



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:45 am GMT

PDB ID : 5B6B  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

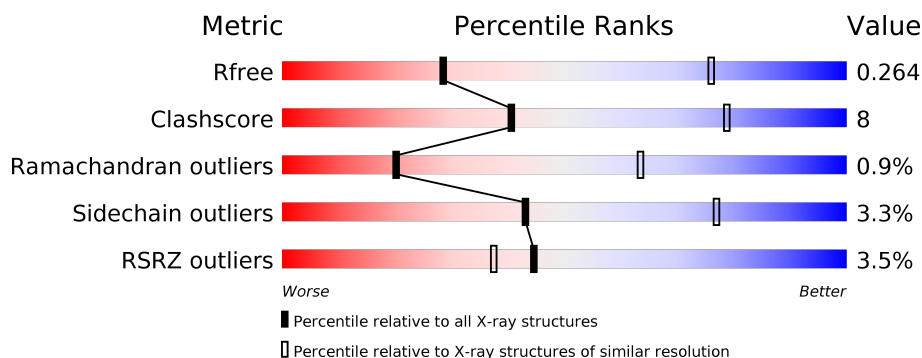
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1286 (3.68-3.40)
Clashscore	112137	1070 (3.66-3.42)
Ramachandran outliers	110173	1033 (3.66-3.42)
Sidechain outliers	110143	1033 (3.66-3.42)
RSRZ outliers	101464	1318 (3.68-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	218	
1	B	218	
1	D	218	
1	F	218	
1	H	218	
1	K	218	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
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

*Continued on next page...*

*Continued from previous page...*

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 (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Zn 1 1	0	0
4	K	1	Total Zn 1 1	0	0

*Continued on next page...*

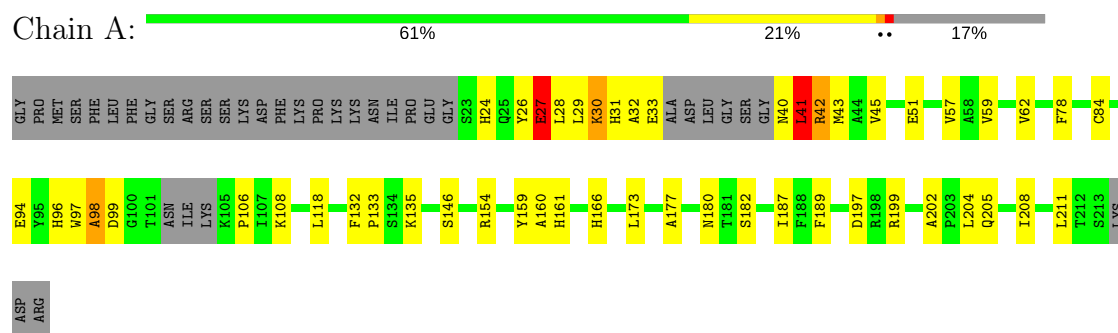
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Zn 1	0	0
4	B	1	Total 1	Zn 1	0	0
4	A	1	Total 1	Zn 1	0	0
4	O	1	Total 1	Zn 1	0	0
4	F	1	Total 1	Zn 1	0	0
4	M	1	Total 1	Zn 1	0	0

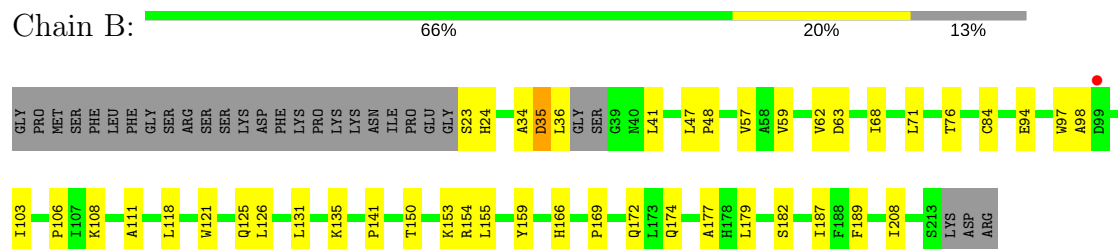
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

