



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:33 PM UTC

PDB ID : 5B6B / pdb_00005b6b
Title : Complex of LATS1 and phosphomimetic MOB1b
Authors : KIM, S.-Y.; Tachioka, Y.; Mori, T.; Hakoshima, T.
Deposited on : 2016-05-26
Resolution : 3.54 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 Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

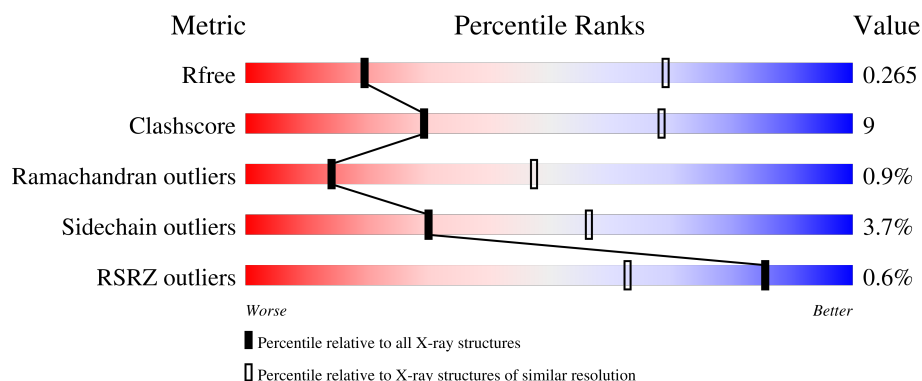
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 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}	180053	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

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	 60% 21% 17% 2%
1	B	218	 65% 21% 13% 1%
1	D	218	 71% 11% 19%
1	F	218	 63% 17% 16% 2%
1	H	218	 58% 22% 16%

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Mol	Chain	Length	Quality of chain
1	K	218	
1	M	218	
1	O	218	
2	C	85	
2	E	85	
2	G	85	
2	I	85	
2	J	85	
2	L	85	
2	N	85	
2	P	85	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16626 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 MOB kinase activator 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1504	977	243	275	9			
1	B	189	Total	C	N	O	S	0	0	0
			1552	1007	253	283	9			
1	D	177	Total	C	N	O	S	0	0	0
			1472	959	236	268	9			
1	F	183	Total	C	N	O	S	0	0	0
			1503	978	241	275	9			
1	H	184	Total	C	N	O	S	0	0	0
			1516	983	245	279	9			
1	K	180	Total	C	N	O	S	0	0	0
			1480	963	238	270	9			
1	M	173	Total	C	N	O	S	0	0	0
			1434	934	231	260	9			
1	O	170	Total	C	N	O	S	0	0	0
			1404	914	225	256	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8BPP0
A	0	PRO	-	expression tag	UNP Q8BPP0
A	12	ASP	THR	engineered mutation	UNP Q8BPP0
A	35	ASP	THR	engineered mutation	UNP Q8BPP0
B	-1	GLY	-	expression tag	UNP Q8BPP0
B	0	PRO	-	expression tag	UNP Q8BPP0
B	12	ASP	THR	engineered mutation	UNP Q8BPP0
B	35	ASP	THR	engineered mutation	UNP Q8BPP0
D	-1	GLY	-	expression tag	UNP Q8BPP0
D	0	PRO	-	expression tag	UNP Q8BPP0
D	12	ASP	THR	engineered mutation	UNP Q8BPP0
D	35	ASP	THR	engineered mutation	UNP Q8BPP0
F	-1	GLY	-	expression tag	UNP Q8BPP0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	PRO	-	expression tag	UNP Q8BPP0
F	12	ASP	THR	engineered mutation	UNP Q8BPP0
F	35	ASP	THR	engineered mutation	UNP Q8BPP0
H	-1	GLY	-	expression tag	UNP Q8BPP0
H	0	PRO	-	expression tag	UNP Q8BPP0
H	12	ASP	THR	engineered mutation	UNP Q8BPP0
H	35	ASP	THR	engineered mutation	UNP Q8BPP0
K	-1	GLY	-	expression tag	UNP Q8BPP0
K	0	PRO	-	expression tag	UNP Q8BPP0
K	12	ASP	THR	engineered mutation	UNP Q8BPP0
K	35	ASP	THR	engineered mutation	UNP Q8BPP0
M	-1	GLY	-	expression tag	UNP Q8BPP0
M	0	PRO	-	expression tag	UNP Q8BPP0
M	12	ASP	THR	engineered mutation	UNP Q8BPP0
M	35	ASP	THR	engineered mutation	UNP Q8BPP0
O	-1	GLY	-	expression tag	UNP Q8BPP0
O	0	PRO	-	expression tag	UNP Q8BPP0
O	12	ASP	THR	engineered mutation	UNP Q8BPP0
O	35	ASP	THR	engineered mutation	UNP Q8BPP0

- Molecule 2 is a protein called Serine/threonine-protein kinase LATS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	71	Total	C	N	O	S	0	0	0
			600	372	115	106	7			
2	C	71	Total	C	N	O	S	0	0	0
			599	370	116	106	7			
2	E	71	Total	C	N	O	S	0	0	0
			603	373	117	106	7			
2	G	74	Total	C	N	O	S	0	0	0
			623	385	120	111	7			
2	I	72	Total	C	N	O	S	0	0	0
			611	379	118	107	7			
2	L	72	Total	C	N	O	S	0	0	0
			608	376	117	108	7			
2	N	65	Total	C	N	O	S	0	0	0
			548	338	108	96	6			
2	P	65	Total	C	N	O	S	0	0	0
			554	343	109	95	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	619	GLY	-	expression tag	UNP Q8BYR2
J	620	PRO	-	expression tag	UNP Q8BYR2
C	619	GLY	-	expression tag	UNP Q8BYR2
C	620	PRO	-	expression tag	UNP Q8BYR2
E	619	GLY	-	expression tag	UNP Q8BYR2
E	620	PRO	-	expression tag	UNP Q8BYR2
G	619	GLY	-	expression tag	UNP Q8BYR2
G	620	PRO	-	expression tag	UNP Q8BYR2
I	619	GLY	-	expression tag	UNP Q8BYR2
I	620	PRO	-	expression tag	UNP Q8BYR2
L	619	GLY	-	expression tag	UNP Q8BYR2
L	620	PRO	-	expression tag	UNP Q8BYR2
N	619	GLY	-	expression tag	UNP Q8BYR2
N	620	PRO	-	expression tag	UNP Q8BYR2
P	619	GLY	-	expression tag	UNP Q8BYR2
P	620	PRO	-	expression tag	UNP Q8BYR2

