O	1:H:206:THR:HG22	2.01	0.61
1:K:107:LEU:HD22	1:K:182:ILE:CD1	2.30	0.61
1:F:74:ILE:O	1:F:75:ASN:CB	2.50	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:F:257:LEU:HD21	1:F:298:VAL:HG11	1.84	0.59
1:J:118:VAL:HG11	1:J:138:MET:CE	2.32	0.59
1:D:328:SER:O	1:D:331:VAL:HG13	2.02	0.59
1:E:257:LEU:HD21	1:E:298:VAL:HG11	1.85	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:B:59:ILE:HD12	1:D:48:VAL:HG21	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:VAL:HG21	1:G:206:THR:HB	1.85	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:HG12	1:B:234:VAL:O	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:B:59:ILE:HG23	1:B:124:TYR:CG	2.40	0.57
1:H:105:VAL:HG12	1:H:136:ILE:CD1	2.33	0.57
1:H:118:VAL:HG23	1:H:205:LEU:O	2.04	0.57
1:A:102:ARG:NH1	1:A:134:LEU:HD11	2.20	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
1:B:177:LEU:HD22	1:B:182:ILE:HG21	1.87	0.56
1:C:48:VAL:HG11	1:K:59:ILE:HD11	1.86	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:A:48:VAL:HG21	1:J:59:ILE:CD1	2.36	0.56
1:J:98:CYS:O	1:J:100:LYS:N	2.38	0.56
1:A:69:VAL:HG22	1:A:79:LEU:CD2	2.33	0.56
1:E:54:ILE:O	1:E:54:ILE:HG23	2.06	0.56
1:J:118:VAL:HG23	1:J:205:LEU:O	2.05	0.56
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:G:253:MET:O	1:G:257:LEU:HD13	2.05	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: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:B:150:ILE:HD12	1:B:158:PHE:CE1	2.42	0.55
1:E:118:VAL:HG23	1:E:205:LEU:O	2.06	0.55
1:G:107:LEU:HD22	1:G:182:ILE:CD1	2.37	0.55
1:L:326:MET:HE3	1:L:327:GLN:NE2	2.20	0.55
1:A:289:PRO:HB3	1:F:162:GLU:CD	2.32	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ILE:O	1:A:75:ASN:CB	2.55	0.55
1:E:147:PHE:HB3	1:E:342:LEU:HD21	1.89	0.55
1:E:59:ILE:CD1	1:E:126:ASN:HD22	2.21	0.54
1:A:48:VAL:HG21	1:J:59:ILE:HD12	1.90	0.54
1:C:111:ALA:HB1	1:C:117:ILE:CD1	2.37	0.54
1:F:107:LEU:HD22	1:F:182:ILE:HD11	1.90	0.54
1:J:118:VAL:HG11	1:J:138:MET:HE2	1.90	0.54
1:G:150:ILE:HD12	1:G:158:PHE:CE1	2.43	0.54
1:L:199:PRO:O	1:L:200:ASN:HB3	2.07	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:B:68:GLN:HG3	1:F:86:THR:HG22	1.90	0.54
1:G:120:ILE:HG22	1:G:138:MET:HG2	1.89	0.54
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:H:301:LEU:HD13	1:H:322:HIS:CD2	2.42	0.53
1:L:170:ILE:HG22	1:L:249:LEU:HD21	1.90	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:D:150:ILE:HD12	1:D:158:PHE:CE1	2.44	0.53
1:I:301:LEU:HD13	1:I:322:HIS:CD2	2.43	0.53
1:J:167:MET:HE2	1:J:253:MET:HE3	1.91	0.53
1:I:118:VAL:CG1	1:I:138:MET:HE2	2.37	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:B:301:LEU:HD12	1:B:314:MET:HE1	1.90	0.52
1:D:298:VAL:HG22	1:D:324:TRP:CD1	2.44	0.52
1:L:54:ILE:HG23	1:L:54:ILE:O	2.10	0.52
1:B:118:VAL:HG11	1:B:138:MET:HE2	1.91	0.52
1:L:98:CYS:O	1:L:100:LYS:N	2.43	0.52
1:L:257:LEU:HA	1:L:336:LEU:HD13	1.91	0.52
1:B:160:GLU:HB2	1:B:334:THR:HG23	1.91	0.52
1:H:108:HIS:CE1	1:H:138:MET:HE2	2.45	0.52
1:F:199:PRO:O	1:F:200:ASN:HB3	2.09	0.52
1:G:234:VAL:HG12	1:G:234:VAL:O	2.10	0.52
1:L:110:ARG:NH2	1:L:182:ILE:HD11	2.25	0.52
1:B:160:GLU:HA	1:B:336:LEU:HD11	1.93	0.51
1:A:150:ILE:HD12	1:A:158:PHE:CE1	2.45	0.51
1:L:92:LEU:HD11	1:L:135:LEU:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:167:MET:HE2	1:L:253:MET:HE3	1.92	0.51
1:C:167:MET:HE2	1:C:253:MET:HE3	1.93	0.51
1:G:48:VAL:HG21	1:I:59:ILE:HD12	1.92	0.51
1:G:111:ALA:HB1	1:G:117:ILE:CD1	2.41	0.51
1:C:191:ASN:O	1:C:206:THR:HG22	2.11	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:172:GLU:HG3	1:F:320:MET:HE1	1.93	0.51
