



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 29, 2016 – 02:07 PM EDT

PDB ID : 5B5V  
Title : Structure of full-length MOB1b  
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Deposited on : 2016-05-24  
Resolution : 2.19 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.

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20027790

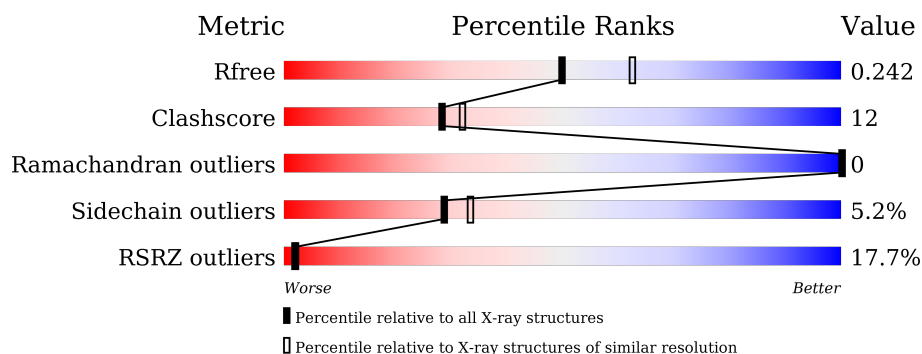
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	<div> <div>17%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>14%</div> </div> </div>
1	B	218	<div> <div>13%</div> <div> <div></div> <div>61%</div> <div>22%</div> <div>16%</div> </div> </div>
1	C	218	<div> <div>17%</div> <div> <div></div> <div>66%</div> <div>20%</div> <div>14%</div> </div> </div>
1	D	218	<div> <div>11%</div> <div> <div></div> <div>62%</div> <div>18%</div> <div>18%</div> </div> </div>
1	E	218	<div> <div>0%</div> <div> <div></div> <div>96%</div> </div> </div>
1	F	218	<div> <div>2%</div> <div> <div></div> <div>96%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6325 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	187	Total	C	N	O	S	0	0	0
			1533	995	248	281	9			
1	B	183	Total	C	N	O	S	0	0	0
			1505	975	243	278	9			
1	C	187	Total	C	N	O	S	0	0	0
			1533	995	248	281	9			
1	D	179	Total	C	N	O	S	0	0	0
			1473	956	239	269	9			
1	E	8	Total	C	N	O		0	0	0
			63	41	11	11				
1	F	8	Total	C	N	O		0	0	0
			63	41	11	11				

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8BPB0
A	0	PRO	-	expression tag	UNP Q8BPB0
B	-1	GLY	-	expression tag	UNP Q8BPB0
B	0	PRO	-	expression tag	UNP Q8BPB0
C	-1	GLY	-	expression tag	UNP Q8BPB0
C	0	PRO	-	expression tag	UNP Q8BPB0
D	-1	GLY	-	expression tag	UNP Q8BPB0
D	0	PRO	-	expression tag	UNP Q8BPB0
E	-1	GLY	-	expression tag	UNP Q8BPB0
E	0	PRO	-	expression tag	UNP Q8BPB0
F	-1	GLY	-	expression tag	UNP Q8BPB0
F	0	PRO	-	expression tag	UNP Q8BPB0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