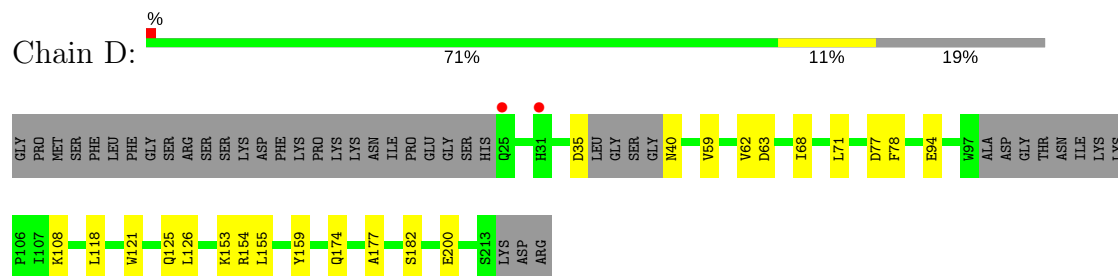
- Molecule 1: MOB kinase activator 1B



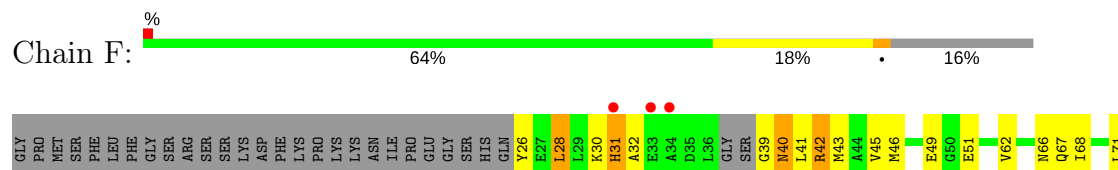
- Molecule 1: MOB kinase activator 1B



- Molecule 1: MOB kinase activator 1B



- Molecule 1: MOB kinase activator 1B







• Molecule 1: MOB kinase activator 1B

Chain H: 59% 22% 16%



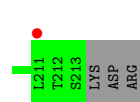
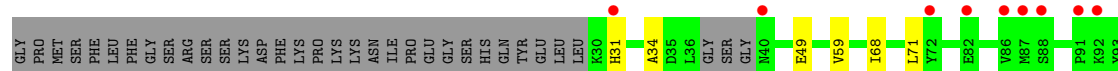
• Molecule 1: MOB kinase activator 1B

Chain K: 68% 14% 17%



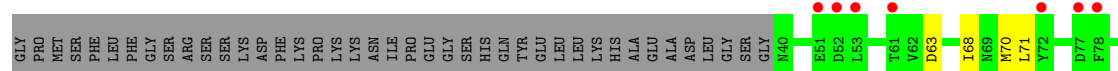
• Molecule 1: MOB kinase activator 1B

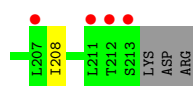
Chain M: 13% 67% 12% 21%



• Molecule 1: MOB kinase activator 1B

Chain O: 12% 63% 14% 22%





- Molecule 2: Serine/threonine-protein kinase LATS1

Chain J: 64% 16% 16%



- Molecule 2: Serine/threonine-protein kinase LATS1

Chain C: 61% 19% 16%



- Molecule 2: Serine/threonine-protein kinase LATS1

Chain E: 66% 15% 16%



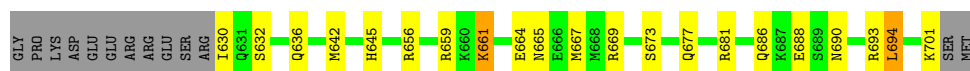
- Molecule 2: Serine/threonine-protein kinase LATS1