1:H:199:PRO:O	1:H:200:ASN:HB3	2.10	0.51
1:K:110:ARG:NH2	1:K:182:ILE:HD11	2.25	0.51
1:B:199:PRO:O	1:B:200:ASN:HB3	2.11	0.50
1:E:72:LEU:HD13	1:E:73:GLY:N	2.26	0.50
1:L:107:LEU:HD22	1:L:182:ILE:CD1	2.36	0.50
1:D:59:ILE:HG23	1:D:124:TYR:CG	2.47	0.50
1:D:98:CYS:O	1:D:99:PRO:C	2.53	0.50
1:G:199:PRO:O	1:G:200:ASN:HB3	2.11	0.50
1:K:98:CYS:O	1:K:99:PRO:C	2.54	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
1:E:174:ILE:HD11	1:E:187:VAL:HG21	1.93	0.50
1:K:54:ILE:HG23	1:K:54:ILE:O	2.12	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:A:105:VAL:HG21	1:A:123:VAL:HG11	1.94	0.49
1:L:146:LEU:HD13	1:L:203:LEU:HD22	1.95	0.49
1:L:118:VAL:CG1	1:L:138:MET:HE2	2.28	0.49
1:K:59:ILE:HG23	1:K:124:TYR:CG	2.48	0.49
1:A:174:ILE:HD11	1:A:187:VAL:HG21	1.95	0.49
1:B:118:VAL:HG23	1:B:205:LEU:O	2.13	0.49
1:C:199:PRO:O	1:C:200:ASN:HB3	2.13	0.49
1:D:111:ALA:CB	1:D:177:LEU:HD21	2.43	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:I:92:LEU:HD11	1:I:135:LEU:HB3	1.95	0.49
1:A:93:LYS:HE2	1:A:95:LEU:HD11	1.94	0.48
1:C:59:ILE:HG23	1:C:124:TYR:CG	2.48	0.48
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:105:VAL:HG21	1:B:123:VAL:HG11	1.95	0.48
1:G:191:ASN:O	1:G:206:THR:HG22	2.13	0.48
1:G:59:ILE:HG23	1:G:124:TYR:CD1	2.48	0.48
1:C:72:LEU:C	1:C:72:LEU:HD13	2.38	0.48
1:C:98:CYS:O	1:C:99:PRO:C	2.55	0.48
1:E:52:LEU:HD11	1:E:123:VAL:HG23	1.96	0.48
1:G:98:CYS:O	1:G:99:PRO:C	2.56	0.48
1:L:120:ILE:HG22	1:L:138:MET:HG2	1.96	0.48
1:B:176:TYR:CE2	1:B:180:ILE:HD13	2.49	0.48
1:C:54:ILE:HG23	1:C:54:ILE:O	2.14	0.48
1:D:54:ILE:HG23	1:D:54:ILE:O	2.14	0.48
1:J:160:GLU:HB2	1:J:334:THR:HG23	1.96	0.48
1:D:75:ASN:CB	1:D:95:LEU:HD12	2.44	0.48
1:H:102:ARG:NH1	1:H:134:LEU:HD11	2.28	0.48
1:K:338:THR:O	1:K:342:LEU:HD13	2.14	0.48
1:B:92:LEU:HD11	1:B:135:LEU:HB3	1.96	0.47
1:B:160:GLU:CB	1:B:334:THR:HG23	2.44	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:I:98:CYS:O	1:I:100:LYS:N	2.47	0.47
1:A:259:GLY:HA2	1:A:338:THR:HG23	1.96	0.47
1:B:146:LEU:HD11	1:B:166:ILE:HD13	1.95	0.47
1:I:54:ILE:HG23	1:I:54:ILE:O	2.14	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:E:301:LEU:HD12	1:E:314:MET:HE1	1.97	0.47
1:A:118:VAL:HB	1:A:138:MET:HE2	1.96	0.47
1:B:301:LEU:CD1	1:B:314:MET:HE1	2.45	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:F:118:VAL:CG1	1:F:138:MET:HE2	2.39	0.47
1:H:98:CYS:O	1:H:100:LYS:N	2.48	0.47
1:L:81:ILE:HD11	1:L:137:VAL:HG13	1.97	0.47
1:C:70:LEU:HD11	1:C:80:GLN:HB2	1.97	0.47
1:J:54:ILE:O	1:J:54:ILE:HG23	2.15	0.47
1:J:92:LEU:HD11	1:J:135:LEU:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD21	1:A:105:VAL:HG22	1.97	0.46
1:H:257:LEU:HA	1:H:336:LEU:HD13	1.97	0.46
1:I:150:ILE:HD12	1:I:158:PHE:CE1	2.50	0.46
1:A:48:VAL:HG13	1:A:48:VAL:O	2.15	0.46
1:B:146:LEU:HD13	1:B:203:LEU:HD22	1.97	0.46
1:G:167:MET:HG3	1:G:253:MET:HE2	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:B:177:LEU:HD22	1:B:182:ILE:CG2	2.46	0.46
1:C:47:HIS:N	1:C:47:HIS:CD2	2.84	0.46
1:D:110:ARG:NH2	1:D:182:ILE:HD11	2.30	0.46
1:F:99:PRO:O	1:F:100:LYS:HB2	2.16	0.46
1:F:202:ILE:HD12	1:F:202:ILE:N	2.30	0.46
1:G:107:LEU:HD22	1:G:182:ILE:HD11	1.97	0.46
1:F:170:ILE:HG22	1:F:249:LEU:HD21	1.97	0.46
1:K:118:VAL:HG23	1:K:205:LEU:O	2.15	0.46
1:I:152:ASP:C	1:J:198:ARG:HG3	2.41	0.46
1:L:146:LEU:HD13	1:L:203:LEU:CD2	2.45	0.46
1:F:234:VAL:HG12	1:F:234:VAL:O	2.16	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: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:B:202:ILE:N	1:B:202:ILE:HD12	2.30	0.45
