



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:28 am GMT

PDB ID : 4UMP  
Title : Structure of MELK in complex with inhibitors  
Authors : Johnson, C.N.; Berdini, V.; Beke, L.; Bonnet, P.; Brehmer, D.; Coyle, J.E.; Day, P.J.; Frederickson, M.; Freyne, E.J.E.; Gilissen, R.A.H.J.; Hamlett, C.C.F.; Howard, S.; Meerpoel, L.; McMenamin, R.; Patel, S.; Rees, D.C.; Sharff, A.; Sommen, F.; Wu, T.; Linders, J.T.M.  
Deposited on : 2014-05-20  
Resolution : 2.30 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28683  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

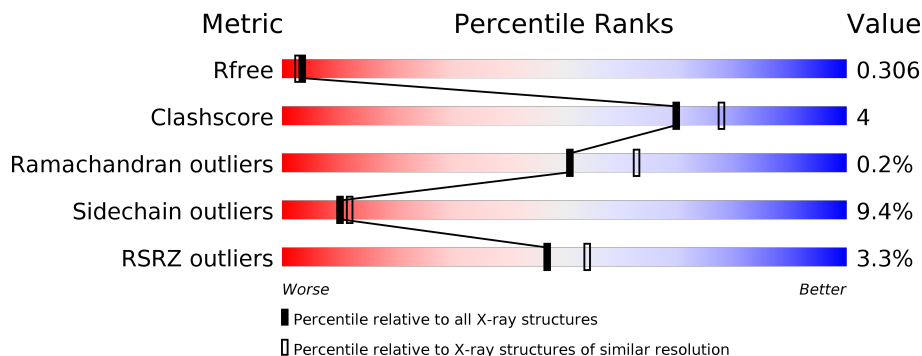
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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  $\geq 3$ , 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	356	<div> <div>0%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	356	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	356	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div></div> <div>13%</div> </div> </div>
1	D	356	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>•</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10944 atoms, of which 36 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 MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	1	0
			2545	1642	430	456	17			
1	B	324	Total	C	N	O	S	0	0	0
			2614	1680	444	472	18			
1	C	311	Total	C	N	O	S	0	1	0
			2536	1636	427	456	17			
1	D	321	Total	C	N	O	S	0	1	0
			2593	1672	439	467	15			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q14680
A	-18	GLY	-	EXPRESSION TAG	UNP Q14680
A	-17	SER	-	EXPRESSION TAG	UNP Q14680
A	-16	SER	-	EXPRESSION TAG	UNP Q14680
A	-15	HIS	-	EXPRESSION TAG	UNP Q14680
A	-14	HIS	-	EXPRESSION TAG	UNP Q14680
A	-13	HIS	-	EXPRESSION TAG	UNP Q14680
A	-12	HIS	-	EXPRESSION TAG	UNP Q14680
A	-11	HIS	-	EXPRESSION TAG	UNP Q14680
A	-10	HIS	-	EXPRESSION TAG	UNP Q14680
A	-9	SER	-	EXPRESSION TAG	UNP Q14680
A	-8	SER	-	EXPRESSION TAG	UNP Q14680
A	-7	GLY	-	EXPRESSION TAG	UNP Q14680
A	-6	LEU	-	EXPRESSION TAG	UNP Q14680
A	-5	VAL	-	EXPRESSION TAG	UNP Q14680
A	-4	PRO	-	EXPRESSION TAG	UNP Q14680
A	-3	ARG	-	EXPRESSION TAG	UNP Q14680
A	-2	GLY	-	EXPRESSION TAG	UNP Q14680
A	-1	SER	-	EXPRESSION TAG	UNP Q14680
A	0	HIS	-	EXPRESSION TAG	UNP Q14680
A	167	ALA	THR	ENGINEERED MUTATION	UNP Q14680

