



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:38 PM GMT

PDB ID : 5AW9  
Title : Kinetics by X-ray crystallography: native E2.MgF42-.2K+ crystal for Rb+ bound crystals  
Authors : Ogawa, H.; Cornelius, F.; Hirata, A.; Toyoshima, C.  
Deposited on : 2015-07-01  
Resolution : 2.80 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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-20026982

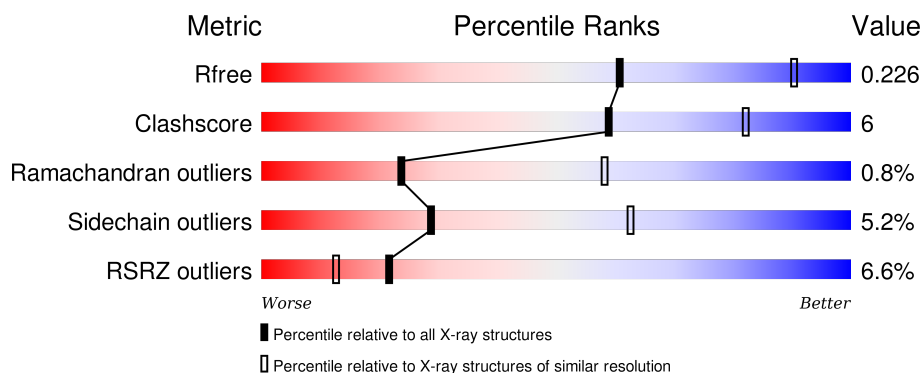
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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>5%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
2	B	305	<div> <div>11%</div> <div>72%</div> <div>14%</div> <div>• 12%</div> </div>
3	G	74	<div> <div>%</div> <div>45%</div> <div>8%</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

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 10362 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		

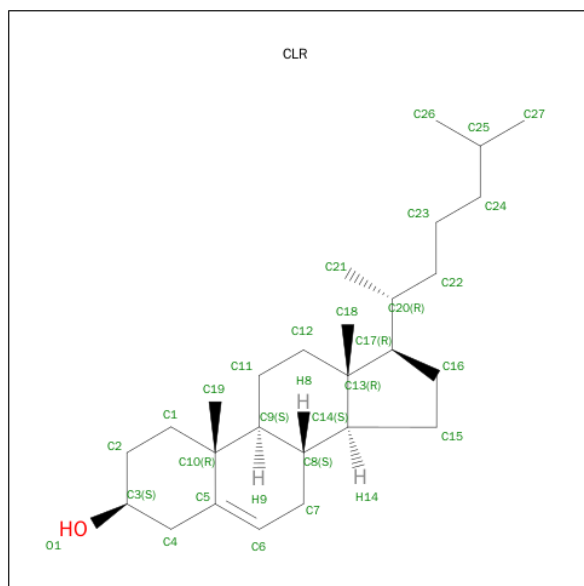
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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	3	Total	K		0	0
			3	3			

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



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

- Molecule 8 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

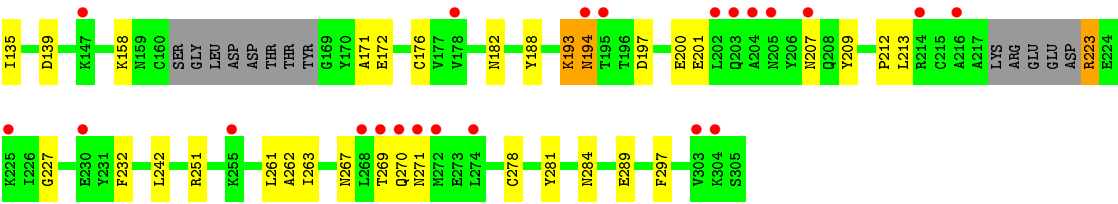
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	129	Total	O	0	0
			129	129		

