



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:26 am GMT

PDB ID : 5AVS  
Title : Kinetics by X-ray crystallography: Tl<sup>+</sup>-substitution of bound K<sup>+</sup> in the E2.MgF42-.2K<sup>+</sup> crystal after 3.5 min  
Authors : Ogawa, H.; Cornelius, F.; Hirata, A.; Toyoshima, C.  
Deposited on : 2015-07-01  
Resolution : 2.90 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

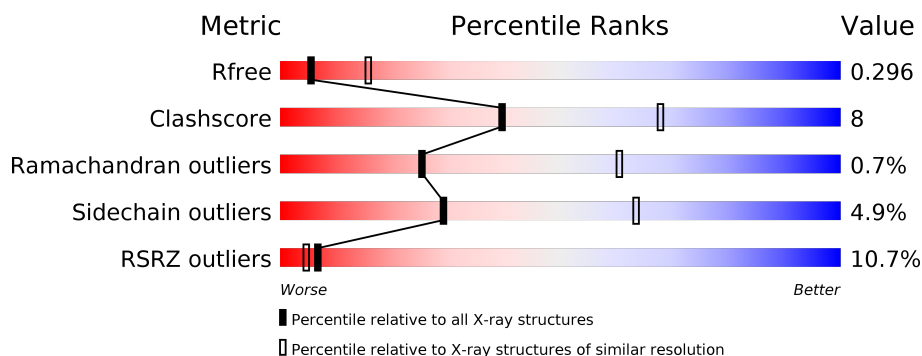
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	1028	<div> <div>8%</div> <div>75%</div> <div>21%</div> <div>• •</div> </div>
2	B	305	<div> <div>18%</div> <div>67%</div> <div>19%</div> <div>• 12%</div> </div>
3	G	74	<div> <div>3%</div> <div>36%</div> <div>16%</div> <div>47%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MF4	A	2001	-	-	-	X
5	MG	A	2002	-	-	-	X
8	CLR	B	3001	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10236 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 Na, K-ATPase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	992	Total	C	N	O	S	0	0	0
			7675	4886	1290	1453	46			

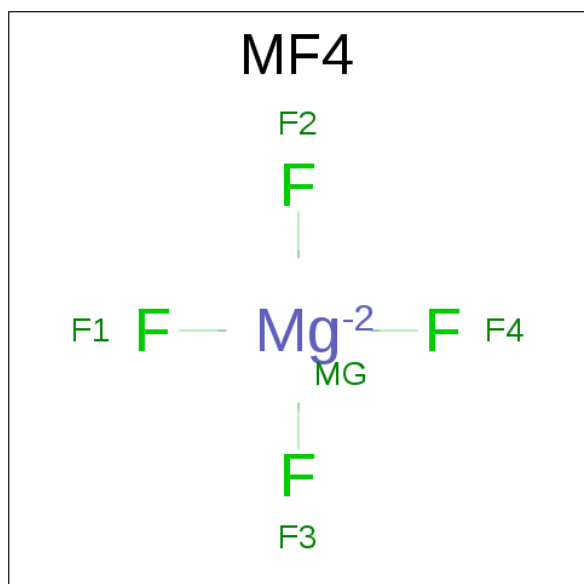
- Molecule 2 is a protein called Na<sup>+</sup>,K<sup>+</sup>-ATPase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	268	Total	C	N	O	S	0	0	0
			2174	1409	358	396	11			

- Molecule 3 is a protein called Phospholemman-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	39	Total	C	N	O	S	0	0	0
			305	200	50	54	1			

- Molecule 4 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F<sub>4</sub>Mg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	F	Mg	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Mg		0	0
			1	1			

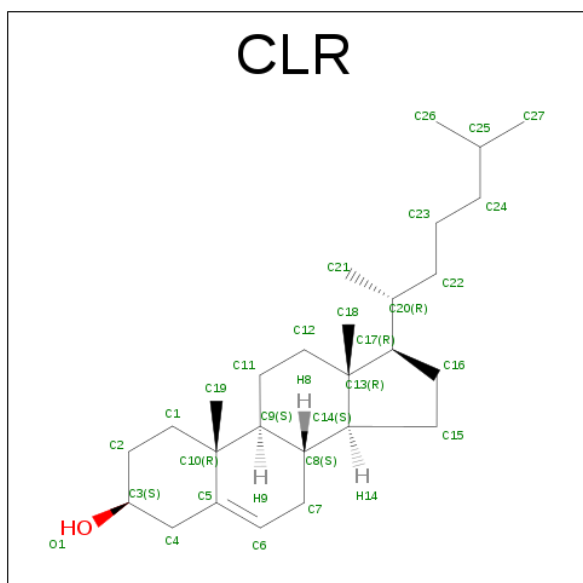
- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	2	Total	K		0	2
			2	2			

- Molecule 7 is THALLIUM (I) ION (three-letter code: TL) (formula: Tl).

