



wwPDB X-ray Structure Validation Summary Report ⓘ

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 wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

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

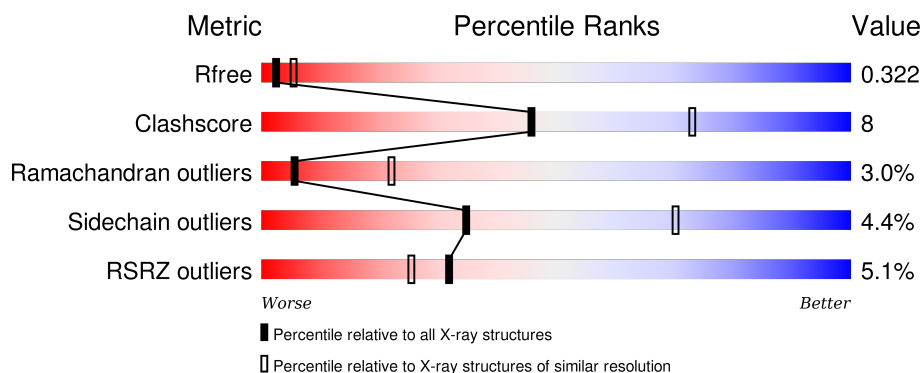
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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 $\leq 5\%$. 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	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>16%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	318	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>19%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	318	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>15%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	318	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>14%</div> <div>•</div> <div>14%</div> </div> </div>
1	E	318	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>17%</div> <div>•</div> <div>14%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	318	
1	G	318	
1	H	318	
1	I	318	
1	J	318	
1	K	318	
1	L	318	

2 Entry composition

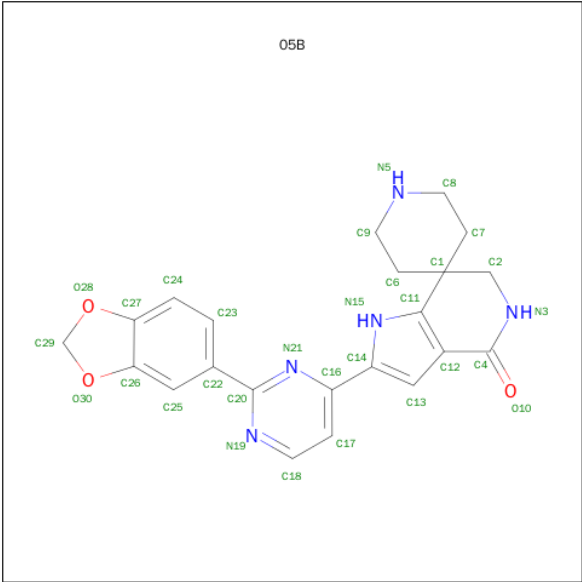
There are 2 unique types of molecules in this entry. The entry contains 26381 atoms, of which 0 are hydrogens and 0 are deuteriums.

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			

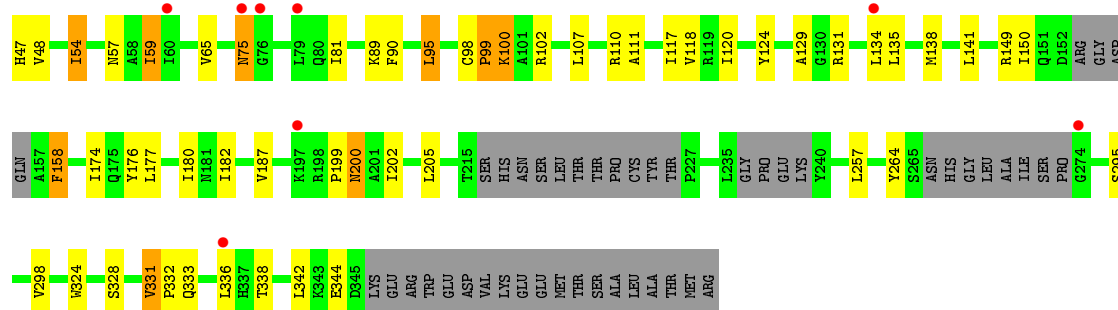
- Molecule 2 is 2'-[2-(1,3-BENZODIOXOL-5-YL)PYRIMIDIN-4-YL]-5',6'-DIHYDROSPIR O[PIPERIDINE-4,7'-PYRROLO[3,2-C]PYRIDIN]-4'(1'H)-ONE (three-letter code: 05B) (formula: C₂₂H₂₁N₅O₃).



