



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2017 – 12:40 PM EDT

PDB ID : 5BRM  
Title : Structural basis for Mob1-dependent activation of the core Mst-Lats kinase cascade in Hippo signaling  
Authors : Luo, X.; Ni, L.  
Deposited on : unknown  
Resolution : 2.65 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
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
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)	:	rb-20029824

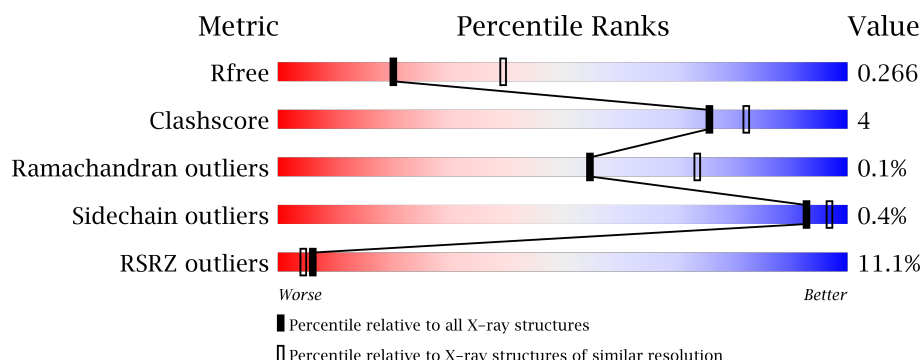
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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	177	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>13%</div> </div> </div>
1	B	177	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>11%</div> </div> </div>
1	C	177	<div> <div>11%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>10%</div> </div> </div>
1	D	177	<div> <div>11%</div> <div> <div></div> <div>72%</div> <div>9%</div> <div>19%</div> </div> </div>
1	E	177	<div> <div>11%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>10%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	177	
2	G	31	
2	H	31	
2	I	31	
2	J	31	
2	K	31	
2	L	31	
2	M	31	
2	N	31	
2	O	31	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17464 atoms, of which 8552 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 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	154	Total	C	H	N	O	S	0	0	0
			2538	842	1247	209	232	8			
1	B	158	Total	C	H	N	O	S	0	0	0
			2586	857	1271	213	237	8			
1	C	160	Total	C	H	N	O	S	0	0	0
			2629	869	1297	216	239	8			
1	D	144	Total	C	H	N	O	S	0	0	0
			2384	796	1166	196	218	8			
1	E	160	Total	C	H	N	O	S	0	0	0
			2628	869	1296	216	239	8			
1	F	160	Total	C	H	N	O	S	0	0	0
			2628	869	1296	216	239	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	GLY	-	expression tag	UNP Q9H8S9
B	40	GLY	-	expression tag	UNP Q9H8S9
C	40	GLY	-	expression tag	UNP Q9H8S9
D	40	GLY	-	expression tag	UNP Q9H8S9
E	40	GLY	-	expression tag	UNP Q9H8S9
F	40	GLY	-	expression tag	UNP Q9H8S9

- Molecule 2 is a protein called Serine/threonine-protein kinase 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	22	Total	C	H	N	O	P	S	0	0
			350	111	167	32	37	1	2		
2	H	17	Total	C	H	N	O	P	S	0	0
			288	92	137	27	29	1	2		
2	I	12	Total	C	H	N	O	P	S	0	0
			207	69	97	16	22	1	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	J	13	Total	C	H	N	O	P	S	0	0	0
			220	73	102	18	24	1	2			
2	K	11	Total	C	H	N	O	P	S	0	0	0
			183	63	84	12	21	1	2			
2	L	12	Total	C	H	N	O	P	S	0	0	0
			208	69	98	17	21	1	2			
2	M	17	Total	C	H	N	O	S		0	0	0
			277	87	136	27	26	1				
2	N	12	Total	C	H	N	O	S		0	0	0
			193	64	92	17	19	1				
2	O	8	Total	C	H	N	O			0	0	0
			133	43	66	13	11					