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	K	1	Total Cl 1 1	0	0
3	M	1	Total Cl 1 1	0	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0

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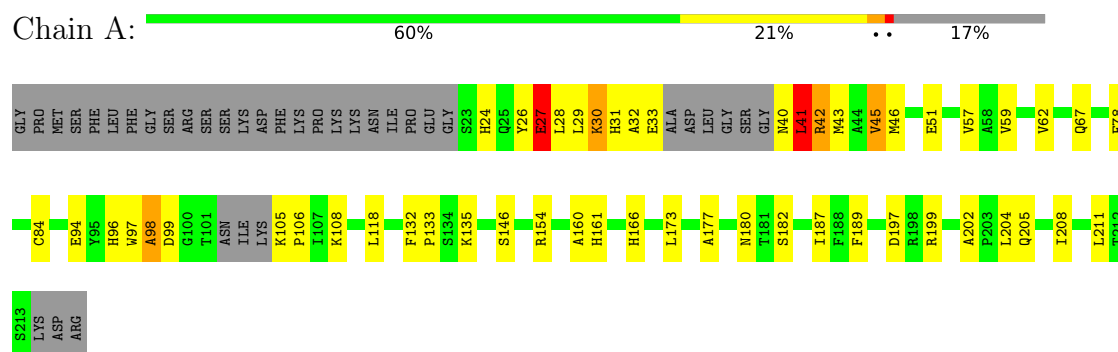
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total 1	Zn 1	0	0
4	F	1	Total 1	Zn 1	0	0
4	H	1	Total 1	Zn 1	0	0
4	K	1	Total 1	Zn 1	0	0
4	M	1	Total 1	Zn 1	0	0
4	O	1	Total 1	Zn 1	0	0

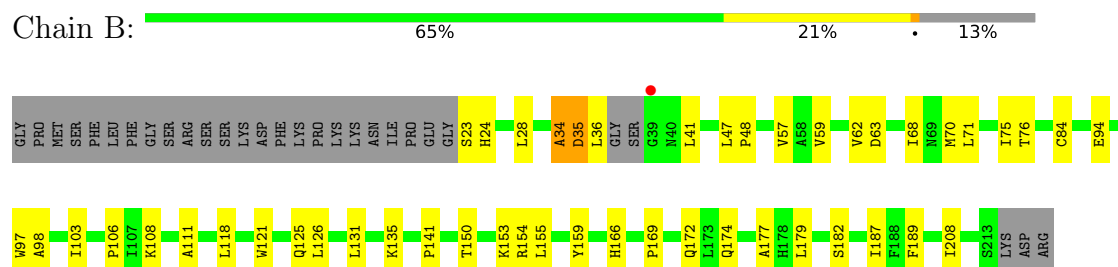
3 Residue-property plots

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.

