



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:22 AM BST

PDB ID : 5AW3  
Title : Kinetics by X-ray crystallography: Tl<sup>+</sup>-substitution of bound K<sup>+</sup> in the E2.MgF42-.2K<sup>+</sup> crystal after 100 min  
Authors : Ogawa, H.; Cornelius, F.; Hirata, A.; Toyoshima, C.  
Deposited on : 2015-07-01  
Resolution : 3.35 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

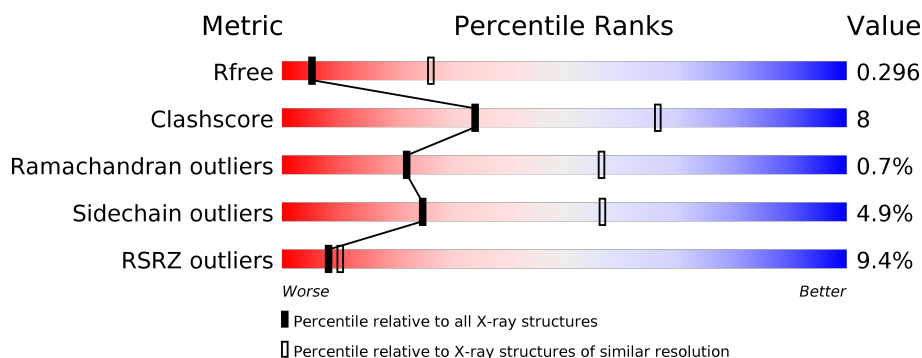
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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))
$R_{free}$	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 respectively. 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> <div></div> <div>75%</div> <div>21%</div> <div>• •</div> </div> </div>
2	B	305	<div> <div>12%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>• 12%</div> </div> </div>
3	G	74	<div> <div>3%</div> <div> <div></div> <div>36%</div> <div>16%</div> <div>47%</div> </div> </div>
4	C	2	<div> <div></div> <div>100%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	B	4021	-	-	-	X
4	NAG	C	2	-	-	-	X
6	MG	A	2002	-	-	-	X
9	CLR	B	3001	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 10235 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.

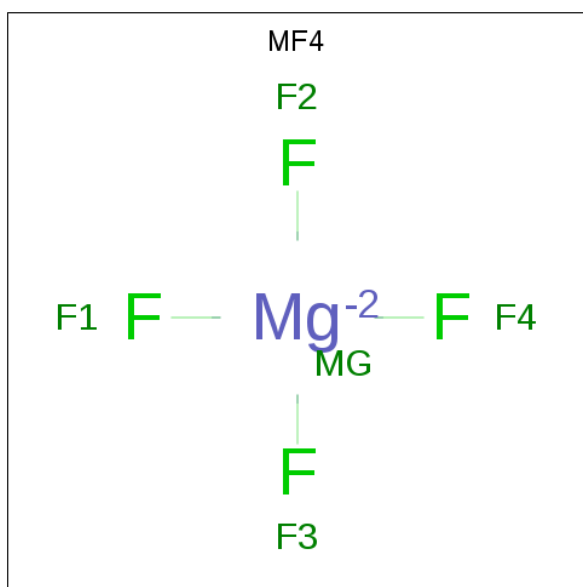
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	39	Total	C	N	O	S	0	0	0
			305	200	50	54	1			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 5 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F<sub>4</sub>Mg).



