



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:32 AM 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 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/ValidationPDFNotes.html>

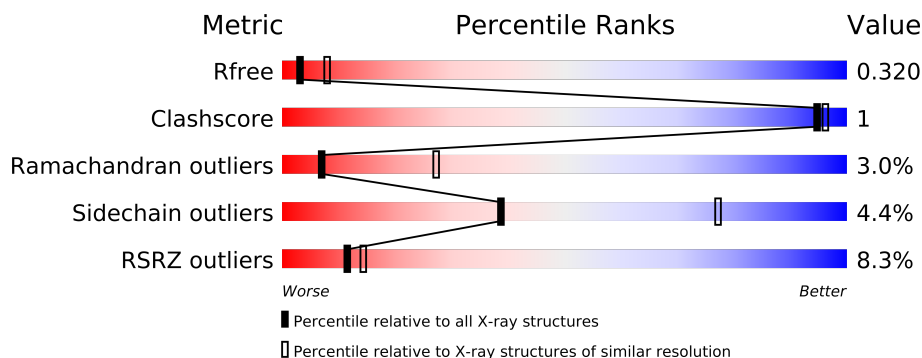
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	318	
1	B	318	
1	C	318	
1	D	318	
1	E	318	
1	F	318	
1	G	318	
1	H	318	
1	I	318	
1	J	318	
1	K	318	
1	L	318	

2 Entry composition

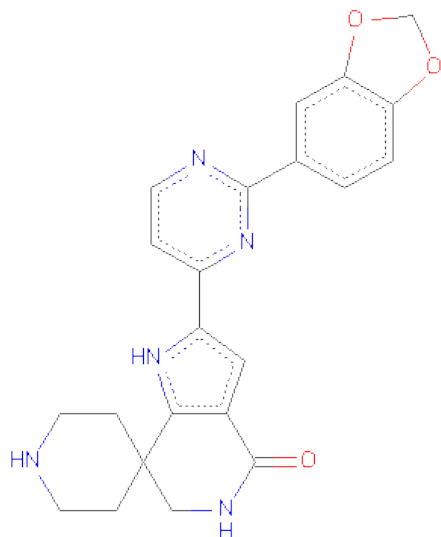
There are 2 unique types of molecules in this entry. The entry contains 26381 atoms, of which 0 are hydrogen and 0 are deuterium.

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).



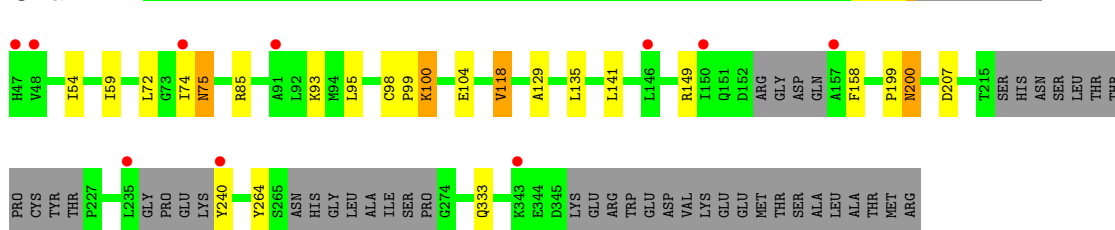
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	22	5	3		
2	B	1	Total	C	N	O	0	0
			30	22	5	3		

3 Residue-property plots

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.

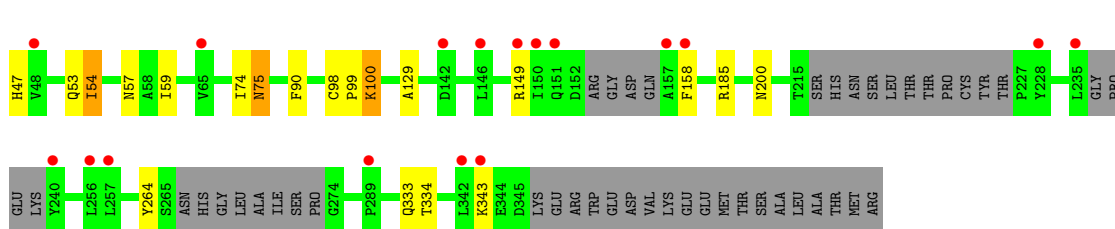
- Molecule 1: MAP kinase-activated protein kinase 2