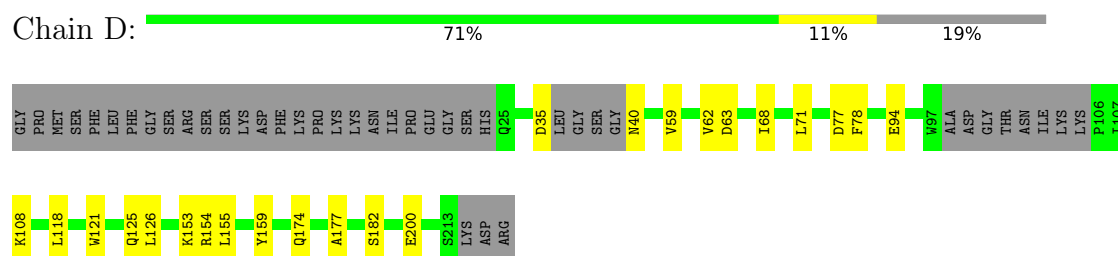
• Molecule 1: MOB kinase activator 1B



• Molecule 1: MOB kinase activator 1B

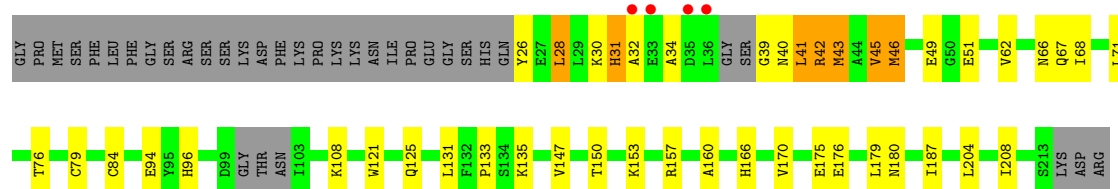


• Molecule 1: MOB kinase activator 1B



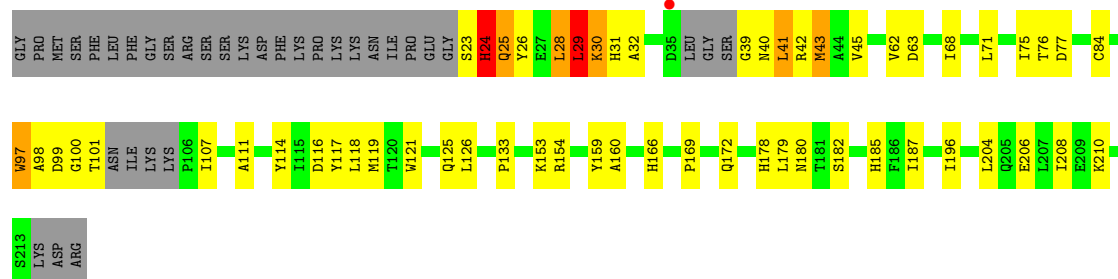
• Molecule 1: MOB kinase activator 1B





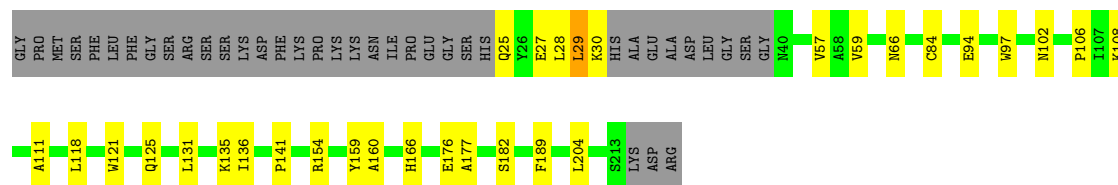
• Molecule 1: MOB kinase activator 1B

Chain H: 58% 22% 16%



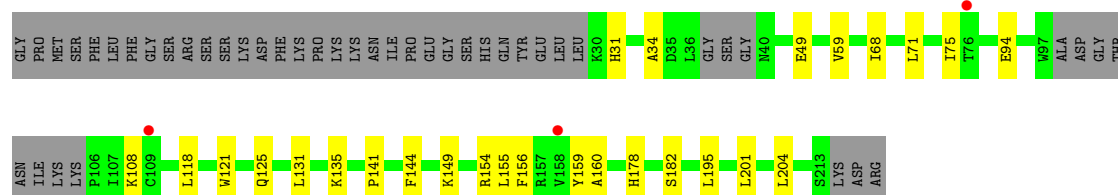
• Molecule 1: MOB kinase activator 1B

Chain K: 68% 14% 17%



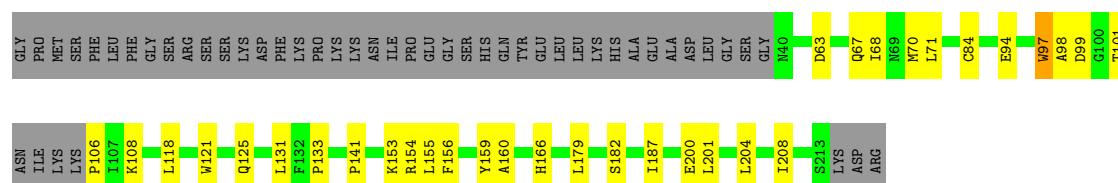
• Molecule 1: MOB kinase activator 1B

Chain M: 67% 12% 21%



• Molecule 1: MOB kinase activator 1B

Chain O: 63% 15% 22%



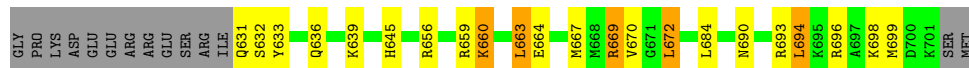
- Molecule 2: Serine/threonine-protein kinase LATS1

Chain J:  62% 19% 16%



- Molecule 2: Serine/threonine-protein kinase LATS1

Chain C:  58% 20% 6% 16%



- Molecule 2: Serine/threonine-protein kinase LATS1

Chain E:  62% 20% 16%



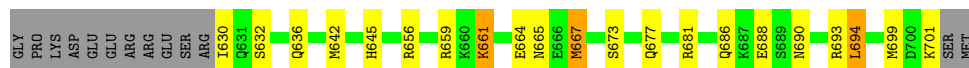
- Molecule 2: Serine/threonine-protein kinase LATS1

Chain G:  65% 19% 13%



- Molecule 2: Serine/threonine-protein kinase LATS1

Chain I:  60% 21% 15%



- Molecule 2: Serine/threonine-protein kinase LATS1

Chain L:  60% 22% 15%

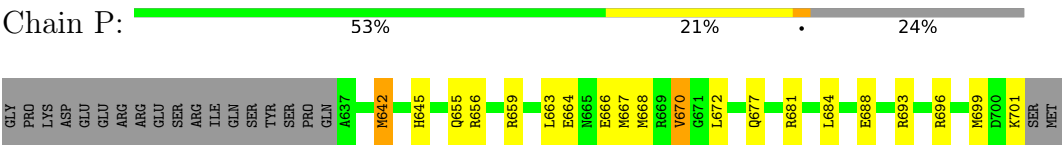


- Molecule 2: Serine/threonine-protein kinase LATS1

Chain N:  2% 54% 16% 6% 24%



● Molecule 2: Serine/threonine-protein kinase LATS1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	168.65Å 301.44Å 127.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.64 – 3.54 48.64 – 3.54	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.64-3.54) 95.2 (48.64-3.54)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.222 , 0.266 0.224 , 0.265	Depositor DCC
R_{free} test set	1998 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	83.4	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 93.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16626	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: ZN, CL

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	0.41	0/1546	0.79	4/2097 (0.2%)
1	B	0.29	0/1595	0.73	1/2163 (0.0%)
1	D	0.28	0/1513	0.70	0/2051
1	F	0.41	0/1544	0.79	4/2095 (0.2%)
1	H	0.39	0/1558	0.81	3/2112 (0.1%)
1	K	0.32	0/1521	0.71	0/2065
1	M	0.27	0/1474	0.68	0/1998
1	O	0.27	0/1444	0.70	0/1960
2	C	0.30	0/607	0.80	1/802 (0.1%)
2	E	0.31	0/611	0.70	0/806
2	G	0.31	0/631	0.71	0/834
2	I	0.31	0/619	0.76	0/817
2	J	0.28	0/608	0.76	0/804
2	L	0.30	0/616	0.70	0/815
2	N	0.36	0/555	0.81	0/734
2	P	0.28	0/560	0.70	0/736
All	All	0.33	0/17002	0.74	13/22889 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	97	TRP	N-CA-C	-8.07	98.57	110.52
1	F	41	LEU	N-CA-C	6.33	118.26	111.36
1	A	45	VAL	N-CA-C	6.15	116.93	110.72
1	H	24	HIS	N-CA-C	-6.07	104.58	111.07
1	F	45	VAL	N-CA-C	5.92	116.70	110.72
1	F	46	MET	N-CA-C	5.92	118.64	110.35
1	A	105	LYS	CA-C-N	5.69	125.70	119.90
1	A	105	LYS	C-N-CA	5.69	125.70	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	29	LEU	N-CA-C	-5.55	105.23	111.28
1	B	34	ALA	N-CA-C	5.36	117.91	108.75
1	A	46	MET	N-CA-C	5.29	118.15	110.42
1	F	34	ALA	N-CA-C	-5.29	106.85	113.72
2	C	669	ARG	N-CA-C	5.00	116.42	110.97

There are no chirality outliers.

There are no planarity outliers.

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	1504	0	1449	41	0
1	B	1552	0	1503	26	0
1	D	1472	0	1426	14	0
1	F	1503	0	1446	36	0
1	H	1516	0	1460	47	0
1	K	1480	0	1425	23	0
1	M	1434	0	1392	18	0
1	O	1404	0	1361	20	0
2	C	599	0	602	12	0
2	E	603	0	613	12	0
2	G	623	0	631	15	0
2	I	611	0	624	15	0
2	J	600	0	607	17	0
2	L	608	0	613	12	0
2	N	548	0	554	12	0
2	P	554	0	571	15	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	1	0
3	H	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
All	All	16626	0	16277	282	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 9.