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Tl	0	1
			3	3		

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	K	0	1
			1	1		

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



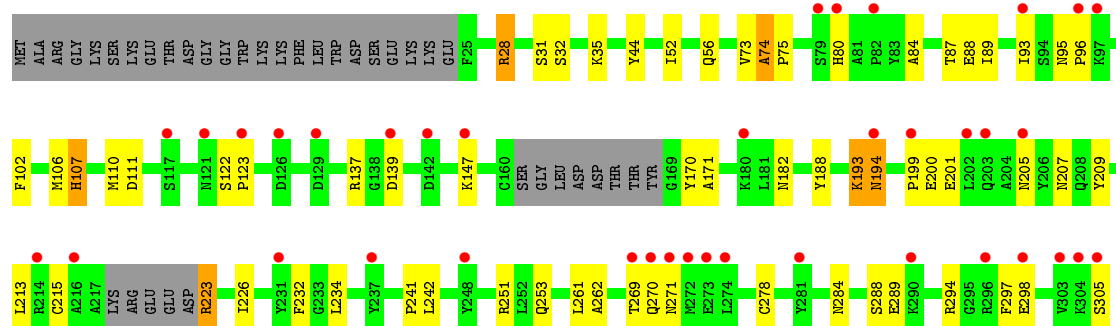
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is water.

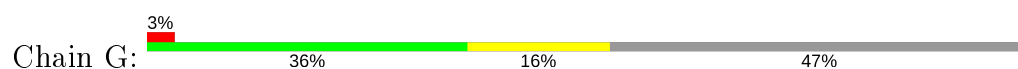
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	O	0	0
			1	1		