Chain G: 65% 19% 13%



- Molecule 2: Serine/threonine-protein kinase LATS1

Chain I: 60% 22% 15%



- Molecule 2: Serine/threonine-protein kinase LATS1

Chain L: 61% 22% 15%



- Molecule 2: Serine/threonine-protein kinase LATS1

Chain N: 4% 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, $\alpha$ , $\beta$ , $\gamma$	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) 95.3 (48.64-3.54)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.04 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.222 , 0.266 0.221 , 0.264	Depositor DCC
$R_{free}$ test set	1996 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	84.9	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 83.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 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 <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.31	0/1546	0.48	0/2097
1	B	0.24	0/1595	0.42	0/2163
1	D	0.23	0/1513	0.40	0/2051
1	F	0.30	0/1544	0.45	0/2095
1	H	0.29	0/1558	0.48	0/2112
1	K	0.27	0/1521	0.42	0/2065
1	M	0.22	0/1474	0.38	0/1998
1	O	0.22	0/1444	0.38	0/1960
2	C	0.26	0/607	0.53	0/802
2	E	0.26	0/611	0.42	0/806
2	G	0.27	0/631	0.44	0/834
2	I	0.27	0/619	0.45	0/817
2	J	0.26	0/608	0.49	0/804
2	L	0.26	0/616	0.42	0/815
2	N	0.28	0/555	0.50	0/734
2	P	0.26	0/560	0.43	0/736
All	All	0.26	0/17002	0.44	0/22889

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

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	40	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	44	0
1	K	1480	0	1425	23	0
1	M	1434	0	1392	17	0
1	O	1404	0	1361	18	0
2	C	599	0	602	12	0
2	E	603	0	613	10	0
2	G	623	0	631	15	0
2	I	611	0	624	15	0
2	J	600	0	607	15	0
2	L	608	0	613	10	0
2	N	548	0	554	11	0
2	P	554	0	571	12	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
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	270	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 8.

