



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2025 – 05:13 PM JST

PDB ID : 9LGU / pdb_00009lgu
Title : Crystal structure of Bcl-xL in complex with stapled HRK peptide
Authors : Wei, H.; Guo, M.; Wang, J.
Deposited on : 2025-01-10
Resolution : 2.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

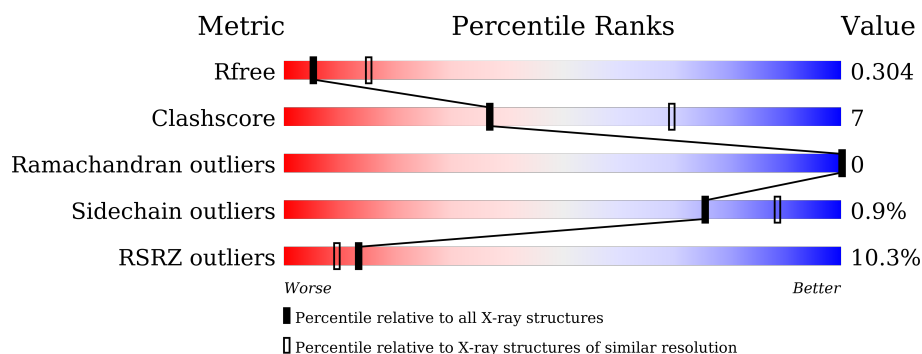
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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}	164625	3360 (3.00-2.96)
Clashscore	180529	3751 (3.00-2.96)
Ramachandran outliers	177936	3628 (3.00-2.96)
Sidechain outliers	177891	3631 (3.00-2.96)
RSRZ outliers	164620	3372 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	218	<div> <div>4%</div> <div>56%</div> <div>10%</div> <div>35%</div> </div>
1	C	218	<div> <div>12%</div> <div>55%</div> <div>11%</div> <div>35%</div> </div>
1	E	218	<div> <div>3%</div> <div>55%</div> <div>9%</div> <div>35%</div> </div>
1	G	218	<div> <div>11%</div> <div>57%</div> <div>8%</div> <div>35%</div> </div>
1	I	218	<div> <div>5%</div> <div>58%</div> <div>8%</div> <div>34%</div> </div>
1	K	218	<div> <div>7%</div> <div>56%</div> <div>9%</div> <div>35%</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	24	<div><div></div><div>67%</div><div>29%</div><div></div></div>
2	D	24	<div><div></div><div>67%</div><div>29%</div><div></div></div>
2	F	24	<div><div>8%</div><div></div><div>71%</div><div>25%</div><div></div></div>
2	H	24	<div><div></div><div>63%</div><div>33%</div><div></div></div>
2	L	24	<div><div></div><div>63%</div><div>29%</div><div></div><div></div></div>
2	M	24	<div><div>29%</div><div></div><div>58%</div><div>38%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8005 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 Bcl-2-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	1	0
			1145	734	190	217	4			
1	C	142	Total	C	N	O	S	3	1	0
			1145	734	190	217	4			
1	E	141	Total	C	N	O	S	0	1	0
			1137	730	188	215	4			
1	G	141	Total	C	N	O	S	0	1	0
			1134	728	188	215	3			
1	I	143	Total	C	N	O	S	3	1	0
			1151	738	190	218	5			
1	K	142	Total	C	N	O	S	0	1	0
			1149	737	190	217	5			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q07817
A	210	LEU	-	expression tag	UNP Q07817
A	211	GLU	-	expression tag	UNP Q07817
A	212	HIS	-	expression tag	UNP Q07817
A	213	HIS	-	expression tag	UNP Q07817
A	214	HIS	-	expression tag	UNP Q07817
A	215	HIS	-	expression tag	UNP Q07817
A	216	HIS	-	expression tag	UNP Q07817
A	217	HIS	-	expression tag	UNP Q07817
C	0	SER	-	expression tag	UNP Q07817
C	210	LEU	-	expression tag	UNP Q07817
C	211	GLU	-	expression tag	UNP Q07817
C	212	HIS	-	expression tag	UNP Q07817
C	213	HIS	-	expression tag	UNP Q07817
C	214	HIS	-	expression tag	UNP Q07817
C	215	HIS	-	expression tag	UNP Q07817
C	216	HIS	-	expression tag	UNP Q07817