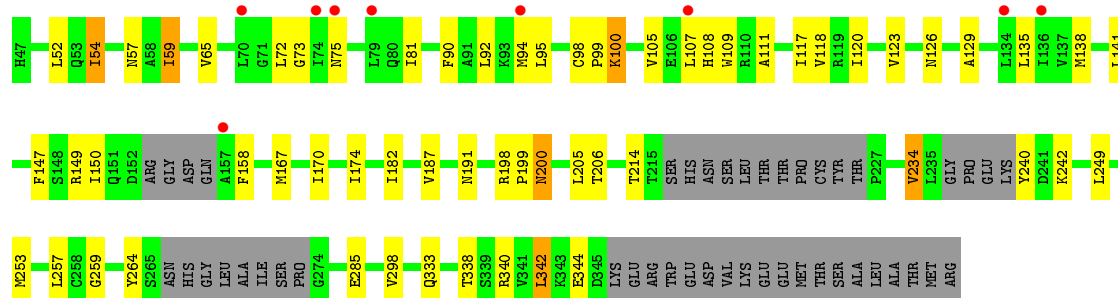
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	22	5	3		
2	B	1	Total	C	N	O	0	0
			30	22	5	3		



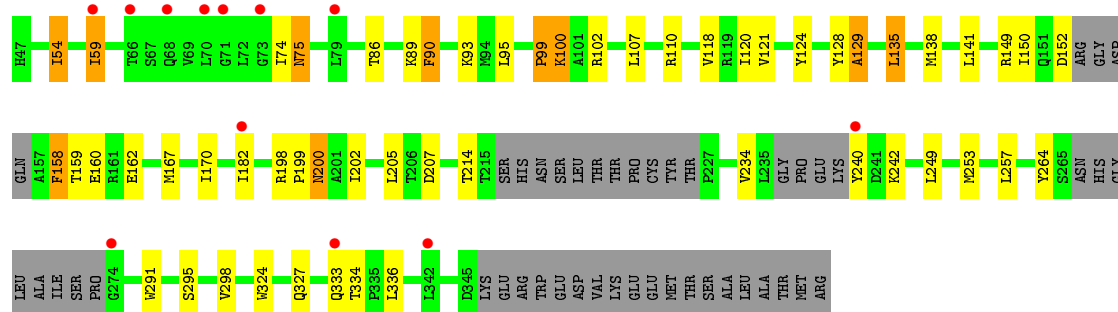
- Molecule 1: MAP kinase-activated protein kinase 2



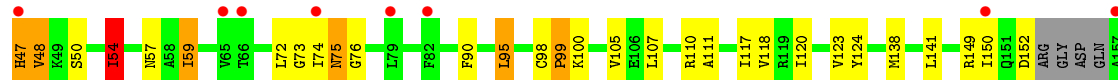
- Molecule 1: MAP kinase-activated protein kinase 2