All (270) 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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:30:LYS:C	1:H:30:LYS:HD2	2.03	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:30:LYS:O	1:H:30:LYS:HD2	1.90	0.72
2:J:695:LYS:HA	2:J:699:MET:HB3	1.71	0.72
2:G:664:GLU:OE1	2:G:681:ARG:NH1	2.24	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:28:LEU:C	1:H:28:LEU:HD12	2.15	0.67
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:H:29:LEU:C	1:H:29:LEU:HD12	2.16	0.66
1:K:29:LEU:C	1:K:29:LEU:HD12	2.15	0.66
1:B:174:GLN:O	2:C:639:LYS:NZ	2.23	0.65
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:HE1	1:A:108:LYS:HG3	1.62	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:F:68:ILE:HD12	1:F:71:LEU:HD23	1.80	0.61
1:A:32:ALA:HB1	2:J:650:LEU:HD22	1.83	0.61
1:H:24:HIS:HB3	1:H:25:GLN:OE1	2.01	0.61
1:H:25:GLN:N	1:H:25:GLN:OE1	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:O:159:TYR:OH	1:O:182:SER:OG	2.16	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:OE2	1:K:27:GLU:HA	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
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:N:656:ARG:HG3	2:N:657:LEU:N	2.19	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
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
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:H:159:TYR:OH	1:H:182:SER:OG	2.25	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:A:159:TYR:OH	1:A:182:SER:OG	2.25	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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:26:TYR:C	1:H:26:TYR:CD2	2.85	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
1:B:35:ASP:CG	1:B:36:LEU:H	2.17	0.48
2:I:659:ARG:NH1	2:I:688:GLU:OE2	2.47	0.48
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:118:LEU:HD11	1:D:154:ARG:HB3	1.97	0.47
1:A:146:SER:HB3	1:F:49:GLU:OE1	2.15	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: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
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:N	1:D:77:ASP:OD1	2.45	0.46
1:F:76:THR:HG21	2:G:632:SER:HB2	1.98	0.46
2:L:630:ILE:O	2:L:631:GLN:HB2	2.16	0.46
1:F:71:LEU:HD21	1:F:179:LEU:HD13	1.98	0.46
2:J:639:LYS:O	2:J:643:GLU:HG3	2.16	0.46
1:A:135:LYS:O	2:J:693:ARG:NH1	2.41	0.45
2:C:660:LYS:HB3	2:C:660:LYS:HE2	1.85	0.45
1:F:131:LEU:HD13	1:F:147:VAL:HG21	1.98	0.45
1:D:159:TYR:OH	1:D:182:SER:OG	2.30	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: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
1:B:62:VAL:HG22	1:B:126:LEU:HD22	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HD11	1:B:154:ARG:HB3	1.99	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: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: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
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:B:174:GLN:HB2	2:C:639:LYS:HZ3	1.83	0.44
1:F:43:MET:HG2	1:F:43:MET:H	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:43:MET:HG2	1:H:43:MET:H	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:TRP:O	1:A:106:PRO:HA	2.19	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:H:160:ALA:HA	1:H:204:LEU:HD11	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:HA	2:E:650:LEU:HD23	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
1:B:76:THR:HG21	2:C:632:SER:HB3	2.02	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:M:49:GLU:HG2	2:N:660:LYS:HZ3	1.85	0.41
1:B:71:LEU:HD21	1:B:179:LEU:HD13	2.02	0.41
2:J:667:MET:HE1	2:J:680:MET:HB2	2.01	0.41
2:P:693:ARG:O	2:P:696:ARG:HG2	2.20	0.41
2:L:663:LEU:HG	2:L:667:MET:SD	2.59	0.41
1:K:136:ILE:HG23	2:L:690:ASN:OD1	2.20	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
1:M:135:LYS:HD3	2:P:701:LYS:HZ1	1.84	0.41
2:N:640:PHE:HZ	2:P:666:GLU:HB3	1.86	0.41
2:C:690:ASN:O	2:C:694:LEU:HD13	2.21	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:M:149:LYS:HG2	1:M:195:LEU:HB3	2.01	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:121:TRP:O	1:O:125:GLN:HG2	2.20	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
1:F:67:GLN:HE21	2:G:645:HIS:CD2	2.39	0.41
1:K:159:TYR:OH	1:K:182:SER:OG	2.38	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
1:B:150:THR:HA	1:B:153:LYS:HE2	2.03	0.40
1:F:31:HIS:HD1	1:F:176:GLU:CD	2.22	0.40
1:H:42:ARG:O	1:H:45:VAL:HG22	2.20	0.40
2:J:675:ASP:O	2:J:679:GLN:HG2	2.21	0.40
2:J:656:ARG:HH11	2:J:656:ARG:HG2	1.85	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
1:A:40:ASN:C	1:A:42:ARG:N	2.75	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

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	176/218 (81%)	162 (92%)	8 (4%)	6 (3%)	4	36
1	B	185/218 (85%)	177 (96%)	5 (3%)	3 (2%)	11	52
1	D	171/218 (78%)	166 (97%)	5 (3%)	0	100	100
1	F	177/218 (81%)	165 (93%)	12 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	178/218 (82%)	169 (95%)	8 (4%)	1 (1%)	28	70
1	K	176/218 (81%)	170 (97%)	5 (3%)	1 (1%)	28	70
1	M	167/218 (77%)	160 (96%)	6 (4%)	1 (1%)	28	70
1	O	166/218 (76%)	160 (96%)	5 (3%)	1 (1%)	28	70
2	C	69/85 (81%)	66 (96%)	2 (3%)	1 (1%)	13	55
2	E	69/85 (81%)	67 (97%)	1 (1%)	1 (1%)	13	55
2	G	72/85 (85%)	68 (94%)	4 (6%)	0	100	100
2	I	70/85 (82%)	68 (97%)	2 (3%)	0	100	100
2	J	69/85 (81%)	65 (94%)	3 (4%)	1 (1%)	13	55
2	L	70/85 (82%)	69 (99%)	1 (1%)	0	100	100
2	N	63/85 (74%)	61 (97%)	0	2 (3%)	5	37
2	P	63/85 (74%)	60 (95%)	3 (5%)	0	100	100
All	All	1941/2424 (80%)	1853 (96%)	70 (4%)	18 (1%)	20	63