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:I:105:VAL:HG21	1:I:123:VAL:HG11	1.98	0.45
1:L:160:GLU:HB2	1:L:334:THR:HG23	1.98	0.45
1:L:59:ILE:HG23	1:L:124:TYR:CD1	2.51	0.45
1:E:234:VAL:HG12	1:E:234:VAL:O	2.17	0.45
1:G:105:VAL:CG2	1:G:123:VAL:HG21	2.47	0.45
1:B:81:ILE:HD11	1:B:137:VAL:HG13	1.98	0.45
1:F:120:ILE:HG22	1:F:138:MET:HG2	1.99	0.45
1:J:301:LEU:HD12	1:J:314:MET:HE1	1.99	0.45
1:K:98:CYS:O	1:K:100:LYS:N	2.50	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:107:LEU:HD22	1:I:182:ILE:HD12	1.99	0.44
1:I:301:LEU:HD12	1:I:314:MET:HE1	1.99	0.44
1:F:298:VAL:HG22	1:F:324:TRP:CD1	2.52	0.44
1:G:301:LEU:HD12	1:G:314:MET:HE1	1.99	0.44
1:I:172:GLU:HG3	1:I:320:MET:HE1	2.00	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:A:118:VAL:HG22	1:A:205:LEU:O	2.18	0.44
1:B:167:MET:HE2	1:B:253:MET:HB2	1.98	0.44
1:C:72:LEU:HD22	1:C:73:GLY:N	2.33	0.44
1:K:214:THR:HG21	1:K:242:LYS:HG3	1.99	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:C:72:LEU:HD22	1:C:73:GLY:H	1.82	0.43
1:D:199:PRO:O	1:D:200:ASN:CB	2.66	0.43
1:G:170:ILE:HG22	1:G:249:LEU:HD21	2.00	0.43
1:I:146:LEU:HD22	1:I:203:LEU:HD21	2.01	0.43
1:L:338:THR:O	1:L:342:LEU:HD23	2.18	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:111:ALA:HB2	1:J:177:LEU:HD21	2.00	0.43
1:A:98:CYS:O	1:A:100:LYS:N	2.52	0.43
1:I:65:VAL:HA	1:I:81:ILE:HG22	2.00	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:J:59:ILE:CD1	1:J:126:ASN:HD22	2.31	0.43
1:A:70:LEU:N	1:A:70:LEU:HD22	2.34	0.43
1:D:338:THR:O	1:D:342:LEU:HD13	2.19	0.43
1:I:59:ILE:HD12	1:I:59:ILE:H	1.83	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:B:118:VAL:CG1	1:B:138:MET:HE2	2.48	0.43
1:H:199:PRO:O	1:H:200:ASN:CB	2.67	0.43
1:L:118:VAL:HG23	1:L:205:LEU:O	2.17	0.43
1:G:54:ILE:O	1:G:54:ILE:CG2	2.67	0.43
1:B:54:ILE:O	1:B:54:ILE:CG2	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:A:54:ILE:HG23	1:A:54:ILE:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:LEU:CD2	1:G:298:VAL:HG11	2.44	0.42
1:C:167:MET:HG3	1:C:253:MET:HE2	2.01	0.42
1:D:176:TYR:CE2	1:D:180:ILE:HD13	2.54	0.42
1:D:202:ILE:HD12	1:D:202:ILE:N	2.34	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:C:58:ALA:HA	1:C:126:ASN:HD21	1.84	0.42
1:C:95:LEU:HD21	1:C:104:GLU:CD	2.44	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:B:59:ILE:HD11	1:D:48:VAL:HG11	2.01	0.42
1:C:257:LEU:HD21	1:C:298:VAL:HG11	2.01	0.42
1:E:98:CYS:O	1:E:100:LYS:N	2.53	0.42
1:F:160:GLU:HA	1:F:336:LEU:HD11	2.01	0.42
1:G:47:HIS:CD2	1:G:47:HIS:N	2.86	0.42
1:L:174:ILE:HD11	1:L:187:VAL:HG21	2.02	0.42
1:E:92:LEU:HD11	1:E:135:LEU:HB3	2.00	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:A:59:ILE:HG23	1:A:124:TYR:CD1	2.55	0.42
1:A:162:GLU:O	1:A:166:ILE:HG12	2.19	0.42
1:J:59:ILE:HG22	1:J:63:TYR:HB2	2.02	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
1:H:145:GLU:HA	1:H:193:LEU:HD23	2.02	0.41
1:E:214:THR:HG21	1:E:242:LYS:HG3	2.01	0.41
1:I:328:SER:O	1:I:331:VAL:HG12	2.19	0.41
1:L:301:LEU:HD22	1:L:322:HIS:CE1	2.54	0.41
1:A:195:THR:HG23	1:A:202:ILE:O	2.20	0.41
1:A:199:PRO:O	1:A:200:ASN:CB	2.68	0.41
1:B:58:ALA:HA	1:B:126:ASN:HD21	1.84	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:F:110:ARG:NH2	1:F:182:ILE:HD11	2.34	0.41
1:L:150:ILE:HD12	1:L:158:PHE:CE1	2.55	0.41
1:C:174:ILE:HD11	1:C:187:VAL:HG21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:VAL:HG23	1:F:205:LEU:O	2.20	0.41
1:G:328:SER:O	1:G:331:VAL:HG12	2.20	0.41