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

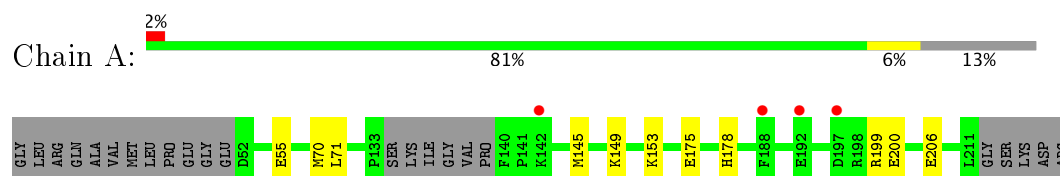
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	F	3	Total	O	0	0
			3	3		

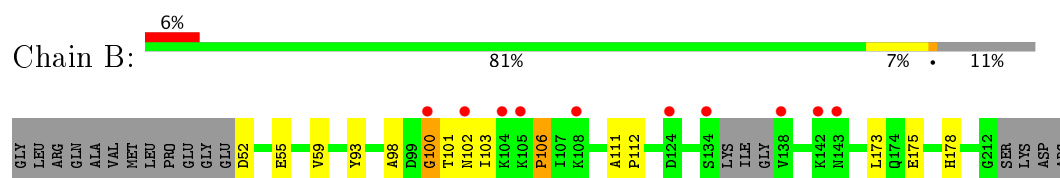
### 3 Residue-property plots [i](#)

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.