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%)	46	79
1	B	170/197 (86%)	167 (98%)	3 (2%)	64	87
1	D	163/197 (83%)	162 (99%)	1 (1%)	89	96
1	F	164/197 (83%)	160 (98%)	4 (2%)	54	83
1	H	167/197 (85%)	158 (95%)	9 (5%)	26	64
1	K	162/197 (82%)	161 (99%)	1 (1%)	89	96
1	M	159/197 (81%)	158 (99%)	1 (1%)	89	96
1	O	156/197 (79%)	155 (99%)	1 (1%)	89	96
2	C	66/80 (82%)	59 (89%)	7 (11%)	8	38
2	E	67/80 (84%)	64 (96%)	3 (4%)	32	70
2	G	69/80 (86%)	65 (94%)	4 (6%)	23	62
2	I	68/80 (85%)	63 (93%)	5 (7%)	16	53
2	J	66/80 (82%)	62 (94%)	4 (6%)	22	61
2	L	67/80 (84%)	62 (92%)	5 (8%)	16	53
2	N	60/80 (75%)	55 (92%)	5 (8%)	13	48
2	P	61/80 (76%)	58 (95%)	3 (5%)	29	67
All	All	1831/2216 (83%)	1770 (97%)	61 (3%)	43	77

All (61) 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	636	GLN
2	J	669	ARG
2	J	694	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	J	699	MET
1	B	23	SER
1	B	24	HIS
1	B	41	LEU
2	C	631	GLN
2	C	636	GLN
2	C	660	LYS
2	C	663	LEU
2	C	669	ARG
2	C	670	VAL
2	C	672	LEU
1	D	40	ASN
2	E	656	ARG
2	E	664	GLU
2	E	694	LEU
1	F	28	LEU
1	F	31	HIS
1	F	40	ASN
1	F	42	ARG
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
2	I	636	GLN
2	I	656	ARG
2	I	661	LYS
2	I	669	ARG
2	I	694	LEU
1	K	29	LEU
2	L	653	HIS
2	L	661	LYS
2	L	663	LEU
2	L	670	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	L	694	LEU
1	M	31	HIS
2	N	640	PHE
2	N	656	ARG
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	F	40	ASN
1	O	67	GLN
2	P	662	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 carbohydrates 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