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Chain	Residue	Modelled	Actual	Comment	Reference
C	217	HIS	-	expression tag	UNP Q07817
E	0	SER	-	expression tag	UNP Q07817
E	210	LEU	-	expression tag	UNP Q07817
E	211	GLU	-	expression tag	UNP Q07817
E	212	HIS	-	expression tag	UNP Q07817
E	213	HIS	-	expression tag	UNP Q07817
E	214	HIS	-	expression tag	UNP Q07817
E	215	HIS	-	expression tag	UNP Q07817
E	216	HIS	-	expression tag	UNP Q07817
E	217	HIS	-	expression tag	UNP Q07817
G	0	SER	-	expression tag	UNP Q07817
G	210	LEU	-	expression tag	UNP Q07817
G	211	GLU	-	expression tag	UNP Q07817
G	212	HIS	-	expression tag	UNP Q07817
G	213	HIS	-	expression tag	UNP Q07817
G	214	HIS	-	expression tag	UNP Q07817
G	215	HIS	-	expression tag	UNP Q07817
G	216	HIS	-	expression tag	UNP Q07817
G	217	HIS	-	expression tag	UNP Q07817
I	0	SER	-	expression tag	UNP Q07817
I	210	LEU	-	expression tag	UNP Q07817
I	211	GLU	-	expression tag	UNP Q07817
I	212	HIS	-	expression tag	UNP Q07817
I	213	HIS	-	expression tag	UNP Q07817
I	214	HIS	-	expression tag	UNP Q07817
I	215	HIS	-	expression tag	UNP Q07817
I	216	HIS	-	expression tag	UNP Q07817
I	217	HIS	-	expression tag	UNP Q07817
K	0	SER	-	expression tag	UNP Q07817
K	210	LEU	-	expression tag	UNP Q07817
K	211	GLU	-	expression tag	UNP Q07817
K	212	HIS	-	expression tag	UNP Q07817
K	213	HIS	-	expression tag	UNP Q07817
K	214	HIS	-	expression tag	UNP Q07817
K	215	HIS	-	expression tag	UNP Q07817
K	216	HIS	-	expression tag	UNP Q07817
K	217	HIS	-	expression tag	UNP Q07817

- Molecule 2 is a protein called Activator of apoptosis harakiri.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	23	Total	C	N	O	S	0	0	0
			188	121	35	31	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	23	Total	C	N	O	S	0	0	0
			188	121	35	31	1			
2	F	24	Total	C	N	O	S	0	0	0
			194	124	36	33	1			
2	H	24	Total	C	N	O	S	0	0	0
			194	124	36	33	1			
2	L	23	Total	C	N	O	S	0	0	0
			188	121	35	31	1			
2	M	23	Total	C	N	O	S	0	0	0
			187	121	35	30	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	33	LEU	THR	conflict	UNP O00198
B	35	MK8	ALA	conflict	UNP O00198
B	39	MK8	ALA	conflict	UNP O00198
D	33	LEU	THR	conflict	UNP O00198
D	35	MK8	ALA	conflict	UNP O00198
D	39	MK8	ALA	conflict	UNP O00198
F	33	LEU	THR	conflict	UNP O00198
F	35	MK8	ALA	conflict	UNP O00198
F	39	MK8	ALA	conflict	UNP O00198
H	33	LEU	THR	conflict	UNP O00198
H	35	MK8	ALA	conflict	UNP O00198
H	39	MK8	ALA	conflict	UNP O00198
L	33	LEU	THR	conflict	UNP O00198
L	35	MK8	ALA	conflict	UNP O00198
L	39	MK8	ALA	conflict	UNP O00198
M	33	LEU	THR	conflict	UNP O00198
M	35	MK8	ALA	conflict	UNP O00198
M	39	MK8	ALA	conflict	UNP O00198

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		

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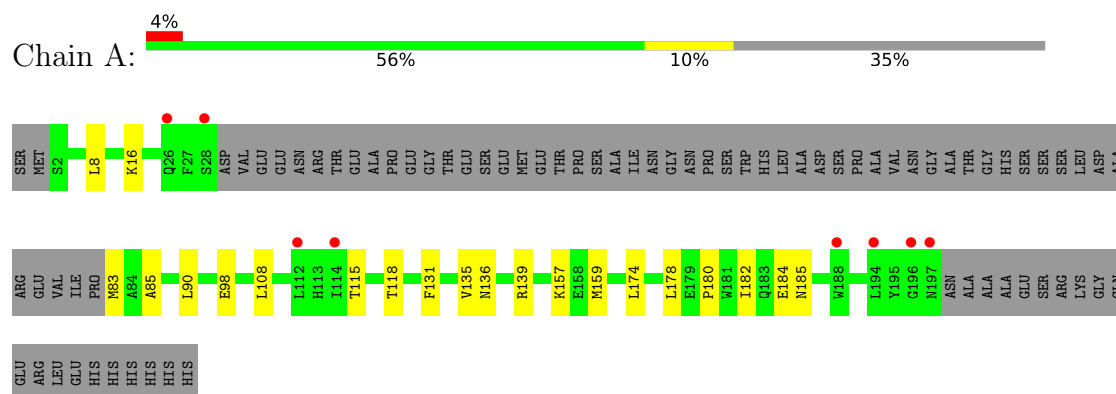
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0