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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A:
- 
- 5% 78% 17%
- 0 100
- MET GLY LYS GLY THR ALA SER ASP LYS TYR GLU PRO ALA ALA THR SER GLU ASN ALA THR LYS SER LYS LYS LYS GLY LYS LYS ASP LYS LYS ARG ASP L32 M41 L46 L51 H52 T57 D58 L59 T60 G62 L63 T64 H65 A66 L72 N78 S76

- Chain B:
- 
- 11% 72% 14% 12%
- MET ALA ARG GLY LYS SER LYS GLU THR ASP GLY GLY TRP LYS PHE LEU TRP ASP SER SER GLU LYS LYS LYS GLU P25 R28 W33 L68 V73 A74 P75 H80 S92 I93 S94 N95 P96 K97 S98 Y99 E100 M106 H107 M110 D111 M121 S122 P123 D126



● 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, $\alpha$ , $\beta$ , $\gamma$	219.97Å 50.67Å 163.07Å 90.00° 104.50° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 35.49 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.9 (15.00-2.80) 93.6 (35.49-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.217 , 0.265 0.218 , 0.226	Depositor DCC
$R_{free}$ test set	2049 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.9	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 40877 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10362	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: K, MG, MF4, NAG, 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	0.47	0/7825	0.68	1/10616 (0.0%)
2	B	0.51	0/2229	0.65	0/3002
3	G	0.52	0/309	0.66	0/419
All	All	0.48	0/10363	0.67	1/14037 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	670	LEU	CA-CB-CG	5.26	127.41	115.30

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	7675	0	7699	92	0
2	B	2174	0	2146	27	0
3	G	305	0	318	2	0
4	A	5	0	0	0	0
5	A	1	0	0	0	0
6	A	3	0	0	0	0
7	B	28	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	42	0	38	0	0
9	A	129	0	0	3	0
All	All	10362	0	10247	118	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 6.