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Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ALA	SER	ENGINEERED MUTATION	UNP Q14680
A	213	THR	ASN	ENGINEERED MUTATION	UNP Q14680
A	214	ALA	VAL	ENGINEERED MUTATION	UNP Q14680
A	215	ALA	MET	ENGINEERED MUTATION	UNP Q14680
A	218	VAL	TYR	ENGINEERED MUTATION	UNP Q14680
A	219	ALA	LYS	ENGINEERED MUTATION	UNP Q14680
B	-19	MET	-	EXPRESSION TAG	UNP Q14680
B	-18	GLY	-	EXPRESSION TAG	UNP Q14680
B	-17	SER	-	EXPRESSION TAG	UNP Q14680
B	-16	SER	-	EXPRESSION TAG	UNP Q14680
B	-15	HIS	-	EXPRESSION TAG	UNP Q14680
B	-14	HIS	-	EXPRESSION TAG	UNP Q14680
B	-13	HIS	-	EXPRESSION TAG	UNP Q14680
B	-12	HIS	-	EXPRESSION TAG	UNP Q14680
B	-11	HIS	-	EXPRESSION TAG	UNP Q14680
B	-10	HIS	-	EXPRESSION TAG	UNP Q14680
B	-9	SER	-	EXPRESSION TAG	UNP Q14680
B	-8	SER	-	EXPRESSION TAG	UNP Q14680
B	-7	GLY	-	EXPRESSION TAG	UNP Q14680
B	-6	LEU	-	EXPRESSION TAG	UNP Q14680
B	-5	VAL	-	EXPRESSION TAG	UNP Q14680
B	-4	PRO	-	EXPRESSION TAG	UNP Q14680
B	-3	ARG	-	EXPRESSION TAG	UNP Q14680
B	-2	GLY	-	EXPRESSION TAG	UNP Q14680
B	-1	SER	-	EXPRESSION TAG	UNP Q14680
B	0	HIS	-	EXPRESSION TAG	UNP Q14680
B	167	ALA	THR	ENGINEERED MUTATION	UNP Q14680
B	171	ALA	SER	ENGINEERED MUTATION	UNP Q14680
B	213	THR	ASN	ENGINEERED MUTATION	UNP Q14680
B	214	ALA	VAL	ENGINEERED MUTATION	UNP Q14680
B	215	ALA	MET	ENGINEERED MUTATION	UNP Q14680
B	218	VAL	TYR	ENGINEERED MUTATION	UNP Q14680
B	219	ALA	LYS	ENGINEERED MUTATION	UNP Q14680
C	-19	MET	-	EXPRESSION TAG	UNP Q14680
C	-18	GLY	-	EXPRESSION TAG	UNP Q14680
C	-17	SER	-	EXPRESSION TAG	UNP Q14680
C	-16	SER	-	EXPRESSION TAG	UNP Q14680
C	-15	HIS	-	EXPRESSION TAG	UNP Q14680
C	-14	HIS	-	EXPRESSION TAG	UNP Q14680
C	-13	HIS	-	EXPRESSION TAG	UNP Q14680
C	-12	HIS	-	EXPRESSION TAG	UNP Q14680
C	-11	HIS	-	EXPRESSION TAG	UNP Q14680