- Molecule 3: Phospholemman-like protein



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.18Å 50.86Å 164.25Å 90.00° 104.17° 90.00°	Depositor
Resolution (Å)	14.97 – 3.35 39.15 – 3.35	Depositor EDS
% Data completeness (in resolution range)	85.6 (14.97-3.35) 93.3 (39.15-3.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 3.32Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.302 , 0.313 0.287 , 0.296	Depositor DCC
$R_{free}$ test set	731 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	98.6	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	10235	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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: 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	0.36	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 [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	123	0
2	B	2174	0	2146	45	0
3	G	305	0	318	8	0
4	C	28	0	25	0	0
5	A	5	0	0	0	0
6	A	1	0	0	0	0
7	A	3	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	46	1	0
10	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	1	0	0	0	0
All	All	10235	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	1.65	0.79
1:A:905:GLN:NE2	2:B:182:ASN:HA	1.98	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	0.68
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	1.77	0.65
1:A:935:ILE:HG23	1:A:944:ILE:HD12	1.77	0.65
1:A:78:ASN:HA	1:A:261:THR:HG23	1.79	0.64
1:A:160:SER:HB3	1:A:741:VAL:HG22	1.80	0.63
1:A:816:MET:O	1:A:820:ILE:HG12	1.97	0.63
2:B:74:ALA:CB	2:B:75:PRO:HD3	2.23	0.63
1:A:52:HIS:HA	1:A:57:THR:HG23	1.80	0.63
2:B:28:ARG:NH1	9:B:3001:CLR:H22	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:O	1:A:110:LEU:HB2	2.03	0.59
3:G:21:VAL:O	3:G:25:ILE:HG12	2.02	0.59
1:A:212:LYS:HB2	1:A:251:GLU:HG2	1.85	0.59
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
2:B:75:PRO:HG2	2:B:294:ARG:HH21	1.68	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
2:B:74:ALA:HB3	2:B:75:PRO:CD	2.29	0.57
1:A:818:PRO:HB3	1:A:934:LEU:HD22	1.87	0.56
2:B:137:ARG:HD2	2:B:147:LYS:HB3	1.87	0.56
2:B:52:ILE:O	2:B:56:GLN:HG2	2.05	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	0.56
1:A:190:LEU:HD11	1:A:206:ILE:HD11	1.88	0.55
2:B:93:ILE:H	2:B:305:SER:HB2	1.71	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
1:A:351:MET:HA	1:A:354:LYS:HG2	1.89	0.55
1:A:596:ARG:HB2	1:A:599:VAL:HG23	1.89	0.55
1:A:261:THR:HG22	1:A:264:ARG:HH21	1.71	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:64:THR:HG22	1:A:66:ALA:N	2.23	0.54
1:A:921:SER:HA	1:A:983:LEU:HD11	1.90	0.53
1:A:424:ILE:HG23	1:A:506:VAL:HB	1.90	0.53
2:B:213:LEU:HD23	2:B:261:LEU:HD13	1.89	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:1016:TRP:HE1	2:B:35:LYS:HE3	1.73	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:766:ARG:HD2	1:A:832:MET:HE2	1.91	0.52
1:A:956:PHE:CE1	3:G:38:LEU:HD22	2.44	0.52
1:A:212:LYS:HD3	1:A:224:PRO:HB2	1.90	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	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:571:PHE:HA	1:A:577:ASN:HD22	1.76	0.50
1:A:359:LYS:HE2	1:A:746:ALA:O	2.12	0.49
1:A:826:GLN:HE22	1:A:950:LYS:HE3	1.78	0.49
2:B:232:PHE:HB2	2:B:262:ALA:HB3	1.93	0.49
1:A:1005:ARG:NH1	1:A:1006:ARG:HG3	2.28	0.49
1:A:905:GLN:HE21	2:B:182:ASN:HA	1.73	0.48
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	0.47
1:A:323:PHE:CE1	1:A:793:PHE:HE2	2.32	0.47
1:A:132:LEU:HD21	1:A:804:THR:HG21	1.97	0.47
1:A:171:VAL:HG12	1:A:191:VAL:HG22	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:87:THR:HB	2:B:298:GLU:O	2.14	0.47
3:G:31:CYS:O	3:G:35:ILE:HG12	2.14	0.47
2:B:80:HIS:HB3	2:B:297:PHE:CZ	2.50	0.47
1:A:924:ILE:HD12	1:A:983:LEU:CD1	2.45	0.46
1:A:127:ASN:HB3	1:A:131:TYR:CD1	2.50	0.46
1:A:336:LEU:HD11	1:A:776:ILE:HG12	1.96	0.46
2:B:226:ILE:HG22	2:B:269:THR:HB	1.96	0.46
2:B:122:SER:HA	2:B:123:PRO:HA	1.75	0.46
2:B:215:CYS:HA	2:B:278:CYS:HA	1.96	0.46
1:A:631:VAL:HG23	1:A:633:ILE:HG12	1.96	0.46
1:A:63:LEU:HD22	1:A:189:ASP:HB3	1.97	0.46
1:A:303:GLY:HA2	1:A:327:ILE:HG21	1.97	0.46
1:A:670:LEU:HD23	1:A:678:LEU:HD21	1.96	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	1.98	0.45
1:A:889:ARG:HD2	1:A:895:ILE:CD1	2.46	0.45
1:A:676:GLU:H	1:A:676:GLU:CD	2.20	0.45
2:B:84:ALA:HB1	2:B:88:GLU:N	2.32	0.45
1:A:631:VAL:CG2	1:A:633:ILE:HG12	2.46	0.45
1:A:722:SER:OG	1:A:723:PRO:HD3	2.17	0.45
1:A:847:GLU:H	1:A:847:GLU:CD	2.20	0.45
1:A:915:GLU:O	1:A:918:CYS:HB2	2.17	0.44
1:A:52:HIS:HE2	1:A:59:LEU:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:246:SER:OG	1:A:267:MET:HG3	2.18	0.44
2:B:234:LEU:HG	2:B:241:PRO:HG3	1.99	0.44
2:B:107:HIS:O	2:B:111:ASP:HB2	2.18	0.43
2:B:107:HIS:ND1	2:B:170:TYR:HE1	2.17	0.43
1:A:273:LEU:O	1:A:277:LEU:HG	2.19	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
2:B:147:LYS:HB2	2:B:253:GLN:HG3	1.99	0.43
3:G:4:GLU:CD	3:G:5:GLY:H	2.22	0.43
1:A:87:PRO:HD2	1:A:90:ILE:HD12	1.99	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	2.00	0.42
1:A:170:LEU:HD21	1:A:177:LYS:HD3	2.00	0.42
1:A:291:PHE:HA	1:A:294:ILE:HD12	2.01	0.42
2:B:188:TYR:O	2:B:284:ASN:ND2	2.53	0.42
1:A:291:PHE:HB3	1:A:845:VAL:HB	2.02	0.42
2:B:74:ALA:CB	2:B:75:PRO:CD	2.92	0.42
2:B:223:ARG:HB2	2:B:223:ARG:HH11	1.84	0.42
2:B:89:ILE:HG22	2:B:102:PHE:CE2	2.55	0.42
2:B:95:ASN:HA	2:B:96:PRO:HD3	1.86	0.42
1:A:784:ILE:N	1:A:785:PRO:HD2	2.35	0.42
2:B:137:ARG:HB3	2:B:147:LYS:HD2	2.01	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	0.42
1:A:502:ARG:HE	1:A:562:GLU:HG2	1.85	0.41
1:A:367:LEU:HD23	1:A:761:GLY:HA3	2.01	0.41
1:A:110:LEU:CD2	1:A:324:LEU:HD12	2.50	0.41
1:A:48:LEU:HD23	1:A:59:LEU:HD11	2.01	0.41
2:B:271:ASN:HD21	2:B:305:SER:N	2.18	0.41
1:A:785:PRO:HB2	1:A:926:ILE:CD1	2.50	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ALA:O	1:A:471:ARG:HD2	2.20	0.41
1:A:44:HIS:HB3	1:A:242:ILE:HD11	2.03	0.41
1:A:540:ASN:N	1:A:540:ASN:HD22	2.18	0.41
1:A:647:ARG:HH21	1:A:648:LEU:HD11	1.86	0.41
1:A:284:ILE:O	1:A:288:ILE:HG12	2.21	0.41
1:A:301:PHE:O	1:A:305:SER:HB2	2.20	0.41
1:A:458:LYS:O	1:A:462:LEU:HB2	2.21	0.41
1:A:423:ARG:O	1:A:427:LEU:HB2	2.21	0.41
1:A:502:ARG:HG3	1:A:562:GLU:HG2	2.02	0.41
1:A:702:VAL:HG13	1:A:712:VAL:HG21	2.03	0.41
1:A:354:LYS:HE2	1:A:760:THR:HB	2.02	0.40
1:A:831:ILE:O	1:A:834:ARG:HG2	2.22	0.40
1:A:900:ASP:OD1	1:A:904:GLN:HB2	2.21	0.40
1:A:925:SER:O	1:A:929:VAL:HG22	2.22	0.40
1:A:199:ILE:HG22	1:A:201:ALA:O	2.22	0.40
1:A:859:MET:HG2	2:B:44:TYR:CE2	2.56	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%)	29	63
2	B	262/305 (86%)	223 (85%)	35 (13%)	4 (2%)	10	39
3	G	37/74 (50%)	33 (89%)	4 (11%)	0	100	100
All	All	1289/1407 (92%)	1198 (93%)	82 (6%)	9 (1%)	22	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	THR