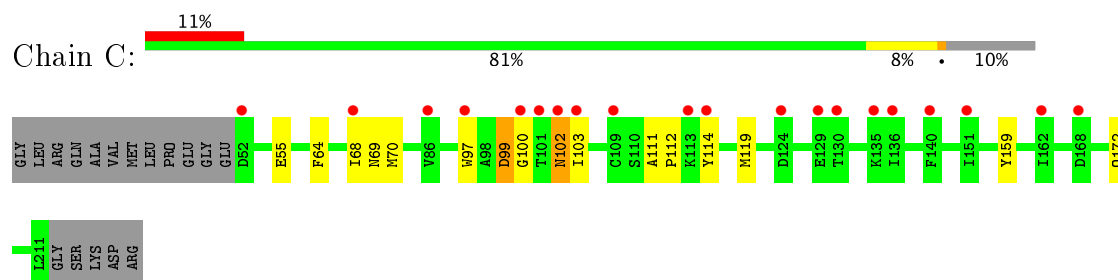
- Molecule 1: MOB kinase activator 1A



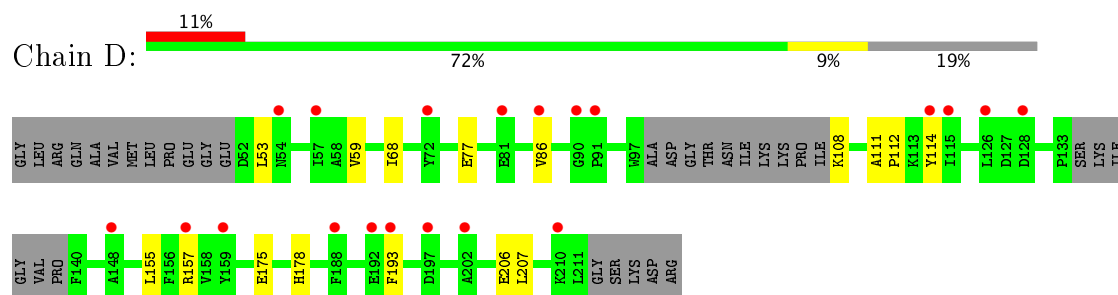
- Molecule 1: MOB kinase activator 1A



- Molecule 1: MOB kinase activator 1A

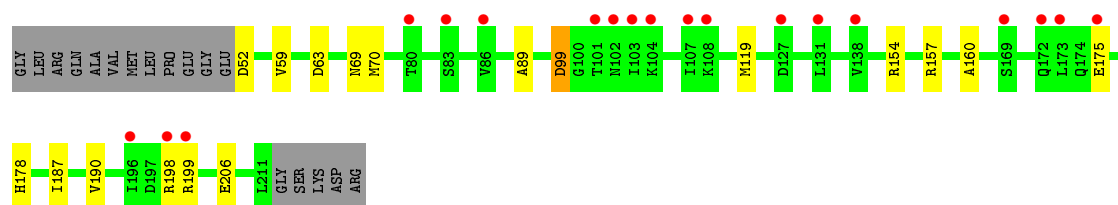


- Molecule 1: MOB kinase activator 1A

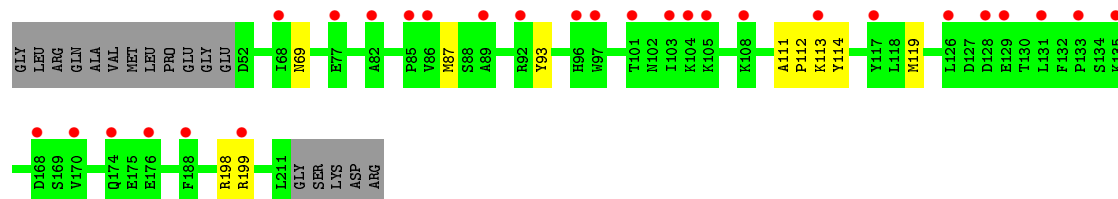
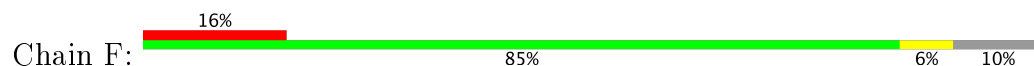


- Molecule 1: MOB kinase activator 1A

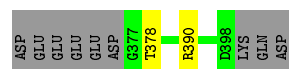




- Molecule 1: MOB kinase activator 1A



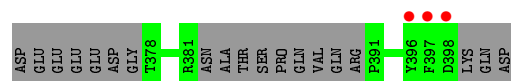
- Molecule 2: Serine/threonine-protein kinase 3



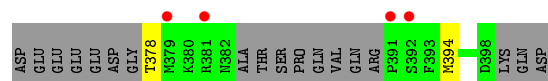
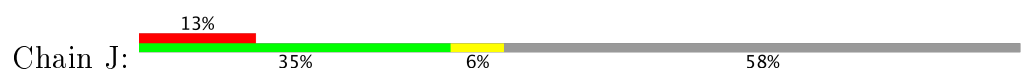
- Molecule 2: Serine/threonine-protein kinase 3



- Molecule 2: Serine/threonine-protein kinase 3

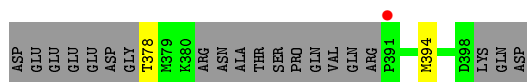


- Molecule 2: Serine/threonine-protein kinase 3

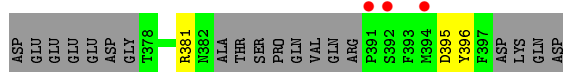


- Molecule 2: Serine/threonine-protein kinase 3

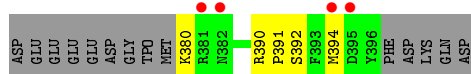




- Molecule 2: Serine/threonine-protein kinase 3



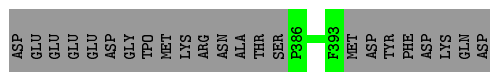
- Molecule 2: Serine/threonine-protein kinase 3



- Molecule 2: Serine/threonine-protein kinase 3



- Molecule 2: Serine/threonine-protein kinase 3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.19Å 142.19Å 135.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.30 – 2.65 39.29 – 2.65	Depositor EDS
% Data completeness (in resolution range)	89.3 (39.30-2.65) 89.3 (39.29-2.65)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.96 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.244 , 0.268 0.243 , 0.266	Depositor DCC
$R_{free}$ test set	2003 reflections (4.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 26.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.067 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	17464	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.26	0/1328	0.47	0/1800
1	B	0.26	0/1353	0.51	1/1835 (0.1%)
1	C	0.26	0/1371	0.46	0/1860
1	D	0.30	0/1253	0.46	0/1697
1	E	0.26	0/1371	0.49	0/1860
1	F	0.29	0/1371	0.49	0/1860
2	G	0.30	0/175	0.43	0/232
2	H	0.31	0/141	0.37	0/181
2	I	0.31	0/101	0.48	0/130
2	J	0.32	0/109	0.53	0/141
2	K	0.35	0/90	0.50	0/116
2	L	0.33	0/101	0.46	0/130
2	M	0.25	0/144	0.55	0/193
2	N	0.25	0/104	0.47	0/140
2	O	0.21	0/69	0.40	0/92
All	All	0.27	0/9081	0.48	1/12267 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	100	GLY	N-CA-C	-6.09	97.87	113.10