Chain A:



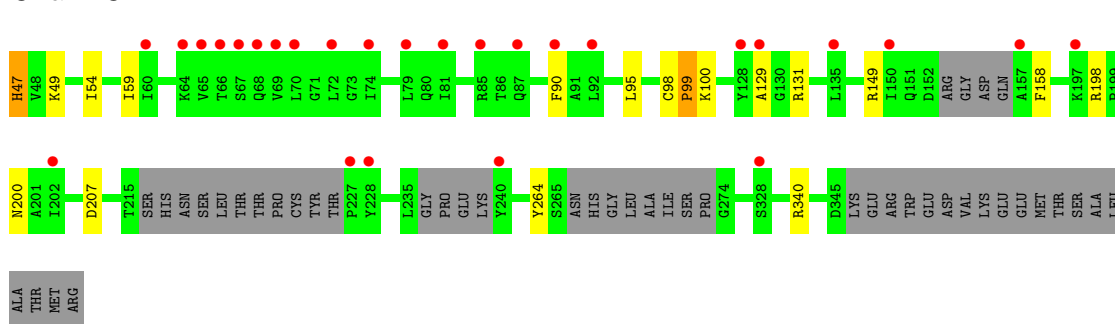
- Molecule 1: MAP kinase-activated protein kinase 2

Chain B:



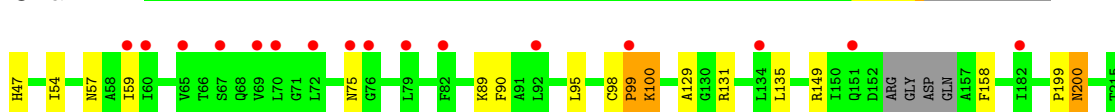
- Molecule 1: MAP kinase-activated protein kinase 2

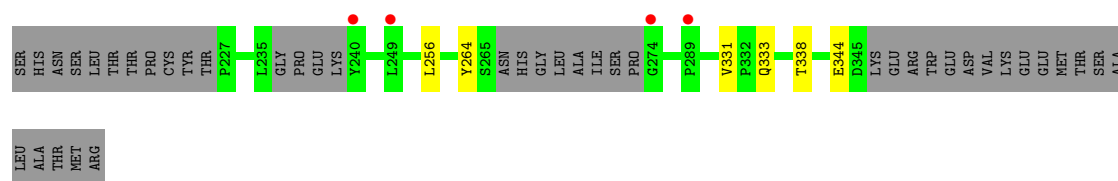
Chain C:



- Molecule 1: MAP kinase-activated protein kinase 2

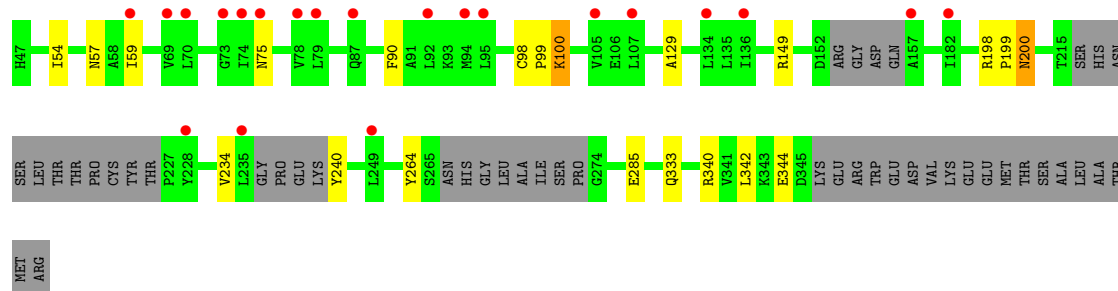
Chain D:





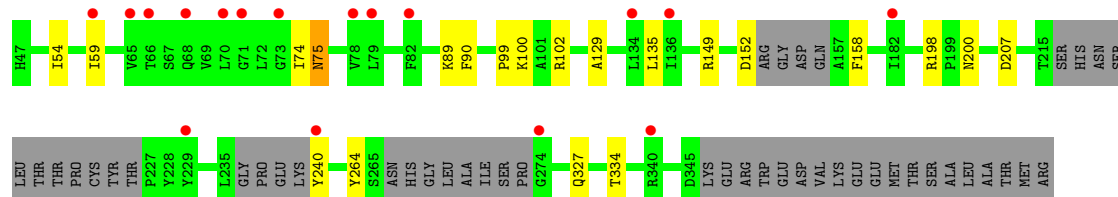
- Molecule 1: MAP kinase-activated protein kinase 2