All (282) 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:F:40:ASN:HD22	1:F:41:LEU:N	1.44	1.16
1:K:25:GLN:O	1:K:176:GLU:OE1	1.63	1.14
1:F:40:ASN:ND2	1:F:41:LEU:H	1.53	1.06
1:O:94:GLU:OE2	1:O:108:LYS:NZ	2.00	0.95
1:K:29:LEU:HB3	1:K:177:ALA:HB1	1.56	0.88
1:H:39:GLY:O	1:H:42:ARG:N	2.08	0.86
1:A:40:ASN:O	1:A:43:MET:N	2.07	0.86
1:K:29:LEU:HD12	1:K:30:LYS:N	1.92	0.83
1:H:30:LYS:HD2	1:H:30:LYS:C	2.03	0.83
1:F:40:ASN:ND2	1:F:41:LEU:N	2.16	0.82
1:A:42:ARG:O	1:A:45:VAL:HG22	1.79	0.81
1:A:41:LEU:O	1:A:45:VAL:HG13	1.79	0.81
1:A:84:CYS:SG	1:A:166:HIS:HE1	1.92	0.81
1:B:94:GLU:OE2	1:B:108:LYS:NZ	2.16	0.78
1:H:133:PRO:HB2	2:I:693:ARG:HH12	1.48	0.78
1:K:28:LEU:HD12	1:K:29:LEU:O	1.83	0.77
1:D:35:ASP:HB3	1:D:177:ALA:HB1	1.67	0.77
2:N:668:MET:O	2:N:670:VAL:N	2.19	0.76
1:H:28:LEU:HD12	1:H:28:LEU:O	1.86	0.75
2:C:667:MET:HG2	2:C:672:LEU:HD11	1.69	0.74
2:I:686:GLN:O	2:I:690:ASN:ND2	2.18	0.73
1:H:29:LEU:O	1:H:29:LEU:HD12	1.89	0.72
1:H:28:LEU:HD12	1:H:28:LEU:C	2.15	0.72
2:J:695:LYS:HA	2:J:699:MET:HB3	1.71	0.72
1:B:174:GLN:O	2:C:639:LYS:NZ	2.23	0.72
1:H:30:LYS:HD2	1:H:30:LYS:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:LEU:HD12	1:H:29:LEU:C	2.16	0.71
2:G:664:GLU:OE1	2:G:681:ARG:NH1	2.24	0.70
1:K:29:LEU:HD12	1:K:29:LEU:C	2.15	0.70
1:M:182:SER:HB2	2:N:642:MET:HE2	1.73	0.70
1:F:42:ARG:O	1:F:45:VAL:HG22	1.90	0.70
1:F:40:ASN:HD22	1:F:41:LEU:H	0.78	0.69
1:A:40:ASN:O	1:A:42:ARG:N	2.25	0.68
1:M:68:ILE:HD12	1:M:71:LEU:HD23	1.73	0.68
1:O:133:PRO:O	2:P:696:ARG:NH2	2.26	0.68
1:H:99:ASP:O	1:H:101:THR:N	2.27	0.67
1:H:39:GLY:O	1:H:42:ARG:HB3	1.95	0.66
1:D:68:ILE:HD12	1:D:71:LEU:HD23	1.80	0.64
1:M:59:VAL:HG22	2:N:696:ARG:HB2	1.78	0.64
1:A:133:PRO:O	2:J:696:ARG:NH2	2.29	0.64
1:D:59:VAL:HG22	2:E:696:ARG:HB2	1.79	0.64
2:C:663:LEU:HD12	2:C:684:LEU:HD22	1.80	0.63
2:I:661:LYS:O	2:I:665:ASN:ND2	2.31	0.63
1:F:94:GLU:OE2	1:F:108:LYS:NZ	2.31	0.63
1:B:68:ILE:HD12	1:B:71:LEU:HD23	1.80	0.63
1:A:96:HIS:HE1	1:A:108:LYS:HG3	1.62	0.63
2:L:683:MET:HE3	2:L:687:LYS:HE3	1.80	0.63
1:O:159:TYR:OH	1:O:182:SER:OG	2.16	0.63
1:O:68:ILE:HD12	1:O:71:LEU:HD23	1.81	0.62
1:K:29:LEU:CB	1:K:177:ALA:HB1	2.28	0.62
1:H:68:ILE:HD12	1:H:71:LEU:HD23	1.81	0.61
1:A:32:ALA:HB1	2:J:650:LEU:HD22	1.83	0.61
1:F:68:ILE:HD12	1:F:71:LEU:HD23	1.80	0.61
1:H:24:HIS:HB3	1:H:25:GLN:OE1	2.01	0.61
1:H:25:GLN:OE1	1:H:25:GLN:N	2.34	0.61
1:F:96:HIS:HE1	1:F:108:LYS:HG3	1.66	0.60
1:F:176:GLU:O	1:F:180:ASN:ND2	2.33	0.60
1:K:84:CYS:SG	1:K:166:HIS:HE1	2.14	0.60
1:A:29:LEU:HB2	1:A:30:LYS:HB2	1.85	0.59
1:O:98:ALA:HB2	1:O:106:PRO:HA	1.85	0.59
1:F:40:ASN:N	2:G:650:LEU:HD22	2.18	0.59
1:H:40:ASN:HA	1:H:43:MET:HG3	1.85	0.58
1:H:116:ASP:HA	2:I:630:ILE:HD12	1.85	0.58
1:K:27:GLU:HA	1:K:27:GLU:OE2	2.04	0.58
2:L:636:GLN:HA	2:L:639:LYS:HD2	1.86	0.58
1:A:94:GLU:OE2	1:A:108:LYS:NZ	2.37	0.57
1:H:97:TRP:O	1:H:107:ILE:N	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:GLU:OE2	1:D:108:LYS:NZ	2.36	0.56
1:B:63:ASP:OD1	2:C:645:HIS:NE2	2.38	0.56
1:K:94:GLU:OE2	1:K:108:LYS:NZ	2.35	0.56
2:C:656:ARG:HA	2:C:659:ARG:NH1	2.19	0.56
1:M:68:ILE:HG21	1:M:155:LEU:HD22	1.86	0.56
2:N:656:ARG:HG3	2:N:657:LEU:N	2.19	0.56
1:B:34:ALA:HB1	1:B:177:ALA:HA	1.88	0.56
1:K:66:ASN:ND2	2:L:699:MET:SD	2.78	0.55
2:P:667:MET:HE2	2:P:677:GLN:HA	1.88	0.55
1:A:59:VAL:HG22	2:J:696:ARG:HB2	1.88	0.55
1:A:160:ALA:HA	1:A:204:LEU:HD11	1.89	0.55
1:A:182:SER:HB2	2:J:642:MET:HE2	1.89	0.54
1:H:159:TYR:OH	1:H:182:SER:OG	2.25	0.54
1:H:26:TYR:C	1:H:26:TYR:CD2	2.85	0.54
2:L:663:LEU:HD13	2:L:684:LEU:HD22	1.89	0.54
1:F:135:LYS:HD3	2:I:701:LYS:NZ	2.23	0.54
1:O:131:LEU:HA	1:O:141:PRO:HG3	1.88	0.54
2:P:656:ARG:HG3	2:P:688:GLU:OE2	2.07	0.54
2:N:683:MET:HG3	2:N:687:LYS:HE2	1.90	0.53
1:A:173:LEU:O	2:J:639:LYS:NZ	2.31	0.53
1:B:35:ASP:CG	1:B:36:LEU:H	2.17	0.53
2:G:678:ASP:OD2	2:G:682:LYS:NZ	2.42	0.53
1:A:187:ILE:HG21	1:A:208:ILE:HG23	1.91	0.52
1:B:84:CYS:SG	1:B:166:HIS:HE1	2.22	0.52
1:H:153:LYS:HG2	1:H:196:ILE:HG23	1.90	0.52
1:M:135:LYS:HD3	2:P:701:LYS:NZ	2.25	0.52
1:A:98:ALA:HB2	1:A:106:PRO:HA	1.92	0.52
1:A:197:ASP:OD2	1:A:199:ARG:NE	2.40	0.52
1:D:68:ILE:HG21	1:D:155:LEU:HD22	1.92	0.52
2:G:663:LEU:HD22	2:G:684:LEU:HD13	1.92	0.52
1:H:29:LEU:HD13	1:H:210:LYS:HG2	1.91	0.51
1:M:94:GLU:OE2	1:M:108:LYS:NZ	2.42	0.51
1:A:27:GLU:HG2	1:A:177:ALA:HB2	1.92	0.51
1:F:133:PRO:O	2:G:696:ARG:NH2	2.40	0.51
