



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:36 pm GMT

PDB ID : 4U42  
Title : MAP4K4 T181E Mutant Bound to inhibitor compound 1  
Authors : Harris, S.F.; Wu, P.; Coons, M.  
Deposited on : 2014-07-23  
Resolution : 2.50 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 : 1.7.2 (RC1), CSD as538be (2017)  
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

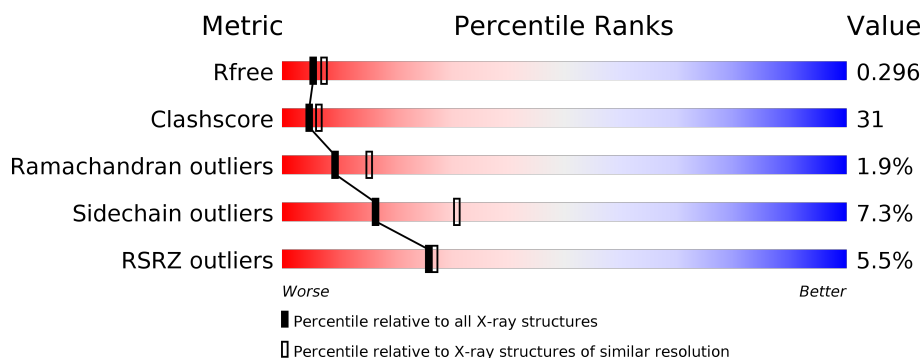
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 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	332	<div> <div>3%</div> <div> <div></div> <div>45%</div> <div>35%</div> <div>5%</div> <div>15%</div> </div> </div>
1	B	332	<div> <div>6%</div> <div> <div></div> <div>45%</div> <div>33%</div> <div>•</div> <div>20%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4530 atoms, of which 2 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 Mitogen-activated protein kinase kinase kinase kinase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2278	1453	400	412	13			
1	B	265	Total	C	N	O	S	0	1	0
			2143	1371	380	379	13			

There are 12 discrepancies between the modelled and reference sequences:

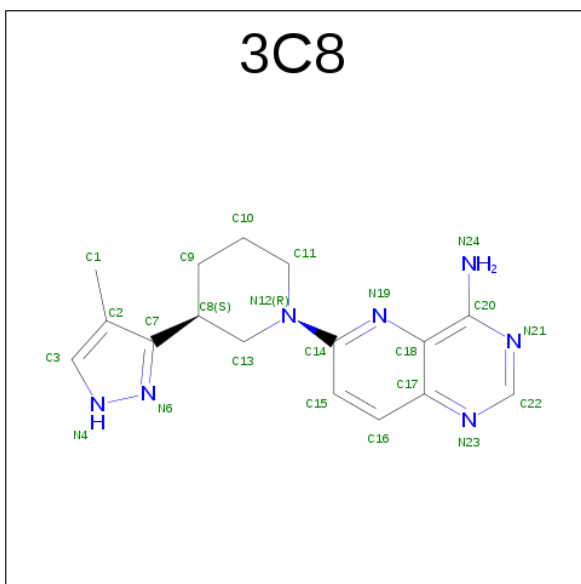
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP O95819
A	1	SER	-	expression tag	UNP O95819
A	181	GLU	THR	engineered mutation	UNP O95819
A	329	GLY	-	expression tag	UNP O95819
A	330	ASN	-	expression tag	UNP O95819
A	331	SER	-	expression tag	UNP O95819
B	0	GLY	-	expression tag	UNP O95819
B	1	SER	-	expression tag	UNP O95819
B	181	GLU	THR	engineered mutation	UNP O95819
B	329	GLY	-	expression tag	UNP O95819
B	330	ASN	-	expression tag	UNP O95819
B	331	SER	-	expression tag	UNP O95819

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is 6-[(3S)-3-(4-methyl-1H-pyrazol-3-yl)piperidin-1-yl]pyrido[3,2-d]pyrimidin-4-amine (three-letter code: 3C8) (formula: C<sub>16</sub>H<sub>19</sub>N<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			24	16	1	7		
3	B	1	Total	C	H	N	0	0
			24	16	1	7		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	22	Total	O	0	0
			22	22		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.45Å 83.67Å 95.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.72 – 2.50 39.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.72-2.50) 99.5 (39.72-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.227 , 0.303 0.218 , 0.296	Depositor DCC
$R_{free}$ test set	1144 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: MG, 3C8, MES

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	0.44	0/2334	0.59	0/3156
1	B	0.43	0/2196	0.56	0/2970
All	All	0.44	0/4530	0.58	0/6126

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	2278	0	2270	156	0
1	B	2143	0	2143	119	0
2	A	12	0	12	0	0
3	A	23	1	19	5	0
3	B	23	1	19	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	25	0	0	1	0
5	B	22	0	0	2	0
All	All	4528	2	4463	274	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 31.