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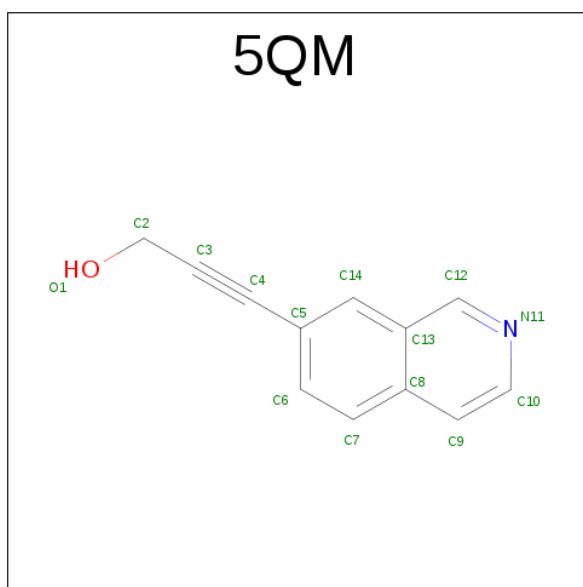
Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	EXPRESSION TAG	UNP Q14680
C	-9	SER	-	EXPRESSION TAG	UNP Q14680
C	-8	SER	-	EXPRESSION TAG	UNP Q14680
C	-7	GLY	-	EXPRESSION TAG	UNP Q14680
C	-6	LEU	-	EXPRESSION TAG	UNP Q14680
C	-5	VAL	-	EXPRESSION TAG	UNP Q14680
C	-4	PRO	-	EXPRESSION TAG	UNP Q14680
C	-3	ARG	-	EXPRESSION TAG	UNP Q14680
C	-2	GLY	-	EXPRESSION TAG	UNP Q14680
C	-1	SER	-	EXPRESSION TAG	UNP Q14680
C	0	HIS	-	EXPRESSION TAG	UNP Q14680
C	167	ALA	THR	ENGINEERED MUTATION	UNP Q14680
C	171	ALA	SER	ENGINEERED MUTATION	UNP Q14680
C	213	THR	ASN	ENGINEERED MUTATION	UNP Q14680
C	214	ALA	VAL	ENGINEERED MUTATION	UNP Q14680
C	215	ALA	MET	ENGINEERED MUTATION	UNP Q14680
C	218	VAL	TYR	ENGINEERED MUTATION	UNP Q14680
C	219	ALA	LYS	ENGINEERED MUTATION	UNP Q14680
D	-19	MET	-	EXPRESSION TAG	UNP Q14680
D	-18	GLY	-	EXPRESSION TAG	UNP Q14680
D	-17	SER	-	EXPRESSION TAG	UNP Q14680
D	-16	SER	-	EXPRESSION TAG	UNP Q14680
D	-15	HIS	-	EXPRESSION TAG	UNP Q14680
D	-14	HIS	-	EXPRESSION TAG	UNP Q14680
D	-13	HIS	-	EXPRESSION TAG	UNP Q14680
D	-12	HIS	-	EXPRESSION TAG	UNP Q14680
D	-11	HIS	-	EXPRESSION TAG	UNP Q14680
D	-10	HIS	-	EXPRESSION TAG	UNP Q14680
D	-9	SER	-	EXPRESSION TAG	UNP Q14680
D	-8	SER	-	EXPRESSION TAG	UNP Q14680
D	-7	GLY	-	EXPRESSION TAG	UNP Q14680
D	-6	LEU	-	EXPRESSION TAG	UNP Q14680
D	-5	VAL	-	EXPRESSION TAG	UNP Q14680
D	-4	PRO	-	EXPRESSION TAG	UNP Q14680
D	-3	ARG	-	EXPRESSION TAG	UNP Q14680
D	-2	GLY	-	EXPRESSION TAG	UNP Q14680
D	-1	SER	-	EXPRESSION TAG	UNP Q14680
D	0	HIS	-	EXPRESSION TAG	UNP Q14680
D	167	ALA	THR	ENGINEERED MUTATION	UNP Q14680
D	171	ALA	SER	ENGINEERED MUTATION	UNP Q14680
D	213	THR	ASN	ENGINEERED MUTATION	UNP Q14680
D	214	ALA	VAL	ENGINEERED MUTATION	UNP Q14680

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Chain	Residue	Modelled	Actual	Comment	Reference
D	215	ALA	MET	ENGINEERED MUTATION	UNP Q14680
D	218	VAL	TYR	ENGINEERED MUTATION	UNP Q14680
D	219	ALA	LYS	ENGINEERED MUTATION	UNP Q14680

- Molecule 2 is 3-(ISOQUINOLIN-7-YL)PROP-2-YN-1-OL (three-letter code: 5QM) (formula: C<sub>12</sub>H<sub>9</sub>NO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			23	12	9	1	1		
2	B	1	Total	C	H	N	O	0	0
			23	12	9	1	1		
2	C	1	Total	C	H	N	O	0	0
			23	12	9	1	1		
2	D	1	Total	C	H	N	O	0	0
			23	12	9	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	143	Total	O	0	0
			143	143		
3	B	162	Total	O	0	0
			162	162		
3	C	130	Total	O	0	0
			130	130		