1:H:63:ASP:OD1	2:I:645:HIS:NE2	2.44	0.51
2:I:690:ASN:O	2:I:694:LEU:HD22	2.10	0.51
1:F:51:GLU:OE2	2:G:656:ARG:NH2	2.31	0.50
1:B:84:CYS:HB2	1:B:111:ALA:HB3	1.94	0.50
1:H:76:THR:HG21	2:I:632:SER:HB3	1.93	0.50
1:A:29:LEU:CA	1:A:30:LYS:HB2	2.42	0.50
1:F:187:ILE:HG21	1:F:208:ILE:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:TRP:NE1	1:H:117:TYR:HB3	2.26	0.50
1:D:63:ASP:OD1	2:E:645:HIS:NE2	2.46	0.49
1:M:159:TYR:OH	1:M:182:SER:OG	2.30	0.49
2:E:699:MET:O	1:K:136:ILE:HG12	2.13	0.49
1:H:84:CYS:SG	1:H:166:HIS:HE1	2.20	0.49
1:H:97:TRP:HB2	1:H:114:TYR:CD2	2.48	0.49
1:B:84:CYS:HB3	1:B:111:ALA:HB2	1.94	0.49
1:K:59:VAL:HG22	2:L:696:ARG:HB2	1.95	0.49
2:G:654:GLN:HG3	2:G:655:GLN:N	2.27	0.49
2:G:700:ASP:OD2	2:G:700:ASP:N	2.33	0.49
1:A:161:HIS:NE2	1:A:166:HIS:CD2	2.79	0.49
1:F:170:VAL:HG13	1:F:175:GLU:HB2	1.95	0.49
1:K:29:LEU:HD12	1:K:30:LYS:CA	2.43	0.48
1:A:96:HIS:HD2	1:D:78:PHE:CZ	2.30	0.48
2:L:673:SER:O	2:L:677:GLN:HG3	2.13	0.48
1:O:84:CYS:SG	1:O:166:HIS:HE1	2.24	0.48
2:E:670:VAL:O	2:E:672:LEU:HG	2.12	0.48
1:H:97:TRP:CD1	1:H:98:ALA:HB2	2.47	0.48
2:I:659:ARG:NH1	2:I:688:GLU:OE2	2.47	0.48
2:J:667:MET:HE1	2:J:680:MET:HB2	1.95	0.48
1:B:70:MET:HE2	2:C:633:TYR:CE2	2.49	0.47
1:H:84:CYS:HB2	1:H:111:ALA:HB3	1.96	0.47
1:M:178:HIS:HB3	2:N:642:MET:HG2	1.96	0.47
1:A:29:LEU:HA	1:A:30:LYS:HB2	1.96	0.47
2:E:690:ASN:O	2:E:694:LEU:HD22	2.15	0.47
1:H:118:LEU:HD11	1:H:154:ARG:HB3	1.96	0.47
1:M:118:LEU:HD11	1:M:154:ARG:HB3	1.97	0.47
2:P:670:VAL:O	2:P:672:LEU:HG	2.14	0.47
1:O:182:SER:HB2	2:P:642:MET:HE3	1.95	0.47
1:A:146:SER:HB3	1:F:49:GLU:OE1	2.15	0.47
1:D:118:LEU:HD11	1:D:154:ARG:HB3	1.97	0.47
2:I:673:SER:O	2:I:677:GLN:HG3	2.14	0.47
1:M:131:LEU:HA	1:M:141:PRO:HG3	1.94	0.47
1:A:67:GLN:CD	2:J:642:MET:HE1	2.40	0.47
1:K:131:LEU:HA	1:K:141:PRO:HG3	1.96	0.47
1:F:40:ASN:H	2:G:650:LEU:HD22	1.78	0.47
1:H:169:PRO:HA	1:H:172:GLN:HG2	1.97	0.47
2:I:667:MET:CG	2:I:677:GLN:HG2	2.44	0.47
2:N:663:LEU:HD13	2:N:684:LEU:HD22	1.95	0.47
1:B:68:ILE:HG21	1:B:155:LEU:HD22	1.97	0.46
1:F:39:GLY:O	1:F:40:ASN:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:160:ALA:HA	1:K:204:LEU:HD11	1.97	0.46
1:F:160:ALA:HA	1:F:204:LEU:HD11	1.97	0.46
1:F:84:CYS:SG	1:F:166:HIS:HE1	2.22	0.46
2:I:664:GLU:OE1	2:I:681:ARG:NH1	2.49	0.46
1:F:66:ASN:ND2	2:G:699:MET:SD	2.88	0.46
1:K:118:LEU:HD11	1:K:154:ARG:HB3	1.98	0.46
1:A:57:VAL:HA	1:A:189:PHE:HZ	1.79	0.46
1:D:62:VAL:HG22	1:D:126:LEU:HD22	1.98	0.46
1:D:77:ASP:OD1	1:D:77:ASP:N	2.45	0.46
1:F:76:THR:HG21	2:G:632:SER:HB2	1.98	0.46
2:J:639:LYS:O	2:J:643:GLU:HG3	2.16	0.46
1:F:71:LEU:HD21	1:F:179:LEU:HD13	1.98	0.46
1:A:135:LYS:O	2:J:693:ARG:NH1	2.41	0.45
2:C:660:LYS:HE2	2:C:660:LYS:HB3	1.85	0.45
1:F:131:LEU:HD13	1:F:147:VAL:HG21	1.98	0.45
1:F:31:HIS:HD1	1:F:176:GLU:CD	2.22	0.45
1:F:62:VAL:HG21	2:G:696:ARG:HG3	1.99	0.45
1:O:68:ILE:HG21	1:O:155:LEU:HD22	1.98	0.45
2:E:673:SER:O	2:E:677:GLN:HG3	2.16	0.45
1:A:40:ASN:C	1:A:42:ARG:N	2.75	0.45
1:F:45:VAL:HG23	1:F:46:MET:N	2.31	0.45
2:E:699:MET:SD	1:K:135:LYS:HG2	2.57	0.45
1:F:28:LEU:O	1:F:32:ALA:HB2	2.17	0.45
1:H:84:CYS:HB3	1:H:111:ALA:HB2	1.98	0.45
2:L:630:ILE:O	2:L:631:GLN:HB2	2.16	0.45
1:B:62:VAL:HG22	1:B:126:LEU:HD22	1.98	0.44
2:J:636:GLN:H	2:J:636:GLN:HG2	1.59	0.44
2:J:690:ASN:O	2:J:694:LEU:HD22	2.17	0.44
1:B:118:LEU:HD11	1:B:154:ARG:HB3	1.99	0.44
1:B:169:PRO:HA	1:B:172:GLN:HG2	1.97	0.44
1:M:135:LYS:O	2:N:693:ARG:NH1	2.43	0.44
1:A:118:LEU:HD11	1:A:154:ARG:HB3	1.99	0.44
2:P:663:LEU:HD22	2:P:684:LEU:HD13	1.99	0.44
1:A:62:VAL:HG21	2:J:696:ARG:HG3	1.99	0.44
1:D:121:TRP:O	1:D:125:GLN:HG2	2.18	0.44
1:H:25:GLN:HG3	1:H:206:GLU:OE2	2.17	0.44
1:M:49:GLU:HB3	2:N:660:LYS:HZ1	1.83	0.44
1:O:63:ASP:OD1	2:P:645:HIS:NE2	2.51	0.44
1:A:132:PHE:HB3	2:J:696:ARG:NH1	2.33	0.44
1:F:28:LEU:H	1:F:28:LEU:HG	1.49	0.44
1:H:62:VAL:HG22	1:H:126:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:97:TRP:O	1:K:106:PRO:HA	2.17	0.44
1:A:78:PHE:N	1:A:78:PHE:CD2	2.86	0.44
1:F:43:MET:H	1:F:43:MET:HG2	1.65	0.44
1:H:77:ASP:OD1	1:H:77:ASP:N	2.44	0.44
2:P:664:GLU:OE2	2:P:681:ARG:NH1	2.51	0.44
1:B:131:LEU:HA	1:B:141:PRO:HG3	1.99	0.43
1:F:150:THR:HA	1:F:153:LYS:HE2	2.00	0.43
1:H:30:LYS:C	1:H:30:LYS:CD	2.85	0.43
1:H:43:MET:H	1:H:43:MET:HG2	1.64	0.43
1:O:99:ASP:OD2	1:O:101:THR:OG1	2.34	0.43
1:F:26:TYR:O	1:F:30:LYS:HG2	2.18	0.43
1:B:159:TYR:OH	1:B:182:SER:OG	2.34	0.43