Chain E:



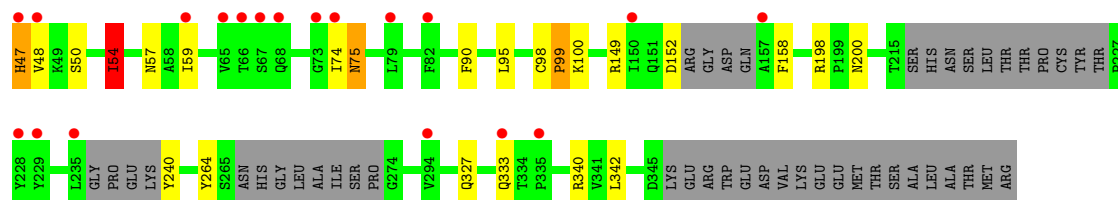
- Molecule 1: MAP kinase-activated protein kinase 2

Chain F:



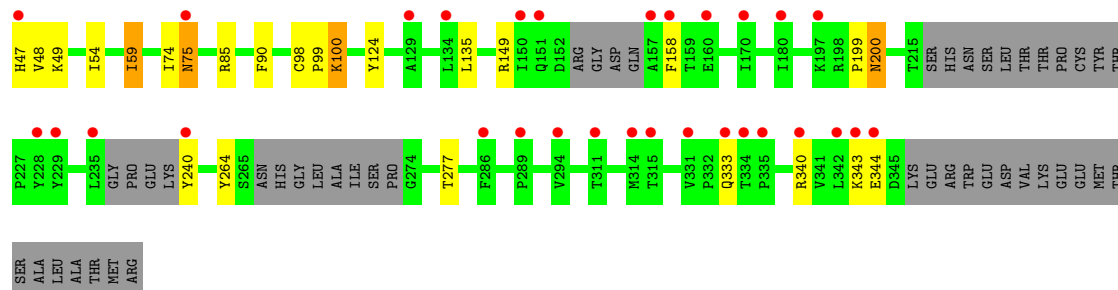
- Molecule 1: MAP kinase-activated protein kinase 2

Chain G:



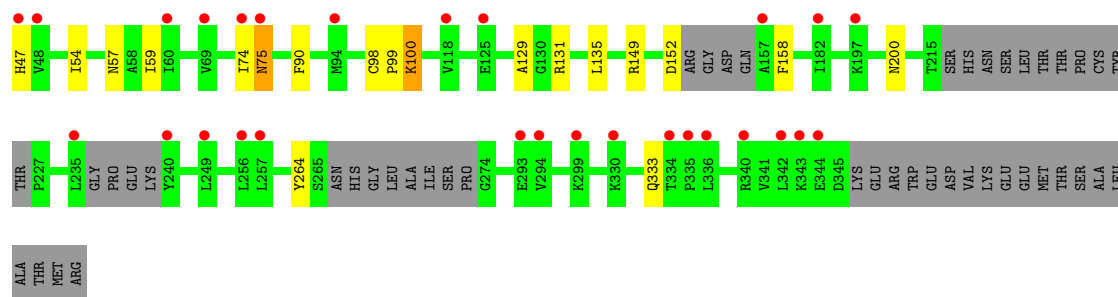
- Molecule 1: MAP kinase-activated protein kinase 2

Chain H:



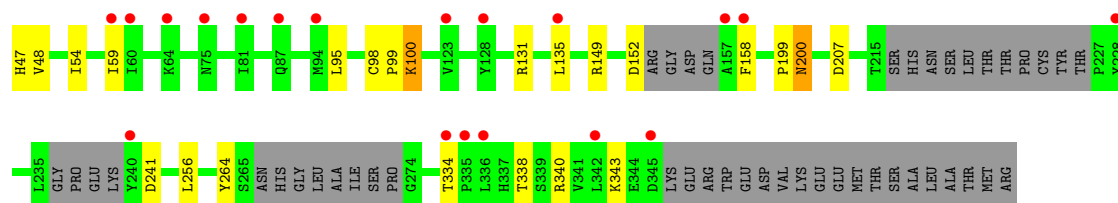
- Molecule 1: MAP kinase-activated protein kinase 2