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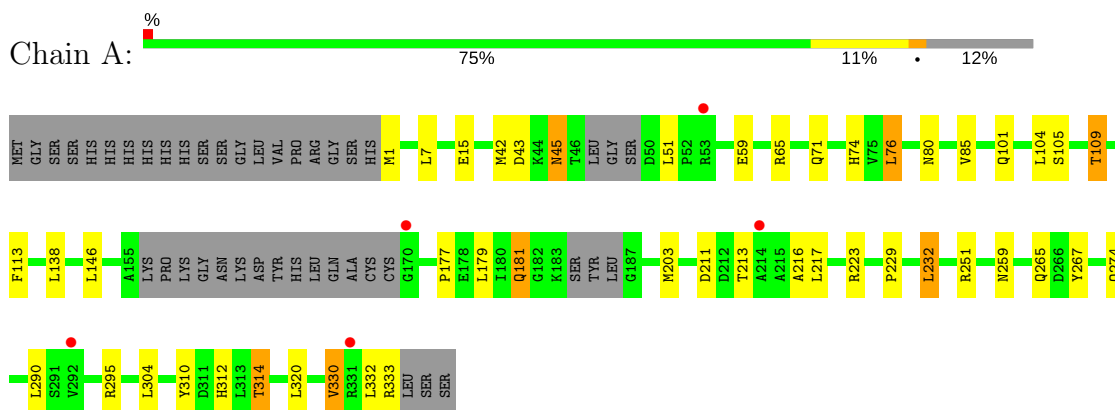
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	129	Total 129	O 129	0	0

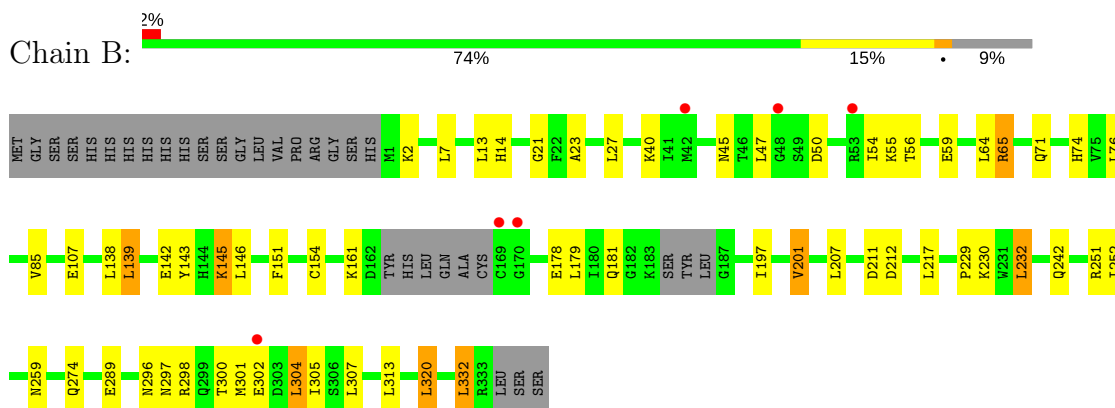
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE



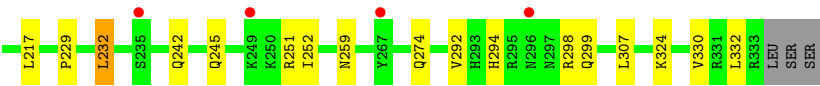
- Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE



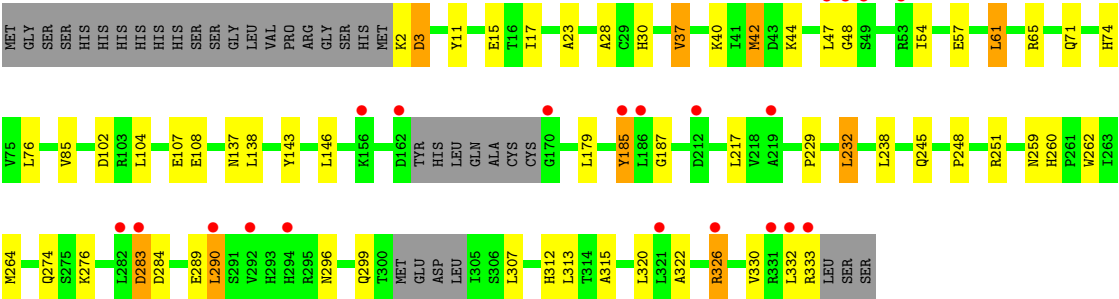
- Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE







● Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.82Å 74.97Å 77.09Å 86.47° 70.06° 89.94°	Depositor
Resolution (Å)	50.38 – 2.30 50.38 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.38-2.30) 94.2 (50.38-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.235 , 0.291 0.243 , 0.306	Depositor DCC
$R_{free}$ test set	2989 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5QM

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	0.58	0/2604	0.74	1/3519 (0.0%)
1	B	0.57	0/2671	0.73	0/3609
1	C	0.55	0/2594	0.71	0/3505
1	D	0.58	0/2653	0.73	0/3587
All	All	0.57	0/10522	0.73	1/14220 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	TYR	CB-CA-C	-5.52	99.37	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	18	GLY	Peptide
1	D	283	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2545	0	2568	18	0
1	B	2614	0	2639	23	0
1	C	2536	0	2555	20	0
1	D	2593	0	2623	27	0
2	A	14	9	9	0	0
2	B	14	9	9	0	0
2	C	14	9	9	0	0
2	D	14	9	9	0	0
3	A	143	0	0	2	0
3	B	162	0	0	0	0
3	C	130	0	0	0	0
3	D	129	0	0	1	0
All	All	10908	36	10421	87	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 4.

All (87) 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:310:TYR:H	1:A:314:THR:HG21	1.47	0.79
1:C:109:THR:HG22	1:C:202:LEU:HB3	1.67	0.75
1:C:138:LEU:HB3	1:C:146:LEU:HD22	1.73	0.69
1:A:104:LEU:HB2	1:A:109:THR:HG22	1.74	0.69
1:A:138:LEU:HB3	1:A:146:LEU:HD22	1.73	0.69
1:B:229:PRO:HD2	1:B:232:LEU:HD22	1.73	0.69
1:D:138:LEU:HB3	1:D:146:LEU:HD22	1.75	0.68
1:B:139:LEU:N	1:B:139:LEU:HD22	2.08	0.67
1:A:213:THR:HG23	1:A:216:ALA:H	1.59	0.66
1:D:229:PRO:HD2	1:D:232:LEU:HD22	1.77	0.66
1:B:289:GLU:HG3	1:B:332:LEU:HD22	1.77	0.65
1:C:245:GLN:HB2	1:C:251:ARG:HG2	1.78	0.65
1:D:40:LYS:HE3	1:D:42:MET:CE	2.27	0.65
1:D:289:GLU:HG3	1:D:330:VAL:O	1.97	0.65
1:C:104:LEU:HB2	1:C:109:THR:HG23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:PRO:HD2	1:C:232:LEU:HD22	1.79	0.63
1:A:229:PRO:HD2	1:A:232:LEU:HD22	1.81	0.62
1:D:322:ALA:HB1	1:D:326:ARG:HH21	1.67	0.60
1:B:201:VAL:HG11	1:B:207:LEU:HD23	1.84	0.59
1:B:151:PHE:O	1:B:154:CYS:HB2	2.03	0.58
1:B:197:ILE:O	1:B:201:VAL:HG13	2.03	0.58
1:D:260:HIS:CD2	1:D:262:TRP:H	2.22	0.57
1:C:131:ARG:HH11	1:C:155:ALA:HB2	1.69	0.57
1:D:248:PRO:HA	1:D:251:ARG:HG3	1.86	0.57
1:D:57:GLU:HG3	1:D:61:LEU:HD23	1.88	0.55
1:D:40:LYS:HE3	1:D:42:MET:HE3	1.88	0.55
1:D:54:ILE:HA	3:D:2018:HOH:O	2.06	0.55
1:C:109:THR:CG2	1:C:202:LEU:HB3	2.37	0.55
1:D:40:LYS:HE3	1:D:42:MET:HE1	1.89	0.54
1:A:330:VAL:O	1:A:330:VAL:CG2	2.55	0.54
1:D:65:ARG:HG3	1:D:71:GLN:HE22	1.73	0.54
1:B:14:HIS:HB2	1:B:27:LEU:O	2.09	0.53
1:B:50:ASP:O	1:B:54:ILE:HG12	2.07	0.53