1:B:187:ILE:HG21	1:B:208:ILE:HG23	2.00	0.43
2:G:630:ILE:H	2:G:630:ILE:HG13	1.54	0.43
1:A:28:LEU:HD11	1:A:211:LEU:HD22	2.01	0.43
1:B:97:TRP:O	1:B:106:PRO:HA	2.18	0.43
2:I:667:MET:HG2	2:I:677:GLN:HG2	2.00	0.43
1:O:118:LEU:HD11	1:O:154:ARG:HB3	1.99	0.43
1:A:51:GLU:OE2	2:J:656:ARG:NH2	2.51	0.43
1:O:187:ILE:HG21	1:O:208:ILE:HG23	1.99	0.43
1:K:121:TRP:O	1:K:125:GLN:HG2	2.18	0.43
2:P:655:GLN:O	2:P:659:ARG:HG3	2.18	0.43
1:A:26:TYR:O	1:A:180:ASN:ND2	2.51	0.43
2:L:655:GLN:O	2:L:659:ARG:HD3	2.19	0.43
1:M:160:ALA:HA	1:M:204:LEU:HD11	2.01	0.43
1:A:96:HIS:CE1	1:A:108:LYS:HG3	2.48	0.43
1:H:71:LEU:HD21	1:H:179:LEU:HD13	2.00	0.43
1:A:97:TRP:O	1:A:106:PRO:HA	2.19	0.42
2:L:667:MET:HE3	2:L:677:GLN:HA	2.01	0.42
1:B:135:LYS:O	2:C:693:ARG:NH1	2.49	0.42
2:L:666:GLU:O	2:L:669:ARG:HB3	2.20	0.42
1:B:57:VAL:HA	1:B:189:PHE:HZ	1.83	0.42
1:M:135:LYS:HD3	2:P:701:LYS:HZ1	1.83	0.42
1:H:160:ALA:HA	1:H:204:LEU:HD11	2.00	0.42
2:E:667:MET:HE3	2:E:677:GLN:HA	2.00	0.42
1:H:187:ILE:HG21	1:H:208:ILE:HG23	2.01	0.42
1:M:141:PRO:HG2	1:M:144:PHE:HB2	2.00	0.42
1:O:97:TRP:CH2	1:O:118:LEU:HA	2.55	0.42
2:E:650:LEU:HD23	2:E:650:LEU:HA	1.85	0.42
1:H:119:MET:HB2	2:I:630:ILE:HD11	2.01	0.42
1:O:71:LEU:HD21	1:O:179:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:THR:HG21	2:C:632:SER:HB3	2.02	0.42
1:D:159:TYR:OH	1:D:182:SER:OG	2.30	0.42
1:H:121:TRP:O	1:H:125:GLN:HG2	2.20	0.42
1:B:47:LEU:HD12	1:B:48:PRO:HD2	2.02	0.41
2:C:667:MET:HG3	2:C:672:LEU:HD21	2.01	0.41
2:E:659:ARG:NH2	2:E:688:GLU:OE1	2.48	0.41
1:M:156:PHE:CE2	1:M:201:LEU:HA	2.54	0.41
1:A:29:LEU:HA	1:A:30:LYS:CB	2.50	0.41
1:D:153:LYS:HD2	1:D:200:GLU:HG3	2.02	0.41
1:H:32:ALA:HA	1:H:180:ASN:ND2	2.35	0.41
1:B:71:LEU:HD21	1:B:179:LEU:HD13	2.02	0.41
2:P:693:ARG:O	2:P:696:ARG:HG2	2.20	0.41
1:K:136:ILE:HG23	2:L:690:ASN:OD1	2.20	0.41
2:L:663:LEU:HG	2:L:667:MET:SD	2.59	0.41
2:N:634:SER:N	2:N:635:PRO:HD2	2.35	0.41
1:O:156:PHE:CE2	1:O:201:LEU:HA	2.56	0.41
1:O:160:ALA:HA	1:O:204:LEU:HD11	2.01	0.41
1:B:121:TRP:O	1:B:125:GLN:HG2	2.21	0.41
1:H:40:ASN:HA	1:H:43:MET:CG	2.48	0.41
1:M:121:TRP:O	1:M:125:GLN:HG2	2.20	0.41
1:F:121:TRP:O	1:F:125:GLN:HG2	2.20	0.41
1:H:41:LEU:CD2	1:H:185:HIS:ND1	2.84	0.41
1:K:57:VAL:HA	1:K:189:PHE:HZ	1.86	0.41
2:N:640:PHE:HZ	2:P:666:GLU:HB3	1.86	0.41
1:A:29:LEU:CB	1:A:30:LYS:HB2	2.49	0.41
1:B:59:VAL:HG22	2:C:696:ARG:HB2	2.03	0.41
2:C:690:ASN:O	2:C:694:LEU:HD13	2.21	0.41
1:F:67:GLN:HE21	2:G:645:HIS:CD2	2.39	0.41
1:F:157:ARG:NH2	3:F:301:CL:CL	2.86	0.41
1:K:84:CYS:HB3	1:K:111:ALA:HB2	2.02	0.41
1:K:159:TYR:OH	1:K:182:SER:OG	2.38	0.41
1:M:149:LYS:HG2	1:M:195:LEU:HB3	2.01	0.41
1:O:121:TRP:O	1:O:125:GLN:HG2	2.20	0.41
1:A:96:HIS:ND1	1:A:108:LYS:HA	2.35	0.41
2:E:656:ARG:HG2	2:E:688:GLU:OE2	2.21	0.41
1:A:202:ALA:HA	1:A:205:GLN:HG3	2.03	0.40
2:J:675:ASP:O	2:J:679:GLN:HG2	2.21	0.40
1:B:150:THR:HA	1:B:153:LYS:HE2	2.03	0.40
1:H:42:ARG:O	1:H:45:VAL:HG22	2.20	0.40
2:J:656:ARG:HG2	2:J:656:ARG:HH11	1.85	0.40
2:E:632:SER:C	2:E:633:TYR:HD2	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:67:GLN:CD	2:P:642:MET:HE1	2.45	0.40
1:H:29:LEU:C	1:H:29:LEU:CD1	2.86	0.40
1:H:178:HIS:HB3	2:I:642:MET:HG3	2.04	0.40
2:N:651:LYS:O	2:N:654:GLN:HG3	2.21	0.40
1:O:153:LYS:HD2	1:O:200:GLU:HG3	2.02	0.40
2:P:659:ARG:NH1	2:P:688:GLU:OE1	2.54	0.40
2:G:694:LEU:O	2:G:698:LYS:HG3	2.21	0.40
1:A:199:ARG:CZ	1:D:174:GLN:HB3	2.51	0.40
1:F:79:CYS:HA	1:F:166:HIS:CE1	2.57	0.40
1:H:25:GLN:N	1:H:25:GLN:CD	2.78	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	176/218 (81%)	162 (92%)	8 (4%)	6 (3%)	3	23
1	B	185/218 (85%)	177 (96%)	5 (3%)	3 (2%)	7	36
1	D	171/218 (78%)	166 (97%)	5 (3%)	0	100	100
1	F	177/218 (81%)	165 (93%)	12 (7%)	0	100	100
1	H	178/218 (82%)	169 (95%)	8 (4%)	1 (1%)	21	55
1	K	176/218 (81%)	170 (97%)	5 (3%)	1 (1%)	21	55
1	M	167/218 (77%)	160 (96%)	6 (4%)	1 (1%)	21	55
1	O	166/218 (76%)	160 (96%)	5 (3%)	1 (1%)	21	55
2	C	69/85 (81%)	66 (96%)	2 (3%)	1 (1%)	9	38
2	E	69/85 (81%)	67 (97%)	1 (1%)	1 (1%)	9	38
2	G	72/85 (85%)	68 (94%)	4 (6%)	0	100	100
2	I	70/85 (82%)	68 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	69/85 (81%)	65 (94%)	3 (4%)	1 (1%)	9	38
2	L	70/85 (82%)	69 (99%)	1 (1%)	0	100	100
2	N	63/85 (74%)	61 (97%)	0	2 (3%)	3	24
2	P	63/85 (74%)	60 (95%)	3 (5%)	0	100	100
All	All	1941/2424 (80%)	1853 (96%)	70 (4%)	18 (1%)	14	47