All (118) 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	1.69	0.75
1:A:677:VAL:HG21	9:A:2222:HOH:O	1.89	0.73
1:A:935:ILE:HG23	1:A:944:ILE:HD12	1.72	0.71
1:A:61:ARG:HB3	1:A:61:ARG:HH11	1.55	0.70
1:A:52:HIS:HA	1:A:57:THR:HG23	1.73	0.70
1:A:78:ASN:HA	1:A:261:THR:HG23	1.74	0.70
1:A:766:ARG:HD2	1:A:832:MET:CE	2.28	0.64
1:A:64:THR:HG22	1:A:66:ALA:H	1.61	0.64
1:A:261:THR:HG21	9:A:2134:HOH:O	1.98	0.63
2:B:74:ALA:CB	2:B:75:PRO:HD3	2.29	0.62
1:A:261:THR:HG22	1:A:264:ARG:HH21	1.62	0.62
1:A:261:THR:HG22	1:A:264:ARG:NH2	2.15	0.62
1:A:994:TYR:HA	1:A:997:ILE:HG22	1.84	0.59
2:B:213:LEU:HD11	2:B:278:CYS:HB3	1.85	0.59
1:A:816:MET:O	1:A:820:ILE:HG12	2.02	0.59
1:A:670:LEU:HD23	1:A:678:LEU:HD21	1.85	0.58
1:A:246:SER:OG	1:A:267:MET:HG3	2.04	0.57
2:B:227:GLY:HA2	2:B:267:ASN:HB3	1.86	0.57
1:A:344:LEU:HB3	1:A:361:LEU:HG	1.86	0.57
1:A:359:LYS:HE2	1:A:746:ALA:O	2.06	0.56
1:A:868:SER:O	1:A:872:ILE:HG12	2.05	0.56
1:A:345:THR:HA	1:A:361:LEU:HD11	1.88	0.56
2:B:270:GLN:HG2	2:B:271:ASN:HD22	1.71	0.55
1:A:483:ASN:HB2	1:A:486:ASN:HB2	1.89	0.55
2:B:80:HIS:HB3	2:B:297:PHE:CZ	2.42	0.55
2:B:25:PHE:HB3	2:B:33:TRP:HE1	1.72	0.54
3:G:29:VAL:O	3:G:33:ILE:HG12	2.07	0.54
1:A:418:TRP:HZ2	1:A:463:CYS:HG	1.56	0.53
1:A:190:LEU:HD11	1:A:206:ILE:HD11	1.90	0.53
1:A:424:ILE:HG23	1:A:506:VAL:HB	1.91	0.53
1:A:417:THR:HA	1:A:522:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:HIS:CE1	1:A:59:LEU:HA	2.44	0.53
2:B:193:LYS:HA	2:B:207:ASN:HD21	1.73	0.52
1:A:631:VAL:HG23	1:A:633:ILE:HG12	1.92	0.52
1:A:351:MET:HA	1:A:354:LYS:HG2	1.91	0.52
1:A:87:PRO:HD2	1:A:90:ILE:HD12	1.92	0.52
1:A:392:TRP:HB3	1:A:588:LEU:HB2	1.92	0.51
1:A:106:ILE:O	1:A:110:LEU:HB2	2.10	0.51
1:A:921:SER:HA	1:A:983:LEU:HD11	1.93	0.51
2:B:158:LYS:HB2	2:B:232:PHE:CD1	2.46	0.51
2:B:107:HIS:O	2:B:111:ASP:HB2	2.11	0.51
2:B:106:MET:O	2:B:110:MET:HG2	2.11	0.50
1:A:818:PRO:HB3	1:A:934:LEU:HD22	1.92	0.50
1:A:339:THR:HG23	1:A:820:ILE:HD13	1.93	0.50
1:A:160:SER:HB3	1:A:741:VAL:HG22	1.93	0.50
1:A:766:ARG:HD2	1:A:832:MET:HE2	1.94	0.50
1:A:323:PHE:O	1:A:327:ILE:HG12	2.12	0.49
2:B:209:TYR:HA	2:B:242:LEU:HD22	1.93	0.49
1:A:475:PRO:HD2	1:A:494:GLU:HB2	1.94	0.49
1:A:714:VAL:HG23	1:A:728:ALA:HB2	1.95	0.49
1:A:596:ARG:HB2	1:A:599:VAL:HG23	1.94	0.48
1:A:871:VAL:HG22	2:B:58:LEU:HD13	1.94	0.48
1:A:110:LEU:HD22	1:A:324:LEU:HD12	1.95	0.48
1:A:940:ARG:HE	1:A:1023:TYR:HB2	1.79	0.48
1:A:847:GLU:H	1:A:847:GLU:CD	2.17	0.48
1:A:423:ARG:HG2	1:A:427:LEU:HD22	1.96	0.47
2:B:194:ASN:N	2:B:194:ASN:HD22	2.12	0.47
1:A:478:VAL:HG21	1:A:571:PHE:HB2	1.96	0.47
2:B:194:ASN:H	2:B:194:ASN:HD22	1.61	0.47
1:A:846:ASN:ND2	1:A:848:ARG:HB2	2.29	0.47
2:B:267:ASN:HB2	2:B:269:THR:HG22	1.96	0.47
1:A:502:ARG:HD2	1:A:503:TYR:H	1.79	0.47