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	1291	1247	1247	7	0
1	B	1315	1271	1271	10	0
1	C	1332	1297	1296	10	0
1	D	1218	1166	1166	15	0
1	E	1332	1296	1296	14	0
1	F	1332	1296	1296	9	0
2	G	183	167	167	2	0
2	H	151	137	138	2	0
2	I	110	97	98	0	0
2	J	118	102	104	3	0
2	K	99	84	85	3	0
2	L	110	98	100	2	0
2	M	141	136	136	4	0
2	N	101	92	92	1	0
2	O	67	66	66	0	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	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	F	3	0	0	0	0
All	All	8912	8552	8558	63	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (63) 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:B:52:ASP:N	1:B:55:GLU:OE2	2.18	0.76
1:E:99:ASP:OD2	2:K:378:TPO:O2P	2.05	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:NH2	1:A:200:GLU:OE2	2.25	0.69
1:E:69:ASN:ND2	1:E:119:MET:SD	2.65	0.69
1:E:175:GLU:OE1	1:E:178:HIS:ND1	2.25	0.68
1:D:77:GLU:OE2	2:L:381:ARG:NH1	2.27	0.68
1:A:153:LYS:NZ	2:G:378:TPO:O3P	2.29	0.65
1:F:69:ASN:ND2	1:F:119:MET:SD	2.71	0.63
1:D:114:TYR:OH	1:D:157:ARG:NH1	2.32	0.62
1:B:175:GLU:OE1	1:B:178:HIS:ND1	2.33	0.61
1:A:175:GLU:OE1	1:A:178:HIS:ND1	2.34	0.61
1:C:99:ASP:N	1:C:100:GLY:HA2	2.16	0.60
1:B:101:THR:OG1	1:B:102:ASN:N	2.33	0.60
1:B:173:LEU:HA	1:E:198:ARG:HD3	1.84	0.59
1:E:206:GLU:HB2	2:K:394:MET:HE2	1.86	0.56
1:E:99:ASP:OD2	1:E:154:ARG:NH2	2.39	0.56
1:D:86:VAL:HB	1:D:108:LYS:CE	2.35	0.55
1:D:175:GLU:OE1	1:D:178:HIS:ND1	2.39	0.55
1:D:207:LEU:HB2	2:J:394:MET:HE2	1.91	0.52
1:A:206:GLU:OE2	2:G:390:ARG:NH2	2.42	0.52
1:B:93:TYR:OH	2:H:381:ARG:NH2	2.43	0.51
1:D:175:GLU:HG3	1:F:198:ARG:HH12	1.76	0.51
2:N:385:SER:N	2:N:386:PRO:CD	2.74	0.50
1:A:55:GLU:N	1:A:55:GLU:OE1	2.42	0.50
1:A:70:MET:HE3	1:A:71:LEU:HG	1.94	0.50
1:C:69:ASN:ND2	1:C:119:MET:SD	2.85	0.50
1:D:53:LEU:CD1	1:D:193:PHE:CZ	2.96	0.49
1:D:175:GLU:CG	1:F:198:ARG:HH12	2.27	0.48
1:B:59:VAL:HG11	1:C:70:MET:HB2	1.96	0.48
1:D:86:VAL:HB	1:D:108:LYS:HE3	1.96	0.48
1:D:111:ALA:HB3	1:D:112:PRO:HD3	1.96	0.47
1:B:111:ALA:HB3	1:B:112:PRO:HD3	1.97	0.47
1:D:206:GLU:HB2	2:J:394:MET:HE1	1.96	0.47
1:F:87:MET:HE2	1:F:114:TYR:HB3	1.96	0.47