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	H	100	GLY
2	N	668	MET
2	N	669	ARG
1	A	30	LYS
1	A	98	ALA
2	J	632	SER
1	B	98	ALA
1	A	24	HIS
1	A	27	GLU
2	E	698	LYS
1	A	99	ASP
1	B	35	ASP
1	K	102	ASN
1	M	34	ALA
2	C	698	LYS
1	O	97	TRP
1	B	103	ILE

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	166/197 (84%)	161 (97%)	5 (3%)	36	60
1	B	170/197 (86%)	165 (97%)	5 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	163/197 (83%)	162 (99%)	1 (1%)	78	80
1	F	164/197 (83%)	160 (98%)	4 (2%)	43	64
1	H	167/197 (85%)	157 (94%)	10 (6%)	17	44
1	K	162/197 (82%)	161 (99%)	1 (1%)	78	80
1	M	159/197 (81%)	157 (99%)	2 (1%)	61	72
1	O	156/197 (79%)	155 (99%)	1 (1%)	78	80
2	C	66/80 (82%)	56 (85%)	10 (15%)	3	16
2	E	67/80 (84%)	65 (97%)	2 (3%)	36	60
2	G	69/80 (86%)	65 (94%)	4 (6%)	18	45
2	I	68/80 (85%)	62 (91%)	6 (9%)	9	33
2	J	66/80 (82%)	63 (96%)	3 (4%)	24	51
2	L	67/80 (84%)	62 (92%)	5 (8%)	12	38
2	N	60/80 (75%)	55 (92%)	5 (8%)	10	35
2	P	61/80 (76%)	57 (93%)	4 (7%)	15	42
All	All	1831/2216 (83%)	1763 (96%)	68 (4%)	30	56