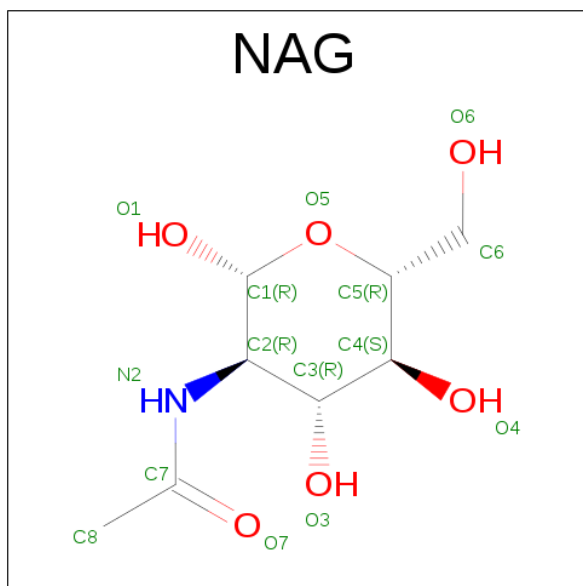
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	3	Total	Tl		0	2
			3	3			

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			28	27	1		

- Molecule 9 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

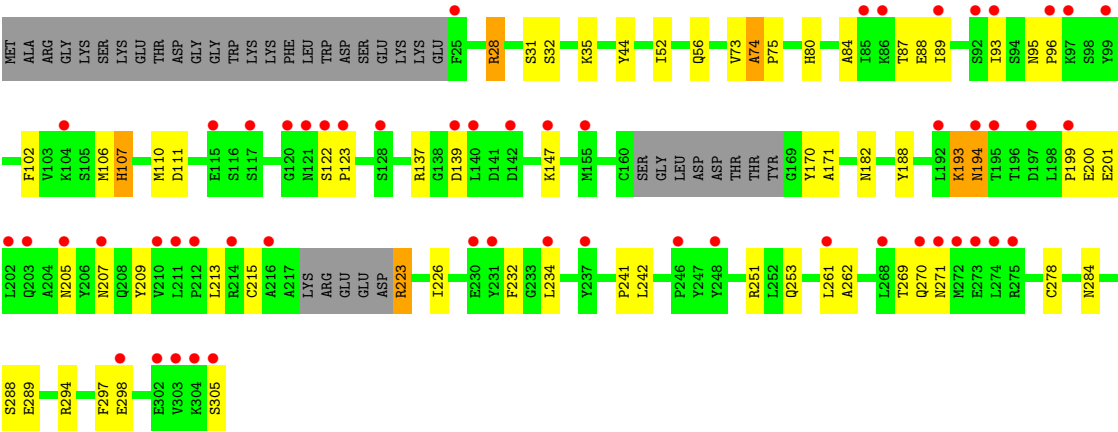


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		

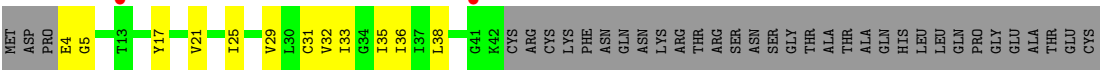
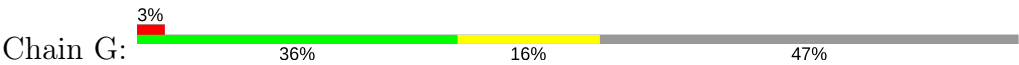
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	O	0	0
			1	1		





● Molecule 3: Phospholemman-like protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	221.90Å 50.87Å 164.19Å 90.00° 104.45° 90.00°	Depositor
Resolution (Å)	14.99 – 2.90 43.55 – 2.90	Depositor EDS
% Data completeness (in resolution range)	70.2 (14.99-2.90) 87.7 (43.55-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.38 (at 2.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.285 , 0.284 0.294 , 0.296	Depositor DCC
$R_{free}$ test set	1106 reflections (3.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.4	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	10236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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, NAG, K, TL, MF4, CLR