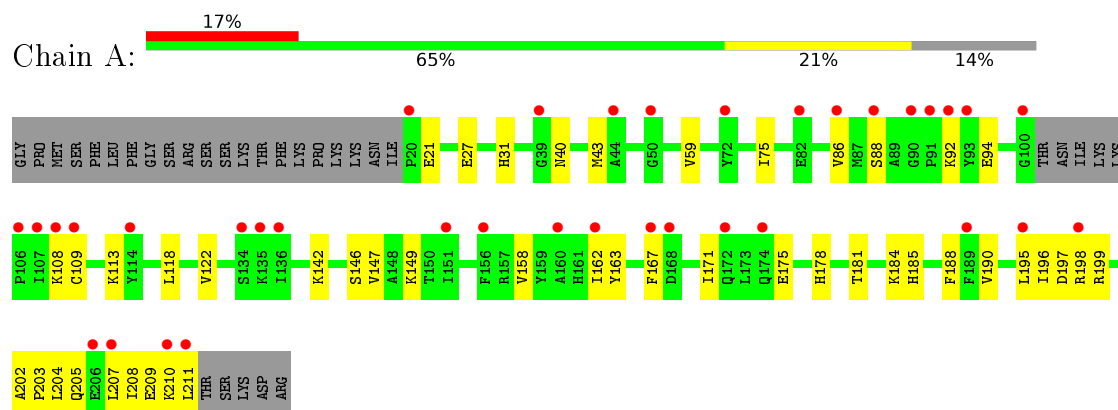
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	30	Total O 30 30	0	0
4	B	47	Total O 47 47	0	0
4	C	34	Total O 34 34	0	0
4	D	38	Total O 38 38	0	0

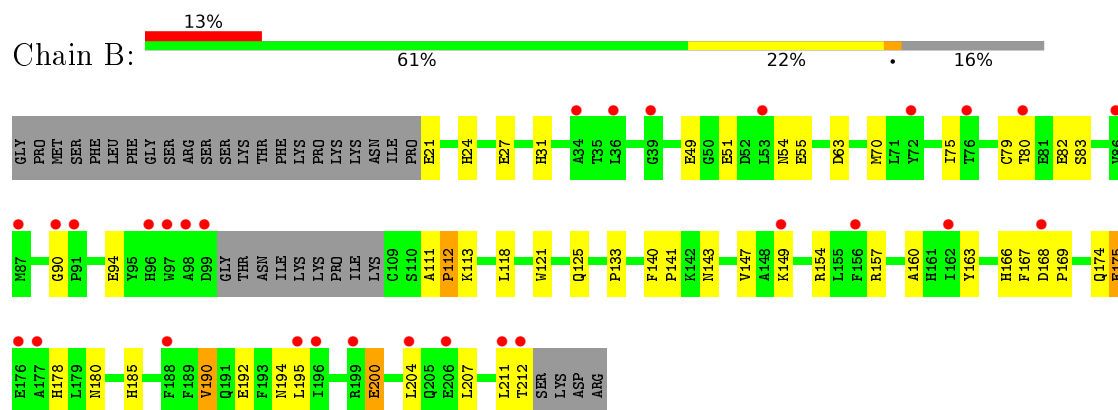
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

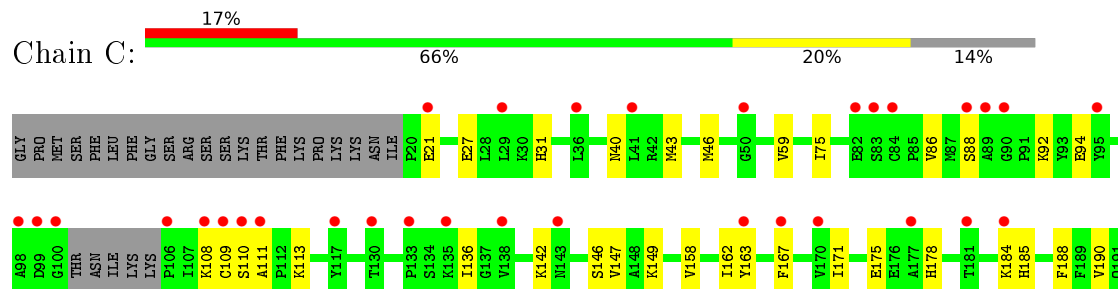
#### • Molecule 1: MOB kinase activator 1B