Chain I:



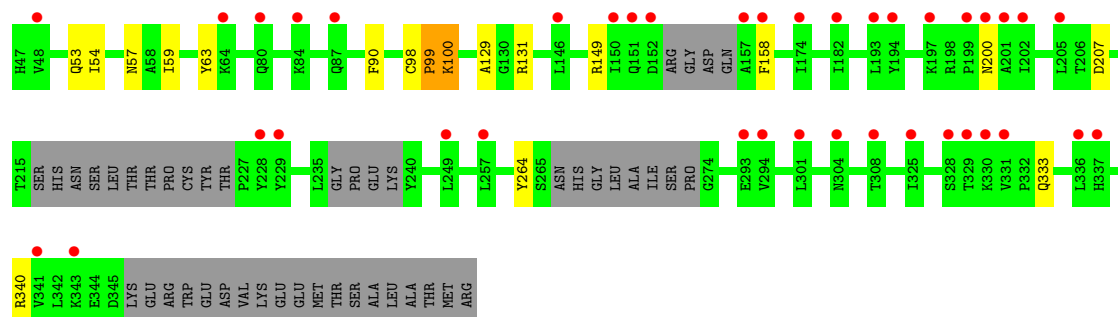
- Molecule 1: MAP kinase-activated protein kinase 2

Chain J:



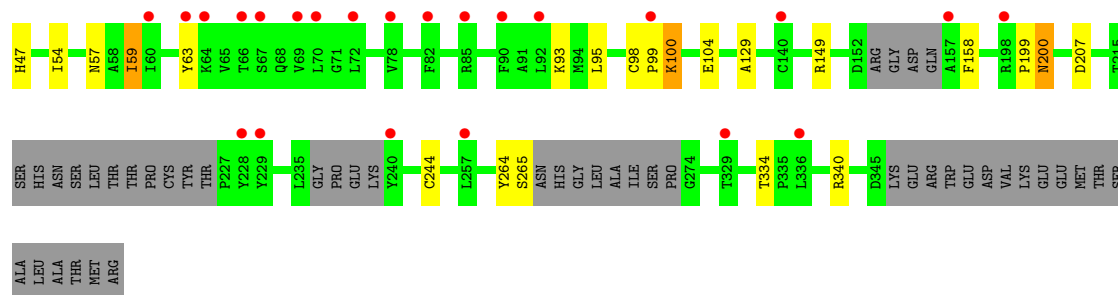
- Molecule 1: MAP kinase-activated protein kinase 2

Chain K:



- Molecule 1: MAP kinase-activated protein kinase 2

Chain L:



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 , 0.320	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 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2194	0	0	5	0
1	B	2197	0	0	3	0
1	C	2197	0	0	2	0
1	D	2193	0	0	4	0
1	E	2198	0	0	3	0
1	F	2191	0	0	1	0
1	G	2191	0	0	4	0
1	H	2187	0	0	5	0
1	I	2181	0	0	2	0
1	J	2195	0	0	3	0
1	K	2196	0	0	3	0
1	L	2201	0	0	4	0
2	A	30	0	21	0	0
2	B	30	0	21	0	0
All	All	26381	0	42	38	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (38) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:74:ILE:O	1:G:75:ASN:CB	2.47	0.63
1:F:74:ILE:O	1:F:75:ASN:CB	2.50	0.60
1:I:74:ILE:O	1:I:75:ASN:CB	2.48	0.60
1:D:98:CYS:O	1:D:100:LYS:N	2.38	0.56
1:J:98:CYS:O	1:J:100:LYS:N	2.38	0.56
1:H:74:ILE:O	1:H:75:ASN:CB	2.53	0.55
1:A:74:ILE:O	1:A:75:ASN:CB	2.55	0.55
1:A:93:LYS:NZ	1:A:104:GLU:OE1	2.41	0.54
1:L:98:CYS:O	1:L:100:LYS:N	2.43	0.52
1:A:118:VAL:CG1	1:A:141:LEU:CD1	2.88	0.51
1:I:98:CYS:O	1:I:100:LYS:N	2.47	0.47
1:H:98:CYS:O	1:H:100:LYS:N	2.48	0.47
1:D:98:CYS:O	1:D:99:PRO:C	2.53	0.46
1:C:47:HIS:CD2	1:C:47:HIS:N	2.84	0.46
1:K:98:CYS:O	1:K:99:PRO:C	2.54	0.46
1:B:54:ILE:CG2	1:B:54:ILE:O	2.64	0.46
1:K:98:CYS:O	1:K:100:LYS:N	2.50	0.45
1:E:200:ASN:ND2	1:H:85:ARG:O	2.50	0.44
1:C:98:CYS:O	1:C:99:PRO:C	2.55	0.44
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:B:74:ILE:O	1:B:75:ASN:CB	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:98:CYS:O	1:A:100:LYS:N	2.52	0.43
1:J:256:LEU:O	1:J:338:THR:OG1	2.37	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:D:256:LEU:O	1:D:338:THR:OG1	2.37	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:L:59:ILE:O	1:L:63:TYR:N	2.53	0.42
1:A:199:PRO:O	1:A:200:ASN:CB	2.68	0.41
1:L:199:PRO:O	1:L:200:ASN:CB	2.68	0.41
1:E:199:PRO:O	1:E:200:ASN:CB	2.69	0.40
1:K:59:ILE:O	1:K:63:TYR:N	2.54	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:J:199:PRO:O	1:J:200:ASN:CB	2.69	0.40
1:L:93:LYS:NZ	1:L:104:GLU:OE1	2.54	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%)	7	26
1	B	262/318 (82%)	237 (90%)	17 (6%)	8 (3%)	7	26
1	C	262/318 (82%)	238 (91%)	16 (6%)	8 (3%)	7	26
1	D	262/318 (82%)	238 (91%)	15 (6%)	9 (3%)	6	23
1	E	262/318 (82%)	239 (91%)	15 (6%)	8 (3%)	7	26
1	F	262/318 (82%)	240 (92%)	12 (5%)	10 (4%)	5	19
1	G	262/318 (82%)	240 (92%)	15 (6%)	7 (3%)	8	30
1	H	262/318 (82%)	239 (91%)	16 (6%)	7 (3%)	8	30
1	I	262/318 (82%)	239 (91%)	15 (6%)	8 (3%)	7	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	262/318 (82%)	243 (93%)	13 (5%)	6 (2%)	10	36
1	K	262/318 (82%)	242 (92%)	12 (5%)	8 (3%)	7	26
1	L	262/318 (82%)	237 (90%)	18 (7%)	7 (3%)	8	30
All	All	3144/3816 (82%)	2867 (91%)	183 (6%)	94 (3%)	7	27

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	L	129	ALA
1	B	158	PHE
1	C	90	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	41	80
1	B	242/287 (84%)	232 (96%)	10 (4%)	41	80
1	C	243/287 (85%)	234 (96%)	9 (4%)	45	84
1	D	241/287 (84%)	230 (95%)	11 (5%)	37	76
1	E	243/287 (85%)	232 (96%)	11 (4%)	38	77
1	F	241/287 (84%)	231 (96%)	10 (4%)	41	80
1	G	241/287 (84%)	225 (93%)	16 (7%)	24	57
1	H	240/287 (84%)	227 (95%)	13 (5%)	31	69
1	I	238/287 (83%)	229 (96%)	9 (4%)	44	83
1	J	242/287 (84%)	229 (95%)	13 (5%)	31	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	242/287 (84%)	235 (97%)	7 (3%)	55	89
1	L	244/287 (85%)	234 (96%)	10 (4%)	41	80
All	All	2899/3444 (84%)	2770 (96%)	129 (4%)	39	77