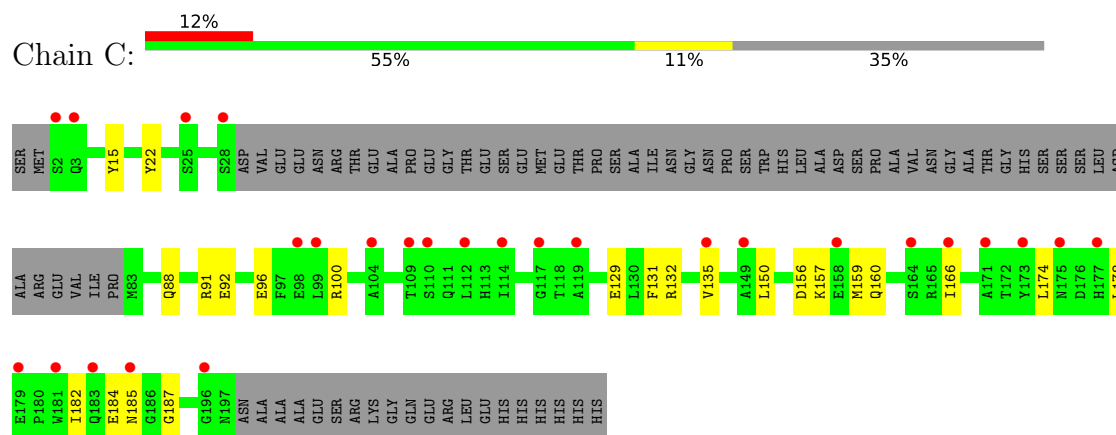
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

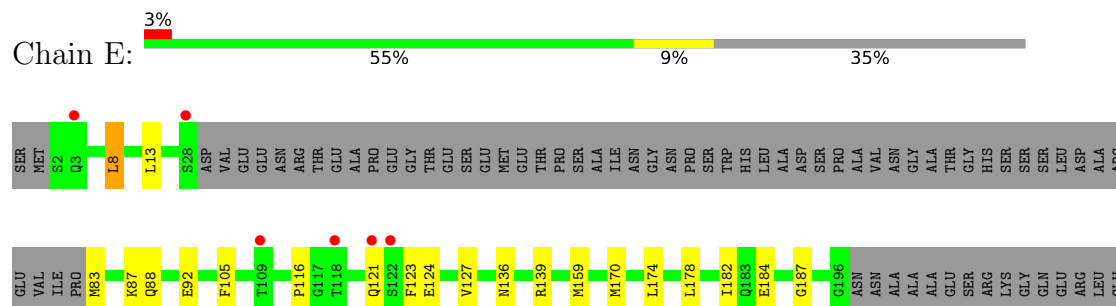
• Molecule 1: Bcl-2-like protein 1



• Molecule 1: Bcl-2-like protein 1



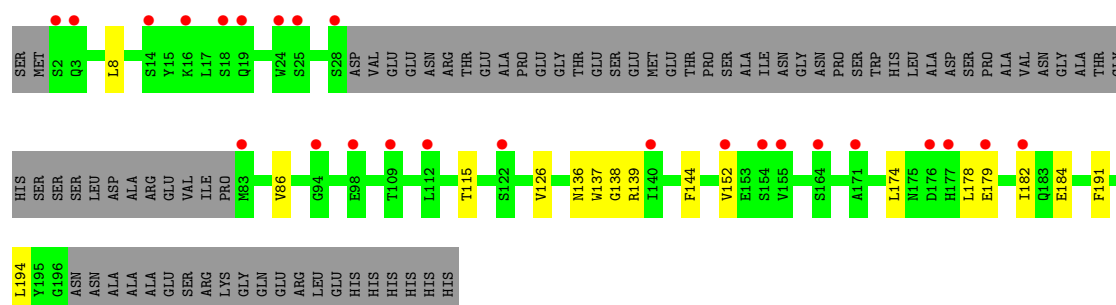
• Molecule 1: Bcl-2-like protein 1



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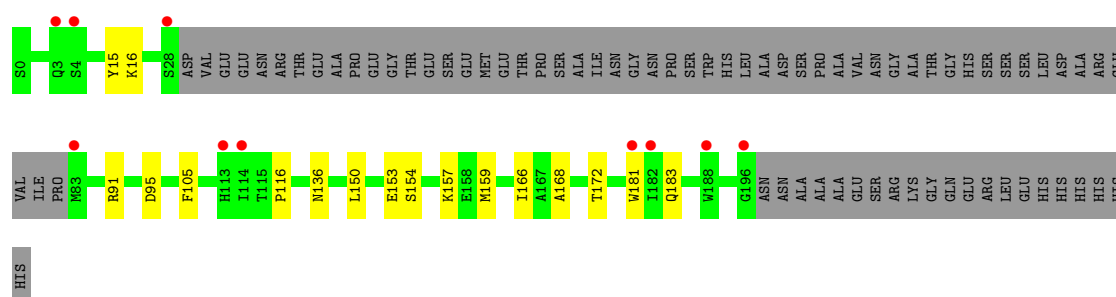
• Molecule 1: Bcl-2-like protein 1

Chain G: 