2:M:392:SER:OG	2:M:394:MET:O	2.31	0.47
1:C:97:TRP:HB2	1:C:114:TYR:CD2	2.50	0.47
1:D:77:GLU:OE2	1:F:93:TYR:OH	2.25	0.46
2:M:390:ARG:CG	2:M:391:PRO:HD2	2.46	0.46
2:M:390:ARG:HG3	2:M:391:PRO:HD2	1.97	0.46
1:F:198:ARG:HG3	1:F:199:ARG:N	2.32	0.45
1:E:157:ARG:NH2	2:K:378:TPO:O3P	2.39	0.44
1:E:187:ILE:HA	1:E:190:VAL:HG22	1.98	0.44
1:E:59:VAL:O	1:E:63:ASP:N	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:395:ASP:OD1	2:L:396:TYR:N	2.50	0.44
1:F:111:ALA:HB3	1:F:112:PRO:HD3	2.01	0.43
1:C:68:ILE:HD11	1:C:159:TYR:CE2	2.53	0.43
1:E:89:ALA:HB1	1:E:160:ALA:HB1	1.99	0.43
1:D:59:VAL:HG21	1:E:70:MET:HB2	2.00	0.42
1:B:100:GLY:HA3	1:B:103:ILE:HD11	2.01	0.42
1:C:64:PHE:O	1:C:68:ILE:HG12	2.19	0.42
1:D:157:ARG:HH22	2:J:378:TPO:P	2.42	0.42
1:F:113:LYS:HE3	2:M:380:LYS:HE2	2.01	0.42
1:C:111:ALA:HB3	1:C:112:PRO:HD3	2.00	0.42
1:C:102:ASN:C	1:C:103:ILE:HG13	2.40	0.42
1:E:52:ASP:N	1:F:198:ARG:HE	2.18	0.42
2:H:390:ARG:NH1	2:H:398:ASP:OD2	2.45	0.42
1:B:98:ALA:HB1	1:B:103:ILE:HD12	2.01	0.41
1:E:99:ASP:HB2	1:E:154:ARG:HH22	1.85	0.41
1:C:55:GLU:OE1	1:E:199:ARG:NH2	2.51	0.41
1:D:68:ILE:CD1	1:D:155:LEU:HB3	2.51	0.41
1:B:98:ALA:HB2	1:B:106:PRO:HB3	2.01	0.41
1:A:145:MET:HG3	1:A:149:LYS:HE3	2.01	0.41
1:C:100:GLY:HA2	1:C:103:ILE:O	2.22	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	150/177 (85%)	146 (97%)	4 (3%)	0	100	100
1	B	154/177 (87%)	148 (96%)	5 (3%)	1 (1%)	28	43
1	C	158/177 (89%)	156 (99%)	2 (1%)	0	100	100
1	D	138/177 (78%)	137 (99%)	1 (1%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	158/177 (89%)	153 (97%)	5 (3%)	0	100	100
1	F	158/177 (89%)	154 (98%)	4 (2%)	0	100	100
2	G	19/31 (61%)	18 (95%)	1 (5%)	0	100	100
2	H	12/31 (39%)	12 (100%)	0	0	100	100
2	I	8/31 (26%)	7 (88%)	1 (12%)	0	100	100
2	J	9/31 (29%)	8 (89%)	1 (11%)	0	100	100
2	K	7/31 (23%)	5 (71%)	2 (29%)	0	100	100
2	L	8/31 (26%)	7 (88%)	1 (12%)	0	100	100
2	M	15/31 (48%)	14 (93%)	1 (7%)	0	100	100
2	N	10/31 (32%)	10 (100%)	0	0	100	100
2	O	6/31 (19%)	6 (100%)	0	0	100	100
All	All	1010/1341 (75%)	981 (97%)	28 (3%)	1 (0%)	55	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	106	PRO