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	0.38	0/7825	0.51	0/10616
2	B	0.35	0/2229	0.49	0/3002
3	G	0.36	0/309	0.46	0/419
All	All	0.38	0/10363	0.51	0/14037

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	7675	0	7699	123	0
2	B	2174	0	2146	45	0
3	G	305	0	318	8	0
4	A	5	0	0	0	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
7	A	3	0	0	0	0
8	B	28	0	46	1	0
9	B	42	0	38	0	0
10	A	1	0	0	0	0
All	All	10236	0	10247	171	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 (171) 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)
2:B:74:ALA:HB3	2:B:75:PRO:HD3	1.47	0.94
1:A:478:VAL:HG21	1:A:571:PHE:HB2	1.64	0.79
1:A:905:GLN:NE2	2:B:182:ASN:HA	1.99	0.78
1:A:497:LYS:HE2	1:A:499:SER:HB2	1.69	0.75
1:A:868:SER:O	1:A:872:ILE:HG12	1.86	0.75
1:A:61:ARG:HH11	1:A:61:ARG:HB3	1.52	0.73
1:A:261:THR:HG22	1:A:264:ARG:NH2	2.02	0.73
1:A:51:LEU:HD13	1:A:204:ARG:HG3	1.69	0.71
2:B:270:GLN:HG2	2:B:271:ASN:HD22	1.58	0.69
1:A:766:ARG:HD2	1:A:832:MET:CE	2.24	0.68
1:A:339:THR:HG23	1:A:820:ILE:HD13	1.77	0.67
2:B:213:LEU:HD11	2:B:278:CYS:HB3	1.78	0.65
1:A:935:ILE:HG23	1:A:944:ILE:HD12	1.77	0.64
1:A:160:SER:HB3	1:A:741:VAL:HG22	1.80	0.64
1:A:78:ASN:HA	1:A:261:THR:HG23	1.79	0.64
2:B:74:ALA:CB	2:B:75:PRO:HD3	2.23	0.63
1:A:816:MET:O	1:A:820:ILE:HG12	1.97	0.63
1:A:52:HIS:HA	1:A:57:THR:HG23	1.80	0.63
2:B:28:ARG:HB2	2:B:32:SER:HB3	1.81	0.63
1:A:673:LEU:HD22	1:A:677:VAL:HG11	1.80	0.62
2:B:193:LYS:HA	2:B:207:ASN:HD21	1.65	0.62
1:A:323:PHE:O	1:A:327:ILE:HG12	2.01	0.61
1:A:64:THR:HG22	1:A:66:ALA:H	1.65	0.61
3:G:29:VAL:O	3:G:33:ILE:HG12	2.00	0.60
1:A:483:ASN:HB2	1:A:486:ASN:HB2	1.82	0.60
1:A:363:ALA:HB1	1:A:730:ILE:HD12	1.83	0.60
2:B:31:SER:O	2:B:35:LYS:HG3	2.01	0.60
2:B:270:GLN:HG2	2:B:271:ASN:ND2	2.16	0.60
1:A:344:LEU:HB3	1:A:361:LEU:HG	1.85	0.59
1:A:392:TRP:HB3	1:A:588:LEU:HB2	1.84	0.59
2:B:84:ALA:HB1	2:B:88:GLU:H	1.67	0.59
2:B:28:ARG:NH1	8:B:3001:CLR:H22	2.16	0.59
3:G:21:VAL:O	3:G:25:ILE:HG12	2.02	0.59
1:A:106:ILE:O	1:A:110:LEU:HB2	2.03	0.59
1:A:212:LYS:HB2	1:A:251:GLU:HG2	1.85	0.58
2:B:106:MET:O	2:B:110:MET:HG2	2.03	0.58
1:A:345:THR:HA	1:A:361:LEU:HD11	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:PRO:HG2	2:B:294:ARG:HH21	1.68	0.57
2:B:74:ALA:HB3	2:B:75:PRO:CD	2.29	0.57
1:A:491:SER:HB3	1:A:493:HIS:NE2	2.19	0.57
2:B:193:LYS:HA	2:B:207:ASN:ND2	2.20	0.57
1:A:818:PRO:HB3	1:A:934:LEU:HD22	1.87	0.56
2:B:52:ILE:O	2:B:56:GLN:HG2	2.05	0.56
2:B:137:ARG:HD2	2:B:147:LYS:HB3	1.88	0.56
1:A:172:ILE:HD13	1:A:177:LYS:HB3	1.87	0.56
1:A:933:ASP:HA	1:A:936:ILE:HG12	1.86	0.55
1:A:190:LEU:HD11	1:A:206:ILE:HD11	1.88	0.55
1:A:157:ILE:HD11	1:A:745:ALA:HA	1.88	0.55
1:A:994:TYR:O	1:A:997:ILE:HG22	2.06	0.55
2:B:93:ILE:H	2:B:305:SER:HB2	1.72	0.55