1:H:160:GLU:HB2	1:H:334:THR:HG23	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:L:332:PRO:HB2	1:L:334:THR:HG22	2.02	0.41
1:A:199:PRO:O	1:A:200:ASN:HB3	2.20	0.41
1:E:52:LEU:HD13	1:E:109:TRP:CE3	2.56	0.41
1:J:202:ILE:N	1:J:202:ILE:HD12	2.36	0.41
1:K:150:ILE:HD12	1:K:158:PHE:CE1	2.55	0.41
1:L:199:PRO:O	1:L:200:ASN:CB	2.68	0.41
1:A:108:HIS:CD2	1:A:120:ILE:HG23	2.55	0.41
1:B:108:HIS:CD2	1:B:120:ILE:HG23	2.55	0.41
1:G:181:ASN:HD22	1:G:215:THR:CG2	2.33	0.41
1:I:166:ILE:CG2	1:I:256:LEU:HD11	2.51	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:94:MET:C	1:A:95:LEU:HD13	2.46	0.41
1:A:192:LEU:HD21	1:A:205:LEU:HD13	2.02	0.41
1:B:102:ARG:NH1	1:B:134:LEU:HD11	2.36	0.41
1:B:259:GLY:O	1:B:342:LEU:HD12	2.20	0.41
1:B:332:PRO:HB2	1:B:334:THR:HG22	2.02	0.41
1:C:202:ILE:N	1:C:202:ILE:HD12	2.35	0.41
1:J:111:ALA:HB1	1:J:117:ILE:CD1	2.50	0.41
1:K:118:VAL:CG2	1:K:141:LEU:HD11	2.41	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
1:E:199:PRO:O	1:E:200:ASN:CB	2.69	0.40
1:H:59:ILE:CG2	1:H:124:TYR:CD1	3.04	0.40
1:B:98:CYS:O	1:B:100:LYS:N	2.55	0.40
1:E:59:ILE:H	1:E:59:ILE:HD12	1.86	0.40
1:F:257:LEU:HD23	1:F:291:TRP:CZ3	2.56	0.40
1:F:327:GLN:C	1:F:329:THR:H	2.29	0.40
1:G:59:ILE:HG23	1:G:124:TYR:CE1	2.57	0.40
1:H:54:ILE:HG23	1:H:54:ILE:O	2.21	0.40
1:H:150:ILE:HD12	1:H:158:PHE:CD1	2.56	0.40
1:J:199:PRO:O	1:J:200:ASN:CB	2.69	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:HD12	1:H:202:ILE:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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	262/318 (82%)	235 (90%)	19 (7%)	8 (3%)	3	14
1	B	262/318 (82%)	237 (90%)	17 (6%)	8 (3%)	3	14
1	C	262/318 (82%)	238 (91%)	16 (6%)	8 (3%)	3	14
1	D	262/318 (82%)	238 (91%)	15 (6%)	9 (3%)	3	12
1	E	262/318 (82%)	239 (91%)	15 (6%)	8 (3%)	3	14
1	F	262/318 (82%)	240 (92%)	12 (5%)	10 (4%)	2	10
1	G	262/318 (82%)	240 (92%)	15 (6%)	7 (3%)	4	16
1	H	262/318 (82%)	239 (91%)	16 (6%)	7 (3%)	4	16
1	I	262/318 (82%)	239 (91%)	15 (6%)	8 (3%)	3	14
1	J	262/318 (82%)	243 (93%)	13 (5%)	6 (2%)	5	19
1	K	262/318 (82%)	242 (92%)	12 (5%)	8 (3%)	3	14
1	L	262/318 (82%)	237 (90%)	18 (7%)	7 (3%)	4	16
All	All	3144/3816 (82%)	2867 (91%)	183 (6%)	94 (3%)	3	14

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	233 (96%)	9 (4%)	30	64
1	B	242/287 (84%)	232 (96%)	10 (4%)	27	61
1	C	243/287 (85%)	234 (96%)	9 (4%)	30	64
1	D	241/287 (84%)	232 (96%)	9 (4%)	30	64
1	E	243/287 (85%)	234 (96%)	9 (4%)	30	64
1	F	241/287 (84%)	229 (95%)	12 (5%)	22	53
1	G	241/287 (84%)	227 (94%)	14 (6%)	18	49
1	H	240/287 (84%)	228 (95%)	12 (5%)	22	53
1	I	238/287 (83%)	228 (96%)	10 (4%)	26	60
1	J	242/287 (84%)	229 (95%)	13 (5%)	20	51
1	K	242/287 (84%)	234 (97%)	8 (3%)	33	67
1	L	244/287 (85%)	234 (96%)	10 (4%)	27	61
All	All	2899/3444 (84%)	2774 (96%)	125 (4%)	26	60

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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	59	ILE
1	C	72	LEU
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
1	D	59	ILE
1	D	95	LEU
1	D	131	ARG
1	D	135	LEU
1	D	149	ARG
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	264	TYR
1	E	333	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	340	ARG
1	E	342	LEU
1	E	344	GLU
1	F	48	VAL
1	F	59	ILE
1	F	135	LEU
1	F	149	ARG
1	F	152	ASP
1	F	198	ARG
1	F	206	THR
1	F	240	TYR
1	F	264	TYR
1	F	326	MET
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	327	GLN
1	G	333	GLN
1	G	340	ARG
1	G	342	LEU
1	H	48	VAL
1	H	49	LYS
1	H	59	ILE
1	H	105	VAL
1	H	135	LEU
1	H	149	ARG