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Mol	Chain	Res	Type
1	A	128	ASP
1	A	576	PRO
2	B	74	ALA
2	B	171	ALA
2	B	201	GLU
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%)	23	55
2	B	234/266 (88%)	224 (96%)	10 (4%)	29	60
3	G	32/62 (52%)	32 (100%)	0	100	100
All	All	1106/1197 (92%)	1052 (95%)	54 (5%)	25	57

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

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Mol	Chain	Res	Type
1	A	250	VAL
1	A	255	ARG
1	A	261	THR
1	A	284	ILE
1	A	309	LEU
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
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 ⓘ

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 ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	1	2,4	14,14,15	0.48	0	17,19,21	0.93	1 (5%)
4	NAG	C	2	4	14,14,15	0.65	0	17,19,21	1.41	1 (5%)

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	NAG	C	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2	NAG	C2-N2-C7	3.92	128.48	122.90
4	C	1	NAG	C1-O5-C5	2.67	115.81	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	NAG	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	C	2	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 5 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	$\# Z  > 2$
10	NAG	B	4021	2	14,14,15	0.59	0	17,19,21	1.25	2 (11%)
5	MF4	A	2001	1	0,4,4	0.00	-	-		
9	CLR	B	3001	-	31,31,31	0.46	0	48,48,48	1.10	5 (10%)