1:A:330:VAL:O	1:A:330:VAL:HG22	2.07	0.53
1:D:245:GLN:HB2	1:D:251:ARG:HG2	1.90	0.52
1:B:297:ASN:O	1:B:301:MET:HB2	2.09	0.52
1:C:65:ARG:HG3	1:C:71:GLN:HE22	1.76	0.51
1:C:32:LEU:HB3	1:C:332:LEU:HD22	1.93	0.51
1:B:298:ARG:O	1:B:302:GLU:HB3	2.10	0.50
1:A:312:HIS:HE1	3:A:2011:HOH:O	1.95	0.50
1:C:197:ILE:O	1:C:201:VAL:HG13	2.13	0.49
1:B:201:VAL:CG1	1:B:207:LEU:HD23	2.43	0.49
1:B:21:GLY:C	1:B:23:ALA:H	2.14	0.49
1:D:290:LEU:HD21	1:D:313:LEU:HD11	1.95	0.48
1:A:310:TYR:H	1:A:314:THR:CG2	2.23	0.48
1:A:65:ARG:HG3	1:A:71:GLN:HE22	1.78	0.48
1:B:143:TYR:HB2	1:B:145:LYS:HD2	1.96	0.48
1:B:178:GLU:HA	1:B:181:GLN:HG2	1.96	0.47
1:C:37:VAL:CG1	1:C:85:VAL:HG13	2.45	0.47
1:A:105:SER:O	1:A:109:THR:HG23	2.16	0.46
1:D:185:TYR:HB2	1:D:187:GLY:H	1.80	0.46
1:A:45:ASN:HD21	1:A:80:ASN:HB3	1.80	0.46
1:B:305:ILE:HA	1:B:313:LEU:HD11	1.98	0.46
1:D:40:LYS:CE	1:D:42:MET:HE1	2.45	0.46
1:B:300:THR:O	1:B:304:LEU:HB2	2.16	0.45
1:D:28:ALA:HB3	1:D:37:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:HIS:HB3	1:B:85:VAL:HB	1.99	0.44
1:D:23:ALA:HB3	1:D:42:MET:HE3	1.98	0.44
1:C:201:VAL:CG1	1:C:207:LEU:HD23	2.47	0.44
1:C:242:GLN:HB3	1:C:252:ILE:HB	2.00	0.44
1:D:2:LYS:O	1:D:3:ASP:HB2	2.18	0.44
1:A:109:THR:HG21	1:A:203:MET:HG3	2.00	0.44
1:B:242:GLN:HB3	1:B:252:ILE:HB	2.00	0.43
1:A:109:THR:O	1:A:113:PHE:HB2	2.19	0.43
1:A:177:PRO:O	1:A:181:GLN:HG2	2.18	0.43
1:C:132:ASP:HB2	1:C:153:LEU:HD12	2.00	0.43
1:C:324:LYS:HD3	1:C:330:VAL:CG2	2.48	0.43
1:B:65:ARG:HG3	1:B:71:GLN:HE22	1.83	0.43
1:C:7:LEU:HD11	1:C:39:ILE:HD13	2.01	0.43
1:C:57:GLU:O	1:C:61:LEU:HD13	2.18	0.42
1:A:74:HIS:HB3	1:A:85:VAL:HB	2.01	0.42
1:D:23:ALA:CB	1:D:42:MET:HE3	2.50	0.42
1:B:320:LEU:HD23	1:B:320:LEU:HA	1.91	0.42
1:D:104:LEU:HB3	1:D:108:GLU:HB3	2.02	0.41
1:B:138:LEU:HB3	1:B:146:LEU:HD22	2.02	0.41
1:A:312:HIS:CE1	3:A:2011:HOH:O	2.73	0.41
1:A:7:LEU:HD23	1:A:76:LEU:HD13	2.02	0.41
1:D:74:HIS:HB3	1:D:85:VAL:HB	2.01	0.41
1:B:21:GLY:H	1:B:40:LYS:NZ	2.19	0.41
1:D:30:HIS:NE2	1:D:312:HIS:CE1	2.89	0.41
1:C:97[B]:TYR:CE2	1:C:144:HIS:HE1	2.39	0.40
1:D:137:ASN:HD22	1:D:137:ASN:HA	1.71	0.40
1:D:74:HIS:HB2	1:D:315:ALA:HB2	2.01	0.40
1:D:11:TYR:CE1	1:D:30:HIS:HD2	2.38	0.40
1:B:13:LEU:HD23	1:C:99:ILE:HD13	2.03	0.40
1:D:40:LYS:CE	1:D:42:MET:CE	2.97	0.40
1:C:74:HIS:HB3	1:C:85:VAL:HB	2.03	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	306/356 (86%)	290 (95%)	16 (5%)	0	100	100
1	B	318/356 (89%)	301 (95%)	17 (5%)	0	100	100
1	C	302/356 (85%)	286 (95%)	16 (5%)	0	100	100
1	D	316/356 (89%)	292 (92%)	22 (7%)	2 (1%)	28	34
All	All	1242/1424 (87%)	1169 (94%)	71 (6%)	2 (0%)	51	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	48	GLY
1	D	3	ASP