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	49	LYS
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	120	ILE
1	J	131	ARG
1	J	135	LEU
1	J	149	ARG
1	J	152	ASP
1	J	190	GLU
1	J	264	TYR
1	J	334	THR
1	J	343	LYS
1	K	53	GLN
1	K	57	ASN
1	K	59	ILE
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	120	ILE
1	L	149	ARG
1	L	244	CYS
1	L	264	TYR
1	L	265	SER
1	L	334	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	B	113	GLN
1	B	126	ASN
1	B	175	GLN
1	B	191	ASN
1	B	304	ASN
1	B	321	ASN
1	C	47	HIS
1	C	57	ASN
1	C	126	ASN
1	C	151	GLN
1	C	175	GLN
1	C	191	ASN
1	C	312	GLN
1	C	321	ASN
1	C	337	HIS
1	D	57	ASN
1	D	126	ASN
1	D	151	GLN
1	D	175	GLN
1	D	191	ASN
1	D	304	ASN
1	D	321	ASN
1	D	333	GLN
1	E	68	GLN
1	E	108	HIS
1	E	126	ASN
1	E	151	GLN
1	E	191	ASN
1	E	283	GLN
1	E	304	ASN
1	E	321	ASN
1	F	57	ASN
1	F	80	GLN
1	F	126	ASN
1	F	151	GLN
1	F	191	ASN
1	F	304	ASN
1	F	312	GLN
1	F	327	GLN
1	F	333	GLN
1	G	47	HIS
1	G	57	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	126	ASN
1	G	175	GLN
1	G	191	ASN
1	G	321	ASN
1	G	327	GLN
1	H	113	GLN
1	H	126	ASN
1	H	151	GLN
1	H	175	GLN
1	H	191	ASN
1	H	304	ASN
1	H	333	GLN
1	I	57	ASN
1	I	126	ASN
1	I	178	HIS
1	I	191	ASN
1	I	304	ASN
1	J	57	ASN
1	J	191	ASN
1	J	304	ASN
1	J	322	HIS
1	J	333	GLN
1	K	53	GLN
1	K	57	ASN
1	K	68	GLN
1	K	151	GLN
1	K	191	ASN
1	K	321	ASN
1	K	333	GLN
1	L	57	ASN
1	L	126	ASN
1	L	151	GLN
1	L	191	ASN
1	L	304	ASN
1	L	312	GLN
1	L	321	ASN
1	L	322	HIS
1	L	327	GLN
1	L	333	GLN
1	L	337	HIS

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 oligosaccharides 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	0.90	1 (3%)	40,52,52	2.27	14 (35%)
2	05B	B	1000	-	33,35,35	0.94	1 (3%)	40,52,52	2.41	14 (35%)

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	-	-	4/8/40/40	0/6/6/6
2	05B	B	1000	-	-	4/8/40/40	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	05B	C11-N15	-3.27	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	05B	C11-N15	-3.16	1.33	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	05B	C1-C11-N15	8.41	130.31	123.09
2	A	1000	05B	C1-C11-N15	6.50	128.68	123.09
2	B	1000	05B	C18-N19-C20	4.83	120.84	116.07
2	A	1000	05B	C18-N19-C20	4.77	120.79	116.07
2	A	1000	05B	N19-C20-N21	-4.44	120.88	125.23
2	B	1000	05B	N19-C20-N21	-4.10	121.21	125.23
2	B	1000	05B	C9-C6-C1	3.69	113.51	109.17
2	A	1000	05B	C17-C16-N21	-3.41	118.94	122.92
2	B	1000	05B	C17-C18-N19	-3.40	119.81	123.97
2	B	1000	05B	C17-C16-N21	-3.38	118.98	122.92
2	A	1000	05B	C22-C20-N19	3.32	120.90	117.34
2	B	1000	05B	C9-N5-C8	3.32	119.77	110.40
2	A	1000	05B	C17-C18-N19	-3.21	120.04	123.97
2	A	1000	05B	C8-C7-C1	3.19	112.92	109.17
2	A	1000	05B	O30-C29-O28	-3.17	103.12	108.09
2	B	1000	05B	C22-C20-N19	3.08	120.64	117.34
2	B	1000	05B	C16-C14-C13	-2.91	127.10	132.61
2	A	1000	05B	C9-N5-C8	2.89	118.55	110.40
2	A	1000	05B	C16-C14-C13	-2.84	127.24	132.61
2	A	1000	05B	O30-C26-C25	2.79	131.57	127.86
2	B	1000	05B	O30-C29-O28	-2.75	103.77	108.09
2	A	1000	05B	C9-C6-C1	2.67	112.31	109.17
2	B	1000	05B	O30-C26-C25	2.51	131.19	127.86
2	B	1000	05B	O10-C4-C12	-2.28	120.95	125.98
2	A	1000	05B	O10-C4-C12	-2.22	121.08	125.98
2	B	1000	05B	O28-C27-C24	2.09	131.75	127.72
2	B	1000	05B	C2-C1-C11	-2.07	109.05	113.04
2	A	1000	05B	O28-C27-C24	2.07	131.71	127.72

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1000	05B	N19-C20-C22-C23
2	B	1000	05B	N19-C20-C22-C25
2	B	1000	05B	N21-C20-C22-C23
2	B	1000	05B	N21-C20-C22-C25

Continued on next page...

Continued from previous page...