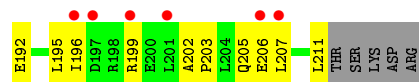


#### • Molecule 1: MOB kinase activator 1B

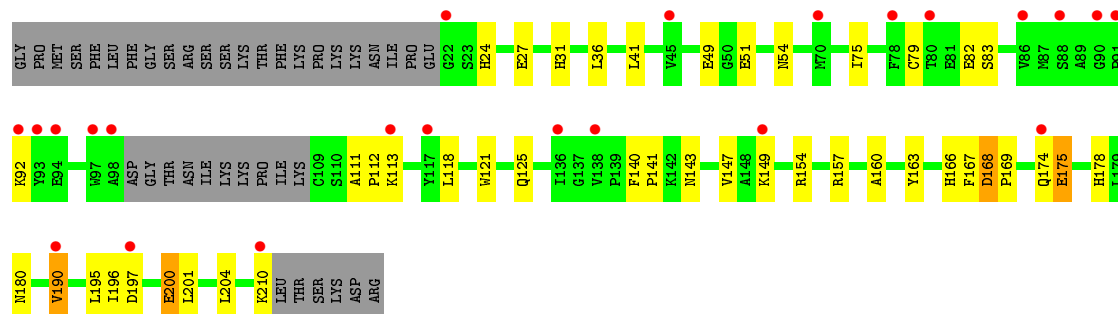


#### • Molecule 1: MOB kinase activator 1B





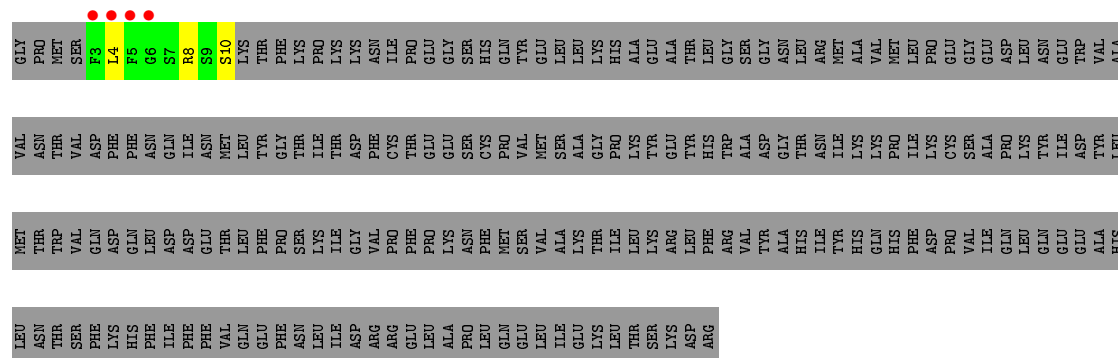
• Molecule 1: MOB kinase activator 1B



• Molecule 1: MOB kinase activator 1B



• Molecule 1: MOB kinase activator 1B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.35Å 127.69Å 59.29Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	29.67 – 2.19 29.74 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.67-2.19) 91.7 (29.74-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.06 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.233 , 0.246 0.229 , 0.242	Depositor DCC
$R_{free}$ test set	2100 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.0	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 4.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.219 for -l,k,h 0.256 for -h,-k,l 0.390 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6325	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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: 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	0.52	0/1577	0.64	0/2138
1	B	0.61	2/1547 (0.1%)	0.65	2/2099 (0.1%)
1	C	0.51	0/1577	0.63	0/2138
1	D	0.62	1/1515 (0.1%)	0.62	1/2055 (0.0%)
1	E	0.86	0/64	0.66	0/83
1	F	0.88	0/64	0.72	0/83
All	All	0.57	3/6344 (0.0%)	0.64	3/8596 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175	GLU	CB-CG	6.97	1.65	1.52
1	B	175	GLU	CB-CG	6.82	1.65	1.52
1	B	112	PRO	N-CD	5.19	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	GLU	CG-CD-OE2	6.05	130.41	118.30
1	B	90	GLY	C-N-CD	6.04	141.09	128.40
1	D	175	GLU	CG-CD-OE2	5.97	130.25	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen



atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1533	0	1481	37	0
1	B	1505	0	1445	42	0
1	C	1533	0	1481	42	1
1	D	1473	0	1417	38	0
1	E	63	0	59	4	0
1	F	63	0	59	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	30	0	0	4	0
4	B	47	0	0	7	0
4	C	34	0	0	4	0
4	D	38	0	0	1	1
All	All	6325	0	5942	141	1

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 12.