1:A:351:MET:HA	1:A:354:LYS:HG2	1.89	0.55
1:A:261:THR:HG22	1:A:264:ARG:HH21	1.71	0.55
1:A:596:ARG:HB2	1:A:599:VAL:HG23	1.89	0.55
1:A:905:GLN:HE21	2:B:182:ASN:HA	1.71	0.54
1:A:64:THR:HG22	1:A:66:ALA:N	2.23	0.54
1:A:924:ILE:HD12	1:A:983:LEU:HD12	1.89	0.54
1:A:994:TYR:HA	1:A:997:ILE:HG22	1.89	0.54
1:A:1016:TRP:HE1	2:B:35:LYS:HE3	1.72	0.54
1:A:921:SER:HA	1:A:983:LEU:HD11	1.90	0.53
2:B:213:LEU:HD23	2:B:261:LEU:HD13	1.89	0.53
1:A:424:ILE:HG23	1:A:506:VAL:HB	1.90	0.53
1:A:51:LEU:CD1	1:A:204:ARG:HG3	2.36	0.53
1:A:161:PHE:HA	1:A:164:MET:HE3	1.90	0.53
1:A:324:LEU:O	1:A:328:ILE:HG12	2.09	0.52
1:A:161:PHE:HA	1:A:164:MET:CE	2.39	0.52
1:A:808:LEU:O	1:A:812:LEU:HB2	2.10	0.52
1:A:212:LYS:HD3	1:A:224:PRO:HB2	1.90	0.52
1:A:766:ARG:HD2	1:A:832:MET:HE2	1.91	0.52
2:B:75:PRO:HG2	2:B:294:ARG:NH2	2.25	0.52
3:G:32:VAL:O	3:G:36:ILE:HG12	2.09	0.52
1:A:82:PRO:HA	1:A:158:MET:HG2	1.93	0.51
1:A:572:ASP:HB3	1:A:577:ASN:HB2	1.92	0.51
1:A:788:THR:N	1:A:789:PRO:HD2	2.26	0.51
3:G:25:ILE:O	3:G:29:VAL:HG23	2.11	0.51
1:A:417:THR:HA	1:A:522:LEU:HD22	1.93	0.51
2:B:288:SER:HB2	2:B:294:ARG:HH11	1.76	0.50
1:A:956:PHE:CE1	3:G:38:LEU:HD22	2.47	0.50
1:A:571:PHE:HA	1:A:577:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LYS:HE2	1:A:746:ALA:O	2.12	0.49
2:B:232:PHE:HB2	2:B:262:ALA:HB3	1.93	0.49
1:A:826:GLN:HE22	1:A:950:LYS:HE3	1.78	0.49
1:A:1005:ARG:NH1	1:A:1006:ARG:HG3	2.28	0.49
2:B:209:TYR:HA	2:B:242:LEU:HD22	1.95	0.48
1:A:502:ARG:CG	1:A:503:TYR:H	2.27	0.48
1:A:442:ILE:O	1:A:445:ARG:HG2	2.14	0.48
1:A:323:PHE:CE1	1:A:793:PHE:HE2	2.32	0.47
1:A:171:VAL:HG12	1:A:191:VAL:HG22	1.97	0.47
1:A:132:LEU:HD21	1:A:804:THR:HG21	1.97	0.47
1:A:797:ASN:HD22	1:A:887:ARG:HD3	1.79	0.47
1:A:814:THR:HB	1:A:961:GLU:HG3	1.96	0.47
2:B:80:HIS:HB3	2:B:297:PHE:CZ	2.50	0.47
3:G:31:CYS:O	3:G:35:ILE:HG12	2.14	0.47
2:B:87:THR:HB	2:B:298:GLU:O	2.14	0.47
1:A:127:ASN:HB3	1:A:131:TYR:CD1	2.50	0.46
1:A:924:ILE:HD12	1:A:983:LEU:CD1	2.45	0.46
2:B:215:CYS:HA	2:B:278:CYS:HA	1.96	0.46
1:A:336:LEU:HD11	1:A:776:ILE:HG12	1.96	0.46
1:A:63:LEU:HD22	1:A:189:ASP:HB3	1.96	0.46
2:B:226:ILE:HG22	2:B:269:THR:HB	1.96	0.46
1:A:631:VAL:HG23	1:A:633:ILE:HG12	1.96	0.46
2:B:122:SER:HA	2:B:123:PRO:HA	1.75	0.46
1:A:670:LEU:HD23	1:A:678:LEU:HD21	1.96	0.46
1:A:303:GLY:HA2	1:A:327:ILE:HG21	1.97	0.46
1:A:784:ILE:HD11	1:A:854:TYR:CG	2.51	0.46
1:A:209:HIS:HB3	1:A:253:THR:HG22	1.98	0.45
1:A:475:PRO:HD2	1:A:494:GLU:HB2	1.99	0.45
1:A:889:ARG:HD2	1:A:895:ILE:CD1	2.46	0.45
1:A:847:GLU:H	1:A:847:GLU:CD	2.20	0.45
2:B:84:ALA:HB1	2:B:88:GLU:N	2.31	0.45
1:A:676:GLU:H	1:A:676:GLU:CD	2.20	0.45
1:A:722:SER:OG	1:A:723:PRO:HD3	2.17	0.45
1:A:631:VAL:CG2	1:A:633:ILE:HG12	2.46	0.45
1:A:52:HIS:HE2	1:A:59:LEU:HD12	1.82	0.44
1:A:915:GLU:O	1:A:918:CYS:HB2	2.17	0.44