All (274) 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:260:LYS:HE2	1:B:260:LYS:HA	1.12	1.04
1:B:92:LYS:HB3	1:B:93:SER:HB3	1.34	1.03
1:B:260:LYS:CE	1:B:260:LYS:HA	1.94	0.96
1:B:236:MET:HG3	1:B:240:ARG:HG2	1.48	0.93
1:B:260:LYS:CA	1:B:260:LYS:HE2	1.99	0.92
1:A:21:PRO:HG2	1:A:91:LYS:HD3	1.51	0.91
1:A:236:MET:HE1	1:A:244:LEU:HD12	1.51	0.90
1:A:90:ILE:HD12	1:A:90:ILE:O	1.71	0.90
1:A:46:LYS:HE3	1:A:46:LYS:HA	1.52	0.90
1:B:18:LEU:HB2	1:B:90:ILE:HD12	1.55	0.87
1:B:56:MET:HE3	1:B:101:LEU:HD23	1.58	0.86
1:A:79:HIS:O	1:A:80:ARG:HB3	1.73	0.86
1:A:308:ARG:HH21	1:A:308:ARG:HB2	1.41	0.86
1:A:64:GLU:HG2	1:A:67:LYS:NZ	1.91	0.86
1:A:236:MET:CE	1:A:244:LEU:HD12	2.07	0.85
1:A:297:GLN:O	1:A:301:GLN:HG3	1.76	0.85
1:B:93:SER:HB2	1:B:94:PRO:CD	2.07	0.85
1:A:29:GLU:O	1:A:30:VAL:HG22	1.78	0.83
1:A:211:ASP:OD1	1:A:213:ARG:HD3	1.77	0.83
1:B:90:ILE:HG21	1:B:92:LYS:HE2	1.61	0.82
1:B:113:ILE:O	1:B:117:VAL:HG23	1.82	0.79
1:A:21:PRO:CG	1:A:91:LYS:HD3	2.12	0.79
1:A:69:GLU:O	1:A:73:LEU:HD12	1.83	0.78
1:B:79:HIS:HD2	1:B:81:ASN:H	1.28	0.78
1:B:116:LEU:HD23	1:B:125:LEU:HD11	1.64	0.78
1:A:59:THR:HG22	1:A:62:GLU:HG3	1.66	0.78
1:B:310:ARG:HB2	1:B:310:ARG:NH1	1.98	0.77
1:A:94:PRO:O	1:A:97:HIS:HB2	1.83	0.77
1:A:117:VAL:HG11	1:A:229:GLY:HA2	1.67	0.76
1:B:305:HIS:O	1:B:309:THR:HG22	1.86	0.76
1:A:70:ILE:O	1:A:74:LYS:HG2	1.86	0.76
1:B:236:MET:CG	1:B:240:ARG:HG2	2.15	0.76
1:A:46:LYS:O	1:A:46:LYS:HE2	1.86	0.75
1:A:296:ARG:HG3	1:A:297:GLN:H	1.52	0.75
1:B:85:TYR:CZ	1:B:87:GLY:HA2	2.22	0.74
1:A:21:PRO:HD2	1:A:91:LYS:HD2	1.69	0.74
1:A:305:HIS:HA	1:A:308:ARG:HD3	1.70	0.73
1:B:305:HIS:NE2	1:B:309:THR:HG21	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:PHE:O	1:B:247:ARG:HD2	1.89	0.73
1:A:308:ARG:HB2	1:A:308:ARG:NH2	2.04	0.72
1:B:56:MET:CE	1:B:101:LEU:HD23	2.19	0.72
1:A:64:GLU:HG2	1:A:67:LYS:HZ3	1.52	0.72
1:B:92:LYS:CB	1:B:93:SER:HB3	2.16	0.71
1:B:36:TYR:HB2	1:B:39:VAL:CG1	2.20	0.71
1:A:56:MET:CE	1:A:101:LEU:HD23	2.20	0.71
1:B:36:TYR:HB2	1:B:39:VAL:HG11	1.71	0.71
1:A:296:ARG:HG3	1:A:297:GLN:N	2.05	0.71
1:B:25:PHE:CE2	1:B:44:HIS:HD2	2.09	0.70
1:A:79:HIS:O	1:A:80:ARG:CB	2.38	0.70
1:B:151:HIS:O	1:B:152:ARG:HB2	1.92	0.70
1:A:38:GLN:HE21	1:A:55:VAL:HG12	1.57	0.69
1:A:59:THR:CG2	1:A:62:GLU:HG3	2.23	0.69
1:A:202:CYS:SG	1:A:204:GLU:HG2	2.33	0.68
1:A:202:CYS:SG	1:A:204:GLU:CG	2.81	0.68
1:B:120:THR:HG21	1:B:124:THR:O	1.93	0.68