All (141) 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:A:197:ASP:OD2	4:A:401:HOH:O	1.68	1.08
1:A:31:HIS:ND1	1:C:175:GLU:OE2	1.91	1.01
1:A:175:GLU:OE2	1:C:31:HIS:ND1	1.92	1.00
1:B:31:HIS:ND1	1:D:175:GLU:OE2	1.98	0.97
1:B:175:GLU:OE2	1:D:31:HIS:ND1	1.96	0.97
1:D:168:ASP:OD1	4:D:401:HOH:O	1.83	0.95
1:A:185:HIS:HD2	4:A:426:HOH:O	1.57	0.87
1:C:175:GLU:OE2	1:C:178:HIS:ND1	2.15	0.79
1:A:175:GLU:OE2	1:A:178:HIS:ND1	2.15	0.79
1:D:175:GLU:OE2	1:D:178:HIS:ND1	2.16	0.78
1:B:175:GLU:OE2	1:B:178:HIS:ND1	2.16	0.75
1:B:175:GLU:CD	1:B:178:HIS:HD1	1.92	0.73
1:B:75:ILE:HD11	1:B:169:PRO:HB2	1.71	0.71
1:C:192:GLU:OE1	4:C:403:HOH:O	2.08	0.71
1:A:203:PRO:HD3	1:E:8:ARG:HH12	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LYS:O	1:E:10:SER:HA	1.90	0.71
1:D:75:ILE:HD11	1:D:169:PRO:HB2	1.71	0.71
1:B:27:GLU:OE2	1:D:175:GLU:OE2	2.11	0.69
1:A:185:HIS:CD2	4:A:426:HOH:O	2.39	0.69
1:C:92:LYS:O	1:F:10:SER:CB	2.42	0.67
1:A:149:LYS:NZ	4:A:401:HOH:O	2.29	0.65
1:B:94:GLU:OE1	4:B:401:HOH:O	2.15	0.65
1:C:206:GLU:HB2	4:C:411:HOH:O	1.96	0.65
1:B:175:GLU:OE2	1:D:27:GLU:OE2	2.15	0.64
1:B:24:HIS:NE2	1:B:51:GLU:OE1	2.28	0.62
1:D:163:TYR:OH	1:D:180:ASN:ND2	2.31	0.62
1:A:149:LYS:HG2	1:A:195:LEU:HA	1.81	0.62
1:B:157:ARG:NH2	1:B:200:GLU:OE2	2.26	0.61
1:B:24:HIS:HE2	1:B:51:GLU:CD	2.03	0.61
1:D:111:ALA:HB3	1:D:112:PRO:HD3	1.81	0.61
1:D:157:ARG:NH2	1:D:200:GLU:OE2	2.26	0.61
1:A:203:PRO:HD3	1:E:8:ARG:NH1	2.15	0.61
1:B:111:ALA:HB3	1:B:112:PRO:HD3	1.81	0.61
1:B:175:GLU:OE1	1:B:178:HIS:HB3	2.01	0.61
1:A:27:GLU:OE2	1:C:175:GLU:OE2	2.20	0.60
1:C:149:LYS:HG2	1:C:195:LEU:HA	1.81	0.60
1:D:175:GLU:OE1	1:D:178:HIS:HB3	2.01	0.60
1:B:163:TYR:OH	1:B:180:ASN:ND2	2.31	0.60
1:C:43:MET:CE	1:C:46:MET:HE2	2.32	0.59
1:C:184:LYS:HG3	1:C:211:LEU:HD13	1.83	0.59
1:C:92:LYS:O	1:F:10:SER:HA	2.02	0.59
1:A:204:LEU:O	1:A:208:ILE:HG13	2.04	0.58
1:C:175:GLU:OE1	1:C:178:HIS:ND1	2.37	0.58
1:B:63:ASP:OD2	4:B:402:HOH:O	2.17	0.58
1:C:158:VAL:O	1:C:162:ILE:HG13	2.04	0.58
1:A:175:GLU:OE1	1:A:178:HIS:ND1	2.37	0.57
1:A:31:HIS:HD1	1:C:175:GLU:CD	2.02	0.57