2:B:188:TYR:O	2:B:284:ASN:ND2	2.48	0.47
1:A:93:CYS:HA	1:A:96:LEU:HD12	1.96	0.46
1:A:497:LYS:HE2	1:A:499:SER:HB2	1.98	0.46
1:A:304:VAL:O	1:A:308:ILE:HG12	2.15	0.46
1:A:905:GLN:NE2	2:B:182:ASN:HA	2.30	0.46
1:A:127:ASN:HB3	1:A:131:TYR:CD1	2.51	0.46
2:B:122:SER:HA	2:B:123:PRO:HA	1.76	0.46
1:A:301:PHE:O	1:A:305:SER:HB2	2.15	0.46
1:A:528:GLU:HB2	1:A:529:PRO:HD2	1.98	0.45
1:A:202:ASP:HB2	1:A:260:TYR:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:LEU:HD21	2:B:263:ILE:HD11	1.99	0.45
1:A:209:HIS:HB3	1:A:253:THR:HG22	1.99	0.45
2:B:223:ARG:HH11	2:B:223:ARG:HB2	1.82	0.45
1:A:675:THR:HA	1:A:678:LEU:HD12	1.98	0.44
3:G:21:VAL:O	3:G:25:ILE:HG12	2.18	0.44
1:A:866:PHE:O	1:A:869:TYR:HB3	2.17	0.44
1:A:170:LEU:HD23	1:A:192:GLU:HB3	1.99	0.44
2:B:74:ALA:CB	2:B:75:PRO:CD	2.96	0.44
1:A:933:ASP:HA	1:A:936:ILE:HG12	1.99	0.44
1:A:236:PRO:HA	1:A:239:THR:HG22	1.99	0.44
1:A:284:ILE:HG12	1:A:365:GLU:HG3	1.98	0.44
1:A:110:LEU:CD2	1:A:324:LEU:HD12	2.48	0.43
1:A:714:VAL:CG2	1:A:728:ALA:HB2	2.47	0.43
1:A:616:VAL:HG12	1:A:698:LYS:HG2	2.00	0.43
1:A:103:LEU:HD11	1:A:296:THR:HG23	2.01	0.43
1:A:204:ARG:NH1	1:A:229:PRO:O	2.45	0.43
1:A:270:ILE:HD12	1:A:695:PRO:HB2	2.00	0.43
1:A:46:LEU:HD12	1:A:51:LEU:HD12	2.00	0.43
2:B:212:PRO:HG2	2:B:281:TYR:HB2	2.00	0.43
1:A:426:ALA:O	1:A:471:ARG:HD2	2.18	0.43
2:B:232:PHE:HB2	2:B:262:ALA:HB3	2.01	0.42
1:A:418:TRP:HZ2	1:A:463:CYS:SG	2.42	0.42
1:A:889:ARG:HD3	1:A:889:ARG:HA	1.83	0.42
2:B:213:LEU:HD23	2:B:261:LEU:HD13	2.01	0.42
1:A:780:LEU:O	1:A:783:ASN:HB2	2.20	0.42
2:B:213:LEU:HD23	2:B:261:LEU:HD22	2.01	0.42
1:A:925:SER:O	1:A:929:VAL:HG22	2.20	0.42
1:A:592:ILE:O	1:A:594:PRO:HD3	2.20	0.42
1:A:784:ILE:HD11	1:A:854:TYR:CG	2.55	0.41
1:A:212:LYS:HB2	1:A:251:GLU:HG2	2.02	0.41
1:A:223:GLU:HB2	9:A:2191:HOH:O	2.21	0.41
1:A:291:PHE:HA	1:A:294:ILE:HD12	2.02	0.41
1:A:785:PRO:HB2	1:A:926:ILE:HD12	2.02	0.41
1:A:531:LYS:HE3	1:A:534:MET:HG2	2.01	0.41
1:A:431:ALA:O	1:A:471:ARG:NH2	2.40	0.41
1:A:702:VAL:HG13	1:A:712:VAL:HG21	2.01	0.41
1:A:502:ARG:HD2	1:A:503:TYR:N	2.36	0.41
1:A:517:ARG:HD3	1:A:580:THR:O	2.20	0.41
1:A:620:HIS:HA	1:A:621:PRO:HD3	1.93	0.41
1:A:64:THR:HA	1:A:174:ASP:OD1	2.21	0.41
1:A:631:VAL:CG2	1:A:633:ILE:HG12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:PHE:HB3	1:A:845:VAL:HB	2.03	0.40
1:A:618:GLY:O	1:A:692:ARG:HD2	2.21	0.40
1:A:905:GLN:HE21	2:B:182:ASN:HA	1.87	0.40
1:A:136:LEU:O	1:A:140:VAL:HG23	2.22	0.40
1:A:440:VAL:HG23	1:A:445:ARG:HB3	2.03	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%)	42 (4%)	6 (1%)	30	65
2	B	262/305 (86%)	227 (87%)	32 (12%)	3 (1%)	17	50
3	G	37/74 (50%)	32 (86%)	4 (11%)	1 (3%)	6	21
All	All	1289/1407 (92%)	1201 (93%)	78 (6%)	10 (1%)	24	58