1:A:212:TYR:CE2	1:A:213:ARG:HD2	2.28	0.68
1:B:204:GLU:CD	1:B:204:GLU:N	2.47	0.68
1:B:28:VAL:O	1:B:29:GLU:HB3	1.93	0.67
1:A:209:THR:O	1:A:209:THR:HG22	1.95	0.67
3:B:401:3C8:H10	3:B:401:3C8:H14	1.76	0.67
1:A:66:ILE:CG2	1:A:101:LEU:HD22	2.26	0.66
1:B:75:LYS:HG2	1:B:75:LYS:O	1.96	0.66
1:A:56:MET:HE3	1:A:101:LEU:HD23	1.78	0.66
1:A:71:ASN:HA	1:A:74:LYS:CG	2.27	0.65
1:B:307:ASP:O	1:B:310:ARG:HG2	1.96	0.65
1:B:18:LEU:HD12	1:B:90:ILE:CD1	2.27	0.65
1:B:79:HIS:HB3	1:B:82:ILE:HD12	1.79	0.65
1:B:94:PRO:HD3	1:B:99:ASP:OD2	1.96	0.65
1:A:85:TYR:CE2	1:A:87:GLY:HA2	2.32	0.64
1:B:79:HIS:CD2	1:B:81:ASN:H	2.14	0.64
1:A:19:ARG:H	1:A:90:ILE:HG13	1.61	0.64
1:A:281:GLU:O	1:A:285:LYS:HG3	1.98	0.64
1:A:204:GLU:HA	5:A:504:HOH:O	1.98	0.64
1:A:296:ARG:NH1	1:A:296:ARG:HB3	2.13	0.64
1:A:59:THR:CG2	1:A:62:GLU:CG	2.75	0.64
1:B:93:SER:HB2	1:B:94:PRO:HD3	1.80	0.64
1:A:114:THR:HG21	1:A:157:GLN:HE21	1.63	0.64
3:A:402:3C8:C1	3:A:402:3C8:H10	2.30	0.62
1:A:151:HIS:O	1:A:152:ARG:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:PHE:HD1	1:B:190:GLY:HA2	1.64	0.62
1:B:24:ILE:HD12	1:B:89:PHE:HE1	1.64	0.62
1:A:28:VAL:H	1:A:29:GLU:HA	1.64	0.61
3:A:402:3C8:H14	3:A:402:3C8:H10	1.81	0.61
1:A:18:LEU:HB2	1:A:90:ILE:HG23	1.82	0.61
1:A:81:ASN:O	1:A:168:LYS:HA	2.00	0.61
3:B:401:3C8:H10	3:B:401:3C8:C1	2.31	0.61
1:A:46:LYS:CE	1:A:46:LYS:HA	2.29	0.60
1:B:80:ARG:NH2	5:B:511:HOH:O	2.34	0.60
1:A:79:HIS:HE1	1:A:81:ASN:HD22	1.49	0.60
1:A:237:HIS:HD2	1:A:239:MET:H	1.49	0.60
1:A:296:ARG:CZ	1:A:296:ARG:CB	2.80	0.60
1:B:90:ILE:CG2	1:B:92:LYS:HE2	2.32	0.59
1:A:27:LEU:HB3	1:A:29:GLU:HB3	1.84	0.59
1:A:28:VAL:C	1:A:29:GLU:HG3	2.23	0.59
1:A:296:ARG:CZ	1:A:296:ARG:HB3	2.33	0.59
1:A:62:GLU:HB2	1:A:66:ILE:HD11	1.84	0.59
1:B:296:ARG:O	1:B:300:ILE:HG13	2.03	0.59
1:B:31:VAL:HG22	1:B:39:VAL:O	2.02	0.59
1:A:59:THR:OG1	1:A:60:GLU:N	2.35	0.59
1:A:237:HIS:CD2	1:A:239:MET:H	2.20	0.58
1:B:117:VAL:HG11	1:B:229:GLY:HA2	1.85	0.58
1:B:32:GLY:O	1:B:35:THR:HB	2.03	0.58
1:B:29:GLU:C	1:B:40:TYR:HD1	2.06	0.58
1:A:117:VAL:CG1	1:A:229:GLY:HA2	2.32	0.58
1:A:147:HIS:O	1:A:148:HIS:HB2	2.02	0.58
1:B:93:SER:HB2	1:B:94:PRO:HD2	1.84	0.58
1:A:106:GLU:OE2	1:A:168:LYS:HE3	2.04	0.58
1:B:204:GLU:CD	1:B:204:GLU:H	2.05	0.58
1:B:36:TYR:CB	1:B:39:VAL:HG11	2.33	0.58
1:A:30:VAL:HG12	1:A:40:TYR:CE1	2.39	0.57
1:A:31:VAL:CG2	1:A:39:VAL:HG12	2.33	0.57