1:A:158:VAL:O	1:A:162:ILE:HG13	2.04	0.57
1:A:175:GLU:OE2	1:C:27:GLU:OE2	2.22	0.57
1:D:197:ASP:O	1:D:201:LEU:HG	2.07	0.54
1:B:143:ASN:O	1:B:147:VAL:HG23	2.08	0.53
1:B:31:HIS:HD1	1:D:175:GLU:CD	2.04	0.53
1:C:43:MET:HE3	1:C:46:MET:CE	2.39	0.53
1:D:143:ASN:O	1:D:147:VAL:HG23	2.08	0.53
1:C:175:GLU:CD	1:C:178:HIS:ND1	2.62	0.52
1:A:92:LYS:HE2	1:E:10:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLU:CD	1:D:31:HIS:HD1	2.04	0.52
1:B:194:ASN:HA	4:B:404:HOH:O	2.09	0.52
1:A:175:GLU:CD	1:A:178:HIS:ND1	2.62	0.52
1:A:209:GLU:C	1:A:211:LEU:N	2.62	0.51
1:D:190:VAL:HG11	1:D:196:ILE:HD12	1.92	0.51
1:A:109:CYS:HB3	1:A:113:LYS:HB3	1.93	0.51
1:A:198:ARG:HH21	1:B:133:PRO:HG2	1.76	0.51
1:C:184:LYS:HE2	1:C:188:PHE:HE2	1.77	0.50
1:C:185:HIS:HE1	4:C:408:HOH:O	1.93	0.50
1:B:118:LEU:HD11	1:B:154:ARG:HB3	1.94	0.50
1:B:192:GLU:OE1	4:B:403:HOH:O	2.19	0.50
1:A:167:PHE:CE2	1:A:171:ILE:HD11	2.47	0.50
1:A:184:LYS:HE2	1:A:188:PHE:HE2	1.77	0.50
1:D:118:LEU:HD11	1:D:154:ARG:HB3	1.94	0.50
1:A:209:GLU:C	1:A:211:LEU:H	2.15	0.50
1:C:43:MET:CE	1:C:46:MET:CE	2.90	0.49
1:D:190:VAL:HG22	1:D:195:LEU:HB2	1.94	0.49
1:C:167:PHE:CE2	1:C:171:ILE:HD11	2.47	0.49
1:D:24:HIS:HE2	1:D:51:GLU:CD	2.15	0.49
1:A:208:ILE:O	1:A:211:LEU:N	2.41	0.49
1:B:190:VAL:HG22	1:B:195:LEU:HB2	1.94	0.49
1:D:121:TRP:O	1:D:125:GLN:HG2	2.13	0.49
1:C:92:LYS:O	1:F:10:SER:CA	2.60	0.49
1:B:160:ALA:HA	1:B:204:LEU:HD11	1.95	0.49
1:A:175:GLU:CD	1:C:31:HIS:HD1	2.04	0.49
1:C:43:MET:HB3	1:C:43:MET:HE3	1.65	0.49
1:B:141:PRO:HB2	1:B:143:ASN:OD1	2.13	0.48
1:C:92:LYS:HD2	1:F:10:SER:HB2	1.95	0.48
1:B:121:TRP:O	1:B:125:GLN:HG2	2.13	0.48
1:C:203:PRO:HD3	1:F:8:ARG:NH2	2.29	0.48
1:D:160:ALA:HA	1:D:204:LEU:HD11	1.96	0.48
1:D:141:PRO:HB2	1:D:143:ASN:OD1	2.13	0.47
1:B:49:GLU:HB3	1:D:174:GLN:HG3	1.97	0.47
1:D:196:ILE:HG21	1:D:201:LEU:HD21	1.95	0.47
1:A:198:ARG:NH1	1:B:55:GLU:OE2	2.48	0.47
1:C:109:CYS:HB3	1:C:113:LYS:HB3	1.97	0.47
1:B:207:LEU:O	1:B:211:LEU:HG	2.15	0.47
1:B:79:CYS:O	1:B:112:PRO:HG3	2.15	0.46
1:C:202:ALA:HA	1:C:205:GLN:HG3	1.98	0.46