1:A:806:THR:HG22	1:A:923:PHE:HB2	2.00	0.44
2:B:194:ASN:N	2:B:194:ASN:HD22	2.15	0.44
1:A:354:LYS:HB2	1:A:354:LYS:HZ2	1.81	0.44
2:B:234:LEU:HG	2:B:241:PRO:HG3	1.99	0.44
1:A:246:SER:OG	1:A:267:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:HIS:O	2:B:111:ASP:HB2	2.18	0.43
1:A:273:LEU:O	1:A:277:LEU:HG	2.19	0.43
2:B:107:HIS:ND1	2:B:170:TYR:HE1	2.17	0.43
1:A:790:PHE:O	1:A:794:ILE:HG12	2.19	0.43
1:A:110:LEU:HD22	1:A:324:LEU:HD12	1.99	0.43
1:A:511:PRO:HG2	1:A:542:TYR:CE1	2.53	0.43
1:A:87:PRO:HD2	1:A:90:ILE:HD12	1.99	0.43
2:B:147:LYS:HB2	2:B:253:GLN:HG3	1.99	0.43
3:G:4:GLU:CD	3:G:5:GLY:H	2.23	0.43
1:A:64:THR:HA	1:A:174:ASP:OD1	2.19	0.42
1:A:940:ARG:HE	1:A:1023:TYR:HB2	1.84	0.42
1:A:300:VAL:O	1:A:304:VAL:HG22	2.19	0.42
1:A:661:LYS:HA	1:A:661:LYS:HE2	2.00	0.42
1:A:797:ASN:HB3	1:A:885:GLY:HA2	2.01	0.42
2:B:188:TYR:O	2:B:284:ASN:ND2	2.53	0.42
2:B:95:ASN:HA	2:B:96:PRO:HD3	1.86	0.42
1:A:170:LEU:HD21	1:A:177:LYS:HD3	2.00	0.42
1:A:291:PHE:HB3	1:A:845:VAL:HB	2.02	0.42
1:A:291:PHE:HA	1:A:294:ILE:HD12	2.01	0.42
2:B:223:ARG:HH11	2:B:223:ARG:HB2	1.85	0.42
2:B:74:ALA:CB	2:B:75:PRO:CD	2.92	0.42
2:B:89:ILE:HG22	2:B:102:PHE:CE2	2.55	0.42
1:A:48:LEU:HD23	1:A:59:LEU:HD11	2.01	0.42
1:A:784:ILE:N	1:A:785:PRO:HD2	2.35	0.42
2:B:194:ASN:HB3	2:B:205:ASN:OD1	2.20	0.42
1:A:378:THR:HA	1:A:382:THR:OG1	2.20	0.41
2:B:137:ARG:HB3	2:B:147:LYS:HD2	2.01	0.41
1:A:110:LEU:CD2	1:A:324:LEU:HD12	2.50	0.41
1:A:367:LEU:HD23	1:A:761:GLY:HA3	2.01	0.41
1:A:785:PRO:HB2	1:A:926:ILE:CD1	2.50	0.41
2:B:271:ASN:HD21	2:B:305:SER:N	2.19	0.41
1:A:502:ARG:HE	1:A:562:GLU:HG2	1.85	0.41
1:A:846:ASN:ND2	1:A:848:ARG:HB2	2.35	0.41
3:G:17:TYR:O	3:G:21:VAL:HG23	2.21	0.41
1:A:44:HIS:HB3	1:A:242:ILE:HD11	2.03	0.41
1:A:920:THR:HG21	1:A:981:TYR:O	2.20	0.41
1:A:342:VAL:HB	1:A:820:ILE:HD12	2.03	0.41
1:A:426:ALA:O	1:A:471:ARG:HD2	2.20	0.41
1:A:502:ARG:HG3	1:A:562:GLU:HG2	2.02	0.41
1:A:540:ASN:N	1:A:540:ASN:HD22	2.18	0.41
1:A:284:ILE:O	1:A:288:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LYS:O	1:A:462:LEU:HB2	2.21	0.41
1:A:859:MET:HG2	2:B:44:TYR:CE2	2.55	0.41
1:A:301:PHE:O	1:A:305:SER:HB2	2.20	0.41
1:A:423:ARG:O	1:A:427:LEU:HB2	2.21	0.41
1:A:647:ARG:HH21	1:A:648:LEU:HD11	1.86	0.41
1:A:702:VAL:HG13	1:A:712:VAL:HG21	2.03	0.41
1:A:831:ILE:O	1:A:834:ARG:HG2	2.22	0.40
1:A:925:SER:O	1:A:929:VAL:HG22	2.21	0.40
1:A:199:ILE:HG22	1:A:201:ALA:O	2.22	0.40
1:A:354:LYS:HE2	1:A:760:THR:HB	2.02	0.40
1:A:900:ASP:OD1	1:A:904:GLN:HB2	2.21	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	990/1028 (96%)	942 (95%)	43 (4%)	5 (0%)	32	68
2	B	262/305 (86%)	223 (85%)	35 (13%)	4 (2%)	12	39
3	G	37/74 (50%)	33 (89%)	4 (11%)	0	100	100
All	All	1289/1407 (92%)	1198 (93%)	82 (6%)	9 (1%)	25	60