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
1	D	57	ASN
1	D	59	ILE
1	D	95	LEU
1	D	131	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	G	264	TYR
1	G	327	GLN
1	G	333	GLN
1	G	340	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	K	131	ARG
1	K	149	ARG
1	K	264	TYR
1	K	333	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	-	35,35,35	0.83	2 (5%)	49,52,52	2.25	15 (30%)
2	05B	B	1000	-	35,35,35	0.85	2 (5%)	49,52,52	2.10	14 (28%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	05B	C11-N15	-2.71	1.33	1.37
2	A	1000	05B	C11-N15	-2.61	1.33	1.37
2	B	1000	05B	C13-C14	-2.04	1.36	1.38
2	A	1000	05B	C13-C14	-2.00	1.36	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	05B	C13-C12-C4	6.71	130.92	126.69
2	B	1000	05B	C13-C12-C4	6.57	130.83	126.69
2	A	1000	05B	C16-N21-C20	5.69	121.42	116.75
2	B	1000	05B	C18-N19-C20	5.66	120.84	115.78
2	A	1000	05B	C18-N19-C20	5.60	120.79	115.78
2	B	1000	05B	C16-N21-C20	5.42	121.19	116.75
2	A	1000	05B	C1-C2-N3	4.04	118.31	111.89
2	A	1000	05B	C14-C16-N21	3.82	119.35	115.09
2	B	1000	05B	C17-C18-N19	-3.67	119.81	123.88
2	A	1000	05B	N19-C20-N21	-3.54	120.88	125.23
2	A	1000	05B	C17-C18-N19	-3.46	120.04	123.88
2	B	1000	05B	N19-C20-N21	-3.27	121.21	125.23
2	B	1000	05B	C14-C16-N21	3.16	118.61	115.09
2	A	1000	05B	C22-C20-N19	3.08	120.90	117.39
2	A	1000	05B	O30-C29-O28	-2.87	103.12	108.09
2	B	1000	05B	C22-C20-N19	2.85	120.64	117.39
2	A	1000	05B	C12-C4-N3	2.81	117.66	115.76
2	B	1000	05B	C9-N5-C8	2.77	119.77	110.14
2	B	1000	05B	C12-C13-C14	-2.74	106.27	109.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	05B	C12-C13-C14	-2.58	106.48	109.86
2	A	1000	05B	O30-C26-C25	2.56	131.57	127.85
2	B	1000	05B	O30-C29-O28	-2.49	103.77	108.09
2	B	1000	05B	O28-C27-C24	2.44	131.75	127.92
2	A	1000	05B	C9-N5-C8	2.42	118.55	110.14
2	A	1000	05B	O28-C27-C24	2.41	131.71	127.92
2	B	1000	05B	C1-C2-N3	2.39	115.69	111.89
2	B	1000	05B	O30-C26-C25	2.30	131.19	127.85
2	A	1000	05B	C17-C16-N21	-2.21	118.94	122.02
2	B	1000	05B	C17-C16-N21	-2.19	118.98	122.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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%)	0.48	10 (3%) 39 47	76, 86, 104, 117	0
1	B	272/318 (85%)	0.59	17 (6%) 19 23	83, 93, 109, 129	0
1	C	272/318 (85%)	0.74	27 (9%) 8 10	80, 95, 122, 131	0
1	D	272/318 (85%)	0.68	20 (7%) 14 17	78, 89, 106, 113	0
1	E	272/318 (85%)	0.59	21 (7%) 13 16	85, 96, 118, 129	0
1	F	272/318 (85%)	0.68	17 (6%) 19 23	76, 89, 105, 115	0
1	G	272/318 (85%)	0.70	19 (6%) 16 19	87, 102, 123, 132	0
1	H	272/318 (85%)	0.81	30 (11%) 6 8	93, 110, 137, 154	0
1	I	272/318 (85%)	0.77	28 (10%) 7 9	101, 112, 125, 141	0
1	J	272/318 (85%)	0.62	19 (6%) 16 19	83, 96, 112, 125	0
1	K	272/318 (85%)	0.93	39 (14%) 3 5	104, 113, 137, 144	0
1	L	272/318 (85%)	0.73	23 (8%) 11 13	90, 105, 126, 138	0
All	All	3264/3816 (85%)	0.69	270 (8%) 11 14	76, 99, 125, 154	0