### 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	277/314 (88%)	248 (90%)	29 (10%)	8	9
1	B	285/314 (91%)	255 (90%)	30 (10%)	8	9
1	C	277/314 (88%)	260 (94%)	17 (6%)	22	29
1	D	282/314 (90%)	252 (89%)	30 (11%)	8	9
All	All	1121/1256 (89%)	1015 (90%)	106 (10%)	10	12

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	15	GLU
1	A	42	MET
1	A	43	ASP
1	A	45	ASN
1	A	51	LEU

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Mol	Chain	Res	Type
1	A	59	GLU
1	A	76	LEU
1	A	101	GLN
1	A	109	THR
1	A	179	LEU
1	A	181	GLN
1	A	211	ASP
1	A	217	LEU
1	A	223	ARG
1	A	232	LEU
1	A	251	ARG
1	A	259	ASN
1	A	265	GLN
1	A	274[A]	GLN
1	A	274[B]	GLN
1	A	290	LEU
1	A	295	ARG
1	A	304	LEU
1	A	314	THR
1	A	320	LEU
1	A	330	VAL
1	A	332	LEU
1	A	333	ARG
1	B	2	LYS
1	B	7	LEU
1	B	45	ASN
1	B	47	LEU
1	B	55	LYS
1	B	56	THR
1	B	59	GLU
1	B	64	LEU
1	B	65	ARG
1	B	76	LEU
1	B	107	GLU
1	B	139	LEU
1	B	142	GLU
1	B	145	LYS
1	B	161	LYS
1	B	179	LEU
1	B	201	VAL
1	B	211	ASP
1	B	212	ASP

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Mol	Chain	Res	Type
1	B	217	LEU
1	B	230	LYS
1	B	232	LEU
1	B	251	ARG
1	B	259	ASN
1	B	274	GLN
1	B	296	ASN
1	B	304	LEU
1	B	307	LEU
1	B	320	LEU
1	B	332	LEU
1	C	15	GLU
1	C	44	LYS
1	C	59	GLU
1	C	76	LEU
1	C	101	GLN
1	C	107	GLU
1	C	154	CYS
1	C	179	LEU
1	C	217	LEU
1	C	232	LEU
1	C	259	ASN
1	C	274	GLN
1	C	292	VAL
1	C	294	HIS
1	C	298	ARG
1	C	299	GLN
1	C	307	LEU
1	D	15	GLU
1	D	17	ILE
1	D	37	VAL
1	D	42	MET
1	D	44	LYS
1	D	47	LEU
1	D	61	LEU
1	D	76	LEU
1	D	102	ASP
1	D	107	GLU
1	D	143	TYR
1	D	179	LEU
1	D	185	TYR
1	D	217	LEU