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	THR
1	A	128	ASP
1	A	576	PRO
2	B	74	ALA
2	B	171	ALA
2	B	201	GLU

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Mol	Chain	Res	Type
1	A	123	ASP
1	A	1014	GLY
2	B	199	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	840/869 (97%)	796 (95%)	44 (5%)	27	61
2	B	234/266 (88%)	224 (96%)	10 (4%)	33	68
3	G	32/62 (52%)	32 (100%)	0	100	100
All	All	1106/1197 (92%)	1052 (95%)	54 (5%)	29	63

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	57	THR
1	A	61	ARG
1	A	63	LEU
1	A	72	LEU
1	A	128	ASP
1	A	165	VAL
1	A	213	VAL
1	A	217	SER
1	A	218	LEU
1	A	226	THR
1	A	231	PHE
1	A	245	PHE
1	A	248	ASN
1	A	250	VAL
1	A	255	ARG
1	A	261	THR
1	A	284	ILE
1	A	309	LEU

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Mol	Chain	Res	Type
1	A	344	LEU
1	A	354	LYS
1	A	391	MET
1	A	413	LYS
1	A	434	GLN
1	A	454	SER
1	A	457	LEU
1	A	524	ASN
1	A	540	ASN
1	A	557	HIS
1	A	581	THR
1	A	636	GLU
1	A	670	LEU
1	A	682	LEU
1	A	712	VAL
1	A	719	VAL
1	A	726	LYS
1	A	806	THR
1	A	811	ASP
1	A	833	LYS
1	A	847	GLU
1	A	880	PRO
1	A	974	THR
1	A	987	TRP
1	A	1019	GLN
2	B	28	ARG
2	B	73	VAL
2	B	107	HIS
2	B	139	ASP
2	B	193	LYS
2	B	194	ASN
2	B	200	GLU
2	B	223	ARG
2	B	251	ARG
2	B	289	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	129	ASN
1	A	163	ASN