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
10	NAG	B	4021	2	-	0/6/23/26	0/1/1/1
9	CLR	B	3001	-	-	2/10/68/68	0/4/4/4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	3001	CLR	C15-C14-C13	2.95	107.39	103.84
10	B	4021	NAG	C1-O5-C5	2.60	115.72	112.19
9	B	3001	CLR	C1-C2-C3	2.56	113.76	110.47
9	B	3001	CLR	C4-C5-C6	-2.51	116.99	120.61
9	B	3001	CLR	C4-C5-C10	2.44	119.66	116.42
10	B	4021	NAG	C4-C3-C2	2.34	114.45	111.02
9	B	3001	CLR	C12-C11-C9	2.08	116.72	113.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

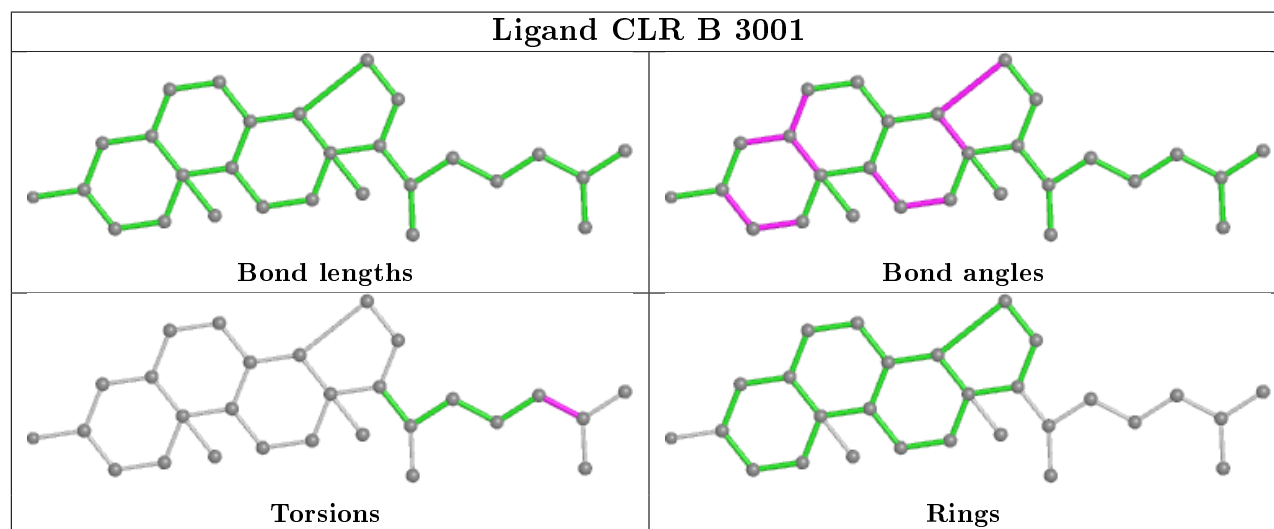
Mol	Chain	Res	Type	Atoms
9	B	3001	CLR	C23-C24-C25-C26
9	B	3001	CLR	C23-C24-C25-C27