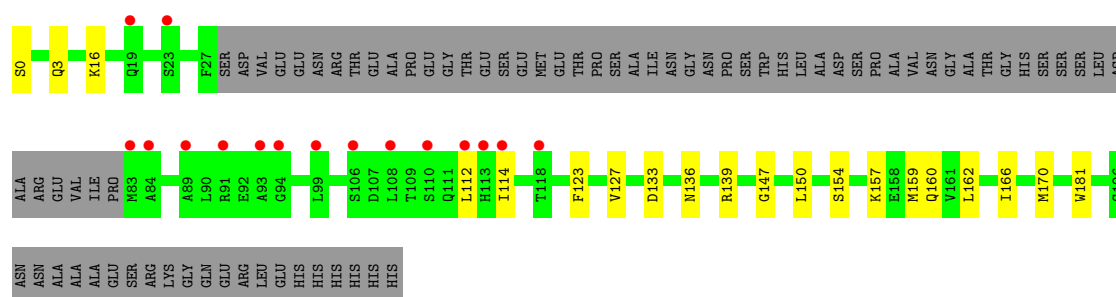
• Molecule 1: Bcl-2-like protein 1

Chain I: 



• Molecule 1: Bcl-2-like protein 1

Chain K: 



• Molecule 2: Activator of apoptosis harakiri

Chain B: 



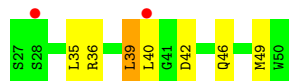
- Molecule 2: Activator of apoptosis harakiri

Chain D:  67% 29% .



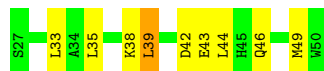
- Molecule 2: Activator of apoptosis harakiri

Chain F:  8% 71% 25% .



- Molecule 2: Activator of apoptosis harakiri

Chain H:  63% 33% .



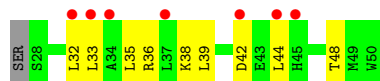
- Molecule 2: Activator of apoptosis harakiri

Chain L:  63% 29% . .



- Molecule 2: Activator of apoptosis harakiri

Chain M:  29% 58% 38% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.59Å 111.91Å 84.14Å 90.00° 109.52° 90.00°	Depositor
Resolution (Å)	29.05 – 2.97 29.05 – 2.97	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.05-2.97) 98.3 (29.05-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.257 , 0.303 0.258 , 0.304	Depositor DCC
R_{free} test set	2000 reflections (7.72%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8005	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 88.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6513e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MK8, MG

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	0.09	0/1176	0.20	0/1592
1	C	0.06	0/1176	0.19	0/1592
1	E	0.07	0/1168	0.20	0/1581
1	G	0.08	0/1165	0.21	0/1578
1	I	0.07	0/1182	0.21	0/1599
1	K	0.07	0/1180	0.21	0/1596
2	B	0.07	0/170	0.20	0/224
2	D	0.06	0/170	0.15	0/224
2	F	0.06	0/176	0.16	0/232
2	H	0.06	0/176	0.15	0/232
2	L	0.09	0/170	0.26	0/224
2	M	0.58	0/169	0.86	0/223
All	All	0.11	0/8078	0.24	0/10897

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	1145	0	1077	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1145	0	1078	13	0
1	E	1137	0	1072	12	0
1	G	1134	0	1065	11	0
1	I	1151	0	1088	11	0
1	K	1149	0	1090	14	0
2	B	188	0	194	8	0
2	D	188	0	194	8	0
2	F	194	0	200	8	0
2	H	194	0	200	11	0
2	L	188	0	195	9	0
2	M	187	0	192	13	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
All	All	8005	0	7645	110	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 7.