1:B:194:ASN:OD1	4:B:404:HOH:O	2.20	0.46
1:B:70:MET:HE2	4:B:412:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:CYS:O	1:D:112:PRO:HG3	2.16	0.46
1:C:92:LYS:O	1:F:10:SER:HB3	2.13	0.46
1:A:202:ALA:HA	1:A:205:GLN:HG3	1.97	0.45
1:B:80:THR:N	1:B:83:SER:OG	2.40	0.45
1:B:163:TYR:O	1:B:167:PHE:HB2	2.17	0.45
1:D:175:GLU:CD	1:D:178:HIS:ND1	2.70	0.45
1:D:196:ILE:HG21	1:D:201:LEU:CD2	2.46	0.45
1:D:163:TYR:O	1:D:167:PHE:HB2	2.17	0.45
1:D:190:VAL:CG2	1:D:196:ILE:HG13	2.46	0.44
1:C:163:TYR:CZ	1:C:207:LEU:HD21	2.52	0.44
1:C:86:VAL:HG21	1:C:94:GLU:OE2	2.18	0.44
1:A:181:THR:HG22	4:C:406:HOH:O	2.16	0.44
1:C:190:VAL:HG11	1:C:196:ILE:HD12	2.00	0.44
1:C:43:MET:HE3	1:C:46:MET:HE2	1.97	0.44
1:B:185:HIS:HD2	4:B:440:HOH:O	2.01	0.44
1:A:86:VAL:HG21	1:A:94:GLU:OE2	2.18	0.43
1:D:54:ASN:HB3	1:D:140:PHE:CD2	2.52	0.43
1:C:40:ASN:OD1	1:C:43:MET:HG2	2.18	0.43
1:B:54:ASN:HB3	1:B:140:PHE:CD2	2.53	0.43
1:B:166:HIS:O	1:B:169:PRO:HD2	2.18	0.43
1:A:190:VAL:HG11	1:A:196:ILE:HD12	2.00	0.43
1:C:211:LEU:HD12	1:C:211:LEU:C	2.39	0.43
1:B:175:GLU:CD	1:D:31:HIS:ND1	2.67	0.43
1:D:175:GLU:OE1	1:D:178:HIS:ND1	2.51	0.43
1:B:149:LYS:HG3	1:B:195:LEU:O	2.19	0.42
1:D:166:HIS:O	1:D:169:PRO:HD2	2.19	0.42
1:B:175:GLU:OE1	1:B:178:HIS:ND1	2.52	0.42
1:C:92:LYS:CD	1:F:10:SER:HB2	2.48	0.42
1:C:110:SER:O	1:C:111:ALA:C	2.57	0.42
1:B:174:GLN:HG3	1:D:49:GLU:HB3	2.00	0.42
1:A:167:PHE:O	1:A:171:ILE:HG12	2.19	0.42
1:D:149:LYS:HG3	1:D:195:LEU:O	2.19	0.42
1:C:92:LYS:CE	1:F:10:SER:HB2	2.50	0.42
1:C:92:LYS:HE2	1:F:10:SER:HB2	2.02	0.41
1:A:163:TYR:CZ	1:A:207:LEU:HD21	2.55	0.41
1:C:109:CYS:HB3	1:C:113:LYS:HE3	2.02	0.41
1:C:167:PHE:O	1:C:171:ILE:HG12	2.20	0.41
1:A:40:ASN:OD1	1:A:43:MET:HG2	2.20	0.41
1:A:86:VAL:HG11	1:A:94:GLU:OE2	2.21	0.41
1:B:31:HIS:ND1	1:D:175:GLU:CD	2.68	0.41
1:D:210:LYS:HA	1:D:210:LYS:HD2	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:LEU:HD22	1:D:41:LEU:HD22	2.04	0.40
1:A:118:LEU:O	1:A:122:VAL:HG23	2.21	0.40
1:C:86:VAL:HG11	1:C:94:GLU:OE2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ILE:CG2	4:D:414:HOH:O[2_658]	2.09	0.11

