



Full wwPDB X-ray Structure Validation Report

Oct 2, 2014 – 09:13 PM EDT

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 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>

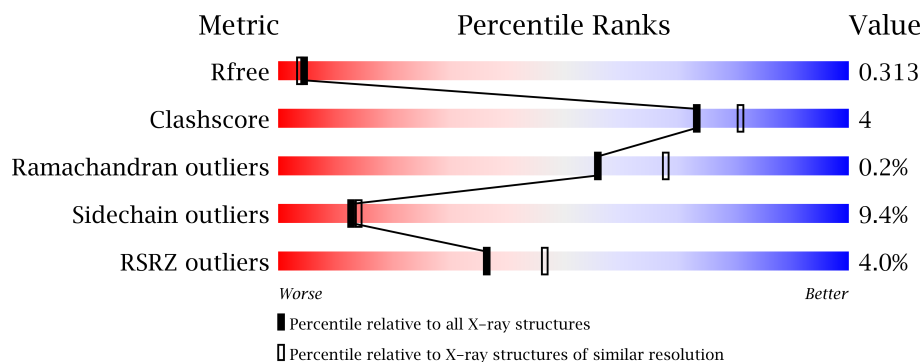
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23828
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) : stable23828

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 ≥ 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	356	
1	B	356	
1	C	356	
1	D	356	

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 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 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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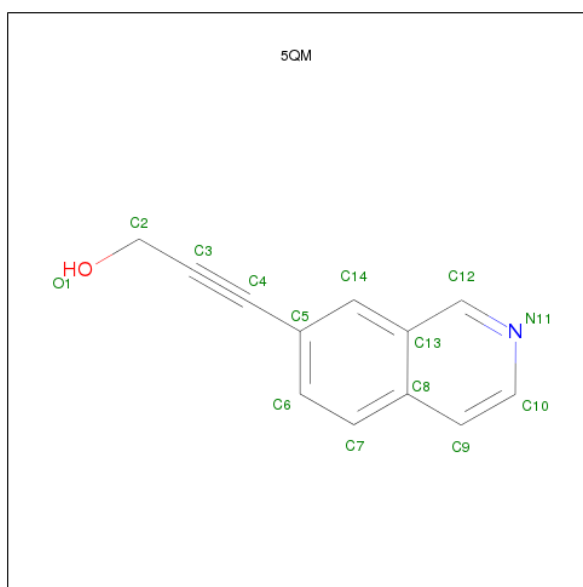
Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	EXPRESSION TAG	UNP Q14680
C	-9	SER	-	EXPRESSION TAG	UNP Q14680
C	-8	SER	-	EXPRESSION TAG	UNP Q14680
C	-7	GLY	-	EXPRESSION TAG	UNP Q14680
C	-6	LEU	-	EXPRESSION TAG	UNP Q14680
C	-5	VAL	-	EXPRESSION TAG	UNP Q14680
C	-4	PRO	-	EXPRESSION TAG	UNP 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: C₁₂H₉NO).



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		

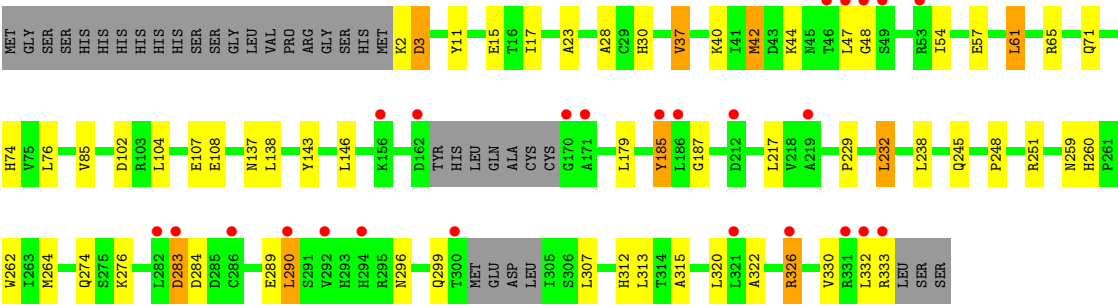
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	129	Total 129	O 129	0	0

● Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 95.8 (50.38-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.235 , 0.291 0.247 , 0.313	Depositor DCC
R_{free} test set	2989 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 58731 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10944	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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($^{\circ}$)	Ideal($^{\circ}$)
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 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	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	0	0	0
2	B	14	9	0	0	0
2	C	14	9	0	0	0
2	D	14	9	0	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	10385	87	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 4.