### 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	142/160 (89%)	142 (100%)	0	100	100
1	B	145/160 (91%)	145 (100%)	0	100	100
1	C	147/160 (92%)	144 (98%)	3 (2%)	60	80
1	D	134/160 (84%)	134 (100%)	0	100	100
1	E	147/160 (92%)	146 (99%)	1 (1%)	87	94
1	F	147/160 (92%)	147 (100%)	0	100	100
2	G	19/28 (68%)	19 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	15/28 (54%)	15 (100%)	0	100	100
2	I	11/28 (39%)	11 (100%)	0	100	100
2	J	12/28 (43%)	12 (100%)	0	100	100
2	K	10/28 (36%)	10 (100%)	0	100	100
2	L	11/28 (39%)	11 (100%)	0	100	100
2	M	16/28 (57%)	16 (100%)	0	100	100
2	N	12/28 (43%)	12 (100%)	0	100	100
2	O	8/28 (29%)	8 (100%)	0	100	100
All	All	976/1212 (80%)	972 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	99	ASP
1	C	102	ASN
1	C	172	GLN
1	E	99	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	TPO	G	378	2	9,10,11	1.21	1 (11%)	10,14,16	1.17	1 (10%)
2	TPO	H	378	2	9,10,11	1.27	1 (11%)	10,14,16	1.27	2 (20%)
2	TPO	I	378	2	9,10,11	1.30	1 (11%)	10,14,16	0.94	0
2	TPO	J	378	2	9,10,11	1.29	1 (11%)	10,14,16	1.31	1 (10%)
2	TPO	K	378	2	9,10,11	1.13	0	10,14,16	1.09	1 (10%)
2	TPO	L	378	2	9,10,11	1.20	0	10,14,16	0.83	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	TPO	G	378	2	-	0/8/11/13	0/0/0/0
2	TPO	H	378	2	-	0/8/11/13	0/0/0/0
2	TPO	I	378	2	-	1/8/11/13	0/0/0/0
2	TPO	J	378	2	-	0/8/11/13	0/0/0/0
2	TPO	K	378	2	-	0/8/11/13	0/0/0/0
2	TPO	L	378	2	-	1/8/11/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	378	TPO	CA-C	2.04	1.52	1.50
2	H	378	TPO	CA-C	2.19	1.53	1.50
2	I	378	TPO	CA-C	2.19	1.53	1.50
2	J	378	TPO	CA-C	2.26	1.53	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	378	TPO	CG2-CB-CA	-3.39	106.92	113.22
2	H	378	TPO	CG2-CB-CA	-3.10	107.45	113.22
2	G	378	TPO	CG2-CB-CA	-2.68	108.23	113.22
2	K	378	TPO	O-C-CA	-2.46	119.41	125.15
2	H	378	TPO	O-C-CA	-2.01	120.45	125.15