## 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	183/218 (84%)	178 (97%)	5 (3%)	0	100	100
1	B	179/218 (82%)	172 (96%)	7 (4%)	0	100	100
1	C	183/218 (84%)	176 (96%)	7 (4%)	0	100	100
1	D	175/218 (80%)	168 (96%)	7 (4%)	0	100	100
1	E	6/218 (3%)	6 (100%)	0	0	100	100
1	F	6/218 (3%)	6 (100%)	0	0	100	100
All	All	732/1308 (56%)	706 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	168/197 (85%)	158 (94%)	10 (6%)	24	26
1	B	165/197 (84%)	158 (96%)	7 (4%)	36	44
1	C	168/197 (85%)	159 (95%)	9 (5%)	27	31
1	D	161/197 (82%)	154 (96%)	7 (4%)	35	43
1	E	7/197 (4%)	6 (86%)	1 (14%)	4	3
1	F	7/197 (4%)	6 (86%)	1 (14%)	4	3
All	All	676/1182 (57%)	641 (95%)	35 (5%)	29	33

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	59	VAL
1	A	75	ILE
1	A	88	SER
1	A	108	LYS
1	A	142	LYS
1	A	146	SER
1	A	147	VAL
1	A	199	ARG
1	A	210	LYS
1	B	21	GLU
1	B	82	GLU
1	B	113	LYS
1	B	168	ASP
1	B	190	VAL
1	B	200	GLU
1	B	212	THR
1	C	21	GLU
1	C	59	VAL
1	C	75	ILE
1	C	88	SER
1	C	108	LYS
1	C	142	LYS
1	C	146	SER
1	C	147	VAL
1	C	199	ARG
1	D	82	GLU