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	182/218 (83%)	-0.34	0 100 100	28, 54, 108, 155	0
1	B	189/218 (86%)	-0.17	1 (0%) 90 86	41, 77, 135, 180	0
1	D	177/218 (81%)	-0.08	2 (1%) 80 73	61, 98, 158, 174	0
1	F	183/218 (83%)	-0.09	3 (1%) 72 64	31, 59, 127, 219	0
1	H	184/218 (84%)	0.01	1 (0%) 90 86	52, 93, 153, 180	0
1	K	180/218 (82%)	-0.15	2 (1%) 80 73	40, 83, 131, 185	0
1	M	173/218 (79%)	0.99	29 (16%) 2 2	113, 175, 217, 241	0
1	O	170/218 (77%)	1.08	26 (15%) 2 3	119, 154, 190, 204	0
2	C	71/85 (83%)	-0.28	0 100 100	42, 75, 111, 129	0
2	E	71/85 (83%)	-0.07	0 100 100	75, 100, 133, 148	0
2	G	74/85 (87%)	-0.31	0 100 100	41, 70, 106, 122	0
2	I	72/85 (84%)	-0.31	0 100 100	46, 83, 117, 144	0
2	J	71/85 (83%)	-0.39	0 100 100	38, 62, 94, 131	0
2	L	72/85 (84%)	-0.15	0 100 100	60, 98, 133, 146	0
2	N	65/85 (76%)	0.21	3 (4%) 33 27	104, 145, 177, 190	0
2	P	65/85 (76%)	0.29	2 (3%) 49 41	125, 164, 202, 216	0
All	All	1999/2424 (82%)	0.06	69 (3%) 44 37	28, 92, 183, 241	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	33	GLU	9.6
1	F	34	ALA	6.5
1	M	113	LYS	6.4
1	F	31	HIS	5.1
1	M	107	ILE	5.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	M	109	CYS	4.8
1	M	112	PRO	4.6
1	M	91	PRO	4.1
1	M	110	SER	3.9
1	O	61	THR	3.8
1	M	31	HIS	3.8
1	M	40	ASN	3.6
1	O	193	PHE	3.6
1	M	114	TYR	3.5
1	M	115	ILE	3.4
1	M	87	MET	3.4
1	M	72	TYR	3.4
1	K	102	ASN	3.2
1	O	97	TRP	3.2
1	K	101	THR	3.2
1	M	211	LEU	3.0
1	M	94	GLU	3.0
1	M	156	PHE	2.9
1	O	77	ASP	2.9
1	D	25	GLN	2.9
1	M	96	HIS	2.9
1	M	108	LYS	2.9
1	O	213	SER	2.9
1	O	199	ARG	2.8
1	O	195	LEU	2.8
1	O	207	LEU	2.8
1	O	201	LEU	2.8
1	O	155	LEU	2.7
1	O	52	ASP	2.6
1	O	200	GLU	2.5
1	O	72	TYR	2.5
2	N	675	ASP	2.5
1	O	53	LEU	2.5
1	M	88	SER	2.4
1	O	96	HIS	2.4
1	M	92	LYS	2.4
1	M	86	VAL	2.4
1	O	189	PHE	2.4
1	O	211	LEU	2.3
1	O	94	GLU	2.3
1	M	180	ASN	2.3
1	O	202	ALA	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	112	PRO	2.3
2	N	676	ALA	2.2
1	M	97	TRP	2.2
1	M	82	GLU	2.2
1	D	31	HIS	2.2
1	O	51	GLU	2.2
1	O	204	LEU	2.2
2	P	701	LYS	2.2
2	N	678	ASP	2.1
1	O	78	PHE	2.1
1	B	99	ASP	2.1
1	M	106	PRO	2.1
1	M	176	GLU	2.1
1	M	154	ARG	2.1
1	O	158	VAL	2.1
1	O	187	ILE	2.1
1	M	158	VAL	2.1
1	O	212	THR	2.1
1	M	160	ALA	2.0
1	O	109	CYS	2.0
1	M	95	TYR	2.0
2	P	692	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	A	302	1/1	0.99	0.25	1.47	167,167,167,167	0
4	ZN	K	302	1/1	0.96	0.20	0.25	100,100,100,100	0
4	ZN	H	302	1/1	0.95	0.10	-1.32	123,123,123,123	0
4	ZN	D	302	1/1	0.91	0.12	-1.60	104,104,104,104	0
4	ZN	F	302	1/1	0.95	0.15	-1.68	69,69,69,69	0
4	ZN	M	302	1/1	0.95	0.12	-1.88	198,198,198,198	0
4	ZN	B	302	1/1	0.92	0.14	-1.90	91,91,91,91	0
4	ZN	O	301	1/1	0.74	0.11	-2.92	188,188,188,188	0
3	CL	M	301	1/1	0.93	0.09	-	89,89,89,89	0
3	CL	K	301	1/1	0.87	0.56	-	56,56,56,56	0
3	CL	H	301	1/1	0.91	0.31	-	54,54,54,54	0
3	CL	F	301	1/1	0.97	0.56	-	30,30,30,30	0
3	CL	D	301	1/1	0.81	0.33	-	75,75,75,75	0
3	CL	B	301	1/1	0.95	0.34	-	57,57,57,57	0
3	CL	A	301	1/1	0.94	0.57	-	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.