1:A:38:GLN:HG2	1:A:55:VAL:HB	1.85	0.57
1:A:212:TYR:CZ	1:A:213:ARG:HD2	2.40	0.57
1:A:21:PRO:HD2	1:A:91:LYS:CD	2.33	0.57
1:A:143:HIS:O	1:A:146:ILE:HG22	2.05	0.57
1:A:18:LEU:HD12	1:A:90:ILE:HG23	1.86	0.57
1:A:29:GLU:O	1:A:30:VAL:CG2	2.51	0.56
1:A:71:ASN:HA	1:A:74:LYS:HG3	1.87	0.56
1:A:228:GLU:CD	1:A:254:LYS:HD2	2.25	0.56
1:B:260:LYS:CE	1:B:260:LYS:CA	2.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:MET:HE2	1:A:101:LEU:HD23	1.86	0.56
1:A:28:VAL:HG21	1:A:41:LYS:HD3	1.87	0.56
1:A:202:CYS:SG	1:A:204:GLU:OE1	2.64	0.56
1:A:86:TYR:HB2	1:A:104:VAL:HG12	1.87	0.55
1:B:194:TRP:CZ2	1:B:231:PRO:HG3	2.42	0.55
1:A:46:LYS:CA	1:A:46:LYS:HE3	2.32	0.55
1:A:237:HIS:CD2	1:A:238:PRO:HD2	2.42	0.55
1:A:28:VAL:C	1:A:29:GLU:CG	2.75	0.54
1:B:233:LEU:O	1:B:236:MET:HB2	2.07	0.54
1:A:20:ASP:OD1	1:A:91:LYS:HD2	2.07	0.54
1:B:126:LYS:O	1:B:129:TRP:HB2	2.08	0.54
1:B:85:TYR:CE2	1:B:87:GLY:HA2	2.42	0.54
1:A:60:GLU:HG2	1:A:61:ASP:N	2.23	0.54
1:A:51:ALA:HA	1:A:107:PHE:HB2	1.89	0.53
1:A:29:GLU:C	1:A:30:VAL:HG22	2.28	0.53
1:B:18:LEU:HD12	1:B:90:ILE:HD11	1.89	0.53
1:B:35:THR:HG22	1:B:36:TYR:CD2	2.43	0.53
1:A:85:TYR:CZ	1:A:87:GLY:HA2	2.43	0.53
1:A:51:ALA:CA	1:A:107:PHE:HB2	2.39	0.53
1:B:57:ASP:HA	1:B:99:ASP:O	2.08	0.53
1:B:279:SER:OG	1:B:282:GLN:HG3	2.10	0.52
1:A:67:LYS:O	1:A:71:ASN:ND2	2.42	0.52
1:B:86:TYR:CE1	1:B:106:GLU:HA	2.45	0.52
1:A:62:GLU:O	1:A:64:GLU:N	2.42	0.52
1:A:188:PHE:CD1	1:B:190:GLY:HA2	2.44	0.52
1:A:64:GLU:HG2	1:A:67:LYS:CE	2.38	0.52
1:B:310:ARG:HB2	1:B:310:ARG:CZ	2.39	0.52
1:B:56:MET:O	1:B:58:VAL:HG13	2.10	0.51
1:A:19:ARG:O	1:A:90:ILE:N	2.41	0.51
1:B:245:ILE:HB	1:B:246:PRO:HD3	1.92	0.51
1:A:20:ASP:CG	1:A:91:LYS:HD2	2.30	0.51
1:A:57:ASP:OD1	1:A:100:GLN:HG2	2.10	0.51
1:B:132:TYR:O	1:B:136:GLU:HG2	2.11	0.51
1:B:110:ALA:HB2	1:B:306:ILE:HD13	1.92	0.51
1:B:305:HIS:CD2	1:B:309:THR:HG21	2.45	0.51
1:A:73:LEU:O	1:A:77:SER:OG	2.25	0.51
1:B:90:ILE:CG2	1:B:92:LYS:CE	2.89	0.51
1:A:308:ARG:CB	1:A:308:ARG:NH2	2.74	0.51
1:A:59:THR:CG2	1:A:62:GLU:HG2	2.41	0.50
1:A:79:HIS:CE1	1:A:81:ASN:HD22	2.29	0.50
1:A:245:ILE:HB	1:A:246:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HG22	1:A:25:PHE:CD2	2.46	0.50
1:A:82:ILE:HD12	1:A:82:ILE:N	2.27	0.50
1:B:225:GLU:O	1:B:229:GLY:N	2.44	0.50
1:A:296:ARG:CG	1:A:297:GLN:H	2.23	0.50
1:A:164:ASN:O	1:A:165:ALA:HB3	2.12	0.49
1:A:118:LYS:HD2	1:A:119:ASN:OD1	2.13	0.49