There are no chirality outliers.

All (2) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	I	378	TPO	OG1-CB-CA-N
2	L	378	TPO	OG1-CB-CA-N

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	378	TPO	1	0
2	J	378	TPO	1	0
2	K	378	TPO	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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, 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	154/177 (87%)	0.49	4 (2%) 56 55	13, 26, 58, 100	0
1	B	158/177 (89%)	0.67	10 (6%) 21 19	14, 31, 80, 109	0
1	C	160/177 (90%)	0.82	20 (12%) 4 3	20, 49, 87, 105	0
1	D	144/177 (81%)	0.95	20 (13%) 3 2	40, 61, 104, 122	0
1	E	160/177 (90%)	0.87	19 (11%) 5 3	26, 50, 98, 128	0
1	F	160/177 (90%)	1.01	28 (17%) 2 1	24, 60, 108, 126	0
2	G	21/31 (67%)	0.61	0 100 100	24, 39, 53, 76	0
2	H	16/31 (51%)	0.74	0 100 100	33, 53, 80, 101	0
2	I	11/31 (35%)	0.81	3 (27%) 1 0	46, 63, 87, 96	0
2	J	12/31 (38%)	1.74	4 (33%) 0 0	70, 86, 119, 130	0
2	K	10/31 (32%)	0.93	1 (10%) 8 6	54, 73, 95, 97	0
2	L	11/31 (35%)	1.30	3 (27%) 1 0	73, 87, 97, 98	0
2	M	17/31 (54%)	1.00	4 (23%) 1 1	31, 60, 98, 129	0
2	N	12/31 (38%)	0.85	1 (8%) 12 10	36, 42, 67, 77	0
2	O	8/31 (25%)	0.81	0 100 100	51, 65, 75, 91	0
All	All	1054/1341 (78%)	0.82	117 (11%) 6 4	13, 49, 96, 130	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	104	LYS	7.3
1	D	91	PRO	6.3
1	F	86	VAL	6.2
1	F	113	LYS	5.6
1	E	107	ILE	4.9
1	E	172	GLN	4.7
1	B	138	VAL	4.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	103	ILE	4.2
2	J	391	PRO	4.2
1	E	108	LYS	4.2
1	F	103	ILE	4.2
1	D	192	GLU	4.0
1	F	131	LEU	3.9
1	F	101	THR	3.9
1	E	138	VAL	3.8
1	B	102	ASN	3.8
2	M	381	ARG	3.8
2	J	381	ARG	3.7
1	E	175	GLU	3.7
1	F	92	ARG	3.7
1	B	105	LYS	3.6
2	K	391	PRO	3.5
1	C	109	CYS	3.5
1	B	100	GLY	3.3
1	B	124	ASP	3.3
2	M	394	MET	3.3
1	D	188	PHE	3.2
1	E	83	SER	3.2
1	E	199	ARG	3.2
1	F	133	PRO	3.1
1	F	129	GLU	3.1
1	C	151	ILE	3.1
1	F	170	VAL	3.0
1	F	168	ASP	3.0
1	C	129	GLU	3.0
1	E	101	THR	3.0
1	F	77	GLU	3.0
1	C	135	LYS	3.0
1	F	105	LYS	2.9
1	A	188	PHE	2.9
1	C	114	TYR	2.9
1	C	168	ASP	2.9
1	B	108	LYS	2.9
1	D	126	LEU	2.9
1	E	104	LYS	2.9
1	A	197	ASP	2.8
1	D	90	GLY	2.8
1	C	124	ASP	2.8
1	C	100	GLY	2.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	101	THR	2.8
1	D	72	TYR	2.7
1	B	134	SER	2.7
1	F	135	LYS	2.7
1	D	193	PHE	2.7
1	F	176	GLU	2.7
1	C	52	ASP	2.7
1	D	202	ALA	2.7
1	C	86	VAL	2.7
1	E	169	SER	2.7
1	E	196	ILE	2.6
1	C	130	THR	2.6
1	E	86	VAL	2.6
1	D	210	LYS	2.5
1	E	127	ASP	2.5
1	D	157	ARG	2.5
1	E	198	ARG	2.5
1	F	126	LEU	2.5
1	D	128	ASP	2.5
1	D	148	ALA	2.5
1	D	159	TYR	2.5
1	F	68	ILE	2.5
2	J	392	SER	2.5
1	B	143	ASN	2.5
2	M	382	ASN	2.5
1	E	173	LEU	2.5
2	L	394	MET	2.5
2	L	391	PRO	2.4
1	D	197	ASP	2.4
1	F	96	HIS	2.4
1	C	113	LYS	2.3
2	I	397	PHE	2.3
1	D	114	TYR	2.3
1	E	80	THR	2.3
1	D	86	VAL	2.3
1	F	199	ARG	2.3
1	F	174	GLN	2.3
1	F	85	PRO	2.3
1	E	131	LEU	2.3
2	L	392	SER	2.3
1	A	142	LYS	2.3
1	F	128	ASP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	192	GLU	2.2
1	F	89	ALA	2.2
1	C	136	ILE	2.2
1	F	117	TYR	2.2
1	F	188	PHE	2.2
1	B	104	LYS	2.2
2	I	396	TYR	2.2
1	C	68	ILE	2.2
1	F	108	LYS	2.2
1	C	162	ILE	2.1
1	D	81	GLU	2.1
1	F	97	TRP	2.1
1	D	57	ILE	2.1
1	C	140	PHE	2.1
1	D	54	ASN	2.1
1	D	115	ILE	2.1
1	C	103	ILE	2.1
1	B	142	LYS	2.1
1	E	102	ASN	2.1
2	J	379	MET	2.1
2	M	395	ASP	2.1
1	F	82	ALA	2.1
2	I	398	ASP	2.1
1	C	102	ASN	2.0
1	C	97	TRP	2.0
2	N	390	ARG	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	TPO	K	378	11/12	0.91	0.14	-	10,32,43,44	0
2	TPO	I	378	11/12	0.88	0.22	-	25,55,83,84	0
2	TPO	H	378	11/12	0.97	0.15	-	25,34,45,47	0
2	TPO	G	378	11/12	0.94	0.21	-	23,28,31,33	0
2	TPO	L	378	11/12	0.85	0.23	-	21,72,102,102	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TPO	J	378	11/12	0.81	0.22	-	18,59,77,84	0

### 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
3	ZN	B	301	1/1	1.00	0.19	0.29	14,14,14,14	0
3	ZN	A	301	1/1	1.00	0.20	0.07	14,14,14,14	0
3	ZN	E	301	1/1	0.97	0.18	-0.81	41,41,41,41	0
3	ZN	F	301	1/1	0.98	0.14	-1.26	77,77,77,77	0
3	ZN	C	301	1/1	0.95	0.14	-1.85	49,49,49,49	0
3	ZN	D	301	1/1	0.95	0.14	-1.86	39,39,39,39	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.