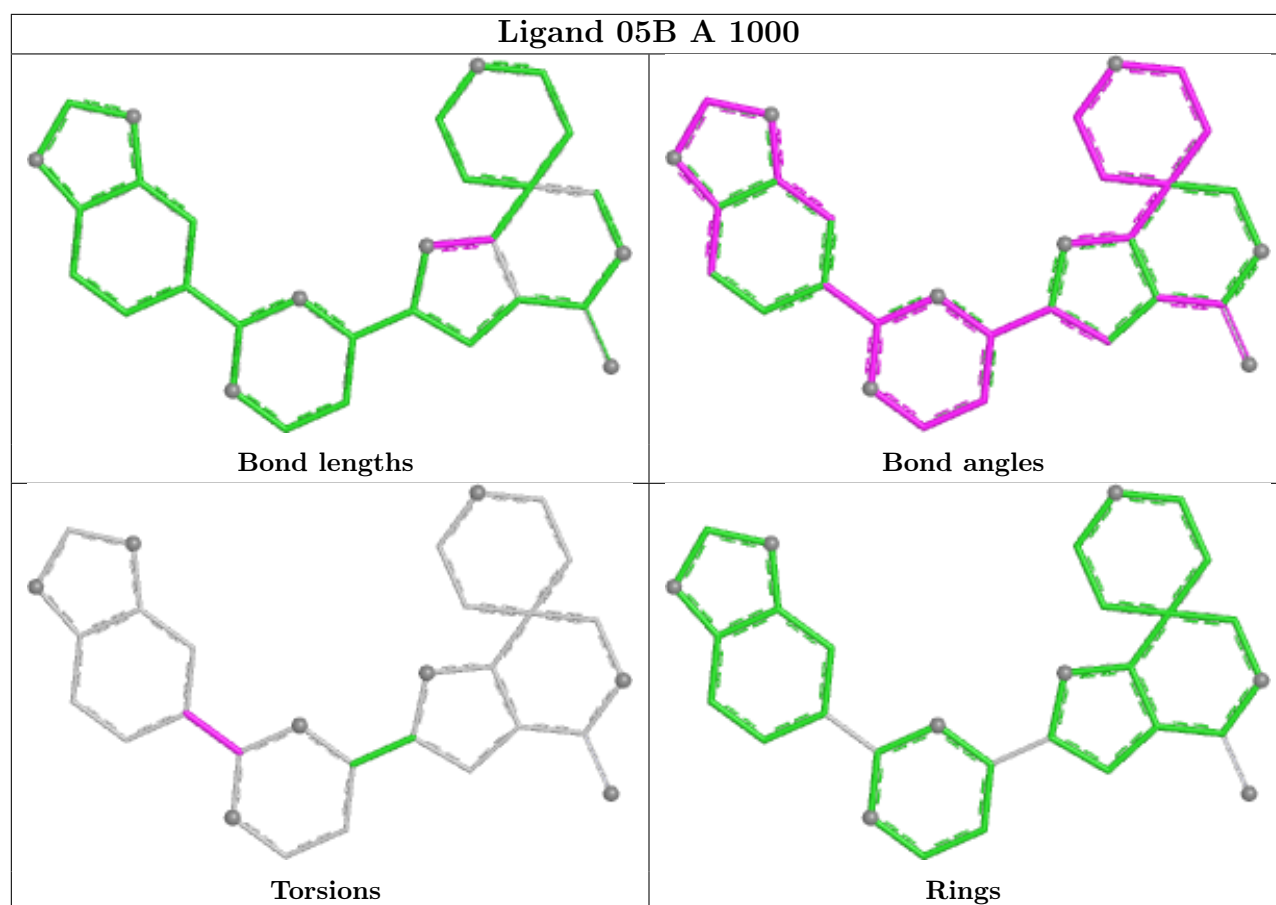
Mol	Chain	Res	Type	Atoms
2	A	1000	05B	N21-C20-C22-C23
2	A	1000	05B	N19-C20-C22-C23
2	A	1000	05B	N19-C20-C22-C25
2	A	1000	05B	N21-C20-C22-C25

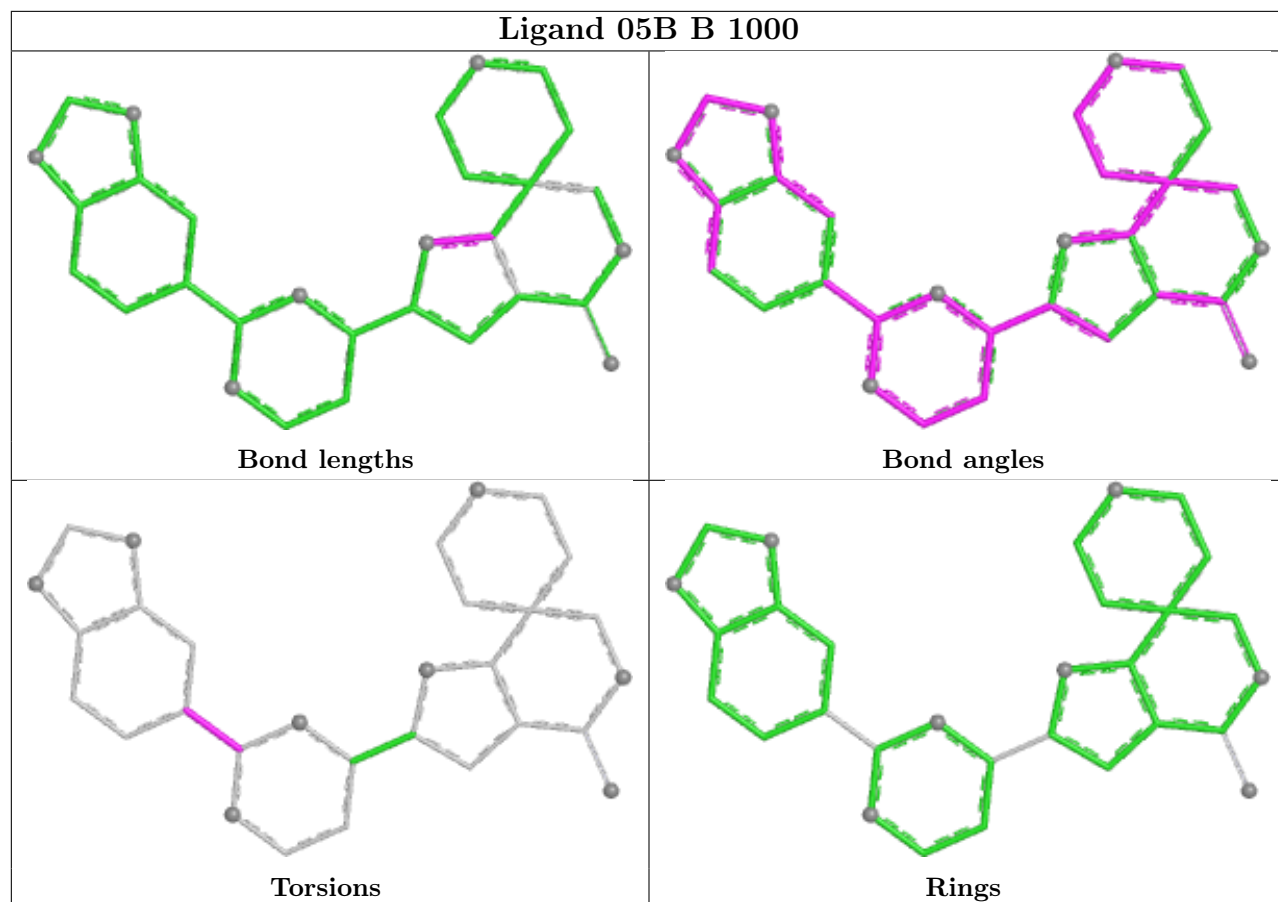
There are no ring outliers.