1:A:154:ILE:O	1:A:218:SER:HB3	2.12	0.49
1:A:228:GLU:OE1	1:A:254:LYS:HD2	2.12	0.49
1:A:71:ASN:HB3	1:A:75:LYS:HE3	1.95	0.49
1:B:251:PRO:HD2	1:B:270:LEU:HD13	1.94	0.49
1:A:30:VAL:HG23	1:A:30:VAL:O	2.13	0.49
1:B:30:VAL:N	1:B:40:TYR:HD1	2.10	0.49
1:A:105:MET:HE3	3:A:402:3C8:C7	2.43	0.48
1:A:28:VAL:HG22	1:A:41:LYS:HB3	1.94	0.48
1:B:85:TYR:CZ	1:B:87:GLY:CA	2.95	0.48
1:A:296:ARG:CG	1:A:297:GLN:N	2.76	0.48
1:A:77:SER:HB3	1:A:84:THR:HA	1.96	0.48
1:A:239:MET:HE3	1:B:201:ALA:HB3	1.95	0.48
1:B:303:LYS:O	1:B:306:ILE:HB	2.12	0.48
1:A:28:VAL:H	1:A:29:GLU:CA	2.26	0.48
1:A:117:VAL:HG21	1:A:226:MET:HA	1.96	0.48
1:A:46:LYS:CA	1:A:46:LYS:CE	2.89	0.48
1:B:310:ARG:HB2	1:B:310:ARG:HH11	1.73	0.48
1:B:82:ILE:CD1	1:B:143:HIS:HD2	2.27	0.47
1:B:216:LEU:O	1:B:219[B]:CYS:HB2	2.14	0.47
1:B:44:HIS:HB3	1:B:47:THR:OG1	2.15	0.47
1:A:202:CYS:O	1:A:205:ASN:N	2.44	0.47
1:A:20:ASP:CG	1:A:21:PRO:HD2	2.34	0.47
1:A:39:VAL:HG21	3:A:402:3C8:H4	1.95	0.47
1:B:211:ASP:HA	5:B:509:HOH:O	2.14	0.47
1:A:136:GLU:HB3	1:A:167:VAL:HB	1.97	0.47
1:A:59:THR:HG23	1:A:62:GLU:CG	2.44	0.47
1:A:71:ASN:HA	1:A:74:LYS:CD	2.44	0.46
1:B:89:PHE:HE2	1:B:104:VAL:HG21	1.80	0.46
1:B:116:LEU:HD23	1:B:125:LEU:CD1	2.39	0.46
1:A:151:HIS:O	1:A:152:ARG:CB	2.64	0.46
1:B:30:VAL:HA	1:B:40:TYR:CD1	2.51	0.46
1:B:59:THR:HG22	1:B:59:THR:O	2.16	0.45
1:B:103:LEU:HD12	1:B:103:LEU:HA	1.70	0.45
1:A:154:ILE:HB	1:A:218:SER:HB2	1.99	0.45
1:B:310:ARG:CB	1:B:310:ARG:CZ	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:HG22	1:A:152:ARG:HG3	1.98	0.45
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.75	0.45
1:B:141:LEU:CD1	1:B:219[B]:CYS:SG	3.05	0.45
1:B:154:ILE:HB	1:B:218:SER:HB2	2.00	0.44
1:B:24:ILE:HD12	1:B:89:PHE:CE1	2.48	0.44
1:A:59:THR:HG23	1:A:62:GLU:HG2	2.00	0.44
1:A:64:GLU:CG	1:A:67:LYS:NZ	2.73	0.44
1:A:135:ARG:HB2	1:A:289:ILE:HG23	1.99	0.44
1:A:121:LYS:HG3	1:A:121:LYS:O	2.16	0.44
1:B:113:ILE:HG23	1:B:159:VAL:O	2.17	0.44
1:B:57:ASP:OD1	1:B:100:GLN:HG2	2.17	0.44
1:B:77:SER:HA	1:B:82:ILE:HG21	1.99	0.44
1:A:64:GLU:HA	1:A:67:LYS:HB2	1.99	0.44
1:B:245:ILE:N	1:B:246:PRO:CD	2.81	0.44
1:B:77:SER:HA	1:B:82:ILE:CG2	2.48	0.44
1:A:28:VAL:N	1:A:29:GLU:CA	2.80	0.43
1:B:35:THR:CG2	1:B:36:TYR:CD2	3.00	0.43
1:B:90:ILE:HG21	1:B:92:LYS:CE	2.38	0.43
1:B:86:TYR:CZ	1:B:106:GLU:HA	2.53	0.43
1:A:238:PRO:HB2	1:B:189:ILE:HG13	2.00	0.43
1:B:21:PRO:HB2	1:B:102:TRP:CZ3	2.53	0.43