All (110) 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)
2:M:32:LEU:HD21	2:M:36:ARG:NH1	1.67	1.09
2:M:32:LEU:HD21	2:M:36:ARG:HH12	1.34	0.91
2:M:32:LEU:CD2	2:M:36:ARG:NH1	2.37	0.86
1:C:184:GLU:HA	2:F:46:GLN:HG3	1.68	0.74
2:F:39:MK8:HB1A	2:F:42:ASP:HB2	1.72	0.71
2:H:39:MK8:HB1A	2:H:42:ASP:HB2	1.74	0.70
2:M:39:MK8:HB1A	2:M:42:ASP:HB2	1.74	0.70
1:A:83:MET:HE2	1:A:85:ALA:H	1.56	0.70
1:A:185:ASN:HA	2:H:49:MET:HG3	1.74	0.69
1:E:8:LEU:HG	1:E:83:MET:HE1	1.74	0.68
1:K:0:SER:HB2	1:K:3:GLN:HB2	1.75	0.67
2:B:39:MK8:HB	2:D:39:MK8:HB	1.76	0.67
1:C:185:ASN:HA	2:F:49:MET:HG3	1.75	0.67
2:L:39:MK8:HB1A	2:L:42:ASP:HB2	1.75	0.67
2:F:39:MK8:HB1B	2:L:39:MK8:HDA	1.76	0.67
2:H:39:MK8:HB1B	2:M:39:MK8:HDA	1.78	0.65
1:I:150:LEU:HB3	1:I:166:ILE:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:43:GLU:OE2	2:M:36:ARG:NH2	2.32	0.62
1:A:184:GLU:HA	2:H:46:GLN:HG3	1.82	0.61
1:E:121:GLN:HA	1:E:124:GLU:HG2	1.82	0.61
1:I:105:PHE:HB3	2:L:36:ARG:HE	1.65	0.61
1:A:16:LYS:NZ	1:A:98:GLU:OE1	2.35	0.59
2:F:39:MK8:HB	2:L:39:MK8:HB	1.85	0.58
2:H:39:MK8:HB	2:M:39:MK8:HB	1.85	0.58
2:M:32:LEU:CD2	2:M:36:ARG:HH11	2.17	0.57
2:D:39:MK8:HB1A	2:D:42:ASP:HB2	1.88	0.56
1:A:115:THR:OG1	1:A:118:THR:OG1	2.24	0.56
1:E:182:ILE:HG23	1:E:187:GLY:HA2	1.86	0.55
1:E:83:MET:HE2	1:E:87:LYS:HE3	1.89	0.55
1:K:150:LEU:HD13	1:K:166:ILE:HD13	1.87	0.55
1:I:153:GLU:OE2	1:I:157:LYS:NZ	2.39	0.55
2:B:39:MK8:HB1A	2:B:42:ASP:HB2	1.89	0.55
1:G:138:GLY:HA2	2:H:44:LEU:HD23	1.89	0.54
2:B:47:ARG:HG3	2:D:32:LEU:HD21	1.89	0.54
1:I:16:LYS:NZ	1:I:95:ASP:OD1	2.35	0.54
1:A:180:PRO:O	1:A:184:GLU:HG3	2.09	0.53
1:G:184:GLU:HA	2:B:46:GLN:HG3	1.91	0.52
2:B:32:LEU:HD21	2:D:47:ARG:HG3	1.90	0.52
1:K:112:LEU:HD11	2:M:33:LEU:CD2	2.40	0.51
1:I:15:TYR:CG	1:I:91:ARG:HD2	2.46	0.51
1:A:178:LEU:O	1:A:182:ILE:HG12	2.12	0.50
1:K:150:LEU:O	1:K:154:SER:OG	2.28	0.50
2:B:39:MK8:HDA	2:D:39:MK8:HB1B	1.94	0.50
1:C:96:GLU:OE2	1:C:100:ARG:NH2	2.45	0.50
1:E:136:ASN:ND2	1:E:139:ARG:HG3	2.27	0.49
1:A:174:LEU:HD12	1:A:178:LEU:HB2	1.95	0.49
1:G:126:VAL:HG21	2:H:33:LEU:HD23	1.95	0.49
1:E:13:LEU:HD21	1:E:170:MET:HE1	1.94	0.48
1:C:160:GLN:CD	1:C:160:GLN:H	2.21	0.48
1:I:150:LEU:O	1:I:154:SER:OG	2.27	0.48
1:A:157:LYS:HB3	1:A:159:MET:HE3	1.96	0.48
1:C:150:LEU:HB3	1:C:166:ILE:HD13	1.95	0.47
2:F:35:MK8:HGA	2:F:35:MK8:HB1B	1.63	0.47
1:I:116:PRO:HG3	1:I:159:MET:HG2	1.97	0.47
2:L:32:LEU:HD11	2:L:36:ARG:NH1	2.30	0.47
1:E:105:PHE:CD2	2:F:36:ARG:HG2	2.49	0.47
2:M:32:LEU:CD2	2:M:36:ARG:HH12	2.14	0.47
1:K:162:LEU:O	1:K:166:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:PRO:HD3	1:E:159:MET:SD	2.55	0.46
2:B:35:MK8:HB1A	2:B:38:LYS:HB2	1.98	0.45
2:L:35:MK8:HB1A	2:L:38:LYS:HB2	1.97	0.45
2:M:35:MK8:HB1A	2:M:38:LYS:HB2	1.98	0.45
1:K:16:LYS:HA	1:K:16:LYS:HD2	1.70	0.45
2:H:35:MK8:HB1A	2:H:38:LYS:HB2	1.98	0.45
2:M:35:MK8:HB1B	2:M:35:MK8:HGA	1.73	0.45
1:E:174:LEU:HA	1:E:178:LEU:HB2	1.98	0.45
1:K:147:GLY:HA2	1:K:150:LEU:HB2	1.99	0.45
2:H:35:MK8:HB1B	2:H:35:MK8:HGA	1.62	0.45
1:G:194:LEU:HD13	2:H:49:MET:HE1	1.97	0.45
1:E:184:GLU:HA	2:D:46:GLN:HG3	1.99	0.45
1:A:108:LEU:HD12	1:A:108:LEU:H	1.82	0.45
1:C:88:GLN:NE2	1:C:92:GLU:OE2	2.41	0.44
2:D:35:MK8:HB1A	2:D:38:LYS:HB2	1.99	0.44
1:G:8:LEU:HD21	1:G:86:VAL:HG12	1.99	0.44
1:I:15:TYR:CD2	1:I:91:ARG:HD2	2.52	0.44
2:D:35:MK8:HGA	2:D:35:MK8:HB1B	1.74	0.44
1:C:129:GLU:OE2	1:C:132:ARG:NH1	2.51	0.44
1:G:136:ASN:ND2	1:G:139:ARG:HG3	2.33	0.44
1:C:157:LYS:HB3	1:C:159:MET:HE3	2.00	0.44
1:A:136:ASN:ND2	1:A:139:ARG:HG3	2.34	0.43
1:G:144:PHE:HZ	1:G:174:LEU:HD11	1.82	0.43
2:L:35:MK8:HGA	2:L:35:MK8:HB1B	1.72	0.43
2:M:44:LEU:O	2:M:48:THR:HG23	2.19	0.43
1:A:8:LEU:HD22	1:A:90:LEU:HD12	2.00	0.43
1:K:123:PHE:O	1:K:127:VAL:HG23	2.18	0.43
1:K:136:ASN:ND2	1:K:139:ARG:HG3	2.34	0.43
1:G:137:TRP:CZ3	1:G:191:PHE:HB2	2.54	0.43
1:A:131:PHE:CD1	1:A:135:VAL:HG22	2.54	0.43
1:C:174:LEU:HD12	1:C:178:LEU:HB2	1.99	0.43
1:G:174:LEU:O	1:G:179:GLU:N	2.52	0.42
1:I:168:ALA:O	1:I:172:THR:OG1	2.30	0.42
1:K:114:ILE:HG22	1:K:157:LYS:HE2	2.02	0.42
2:L:40:LEU:HD23	2:L:40:LEU:HA	1.83	0.42
2:F:40:LEU:HD23	2:F:40:LEU:HA	1.88	0.42
1:K:157:LYS:HB3	1:K:159:MET:HE3	2.01	0.42
1:K:170:MET:HB3	1:K:170:MET:HE2	1.72	0.42
1:C:182:ILE:HG22	1:C:187:GLY:HA2	2.02	0.41
1:E:88:GLN:O	1:E:92:GLU:HG3	2.21	0.41
1:I:150:LEU:HD23	1:I:150:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:PHE:O	1:E:127:VAL:HG23	2.20	0.41
1:K:136:ASN:HA	1:K:181:TRP:CZ2	2.55	0.41
2:L:32:LEU:HD13	2:L:36:ARG:HD2	2.03	0.41
2:B:35:MK8:HGA	2:B:35:MK8:HB1B	1.74	0.41
1:C:15:TYR:CD2	1:C:91:ARG:HG2	2.56	0.41
1:C:22:TYR:OH	1:C:156:ASP:OD1	2.22	0.41
1:G:174:LEU:HA	1:G:178:LEU:HB2	2.02	0.41
1:C:131:PHE:CD1	1:C:135:VAL:HG22	2.56	0.41
1:K:150:LEU:HA	1:K:150:LEU:HD23	1.81	0.40
1:G:182:ILE:HD13	1:G:182:ILE:HA	1.92	0.40
1:I:136:ASN:HA	1:I:181:TRP:CZ2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	139/218 (64%)	134 (96%)	5 (4%)	0	100	100
1	C	139/218 (64%)	136 (98%)	3 (2%)	0	100	100
1	E	138/218 (63%)	135 (98%)	3 (2%)	0	100	100
1	G	138/218 (63%)	136 (99%)	2 (1%)	0	100	100
1	I	140/218 (64%)	134 (96%)	6 (4%)	0	100	100
1	K	139/218 (64%)	133 (96%)	6 (4%)	0	100	100
2	B	19/24 (79%)	19 (100%)	0	0	100	100
2	D	19/24 (79%)	18 (95%)	1 (5%)	0	100	100
2	F	20/24 (83%)	19 (95%)	1 (5%)	0	100	100
2	H	20/24 (83%)	19 (95%)	1 (5%)	0	100	100
2	L	19/24 (79%)	18 (95%)	1 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	19/24 (79%)	18 (95%)	1 (5%)	0	100	100
All	All	949/1452 (65%)	919 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	120/183 (66%)	120 (100%)	0	100	100
1	C	120/183 (66%)	120 (100%)	0	100	100
1	E	119/183 (65%)	118 (99%)	1 (1%)	79	90
1	G	118/183 (64%)	116 (98%)	2 (2%)	56	80
1	I	121/183 (66%)	120 (99%)	1 (1%)	79	90
1	K	121/183 (66%)	119 (98%)	2 (2%)	56	80
2	B	17/18 (94%)	17 (100%)	0	100	100
2	D	17/18 (94%)	17 (100%)	0	100	100
2	F	18/18 (100%)	18 (100%)	0	100	100
2	H	18/18 (100%)	18 (100%)	0	100	100
2	L	17/18 (94%)	16 (94%)	1 (6%)	16	45
2	M	16/18 (89%)	16 (100%)	0	100	100
All	All	822/1206 (68%)	815 (99%)	7 (1%)	75	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	8	LEU
1	G	115	THR
1	G	152	VAL
1	I	183	GLN
1	K	133	ASP