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	31	HIS
1	A	33	GLU
1	A	41	LEU
1	A	42	ARG
2	J	669	ARG
2	J	694	LEU
2	J	699	MET
1	B	23	SER
1	B	24	HIS
1	B	28	LEU
1	B	41	LEU
1	B	75	ILE
2	C	631	GLN
2	C	636	GLN
2	C	660	LYS
2	C	663	LEU
2	C	664	GLU

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Mol	Chain	Res	Type
2	C	669	ARG
2	C	670	VAL
2	C	672	LEU
2	C	694	LEU
2	C	699	MET
1	D	40	ASN
2	E	664	GLU
2	E	694	LEU
1	F	28	LEU
1	F	31	HIS
1	F	42	ARG
1	F	43	MET
2	G	630	ILE
2	G	654	GLN
2	G	660	LYS
2	G	700	ASP
1	H	23	SER
1	H	24	HIS
1	H	25	GLN
1	H	28	LEU
1	H	29	LEU
1	H	30	LYS
1	H	31	HIS
1	H	41	LEU
1	H	43	MET
1	H	75	ILE
2	I	636	GLN
2	I	656	ARG
2	I	661	LYS
2	I	667	MET
2	I	694	LEU
2	I	699	MET
1	K	29	LEU
2	L	661	LYS
2	L	663	LEU
2	L	670	VAL
2	L	694	LEU
2	L	699	MET
1	M	31	HIS
1	M	75	ILE
2	N	640	PHE
2	N	656	ARG

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Mol	Chain	Res	Type
2	N	669	ARG
2	N	670	VAL
2	N	694	LEU
1	O	70	MET
2	P	642	MET
2	P	668	MET
2	P	670	VAL
2	P	699	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	143	ASN
1	A	178	HIS
1	A	180	ASN
2	J	645	HIS
2	J	658	HIS
1	B	123	GLN
1	B	165	GLN
2	C	653	HIS
1	D	165	GLN
1	D	178	HIS
2	E	679	GLN
1	F	40	ASN
1	F	194	ASN
2	G	654	GLN
2	G	658	HIS
2	G	679	GLN
1	H	165	GLN
2	I	636	GLN
2	L	636	GLN
2	L	677	GLN
1	M	67	GLN
2	N	644	GLN
2	N	662	GLN
1	O	123	GLN
1	O	165	GLN
2	P	662	GLN
2	P	686	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 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	182/218 (83%)	-0.36	0 100 100	28, 54, 108, 155	0
1	B	189/218 (86%)	-0.23	1 (0%) 87 66	41, 77, 135, 180	0
1	D	177/218 (81%)	-0.07	0 100 100	61, 98, 158, 174	0
1	F	183/218 (83%)	-0.15	4 (2%) 62 34	31, 59, 127, 219	0
1	H	184/218 (84%)	-0.12	1 (0%) 87 66	52, 93, 153, 180	0
1	K	180/218 (82%)	-0.07	0 100 100	40, 83, 131, 185	0
1	M	173/218 (79%)	0.25	3 (1%) 69 40	113, 175, 217, 241	0
1	O	170/218 (77%)	-0.01	0 100 100	119, 154, 190, 204	0
2	C	71/85 (83%)	-0.23	0 100 100	42, 75, 111, 129	0
2	E	71/85 (83%)	-0.04	0 100 100	75, 100, 133, 148	0
2	G	74/85 (87%)	-0.06	0 100 100	41, 70, 106, 122	0
2	I	72/85 (84%)	-0.07	0 100 100	46, 83, 117, 144	0
2	J	71/85 (83%)	-0.27	0 100 100	38, 62, 94, 131	0
2	L	72/85 (84%)	0.12	0 100 100	60, 98, 133, 146	0
2	N	65/85 (76%)	0.24	2 (3%) 51 28	104, 145, 177, 190	0
2	P	65/85 (76%)	0.14	0 100 100	125, 164, 202, 216	0
All	All	1999/2424 (82%)	-0.08	11 (0%) 85 63	28, 92, 183, 241	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	33	GLU	3.1
1	B	39	GLY	2.7
1	M	158	VAL	2.3
1	M	109	CYS	2.3
1	F	35	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	35	ASP	2.2
2	N	670	VAL	2.2
1	M	76	THR	2.2
1	F	36	LEU	2.1
1	F	32	ALA	2.1
2	N	634	SER	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 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(Å ²)	Q<0.9
3	CL	M	301	1/1	0.88	0.05	89,89,89,89	0
3	CL	D	301	1/1	0.90	0.08	75,75,75,75	0
3	CL	B	301	1/1	0.90	0.17	57,57,57,57	0
4	ZN	O	301	1/1	0.92	0.09	188,188,188,188	0
4	ZN	F	302	1/1	0.93	0.08	69,69,69,69	0
3	CL	A	301	1/1	0.93	0.21	40,40,40,40	0
4	ZN	D	302	1/1	0.95	0.06	104,104,104,104	0
3	CL	K	301	1/1	0.95	0.18	56,56,56,56	0
4	ZN	H	302	1/1	0.95	0.07	123,123,123,123	0
3	CL	H	301	1/1	0.95	0.12	54,54,54,54	0
3	CL	F	301	1/1	0.96	0.19	30,30,30,30	0
4	ZN	K	302	1/1	0.96	0.09	100,100,100,100	0
4	ZN	M	302	1/1	0.96	0.08	198,198,198,198	0
4	ZN	B	302	1/1	0.96	0.07	91,91,91,91	0
4	ZN	A	302	1/1	0.97	0.14	167,167,167,167	0

6.5 Other polymers [i](#)

There are no such residues in this entry.