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	272/318 (85%)	0.32	9 (3%)	49	40	76, 86, 104, 117	0
1	B	272/318 (85%)	0.28	7 (2%)	57	48	83, 93, 109, 129	0
1	C	272/318 (85%)	0.27	10 (3%)	45	37	80, 95, 122, 131	0
1	D	272/318 (85%)	0.27	9 (3%)	49	40	78, 89, 106, 113	0
1	E	272/318 (85%)	0.32	9 (3%)	49	40	85, 96, 118, 129	0
1	F	272/318 (85%)	0.39	13 (4%)	35	28	76, 89, 105, 115	0
1	G	272/318 (85%)	0.29	10 (3%)	45	37	87, 102, 123, 132	0
1	H	272/318 (85%)	0.28	4 (1%)	72	64	93, 110, 137, 154	0
1	I	272/318 (85%)	0.37	12 (4%)	39	30	101, 112, 125, 141	0
1	J	272/318 (85%)	0.38	12 (4%)	39	30	83, 96, 112, 125	0
1	K	272/318 (85%)	0.26	5 (1%)	67	59	104, 113, 137, 144	0
1	L	272/318 (85%)	0.23	9 (3%)	49	40	90, 105, 126, 138	0
All	All	3264/3816 (85%)	0.30	109 (3%)	49	40	76, 99, 125, 154	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	94	MET	4.9
1	A	282	GLY	4.6
1	J	75	ASN	4.2
1	A	274	GLY	3.8
1	B	274	GLY	3.8
1	F	73	GLY	3.7
1	L	228	TYR	3.7
1	F	175	GLN	3.6
1	C	74	ILE	3.5
1	A	74	ILE	3.4
1	I	294	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	74	ILE	3.2
1	B	74	ILE	3.2
1	B	136	ILE	3.2
1	A	234	VAL	3.1
1	C	59	ILE	3.0
1	B	47	HIS	3.0
1	I	127	LEU	3.0
1	C	240	TYR	2.9
1	H	75	ASN	2.9
1	A	265	SER	2.9
1	F	209	GLY	2.8
1	E	74	ILE	2.8
1	C	73	GLY	2.8
1	L	75	ASN	2.8
1	G	67	SER	2.8
1	E	274	GLY	2.8
1	K	130	GLY	2.8
1	A	54	ILE	2.7
1	F	274	GLY	2.7
1	E	58	ALA	2.7
1	G	66	THR	2.7
1	F	328	SER	2.7
1	J	67	SER	2.7
1	G	48	VAL	2.7
1	K	205	LEU	2.7
1	J	135	LEU	2.6
1	K	81	ILE	2.6
1	D	274	GLY	2.6
1	I	94	MET	2.6
1	G	65	VAL	2.6
1	F	71	GLY	2.6
1	C	99	PRO	2.5
1	I	274	GLY	2.4
1	J	228	TYR	2.4
1	H	54	ILE	2.4