All (87) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:B:74:HIS:HB3	1:B:85:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	33	39
All	All	1242/1424 (87%)	1169 (94%)	71 (6%)	2 (0%)	56	68

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%)	10	11
1	B	285/314 (91%)	255 (90%)	30 (10%)	10	11
1	C	277/314 (88%)	260 (94%)	17 (6%)	26	34
1	D	282/314 (90%)	252 (89%)	30 (11%)	10	10
All	All	1121/1256 (89%)	1015 (90%)	106 (10%)	13	14

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
1	A	59	GLU
1	A	76	LEU
1	A	101	GLN
1	A	109	THR

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Mol	Chain	Res	Type
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
1	B	217	LEU
1	B	230	LYS
1	B	232	LEU
1	B	251	ARG

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Mol	Chain	Res	Type
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
1	D	232	LEU
1	D	238	LEU
1	D	259	ASN
1	D	264	MET

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

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Mol	Chain	Res	Type
1	D	312	HIS

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 ⓘ

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	19,19,19	0.59	0
2	5QM	B	1334	-	15,15,15	0.68	0	19,19,19	0.60	0
2	5QM	C	1334	-	15,15,15	0.57	0	19,19,19	0.60	0
2	5QM	D	1334	-	15,15,15	0.72	0	19,19,19	0.61	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	-	-	0/3/4/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5QM	B	1334	-	-	0/3/4/4	0/2/2/2
2	5QM	C	1334	-	-	0/3/4/4	0/2/2/2
2	5QM	D	1334	-	-	0/3/4/4	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.

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	313/356 (87%)	0.12	5 (1%) 68 77	35, 56, 86, 112	0
1	B	324/356 (91%)	0.25	9 (2%) 50 60	37, 57, 91, 121	0
1	C	311/356 (87%)	0.26	12 (3%) 37 48	38, 59, 89, 134	0
1	D	321/356 (90%)	0.38	25 (7%) 13 19	37, 60, 106, 138	0
All	All	1269/1424 (89%)	0.25	51 (4%) 36 47	35, 58, 93, 138	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	47	LEU	7.1
1	D	186	LEU	7.0
1	A	214	ALA	4.2
1	D	49	SER	4.2
1	C	296	ASN	4.0
1	C	45	ASN	4.0
1	C	182	GLY	3.8
1	B	48	GLY	3.8
1	D	282	LEU	3.6
1	D	219	ALA	3.6
1	D	170	GLY	3.5
1	C	235	SER	3.5
1	B	170	GLY	3.5
1	D	326	ARG	3.4
1	D	331	ARG	3.2
1	D	292	VAL	3.2
1	B	169	CYS	3.1
1	D	290	LEU	3.0
1	D	212	ASP	3.0
1	B	42	MET	3.0
1	D	48	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	332	LEU	2.7
1	D	321	LEU	2.7
1	D	283	ASP	2.6
1	C	180	ILE	2.6
1	B	76	LEU	2.5
1	D	162	ASP	2.5
1	C	267	TYR	2.5
1	D	53	ARG	2.5
1	A	331	ARG	2.4
1	D	46	THR	2.3
1	A	128	TYR	2.3
1	C	249	LYS	2.3
1	C	328	LYS	2.3
1	D	286	CYS	2.3
1	D	171	ALA	2.3
1	B	171	ALA	2.2
1	B	302	GLU	2.2
1	B	49	SER	2.2
1	D	156	LYS	2.1
1	D	294	HIS	2.1
1	C	51	LEU	2.1
1	C	49	SER	2.1
1	C	330	VAL	2.1
1	B	299	GLN	2.1
1	D	300	THR	2.1
1	D	333	ARG	2.1
1	A	292	VAL	2.0
1	C	50	ASP	2.0
1	D	185	TYR	2.0
1	A	172	LEU	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	5QM	C	1334	14/14	0.16	1.40	38,47,53,53	0
2	5QM	B	1334	14/14	0.14	0.22	38,45,50,50	23
2	5QM	D	1334	14/14	0.11	-0.64	36,46,55,57	0
2	5QM	A	1334	14/14	0.10	-1.13	35,43,49,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.