1:B:35:THR:CG2	1:B:36:TYR:N	2.81	0.43
1:A:55:VAL:HA	1:A:101:LEU:O	2.18	0.43
1:A:237:HIS:CD2	1:A:239:MET:HB3	2.53	0.43
1:A:66:ILE:HG23	1:A:101:LEU:HD22	2.00	0.43
1:B:217:TRP:C	1:B:217:TRP:CD1	2.92	0.43
1:B:19:ARG:HD2	1:B:24:ILE:CD1	2.49	0.43
1:B:79:HIS:HD2	1:B:81:ASN:N	2.06	0.43
1:B:89:PHE:CE2	1:B:104:VAL:HG21	2.53	0.43
1:A:304:ASP:O	1:A:308:ARG:HG3	2.18	0.43
1:A:230:ALA:HB1	1:A:231:PRO:HD2	2.01	0.43
1:B:237:HIS:CE1	1:B:239:MET:HB3	2.53	0.43
1:B:202:CYS:HB2	1:B:247:ARG:HH12	1.83	0.43
1:A:82:ILE:HG22	1:A:83:ALA:O	2.19	0.42
1:A:90:ILE:HD13	1:A:92:LYS:HE2	2.01	0.42
1:B:130:ILE:HG23	1:B:226:MET:HE3	2.00	0.42
1:A:71:ASN:HA	1:A:74:LYS:HD3	2.01	0.42
1:B:248:ASN:O	1:B:272:LYS:HE3	2.20	0.42
1:A:240:ARG:NH1	1:B:206:PRO:O	2.53	0.42
1:A:55:VAL:HG22	1:A:102:TRP:CD1	2.54	0.42
1:A:279:SER:OG	1:A:282:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ILE:HD13	1:B:159:VAL:CG1	2.49	0.42
1:B:237:HIS:ND1	1:B:239:MET:HB3	2.35	0.42
1:A:237:HIS:HD2	1:A:239:MET:N	2.17	0.42
1:B:241:ALA:O	1:B:245:ILE:HG13	2.20	0.42
1:B:250:PRO:HA	1:B:251:PRO:HD3	1.84	0.42
1:A:38:GLN:HG2	1:A:55:VAL:O	2.20	0.41
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.50	0.41
1:A:54:LYS:HB2	3:A:402:3C8:C3	2.50	0.41
1:A:150:ILE:HG22	1:A:152:ARG:CG	2.51	0.41
1:B:155:LYS:HB3	1:B:194:TRP:CG	2.56	0.41
1:B:81:ASN:ND2	1:B:139:ARG:HB3	2.35	0.41
1:B:77:SER:HB2	1:B:84:THR:HA	2.02	0.41
1:B:85:TYR:OH	1:B:87:GLY:HA2	2.19	0.41
1:A:88:ALA:HA	1:A:102:TRP:O	2.20	0.41
1:A:90:ILE:HD12	1:A:90:ILE:C	2.39	0.41
1:A:232:PRO:O	1:A:233:LEU:HB2	2.21	0.41
1:A:245:ILE:N	1:A:246:PRO:CD	2.83	0.41
1:A:248:ASN:HB3	1:A:249:PRO:HD2	2.03	0.41
1:A:69:GLU:O	1:A:72:MET:HB3	2.21	0.41
1:A:236:MET:HE3	1:A:240:ARG:HG3	2.03	0.41
1:A:90:ILE:HD13	1:A:92:LYS:CE	2.50	0.41
1:B:30:VAL:N	1:B:40:TYR:CD1	2.89	0.41
1:A:135:ARG:HD3	1:A:292:GLN:NE2	2.36	0.40
1:B:302:LEU:O	1:B:306:ILE:HG13	2.22	0.40
1:B:309:THR:O	1:B:310:ARG:C	2.59	0.40
1:A:38:GLN:HE21	1:A:55:VAL:CG1	2.31	0.40
1:B:81:ASN:HD22	1:B:139:ARG:HB3	1.87	0.40
1:A:269:CYS:O	1:A:277:ARG:HD3	2.22	0.40
1:B:146:ILE:HD12	1:B:146:ILE:HA	1.74	0.40
1:B:132:TYR:HA	1:B:292:GLN:HE22	1.87	0.40
1:B:31:VAL:CG2	1:B:39:VAL:O	2.66	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	278/332 (84%)	250 (90%)	21 (8%)	7 (2%)	6	10
1	B	258/332 (78%)	235 (91%)	20 (8%)	3 (1%)	15	27
All	All	536/664 (81%)	485 (90%)	41 (8%)	10 (2%)	9	15