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Mol	Chain	Res	Type
1	A	225	GLN
1	A	290	HIS
1	A	434	GLN
1	A	524	ASN
1	A	540	ASN
1	A	557	HIS
1	A	577	ASN
1	A	754	ASN
1	A	797	ASN
1	A	826	GLN
1	A	905	GLN
1	A	1019	GLN
2	B	80	HIS
2	B	194	ASN
2	B	207	ASN
2	B	264	GLN
2	B	271	ASN
2	B	284	ASN

### 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 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	$\# Z  > 2$
4	MF4	A	2001	1	0,4,4	0.00	-	0,6,6	0.00	-
8	CLR	B	3001	-	31,31,31	0.45	0	48,48,48	1.07	5 (10%)
9	NAG	B	4001	9,2	14,14,15	0.49	0	15,19,21	0.92	1 (6%)
9	NAG	B	4002	9	14,14,15	0.65	0	15,19,21	1.39	1 (6%)
9	NAG	B	4021	2	14,14,15	0.61	0	15,19,21	1.30	3 (20%)

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
4	MF4	A	2001	1	-	0/0/0/0	0/0/0/0
8	CLR	B	3001	-	-	0/10/68/68	0/4/4/4
9	NAG	B	4001	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	4002	9	-	0/6/23/26	0/1/1/1
9	NAG	B	4021	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	3001	CLR	C4-C5-C6	-2.32	117.05	120.59
9	B	4021	NAG	O5-C1-C2	-2.31	108.25	111.47
8	B	3001	CLR	C12-C11-C9	2.00	116.61	113.12
9	B	4021	NAG	C4-C3-C2	2.30	114.39	111.02
8	B	3001	CLR	C4-C5-C10	2.39	119.69	116.41
9	B	4021	NAG	C1-O5-C5	2.53	115.66	112.17
8	B	3001	CLR	C1-C2-C3	2.61	113.75	110.42
9	B	4001	NAG	C1-O5-C5	2.66	115.83	112.17
8	B	3001	CLR	C15-C14-C13	2.86	107.36	103.83
9	B	4002	NAG	C2-N2-C7	3.84	128.54	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	3001	CLR	1	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	992/1028 (96%)	0.58	82 (8%) 12 9	54, 76, 117, 142	0
2	B	268/305 (87%)	1.10	55 (20%) 1 1	74, 125, 150, 160	0
3	G	39/74 (52%)	0.41	2 (5%) 29 24	71, 80, 123, 127	0
All	All	1299/1407 (92%)	0.68	139 (10%) 7 5	54, 81, 138, 160	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	TRP	6.1
2	B	93	ILE	5.8
2	B	214	ARG	5.7
1	A	562	GLU	5.5
1	A	41	MET	5.4
1	A	573	ALA	5.4
2	B	231	TYR	5.3
1	A	79	SER	4.9
2	B	304	LYS	4.8
1	A	534	MET	4.8
2	B	121	ASN	4.8
2	B	195	THR	4.4
2	B	216	ALA	4.3
1	A	563	ASP	4.2
1	A	579	PRO	4.2
2	B	123	PRO	4.1
2	B	117	SER	4.1
1	A	496	GLU	4.1
1	A	578	PHE	4.1
1	A	72	LEU	4.1
1	A	57	THR	3.9
1	A	585	PHE	3.9
1	A	260	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	122	GLU	3.9
1	A	894	TRP	3.9
1	A	121	THR	3.8
2	B	271	ASN	3.8
2	B	122	SER	3.7
2	B	305	SER	3.7
2	B	303	VAL	3.7
1	A	498	SER	3.7
1	A	502	ARG	3.6
1	A	504	LEU	3.6
2	B	273	GLU	3.6
2	B	298	GLU	3.5
2	B	203	GLN	3.5
1	A	464	CYS	3.4
1	A	42	ASP	3.4