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Mol	Chain	Res	Type
1	K	160	GLN
2	L	33	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	5	ASN
1	G	177	HIS
1	G	185	ASN
1	I	183	GLN
2	B	46	GLN
2	D	31	GLN
2	D	46	GLN
2	F	31	GLN
2	L	46	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	MK8	F	39	2	5,8,9	0.98	1 (20%)	4,10,12	0.98	0
2	MK8	M	39	2	5,8,9	0.97	0	4,10,12	0.93	0
2	MK8	M	35	2	5,8,9	0.90	0	4,10,12	0.98	0
2	MK8	B	39	2	5,8,9	0.96	0	4,10,12	0.89	0
2	MK8	B	35	2	5,8,9	0.94	0	4,10,12	0.98	0
2	MK8	H	35	2	5,8,9	0.93	0	4,10,12	0.92	0
2	MK8	L	39	2	5,8,9	0.97	1 (20%)	4,10,12	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MK8	H	39	2	5,8,9	0.98	1 (20%)	4,10,12	1.01	0
2	MK8	D	39	2	5,8,9	0.96	0	4,10,12	0.85	0
2	MK8	F	35	2	5,8,9	0.91	0	4,10,12	0.93	0
2	MK8	L	35	2	5,8,9	0.90	0	4,10,12	0.96	0
2	MK8	D	35	2	5,8,9	0.93	0	4,10,12	0.99	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	MK8	F	39	2	-	4/6/8/11	-
2	MK8	M	39	2	-	3/6/8/11	-
2	MK8	M	35	2	-	1/6/8/11	-
2	MK8	B	39	2	-	3/6/8/11	-
2	MK8	B	35	2	-	1/6/8/11	-
2	MK8	H	35	2	-	2/6/8/11	-
2	MK8	L	39	2	-	3/6/8/11	-
2	MK8	H	39	2	-	4/6/8/11	-
2	MK8	D	39	2	-	3/6/8/11	-
2	MK8	F	35	2	-	2/6/8/11	-
2	MK8	L	35	2	-	1/6/8/11	-
2	MK8	D	35	2	-	1/6/8/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	39	MK8	O-C	2.01	1.26	1.19
2	H	39	MK8	O-C	2.01	1.26	1.19
2	L	39	MK8	O-C	2.00	1.26	1.19