All (270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	228	TYR	6.3
1	K	157	ALA	6.0
1	I	294	VAL	5.8
1	G	66	THR	5.7
1	H	228	TYR	5.4
1	K	199	PRO	5.2
1	L	67	SER	4.9
1	H	157	ALA	4.7
1	I	75	ASN	4.7
1	E	74	ILE	4.7
1	L	66	THR	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	65	VAL	4.5
1	J	94	MET	4.4
1	C	66	THR	4.3
1	E	79	LEU	4.3
1	J	240	TYR	4.2
1	I	47	HIS	4.1
1	K	150	ILE	4.1
1	J	334	THR	4.1
1	F	73	GLY	4.1
1	K	146	LEU	4.1
1	E	157	ALA	4.1
1	F	59	ILE	4.0
1	G	235	LEU	3.9
1	H	343	LYS	3.9
1	I	336	LEU	3.9
1	J	157	ALA	3.8
1	H	334	THR	3.8
1	F	71	GLY	3.8
1	K	48	VAL	3.8
1	F	66	THR	3.8
1	J	345	ASP	3.8
1	C	81	ILE	3.7
1	H	229	TYR	3.7
1	H	158	PHE	3.7
1	H	150	ILE	3.7
1	C	74	ILE	3.7
1	C	70	LEU	3.7
1	J	335	PRO	3.6
1	C	67	SER	3.6
1	G	82	PHE	3.6
1	C	69	VAL	3.6
1	B	146	LEU	3.6
1	K	294	VAL	3.6
1	L	157	ALA	3.6
1	K	228	TYR	3.5
1	G	79	LEU	3.5
1	G	68	GLN	3.4
1	K	201	ALA	3.4
1	H	47	HIS	3.4
1	F	70	LEU	3.4
1	A	48	VAL	3.4
1	K	328	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	74	ILE	3.3
1	K	202	ILE	3.3
1	F	79	LEU	3.3
1	K	158	PHE	3.3
1	I	240	TYR	3.3
1	K	343	LYS	3.3
1	J	228	TYR	3.3
1	G	294	VAL	3.3
1	D	76	GLY	3.3
1	C	157	ALA	3.3
1	L	85	ARG	3.2
1	E	87	GLN	3.2
1	G	48	VAL	3.2
1	I	330	LYS	3.2
1	C	87	GLN	3.1
1	D	82	PHE	3.1
1	K	337	HIS	3.1
1	D	69	VAL	3.1
1	K	331	VAL	3.1
1	H	342	LEU	3.1
1	L	99	PRO	3.1
1	K	329	THR	3.1
1	L	82	PHE	3.0
1	A	47	HIS	3.0
1	E	69	VAL	3.0
1	C	92	LEU	3.0
1	B	342	LEU	3.0
1	H	129	ALA	3.0
1	J	123	VAL	3.0
1	C	135	LEU	2.9
1	D	79	LEU	2.9
1	K	229	TYR	2.9
1	D	70	LEU	2.9
1	I	235	LEU	2.9
1	J	64	LYS	2.9
1	L	92	LEU	2.9
1	C	150	ILE	2.9
1	A	235	LEU	2.9
1	A	91	ALA	2.8
1	C	79	LEU	2.8
1	H	294	VAL	2.8
1	J	342	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	197	LYS	2.8
1	E	70	LEU	2.8
1	E	92	LEU	2.8
1	K	257	LEU	2.8
1	A	240	TYR	2.8
1	G	228	TYR	2.8
1	G	229	TYR	2.8
1	J	135	LEU	2.7
1	I	299	LYS	2.7
1	E	75	ASN	2.7
1	J	75	ASN	2.7
1	C	72	LEU	2.7
1	D	134	LEU	2.7
1	L	70	LEU	2.7
1	L	336	LEU	2.7
1	F	65	VAL	2.7
1	H	75	ASN	2.7
1	H	240	TYR	2.7
1	E	94	MET	2.7
1	J	158	PHE	2.6
1	B	289	PRO	2.6
1	K	293	GLU	2.6
1	L	63	TYR	2.6
1	H	235	LEU	2.6
1	F	68	GLN	2.6
1	C	328	SER	2.6
1	L	329	THR	2.6
1	G	47	HIS	2.6
1	K	336	LEU	2.6
1	D	60	ILE	2.6
1	K	301	LEU	2.6
1	I	48	VAL	2.6
1	K	200	ASN	2.6
1	I	60	ILE	2.6
1	I	94	MET	2.6
1	D	65	VAL	2.6
1	I	343	LYS	2.6
1	H	289	PRO	2.6
1	E	95	LEU	2.6
1	L	72	LEU	2.6
1	B	150	ILE	2.6
1	B	235	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	235	LEU	2.5
1	C	202	ILE	2.5