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	63	GLU
1	A	80	ARG
1	A	97	HIS
1	B	173	GLY
1	B	308	ARG
1	A	95	PRO
1	A	208	ALA
1	A	30	VAL
1	B	29	GLU

### 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	248/290 (86%)	229 (92%)	19 (8%)	15	28
1	B	233/290 (80%)	217 (93%)	16 (7%)	18	34
All	All	481/580 (83%)	446 (93%)	35 (7%)	16	31

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

Mol	Chain	Res	Type
1	A	28	VAL
1	A	29	GLU
1	A	33	ASN

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Mol	Chain	Res	Type
1	A	35	THR
1	A	38	GLN
1	A	46	LYS
1	A	59	THR
1	A	60	GLU
1	A	62	GLU
1	A	68	LEU
1	A	74	LYS
1	A	103	LEU
1	A	118	LYS
1	A	124	THR
1	A	157	GLN
1	A	199	VAL
1	A	261	LYS
1	A	296	ARG
1	A	310	ARG
1	B	31	VAL
1	B	35	THR
1	B	49	GLN
1	B	103	LEU
1	B	146	ILE
1	B	163	GLU
1	B	164	ASN
1	B	203	ASP
1	B	209	THR
1	B	234	CYS
1	B	240	ARG
1	B	260	LYS
1	B	280	THR
1	B	302	LEU
1	B	304	ASP
1	B	310	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	71	ASN
1	A	81	ASN
1	A	157	GLN
1	A	237	HIS
1	B	33	ASN

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Mol	Chain	Res	Type
1	B	38	GLN
1	B	44	HIS
1	B	79	HIS
1	B	81	ASN
1	B	143	HIS
1	B	292	GLN
1	B	297	GLN

### 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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	MES	A	401	-	12,12,12	1.27	2 (16%)	14,16,16	1.71	4 (28%)
3	3C8	A	402	-	24,26,26	0.91	1 (4%)	25,37,37	2.85	9 (36%)
3	3C8	B	401	-	24,26,26	0.93	1 (4%)	25,37,37	2.80	12 (48%)