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	39	MK8	C-CA-CB-CG
2	B	39	MK8	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	B	39	MK8	CB1-CA-CB-CG
2	D	39	MK8	C-CA-CB-CG
2	D	39	MK8	N-CA-CB-CG
2	D	39	MK8	CB1-CA-CB-CG
2	F	39	MK8	C-CA-CB-CG
2	F	39	MK8	N-CA-CB-CG
2	F	39	MK8	CB1-CA-CB-CG
2	H	39	MK8	C-CA-CB-CG
2	H	39	MK8	N-CA-CB-CG
2	H	39	MK8	CB1-CA-CB-CG
2	L	39	MK8	C-CA-CB-CG
2	L	39	MK8	N-CA-CB-CG
2	L	39	MK8	CB1-CA-CB-CG
2	M	39	MK8	C-CA-CB-CG
2	M	39	MK8	N-CA-CB-CG
2	M	39	MK8	CB1-CA-CB-CG
2	B	35	MK8	CA-CB-CG-CD
2	D	35	MK8	CA-CB-CG-CD
2	H	35	MK8	CA-CB-CG-CD
2	L	35	MK8	CA-CB-CG-CD
2	F	35	MK8	CA-CB-CG-CD
2	M	35	MK8	CA-CB-CG-CD
2	H	39	MK8	CE-CD-CG-CB
2	F	39	MK8	CE-CD-CG-CB
2	F	35	MK8	CB1-CA-CB-CG
2	H	35	MK8	CB1-CA-CB-CG