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Mol	Chain	Res	Type
1	D	83	SER
1	D	92	LYS
1	D	113	LYS
1	D	168	ASP
1	D	190	VAL
1	D	200	GLU
1	E	10	SER
1	F	4	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	180	ASN
1	D	180	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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

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	187/218 (85%)	1.38	36 (19%) <b>2</b> <b>1</b>	38, 57, 82, 93	0
1	B	183/218 (83%)	1.22	29 (15%) <b>3</b> <b>2</b>	38, 56, 78, 95	0
1	C	187/218 (85%)	1.26	38 (20%) <b>1</b> <b>1</b>	39, 58, 82, 94	0
1	D	179/218 (82%)	1.18	23 (12%) <b>5</b> <b>4</b>	38, 56, 77, 85	0
1	E	8/218 (3%)	1.82	3 (37%) <b>0</b> <b>0</b>	66, 75, 83, 87	0
1	F	8/218 (3%)	1.55	4 (50%) <b>0</b> <b>0</b>	71, 77, 85, 89	0
All	All	752/1308 (57%)	1.27	133 (17%) <b>2</b> <b>2</b>	38, 57, 81, 95	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	97	TRP	9.1
1	C	100	GLY	8.8
1	C	89	ALA	7.3
1	B	97	TRP	6.7
1	B	211	LEU	5.3
1	A	100	GLY	5.1
1	B	90	GLY	5.1
1	B	91	PRO	5.0
1	D	113	LYS	5.0
1	C	167	PHE	4.8
1	A	108	LYS	4.7
1	D	22	GLY	4.7
1	A	107	ILE	4.5
1	A	160	ALA	4.4
1	D	117	TYR	4.3
1	C	88	SER	4.1
1	A	211	LEU	4.0
1	A	168	ASP	3.9
1	A	172	GLN	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	86	VAL	3.9
1	B	212	THR	3.9
1	A	109	CYS	3.8
1	C	170	VAL	3.7
1	C	184	LYS	3.7
1	E	3	PHE	3.7
1	C	29	LEU	3.7
1	C	117	TYR	3.6
1	C	36	LEU	3.6
1	E	5	PHE	3.6
1	C	201	LEU	3.6
1	B	86	VAL	3.6
1	D	197	ASP	3.6
1	D	88	SER	3.6
1	D	210	LYS	3.5
1	A	92	LYS	3.5
1	D	93	TYR	3.5
1	A	20	PRO	3.5
1	B	96	HIS	3.4
1	D	91	PRO	3.4
1	D	78	PHE	3.4
1	A	86	VAL	3.4
1	C	50	GLY	3.3
1	C	163	TYR	3.3
1	A	207	LEU	3.3
1	B	98	ALA	3.2
1	B	53	LEU	3.2
1	C	41	LEU	3.2
1	A	174	GLN	3.2
1	D	80	THR	3.2
1	D	98	ALA	3.2
1	F	3	PHE	3.1
1	C	130	THR	3.1
1	A	134	SER	3.1
1	B	39	GLY	3.0
1	D	45	VAL	3.0
1	C	106	PRO	3.0
1	C	111	ALA	2.9
1	B	188	PHE	2.9
1	F	4	LEU	2.9
1	A	156	PHE	2.9
1	B	162	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	143	ASN	2.8
1	B	87	MET	2.8
1	D	138	VAL	2.8
1	B	199	ARG	2.7
1	C	84	CYS	2.7
1	C	99	ASP	2.7
1	D	174	GLN	2.7
1	C	197	ASP	2.7
1	B	195	LEU	2.7
1	B	99	ASP	2.6
1	A	151	ILE	2.6
1	A	50	GLY	2.6
1	E	4	LEU	2.6
1	C	83	SER	2.6
1	B	206	GLU	2.5
1	C	199	ARG	2.5
1	A	82	GLU	2.5
1	B	76	THR	2.5
1	A	39	GLY	2.5
1	B	177	ALA	2.5
1	B	196	ILE	2.5
1	C	177	ALA	2.5
1	A	206	GLU	2.5
1	A	88	SER	2.4
1	B	72	TYR	2.4
1	C	95	TYR	2.4
1	A	44	ALA	2.4
1	B	34	ALA	2.4
1	C	98	ALA	2.4
1	A	167	PHE	2.4
1	D	94	GLU	2.4
1	A	189	PHE	2.4
1	C	181	THR	2.3
1	A	198	ARG	2.3
1	C	133	PRO	2.3
1	C	90	GLY	2.3
1	D	92	LYS	2.3
1	F	5	PHE	2.3
1	C	82	GLU	2.3
1	C	138	VAL	2.3
1	C	196	ILE	2.3
1	A	93	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	176	GLU	2.2
1	B	36	LEU	2.2
1	D	190	VAL	2.2
1	A	90	GLY	2.2
1	B	168	ASP	2.2
1	B	149	LYS	2.2
1	A	106	PRO	2.2
1	C	110	SER	2.2
1	D	149	LYS	2.2
1	A	195	LEU	2.2
1	A	210	LYS	2.2
1	A	114	TYR	2.2
1	B	156	PHE	2.2
1	C	108	LYS	2.2
1	C	207	LEU	2.1
1	C	206	GLU	2.1
1	B	204	LEU	2.1
1	C	21	GLU	2.1
1	D	136	ILE	2.1
1	A	72	TYR	2.1
1	F	6	GLY	2.1
1	A	136	ILE	2.1
1	A	91	PRO	2.1
1	C	135	LYS	2.1
1	D	70	MET	2.0
1	A	162	ILE	2.0
1	A	135	LYS	2.0
1	B	80	THR	2.0
1	C	109	CYS	2.0
1	D	90	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [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	ZN	D	301	1/1	0.95	0.11	-1.80	58,58,58,58	0
2	ZN	C	301	1/1	0.85	0.11	-1.88	60,60,60,60	0
3	CL	A	302	1/1	0.77	0.11	-2.33	70,70,70,70	0
3	CL	C	302	1/1	0.97	0.12	-2.64	69,69,69,69	0
2	ZN	A	301	1/1	0.92	0.08	-4.34	61,61,61,61	0
2	ZN	B	301	1/1	0.92	0.07	-4.75	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.