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	MES	A	401	-	-	0/6/14/14	0/1/1/1
3	3C8	A	402	-	-	0/4/18/18	0/4/4/4
3	3C8	B	401	-	-	0/4/18/18	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	MES	C8-S	-2.27	1.74	1.77
3	B	401	3C8	C7-N6	-2.23	1.31	1.33
2	A	401	MES	O2S-S	2.01	1.51	1.45
3	A	402	3C8	C3-N4	2.25	1.35	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	3C8	N23-C22-N21	-7.54	122.29	128.86
3	A	402	3C8	N23-C22-N21	-6.75	122.98	128.86
3	A	402	3C8	C13-N12-C14	-5.62	107.08	120.33
3	A	402	3C8	C11-N12-C14	-5.49	107.39	120.33
3	B	401	3C8	C11-N12-C14	-4.36	110.06	120.33
3	B	401	3C8	C10-C9-C8	-3.94	104.08	111.58
3	A	402	3C8	C10-C9-C8	-3.92	104.12	111.58
3	B	401	3C8	C13-N12-C14	-3.82	111.33	120.33
3	A	402	3C8	C9-C10-C11	-3.67	106.13	110.96
3	B	401	3C8	C18-C17-N23	-2.08	118.76	121.76
3	B	401	3C8	C15-C16-C17	-2.07	118.30	120.84
3	A	402	3C8	C11-N12-C13	2.07	117.11	113.14
3	B	401	3C8	C10-C11-N12	2.10	115.24	111.09
2	A	401	MES	C2-C3-N4	2.16	113.13	110.11
2	A	401	MES	C7-N4-C3	2.17	116.83	111.26
3	B	401	3C8	C11-N12-C13	2.20	117.36	113.14
3	B	401	3C8	C16-C17-N23	2.41	122.44	118.53
3	B	401	3C8	C8-C13-N12	2.45	114.58	110.21
2	A	401	MES	C6-C5-N4	2.52	113.64	110.11
3	A	402	3C8	C16-C17-N23	2.55	122.67	118.53
3	A	402	3C8	C14-N19-C18	3.03	121.31	118.19
3	B	401	3C8	C14-N19-C18	3.20	121.49	118.19
2	A	401	MES	C5-N4-C3	3.57	116.96	108.87
3	A	402	3C8	C22-N23-C17	4.84	120.34	115.27
3	B	401	3C8	C22-N23-C17	5.75	121.30	115.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	3C8	5	0
3	B	401	3C8	2	0

## 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	282/332 (84%)	0.05	9 (3%)	48	51	39, 63, 98, 130	0
1	B	265/332 (79%)	0.32	21 (7%)	13	13	42, 63, 102, 132	0
All	All	547/664 (82%)	0.18	30 (5%)	26	27	39, 63, 101, 132	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	VAL	7.1
1	B	95	PRO	5.0
1	B	101	LEU	4.6
1	B	85	TYR	4.3
1	B	23	GLY	3.8
1	A	93	SER	3.7
1	B	93	SER	3.7
1	A	61	ASP	3.0
1	B	89	PHE	3.0
1	A	95	PRO	2.9
1	B	17	SER	2.9
1	B	45	VAL	2.9
1	B	33	ASN	2.8
1	B	59	THR	2.8
1	B	188	PHE	2.8
1	A	92	LYS	2.6
1	B	309	THR	2.5
1	A	60	GLU	2.5
1	A	38	GLN	2.4
1	B	102	TRP	2.4
1	B	121	LYS	2.4
1	B	94	PRO	2.3
1	B	75	LYS	2.3
1	B	18	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	58	VAL	2.3
1	B	56	MET	2.3
1	A	94	PRO	2.3
1	B	76	TYR	2.2
1	B	308	ARG	2.2
1	A	66	ILE	2.2

## 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
2	MES	A	401	12/12	0.98	0.14	1.01	58,61,70,71	0
3	3C8	A	402	23/23	0.94	0.18	0.40	58,67,78,93	0
3	3C8	B	401	23/23	0.92	0.18	0.17	63,69,76,92	0
4	MG	A	403	1/1	0.88	0.14	-0.12	79,79,79,79	0
4	MG	B	402	1/1	0.92	0.15	-0.23	65,65,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.