1	A	125	PRO	3.4
1	A	86	THR	3.4
2	B	194	ASN	3.4
1	A	183	GLU	3.4
1	A	986	SER	3.3
2	B	192	LEU	3.2
1	A	474	ASN	3.2
1	A	576	PRO	3.2
1	A	571	PHE	3.2
1	A	470	MET	3.1
2	B	268	LEU	3.1
1	A	499	SER	3.1
1	A	675	THR	3.1
1	A	126	ALA	3.0
1	A	411	PHE	3.0
1	A	131	TYR	3.0
1	A	439	ASN	3.0
2	B	142	ASP	3.0
1	A	127	ASN	2.9
2	B	272	MET	2.9
2	B	199	PRO	2.9
3	G	41	GLY	2.9
2	B	234	LEU	2.9
1	A	97	PHE	2.8
1	A	84	PRO	2.8
1	A	574	ASP	2.8
1	A	90	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	129	ASN	2.7
1	A	114	ALA	2.7
2	B	99	TYR	2.7
2	B	147	LYS	2.7
1	A	521	ILE	2.6
1	A	568	GLY	2.6
2	B	115	GLU	2.5
1	A	75	ASP	2.5
2	B	120	GLY	2.5
1	A	94	ARG	2.5
2	B	104	LYS	2.5
2	B	248	TYR	2.5
2	B	97	LYS	2.5
1	A	117	ILE	2.5
1	A	427	LEU	2.5
2	B	261	LEU	2.5
2	B	230	GLU	2.5
2	B	212	PRO	2.5
2	B	207	ASN	2.5
2	B	128	SER	2.4
2	B	96	PRO	2.4
1	A	989	PHE	2.4
1	A	567	GLU	2.4
1	A	71	ILE	2.4
2	B	85	ILE	2.4
2	B	140	LEU	2.4
1	A	493	HIS	2.4
2	B	92	SER	2.4
1	A	98	GLY	2.3
1	A	467	VAL	2.3
1	A	82	PRO	2.3
1	A	815	ASP	2.3
2	B	205	ASN	2.3
2	B	89	ILE	2.3
1	A	829	SER	2.3
1	A	492	ILE	2.3
1	A	1004	MET	2.3
1	A	779	THR	2.2
1	A	80	LEU	2.2
1	A	149	TYR	2.2
2	B	86	LYS	2.2
2	B	139	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1023	TYR	2.2
1	A	83	PRO	2.2
1	A	990	CYS	2.2
2	B	202	LEU	2.2
1	A	120	ALA	2.2
1	A	927	VAL	2.2
2	B	275	ARG	2.2
1	A	153	LYS	2.2
1	A	575	GLU	2.1
2	B	210	VAL	2.1
2	B	237	TYR	2.1
1	A	32	LEU	2.1
1	A	36	LYS	2.1
1	A	468	GLN	2.1
2	B	197	ASP	2.1
1	A	804	THR	2.1
2	B	25	PHE	2.1
2	B	274	LEU	2.1
1	A	412	ASP	2.1
1	A	482	PHE	2.1
1	A	880	PRO	2.1
3	G	13	THR	2.1
1	A	536	GLU	2.1
1	A	925	SER	2.0
2	B	155	MET	2.0
1	A	263	ASP	2.0
1	A	518	CYS	2.0
2	B	302	GLU	2.0
2	B	270	GLN	2.0
1	A	548	LEU	2.0
2	B	211	LEU	2.0
2	B	246	PRO	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

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
5	MG	A	2002	1/1	0.91	0.38	5.84	56,56,56,56	0
4	MF4	A	2001	5/5	0.95	0.26	2.03	59,61,62,62	0
8	CLR	B	3001	28/28	0.80	0.29	2.01	118,118,118,118	0
7	TL	A	2007[B]	1/1	0.99	0.07	-2.80	72,72,72,72	1
6	K	A	2006[A]	1/1	0.99	0.07	-2.80	72,72,72,72	1
6	K	A	2003[A]	1/1	0.98	0.10	-3.06	77,77,77,77	1
7	TL	A	2004[B]	1/1	0.98	0.10	-3.06	77,77,77,77	1
7	TL	A	2005	1/1	0.97	0.05	-5.75	77,77,77,77	0
9	NAG	B	4001	14/15	0.80	0.23	-	132,135,136,137	0
9	NAG	B	4021	14/15	0.71	0.63	-	138,139,139,139	0
9	NAG	B	4002	14/15	0.48	0.40	-	139,139,140,140	0

## 6.5 Other polymers

There are no such residues in this entry.