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	39	MK8	3	0
2	M	39	MK8	3	0
2	M	35	MK8	2	0
2	B	39	MK8	3	0
2	B	35	MK8	2	0
2	H	35	MK8	2	0
2	L	39	MK8	3	0
2	H	39	MK8	3	0
2	D	39	MK8	3	0
2	F	35	MK8	1	0
2	L	35	MK8	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	35	MK8	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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, 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	142/218 (65%)	0.46	8 (5%) 31 20	17, 30, 56, 84	1 (0%)
1	C	142/218 (65%)	1.27	27 (19%) 4 3	25, 49, 55, 70	1 (0%)
1	E	141/218 (64%)	0.45	6 (4%) 40 27	17, 32, 52, 68	1 (0%)
1	G	141/218 (64%)	1.20	25 (17%) 4 4	20, 45, 62, 77	1 (0%)
1	I	143/218 (65%)	0.69	10 (6%) 24 16	20, 40, 62, 77	1 (0%)
1	K	142/218 (65%)	0.80	16 (11%) 11 8	16, 42, 57, 71	1 (0%)
2	B	21/24 (87%)	0.95	0 100 100	39, 43, 49, 51	0
2	D	21/24 (87%)	0.04	0 100 100	20, 25, 31, 40	0
2	F	22/24 (91%)	1.32	2 (9%) 16 11	39, 45, 48, 49	0
2	H	22/24 (91%)	0.06	0 100 100	24, 28, 37, 40	0
2	L	21/24 (87%)	0.21	0 100 100	24, 28, 36, 45	0
2	M	21/24 (87%)	1.74	7 (33%) 1 1	51, 52, 56, 58	0
All	All	979/1452 (67%)	0.80	101 (10%) 13 9	16, 41, 60, 84	6 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	28	SER	4.4
1	C	119	ALA	4.3
1	G	179	GLU	4.0
1	E	122	SER	3.7
1	G	28	SER	3.7
1	G	3	GLN	3.5
2	M	42	ASP	3.5
1	K	23	SER	3.5
1	I	4	SER	3.5
1	K	114	ILE	3.3
1	E	121	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	154	SER	3.2
1	G	14	SER	3.1
1	C	112	LEU	3.1
1	G	2	SER	3.1
1	G	164	SER	3.1
1	C	135	VAL	3.0
1	C	99	LEU	3.0
1	K	118	THR	3.0
1	G	18	SER	3.0
1	I	188	TRP	2.9
2	M	37	LEU	2.9
1	C	98	GLU	2.7
1	C	114	ILE	2.7
1	G	83	MET	2.7
1	K	110	SER	2.7
1	C	109	THR	2.7
1	I	113	HIS	2.7
1	C	104	ALA	2.6
1	A	194	LEU	2.6
1	A	197	ASN	2.6
1	C	171	ALA	2.6
1	G	171	ALA	2.6
1	K	89	ALA	2.6
2	M	33	LEU	2.6
1	K	106	SER	2.5
1	I	3	GLN	2.5
1	C	158	GLU	2.5
1	K	93	ALA	2.5
1	G	182	ILE	2.5
1	G	176	ASP	2.4
1	K	112	LEU	2.4
1	G	16	LYS	2.4
1	C	185	ASN	2.4
2	F	28	SER	2.4
1	C	179	GLU	2.4
1	G	109	THR	2.4
1	C	2	SER	2.3
1	G	98	GLU	2.3
1	I	83	MET	2.3
2	F	40	LEU	2.3
1	C	177	HIS	2.3
1	A	188	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	28	SER	2.3
1	G	112	LEU	2.3
1	G	152	VAL	2.3
1	C	166	ILE	2.3
1	E	28	SER	2.3
1	G	25	SER	2.3
1	C	3	GLN	2.3
1	E	118	THR	2.3
1	A	196	GLY	2.2
1	G	155	VAL	2.2
1	I	196	GLY	2.2
1	A	112	LEU	2.2
1	C	196	GLY	2.2
1	E	3	GLN	2.2
1	K	83	MET	2.2
1	C	164	SER	2.2
1	A	114	ILE	2.2
1	K	19	GLN	2.2
2	M	44	LEU	2.2
1	E	109	THR	2.2
1	A	28	SER	2.2
1	I	114	ILE	2.2
1	C	173	TYR	2.1
1	C	149	ALA	2.1
1	K	99	LEU	2.1
2	M	34	ALA	2.1
1	C	25	SER	2.1
1	C	117	GLY	2.1
1	G	122	SER	2.1
1	K	94	GLY	2.1
2	M	45	HIS	2.1
1	C	181	TRP	2.1
1	K	91	ARG	2.1
1	C	110	SER	2.1
1	G	19	GLN	2.1
1	I	182	ILE	2.1
1	C	183	GLN	2.1
2	M	32	LEU	2.1
1	C	175	ASN	2.1
1	I	181	TRP	2.0
1	G	94	GLY	2.0
1	K	108	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	26	GLN	2.0
1	K	84	ALA	2.0
1	G	140	ILE	2.0
1	G	24	TRP	2.0
1	G	177	HIS	2.0
1	K	113	HIS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MK8	F	39	9/10	0.80	0.26	46,47,48,48	0
2	MK8	L	35	9/10	0.85	0.16	15,21,31,33	0
2	MK8	M	35	9/10	0.86	0.21	51,52,52,52	0
2	MK8	H	39	9/10	0.86	0.16	24,30,38,39	0
2	MK8	B	39	9/10	0.87	0.20	39,40,43,45	0
2	MK8	M	39	9/10	0.87	0.25	50,51,51,52	0
2	MK8	L	39	9/10	0.91	0.13	19,24,30,33	0
2	MK8	H	35	9/10	0.91	0.11	19,21,28,32	0
2	MK8	F	35	9/10	0.92	0.12	40,41,42,42	0
2	MK8	B	35	9/10	0.93	0.14	41,42,44,45	0
2	MK8	D	39	9/10	0.93	0.12	15,19,30,30	0
2	MK8	D	35	9/10	0.94	0.09	13,19,24,26	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	101	1/1	0.80	0.22	28,28,28,28	0
3	MG	D	101	1/1	0.82	0.16	22,22,22,22	0
3	MG	I	301	1/1	0.89	0.14	21,21,21,21	0
3	MG	A	301	1/1	0.90	0.16	26,26,26,26	0
3	MG	C	301	1/1	0.92	0.27	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.