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	3001	CLR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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%) 11 13	105, 126, 167, 192	0
2	B	268/305 (87%)	0.76	38 (14%) 2 3	125, 176, 200, 210	0
3	G	39/74 (52%)	0.25	2 (5%) 28 30	121, 130, 174, 177	0
All	All	1299/1407 (92%)	0.60	122 (9%) 8 10	105, 131, 188, 210	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	579	PRO	7.0
1	A	79	SER	7.0
1	A	573	ALA	6.1
1	A	260	TYR	5.7
1	A	530	LEU	5.5
1	A	183	GLU	5.3
1	A	578	PHE	5.1
1	A	571	PHE	5.1
2	B	123	PRO	5.0
1	A	580	THR	4.9
1	A	534	MET	4.9
1	A	504	LEU	4.7
1	A	57	THR	4.6
1	A	72	LEU	4.5
1	A	894	TRP	4.3
1	A	41	MET	4.2
1	A	815	ASP	4.2
2	B	214	ARG	4.2
1	A	42	ASP	4.0
1	A	86	THR	4.0
1	A	185	VAL	3.9
1	A	567	GLU	3.9
2	B	298	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	563	ASP	3.8
1	A	503	TYR	3.8
1	A	779	THR	3.7
1	A	585	PHE	3.7
2	B	121	ASN	3.6
1	A	533	ASP	3.6
1	A	90	ILE	3.6
2	B	216	ALA	3.5
2	B	270	GLN	3.4
2	B	272	MET	3.4
2	B	79	SER	3.4
1	A	427	LEU	3.3
1	A	562	GLU	3.3
1	A	880	PRO	3.3
2	B	303	VAL	3.3
2	B	93	ILE	3.3
2	B	180	LYS	3.2
1	A	78	ASN	3.2
2	B	273	GLU	3.2
2	B	305	SER	3.1
2	B	194	ASN	3.1
1	A	426	ALA	3.1
2	B	80	HIS	3.0
1	A	568	GLY	2.9
2	B	274	LEU	2.9
1	A	814	THR	2.9
1	A	186	VAL	2.9
1	A	84	PRO	2.8
1	A	317	TRP	2.8
1	A	528	GLU	2.8
1	A	565	TYR	2.8
1	A	883	LEU	2.8
1	A	782	SER	2.7
2	B	271	ASN	2.7
2	B	129	ASP	2.7
2	B	199	PRO	2.7
1	A	480	ILE	2.7
1	A	87	PRO	2.6
1	A	778	TYR	2.6
2	B	290	LYS	2.6
1	A	77	PRO	2.6
1	A	75	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	781	THR	2.6
2	B	203	GLN	2.6
1	A	660	ALA	2.5
1	A	1002	ASP	2.5
1	A	220	GLY	2.5
2	B	237	TYR	2.4
1	A	312	ILE	2.4
1	A	505	LEU	2.4
2	B	126	ASP	2.4
1	A	55	TYR	2.4
1	A	896	SER	2.4
1	A	521	ILE	2.4
1	A	439	ASN	2.4
2	B	202	LEU	2.4
1	A	529	PRO	2.4
1	A	576	PRO	2.4
2	B	147	LYS	2.4
2	B	142	ASP	2.4
1	A	654	GLN	2.3
1	A	930	GLN	2.3
1	A	675	THR	2.3
1	A	99	GLY	2.3
1	A	538	PHE	2.3
1	A	574	ASP	2.3
2	B	231	TYR	2.3
1	A	223	GLU	2.3
1	A	76	GLY	2.3
1	A	189	ASP	2.3
1	A	446	SER	2.3
1	A	206	ILE	2.3
3	G	14	TYR	2.3
1	A	171	VAL	2.3
2	B	96	PRO	2.3
1	A	98	GLY	2.2
1	A	80	LEU	2.2
1	A	82	PRO	2.2
2	B	304	LYS	2.2
2	B	296	ARG	2.2
2	B	248	TYR	2.2
1	A	493	HIS	2.2
1	A	492	ILE	2.2
2	B	139	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	G	15	ASP	2.2
1	A	813	GLY	2.2
1	A	558	PHE	2.1
1	A	378	THR	2.1
2	B	82	PRO	2.1
1	A	909	GLU	2.1
1	A	443	LEU	2.1
2	B	117	SER	2.1
2	B	281	TYR	2.1
2	B	97	LYS	2.1
1	A	85	THR	2.1
2	B	205	ASN	2.1
2	B	269	THR	2.0
1	A	91	LYS	2.0
1	A	36	LYS	2.0

## 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](#)

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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	C	2	14/15	0.47	0.41	189,190,190,191	0
4	NAG	C	1	14/15	0.88	0.28	183,185,186,188	0