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	74	ALA
1	A	524	ASN
2	B	201	GLU
1	A	121	THR
1	A	128	ASP
2	B	171	ALA
1	A	123	ASP
1	A	576	PRO
1	A	1014	GLY
3	G	5	GLY

### 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%)	29	62
2	B	234/266 (88%)	221 (94%)	13 (6%)	26	59
3	G	32/62 (52%)	31 (97%)	1 (3%)	47	81
All	All	1106/1197 (92%)	1048 (95%)	58 (5%)	29	62

All (58) 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	110	LEU
1	A	128	ASP
1	A	213	VAL
1	A	226	THR
1	A	231	PHE
1	A	245	PHE
1	A	248	ASN
1	A	261	THR
1	A	275	SER
1	A	284	ILE
1	A	309	LEU
1	A	318	LEU
1	A	344	LEU
1	A	354	LYS
1	A	413	LYS
1	A	434	GLN
1	A	457	LEU
1	A	513	ARG
1	A	515	LEU
1	A	524	ASN
1	A	530	LEU

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Mol	Chain	Res	Type
1	A	531	LYS
1	A	557	HIS
1	A	670	LEU
1	A	682	LEU
1	A	696	GLN
1	A	719	VAL
1	A	726	LYS
1	A	806	THR
1	A	811	ASP
1	A	822	LEU
1	A	833	LYS
1	A	847	GLU
1	A	880	PRO
1	A	886	LYS
1	A	968	LEU
1	A	974	THR
1	A	987	TRP
1	A	1019	GLN
2	B	28	ARG
2	B	73	VAL
2	B	135	ILE
2	B	139	ASP
2	B	172	GLU
2	B	176	CYS
2	B	193	LYS
2	B	194	ASN
2	B	197	ASP
2	B	200	GLU
2	B	223	ARG
2	B	251	ARG
2	B	289	GLU
3	G	4	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	129	ASN
1	A	225	GLN
1	A	524	ASN
1	A	540	ASN
1	A	577	ASN

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Mol	Chain	Res	Type
1	A	754	ASN
1	A	797	ASN
1	A	1019	GLN
2	B	194	ASN
2	B	207	ASN
2	B	258	GLN
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 9 ligands modelled in this entry, 4 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	-
7	CLR	B	3001	-	31,31,31	0.77	0	48,48,48	1.40	9 (18%)
8	NAG	B	4001	8,2	14,14,15	0.57	0	15,19,21	1.56	1 (6%)
8	NAG	B	4002	8	14,14,15	0.83	1 (7%)	15,19,21	1.95	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	B	4021	2	14,14,15	0.75	0	15,19,21	1.12	1 (6%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	4002	NAG	C1-C2	2.23	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	3001	CLR	C4-C5-C6	-2.71	116.13	120.60
7	B	3001	CLR	C21-C20-C22	-2.15	106.84	110.33
7	B	3001	CLR	C10-C9-C8	2.02	115.94	112.72
7	B	3001	CLR	C22-C20-C17	2.08	114.62	110.24
7	B	3001	CLR	C15-C14-C13	2.23	106.44	103.83
8	B	4021	NAG	C1-O5-C5	2.41	115.68	112.14
7	B	3001	CLR	C2-C1-C10	2.51	118.08	112.78
7	B	3001	CLR	C16-C17-C13	2.78	107.08	103.83
7	B	3001	CLR	C4-C5-C10	3.50	121.48	116.41
8	B	4002	NAG	C1-O5-C5	3.94	117.93	112.14
7	B	3001	CLR	C1-C2-C3	4.18	115.98	110.41
8	B	4001	NAG	C1-O5-C5	5.33	119.98	112.14
8	B	4002	NAG	C2-N2-C7	5.65	130.45	123.11