1	L	99	PRO	2.4
1	G	274	GLY	2.4
1	E	198	ARG	2.4
1	H	129	ALA	2.4
1	E	59	ILE	2.4
1	F	74	ILE	2.4
1	D	144	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	250	GLY	2.4
1	D	67	SER	2.4
1	D	265	SER	2.4
1	A	73	GLY	2.3
1	E	265	SER	2.3
1	J	123	VAL	2.3
1	L	73	GLY	2.3
1	J	87	GLN	2.3
1	D	240	TYR	2.3
1	J	308	THR	2.3
1	I	75	ASN	2.2
1	J	240	TYR	2.2
1	K	176	TYR	2.2
1	L	243	SER	2.2
1	C	157	ALA	2.2
1	B	342	LEU	2.2
1	J	345	ASP	2.2
1	A	48	VAL	2.2
1	C	227	PRO	2.2
1	F	240	TYR	2.2
1	I	108	HIS	2.2
1	E	94	MET	2.2
1	G	73	GLY	2.2
1	I	120	ILE	2.2
1	D	75	ASN	2.2
1	K	228	TYR	2.2
1	L	240	TYR	2.2
1	G	54	ILE	2.1
1	I	66	THR	2.1
1	I	334	THR	2.1
1	F	72	LEU	2.1
1	E	228	TYR	2.1
1	B	265	SER	2.1
1	D	157	ALA	2.1
1	D	328	SER	2.1
1	H	74	ILE	2.1
1	L	135	LEU	2.1
1	G	80	GLN	2.1
1	F	48	VAL	2.1
1	I	118	VAL	2.1
1	J	334	THR	2.1
1	C	229	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	78	VAL	2.1
1	C	75	ASN	2.1
1	I	249	LEU	2.1
1	D	106	GLU	2.1
1	C	264	TYR	2.1
1	J	113	GLN	2.0
1	F	304	ASN	2.0
1	F	76	GLY	2.0
1	B	201	ALA	2.0
1	I	53	GLN	2.0
1	E	249	LEU	2.0
1	G	76	GLY	2.0
1	F	59	ILE	2.0
1	A	330	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

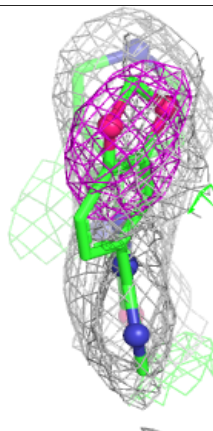
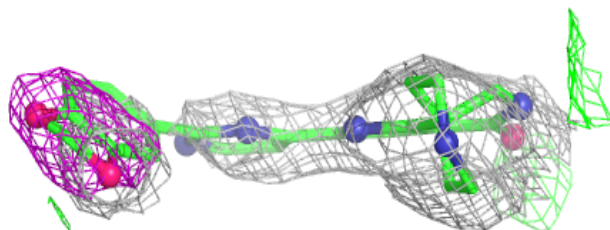
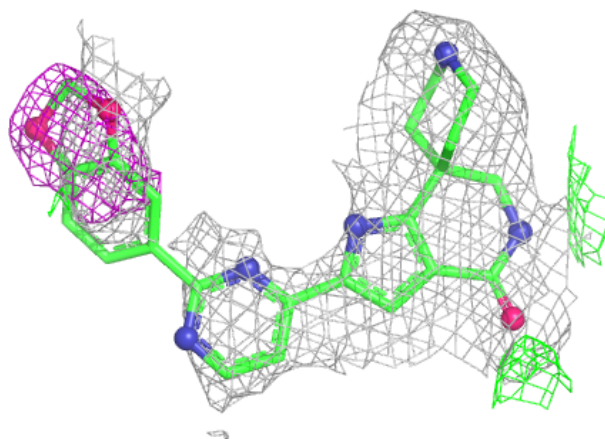
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

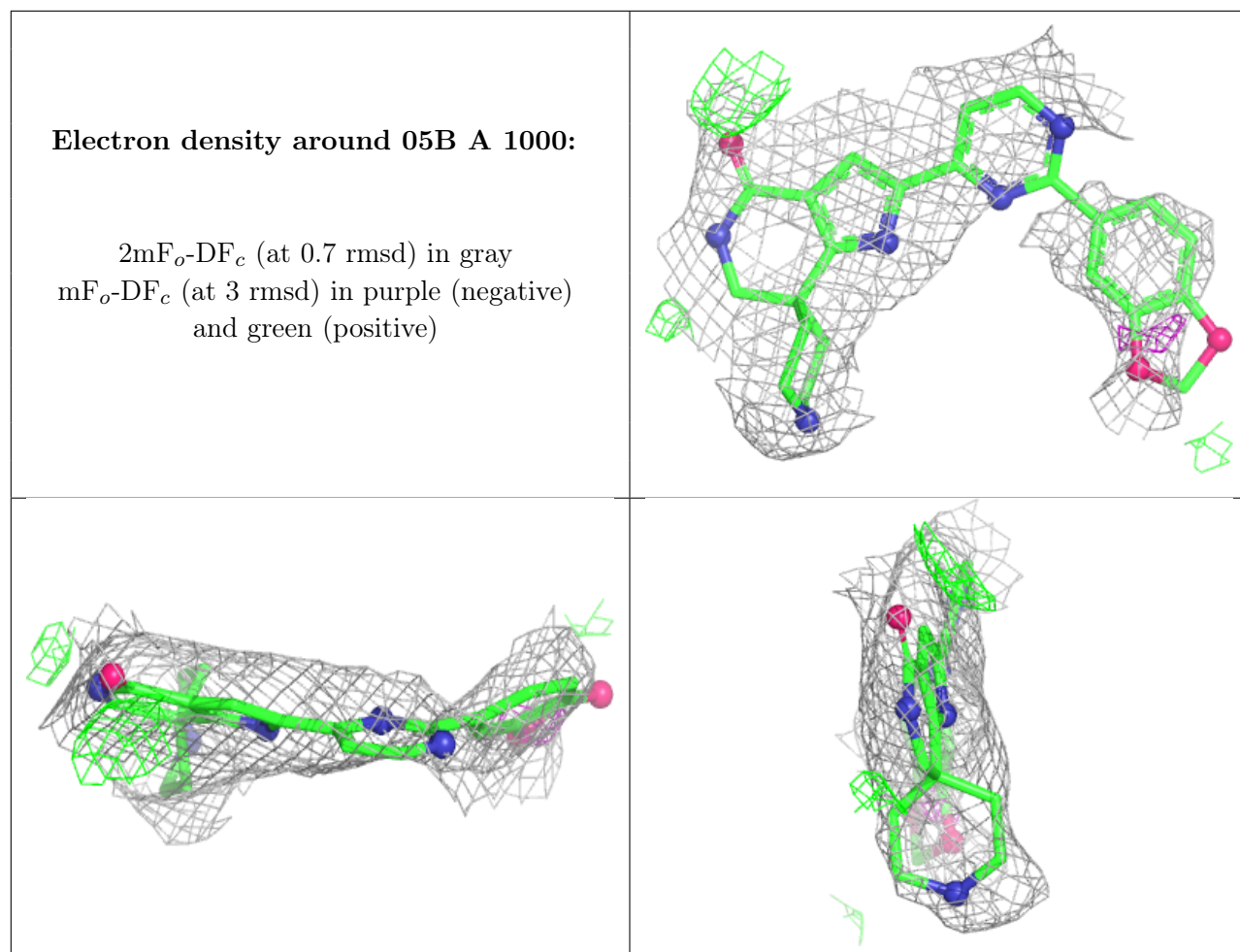
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	05B	B	1000	30/30	0.86	0.12	85,86,91,91	0
2	05B	A	1000	30/30	0.88	0.13	88,89,91,91	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 05B B 1000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.