- Molecule 1: MAP kinase-activated protein kinase 2



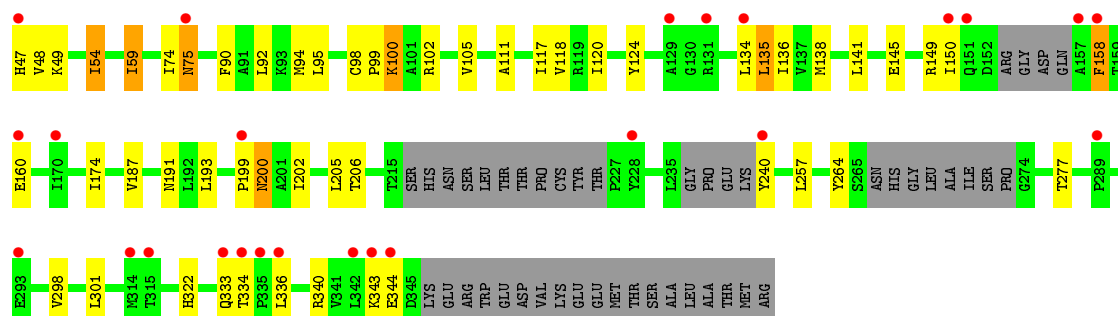
- Molecule 1: MAP kinase-activated protein kinase 2



- Molecule 1: MAP kinase-activated protein kinase 2



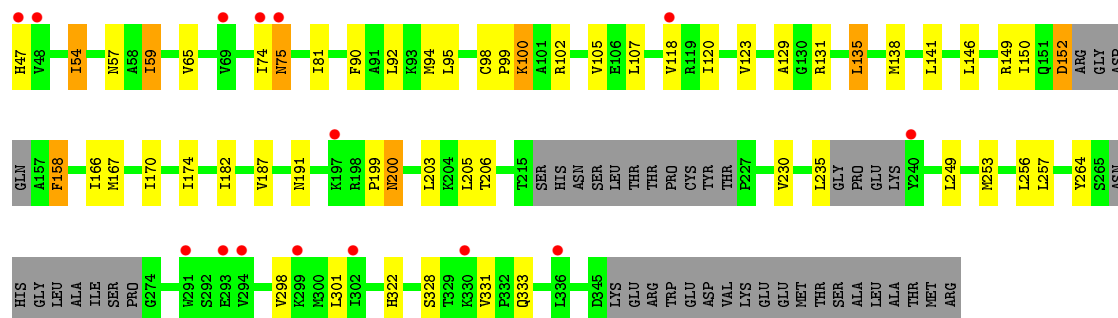
Chain H:



- Molecule 1: MAP kinase-activated protein kinase 2



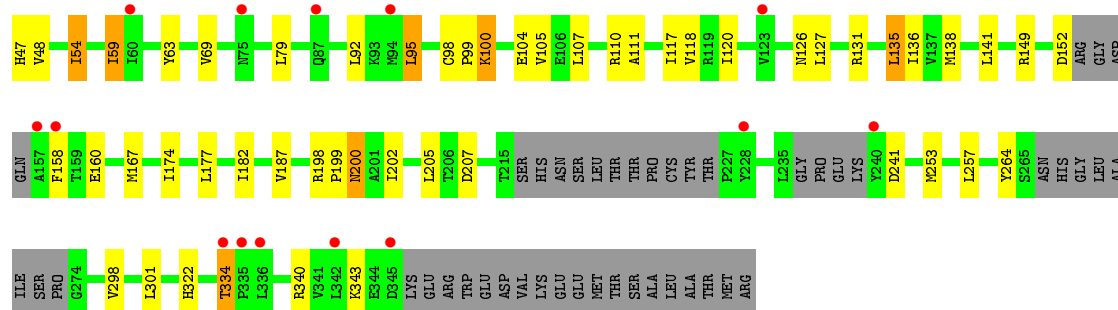
Chain I:



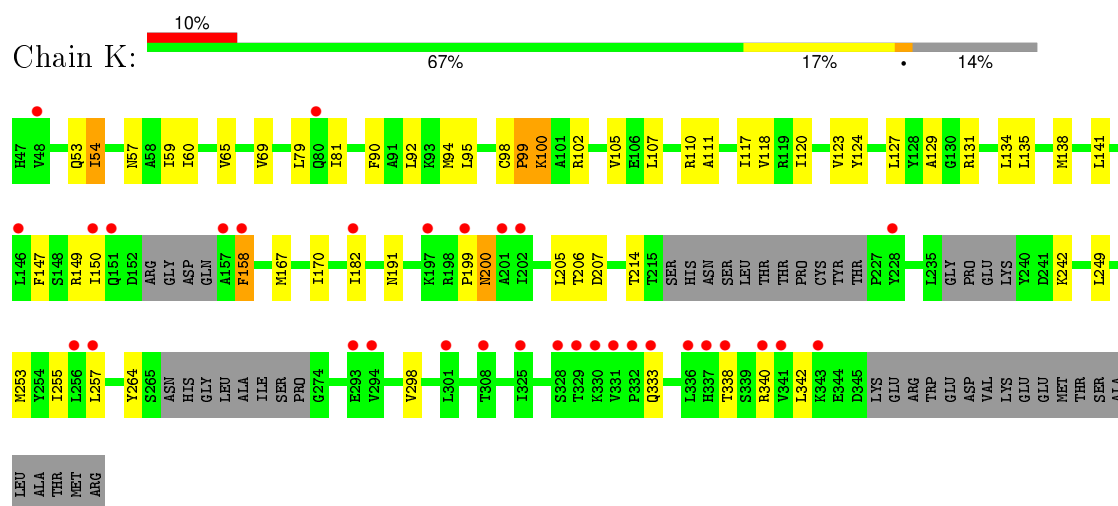
- Molecule 1: MAP kinase-activated protein kinase 2



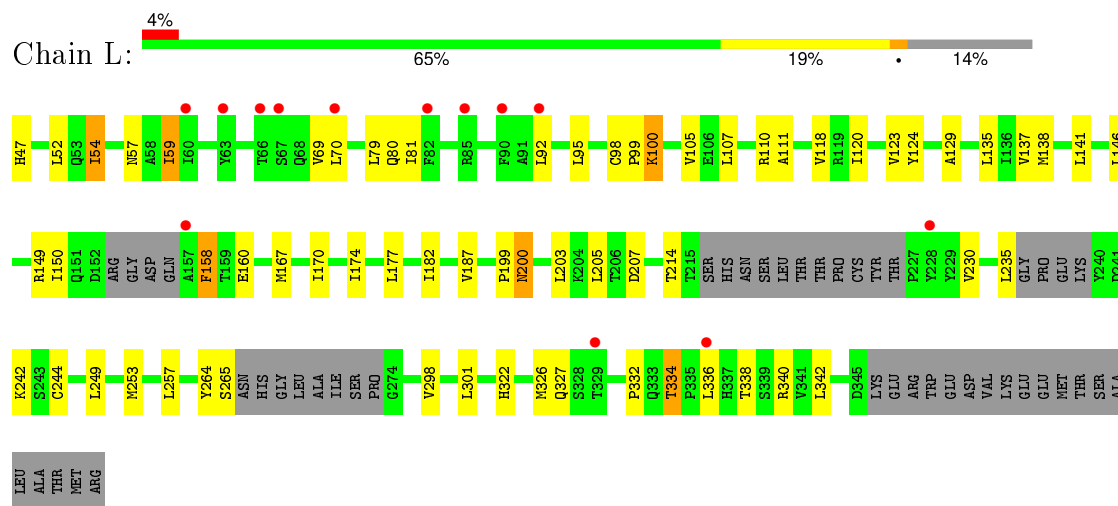
Chain J:



- 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 (5.28%)	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	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 [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	45	0

Continued on next page...

Continued from previous page...

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.

The worst 5 of 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

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%)	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
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

5 of 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

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%)	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	264	TYR
1	G	264	TYR
1	L	47	HIS
1	F	334	THR
1	G	57	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	47	HIS
1	H	191	ASN
1	L	126	ASN
1	G	57	ASN
1	G	191	ASN

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

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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 [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%)	0.37	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

The worst 5 of 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

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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	LLDF	B-factors(\AA^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.