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	992/1028 (96%)	0.14	51 (5%) 32 21	46, 77, 133, 193	0
2	B	268/305 (87%)	0.66	34 (12%) 5 2	63, 123, 159, 173	0
3	G	39/74 (52%)	-0.21	1 (2%) 59 47	63, 75, 136, 153	0
All	All	1299/1407 (92%)	0.23	86 (6%) 22 13	46, 84, 149, 193	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	93	ILE	6.5
1	A	562	GLU	5.9
1	A	567	GLU	4.9
2	B	99	TYR	4.7
1	A	568	GLY	4.7
2	B	304	LYS	4.6
1	A	563	ASP	4.6
2	B	214	ARG	4.5
1	A	579	PRO	4.4
2	B	268	LEU	4.3
2	B	96	PRO	4.3
1	A	84	PRO	4.1
1	A	90	ILE	4.0
1	A	317	TRP	4.0
1	A	32	LEU	3.9
1	A	498	SER	3.8
1	A	503	TYR	3.8
1	A	566	ASN	3.8
1	A	534	MET	3.7
2	B	121	ASN	3.7
1	A	573	ALA	3.7
1	A	313	LEU	3.7
1	A	570	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	195	THR	3.7
2	B	202	LEU	3.6
1	A	574	ASP	3.6
2	B	25	PHE	3.6
1	A	578	PHE	3.5
1	A	571	PHE	3.4
2	B	123	PRO	3.4
2	B	194	ASN	3.3
2	B	271	ASN	3.2
1	A	126	ALA	3.2
2	B	216	ALA	3.1
1	A	89	TRP	3.0
1	A	779	THR	3.0
1	A	312	ILE	2.9
2	B	272	MET	2.9
2	B	204	ALA	2.8
1	A	127	ASN	2.8
2	B	100	GLU	2.8
2	B	230	GLU	2.8
1	A	675	THR	2.7
2	B	92	SER	2.7
1	A	120	ALA	2.7
1	A	530	LEU	2.7
1	A	815	ASP	2.7
1	A	502	ARG	2.6
2	B	97	LYS	2.6
2	B	225	LYS	2.6
2	B	203	GLN	2.6
2	B	269	THR	2.6
1	A	782	SER	2.6
2	B	270	GLN	2.5
1	A	122	GLU	2.5
2	B	147	LYS	2.5
1	A	41	MET	2.4
1	A	576	PRO	2.4
1	A	894	TRP	2.4
2	B	274	LEU	2.4
3	G	41	GLY	2.3
2	B	207	ASN	2.3
1	A	330	ALA	2.3
2	B	303	VAL	2.3
1	A	117	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	79	SER	2.3
1	A	1016	TRP	2.3
1	A	529	PRO	2.3
1	A	564	LYS	2.3
1	A	569	TYR	2.3
2	B	255	LYS	2.3
1	A	121	THR	2.2
1	A	580	THR	2.2
2	B	94	SER	2.2
1	A	113	LEU	2.2
1	A	439	ASN	2.2
2	B	205	ASN	2.2
2	B	80	HIS	2.1
1	A	86	THR	2.1
1	A	536	GLU	2.1
2	B	126	ASP	2.1
2	B	178	VAL	2.1
1	A	116	GLY	2.0
1	A	785	PRO	2.0
1	A	411	PHE	2.0
1	A	441	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
4	MF4	A	2001	5/5	0.97	0.30	2.03	48,48,50,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	K	A	2004	1/1	0.98	0.36	1.75	76,76,76,76	0
7	CLR	B	3001	28/28	0.89	0.20	0.23	105,113,128,129	0
5	MG	A	2002	1/1	0.98	0.24	-0.02	53,53,53,53	0
6	K	A	2003	1/1	0.97	0.32	-0.49	70,70,70,70	0
6	K	A	2005	1/1	0.98	0.16	-1.66	69,69,69,69	0
8	NAG	B	4001	14/15	0.91	0.26	-	122,139,146,150	0
8	NAG	B	4021	14/15	0.79	0.34	-	133,144,149,157	0
8	NAG	B	4002	14/15	0.62	0.46	-	121,153,160,161	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.