1	C	68	GLN	2.5
1	D	75	ASN	2.5
1	H	151	GLN	2.5
1	J	336	LEU	2.5
1	C	128	TYR	2.5
1	C	60	ILE	2.5
1	I	69	VAL	2.5
1	G	157	ALA	2.5
1	E	78	VAL	2.5
1	E	134	LEU	2.5
1	I	340	ARG	2.5
1	E	107	LEU	2.5
1	L	60	ILE	2.5
1	I	342	LEU	2.5
1	B	158	PHE	2.5
1	H	134	LEU	2.5
1	C	129	ALA	2.4
1	L	229	TYR	2.4
1	A	343	LYS	2.4
1	A	74	ILE	2.4
1	F	240	TYR	2.4
1	B	142	ASP	2.4
1	G	150	ILE	2.4
1	B	343	LYS	2.4
1	K	205	LEU	2.4
1	F	136	ILE	2.4
1	E	228	TYR	2.4
1	F	229	TYR	2.4
1	L	240	TYR	2.4
1	L	90	PHE	2.3
1	C	64	LYS	2.3
1	K	330	LYS	2.3
1	F	78	VAL	2.3
1	I	118	VAL	2.3
1	L	78	VAL	2.3
1	K	304	ASN	2.3
1	B	256	LEU	2.3
1	K	325	ILE	2.3
1	J	60	ILE	2.3
1	H	314	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	48	VAL	2.3
1	B	228	TYR	2.3
1	D	274	GLY	2.3
1	L	69	VAL	2.3
1	F	182	ILE	2.3
1	K	87	GLN	2.3
1	B	157	ALA	2.3
1	C	90	PHE	2.3
1	K	84	LYS	2.2
1	B	257	LEU	2.2
1	J	87	GLN	2.2
1	K	151	GLN	2.2
1	K	182	ILE	2.2
1	D	92	LEU	2.2
1	H	286	PHE	2.2
1	E	249	LEU	2.2
1	H	197	LYS	2.2
1	I	74	ILE	2.2
1	C	227	PRO	2.2
1	G	335	PRO	2.2
1	H	315	THR	2.2
1	E	59	ILE	2.2
1	E	136	ILE	2.2
1	D	99	PRO	2.2
1	A	157	ALA	2.2
1	K	341	VAL	2.2
1	K	174	ILE	2.2
1	F	340	ARG	2.2
1	L	140	CYS	2.2
1	A	150	ILE	2.2
1	H	180	ILE	2.2
1	I	334	THR	2.2
1	F	134	LEU	2.2
1	H	344	GLU	2.2
1	I	157	ALA	2.2
1	G	59	ILE	2.2
1	K	64	LYS	2.2
1	K	197	LYS	2.2
1	B	149	ARG	2.1
1	D	151	GLN	2.1
1	H	333	GLN	2.1
1	I	293	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	65	VAL	2.1
1	B	240	TYR	2.1
1	D	59	ILE	2.1
1	E	182	ILE	2.1
1	H	170	ILE	2.1
1	H	340	ARG	2.1
1	G	67	SER	2.1
1	C	228	TYR	2.1
1	L	198	ARG	2.1
1	L	257	LEU	2.1
1	D	240	TYR	2.1
1	C	85	ARG	2.1
1	B	151	GLN	2.1
1	K	308	THR	2.1
1	D	182	ILE	2.1
1	J	81	ILE	2.1
1	K	194	TYR	2.1
1	G	333	GLN	2.1
1	I	344	GLU	2.1
1	L	64	LYS	2.1
1	C	65	VAL	2.1
1	H	160	GLU	2.1
1	A	146	LEU	2.1
1	D	249	LEU	2.1
1	K	193	LEU	2.1
1	D	289	PRO	2.1
1	I	182	ILE	2.1
1	I	249	LEU	2.1
1	I	257	LEU	2.1
1	E	105	VAL	2.0
1	H	331	VAL	2.0
1	K	152	ASP	2.0
1	J	128	TYR	2.0
1	D	72	LEU	2.0
1	I	256	LEU	2.0
1	K	80	GLN	2.0
1	C	240	TYR	2.0
1	I	197	LYS	2.0
1	J	59	ILE	2.0
1	E	73	GLY	2.0
1	F	274	GLY	2.0
1	K	249	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	67	SER	2.0
1	H	335	PRO	2.0
1	I	335	PRO	2.0
1	I	125	GLU	2.0
1	H	311	THR	2.0
1	F	82	PHE	2.0
1	G	73	GLY	2.0

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	05B	B	1000	30/30	0.29	0.98	85,86,91,91	0
2	05B	A	1000	30/30	0.22	0.03	88,89,91,91	0

6.5 Other polymers ⓘ

There are no such residues in this entry.