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Mol	Chain	Res	Type
1	D	232	LEU
1	D	238	LEU
1	D	259	ASN
1	D	264	MET
1	D	274	GLN
1	D	276	LYS
1	D	283	ASP
1	D	284	ASP
1	D	290	LEU
1	D	296	ASN
1	D	299	GLN
1	D	307	LEU
1	D	320	LEU
1	D	326	ARG
1	D	332	LEU
1	D	333	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	71	GLN
1	A	137	ASN
1	A	259	ASN
1	A	277	ASN
1	B	71	GLN
1	B	80	ASN
1	B	137	ASN
1	B	259	ASN
1	B	274	GLN
1	B	277	ASN
1	C	71	GLN
1	C	101	GLN
1	C	137	ASN
1	C	144	HIS
1	C	259	ASN
1	C	265	GLN
1	C	274	GLN
1	C	277	ASN
1	C	312	HIS
1	D	71	GLN
1	D	80	ASN

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Mol	Chain	Res	Type
1	D	137	ASN
1	D	259	ASN
1	D	260	HIS
1	D	274	GLN
1	D	312	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	5QM	A	1334	-	15,15,15	0.65	0	18,19,19	0.49	0
2	5QM	B	1334	-	15,15,15	0.67	0	18,19,19	0.49	0
2	5QM	C	1334	-	15,15,15	0.56	0	18,19,19	0.50	0
2	5QM	D	1334	-	15,15,15	0.69	0	18,19,19	0.51	0

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	5QM	A	1334	-	-	0/2/4/4	0/2/2/2
2	5QM	B	1334	-	-	0/2/4/4	0/2/2/2
2	5QM	C	1334	-	-	0/2/4/4	0/2/2/2
2	5QM	D	1334	-	-	0/2/4/4	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	313/356 (87%)	-0.03	5 (1%) 72 77	35, 56, 86, 112	0
1	B	324/356 (91%)	0.09	6 (1%) 67 73	37, 57, 91, 121	0
1	C	311/356 (87%)	0.09	10 (3%) 48 55	38, 59, 89, 134	0
1	D	321/356 (90%)	0.24	21 (6%) 20 26	37, 60, 106, 138	0
All	All	1269/1424 (89%)	0.10	42 (3%) 47 54	35, 58, 93, 138	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	186	LEU	7.6
1	D	47	LEU	6.3
1	D	49	SER	4.3
1	D	331	ARG	4.2
1	A	214	ALA	3.7
1	D	219	ALA	3.6
1	D	170	GLY	3.5
1	C	296	ASN	3.4
1	D	282	LEU	3.3
1	B	170	GLY	3.3
1	C	182	GLY	3.3
1	C	45	ASN	3.2
1	D	292	VAL	3.2
1	D	212	ASP	3.2
1	B	48	GLY	3.1
1	B	169	CYS	3.1
1	C	51	LEU	3.1
1	C	235	SER	2.9
1	C	180	ILE	2.9
1	D	326	ARG	2.8
1	C	49	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	332	LEU	2.7
1	D	294	HIS	2.7
1	D	53	ARG	2.6
1	C	249	LYS	2.5
1	D	290	LEU	2.4
1	D	283	ASP	2.4
1	A	331	ARG	2.4
1	C	267	TYR	2.3
1	D	185	TYR	2.3
1	D	162	ASP	2.3
1	D	321	LEU	2.3
1	B	42	MET	2.2
1	D	156	LYS	2.2
1	A	170	GLY	2.1
1	B	53	ARG	2.1
1	A	292	VAL	2.1
1	A	53	ARG	2.1
1	C	50	ASP	2.0
1	D	333	ARG	2.0
1	D	48	GLY	2.0
1	B	302	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	5QM	C	1334	14/14	0.93	0.15	1.21	38,47,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	5QM	B	1334	14/14	0.95	0.13	0.31	38,45,50,50	23
2	5QM	D	1334	14/14	0.95	0.11	-0.63	36,46,55,57	0
2	5QM	A	1334	14/14	0.96	0.10	-0.79	35,43,49,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.