## 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. 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.

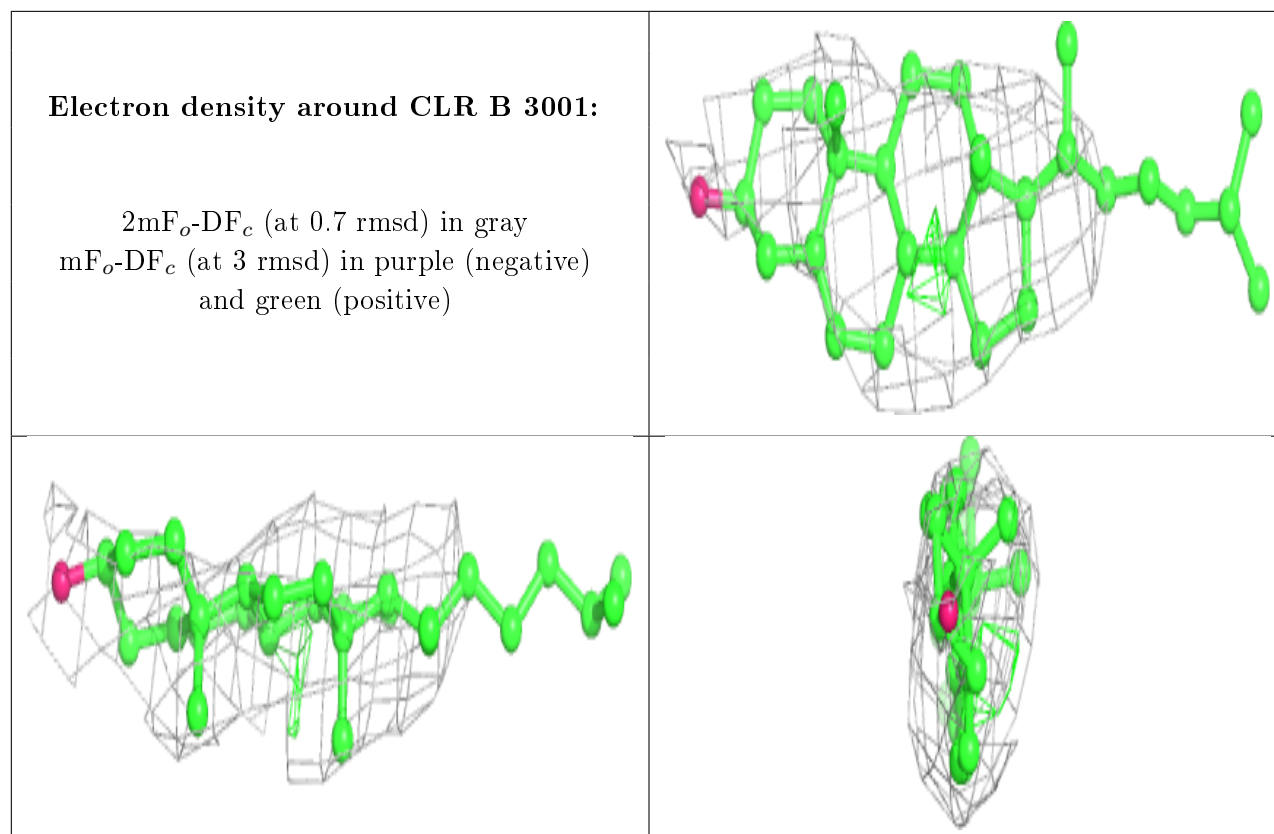
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	NAG	B	4021	14/15	0.70	0.60	188,189,189,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	A	2002	1/1	0.71	0.49	106,106,106,106	0
9	CLR	B	3001	28/28	0.77	0.41	168,168,169,169	0
5	MF4	A	2001	5/5	0.88	0.50	110,111,112,113	0
7	TL	A	2003	1/1	0.96	0.08	127,127,127,127	0
7	TL	A	2006[B]	1/1	0.96	0.04	123,123,123,123	1
8	K	A	2005[A]	1/1	0.96	0.04	123,123,123,123	1
7	TL	A	2004	1/1	0.97	0.14	127,127,127,127	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.