



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:57 PM GMT

PDB ID : 5AVY
Title : Kinetics by X-ray crystallography: Tl⁺-substitution of bound K⁺ in the E2.MgF₄2-.2K⁺ crystal after 20 min
Authors : Ogawa, H.; Cornelius, F.; Hirata, A.; Toyoshima, C.
Deposited on : 2015-07-01
Resolution : 3.45 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

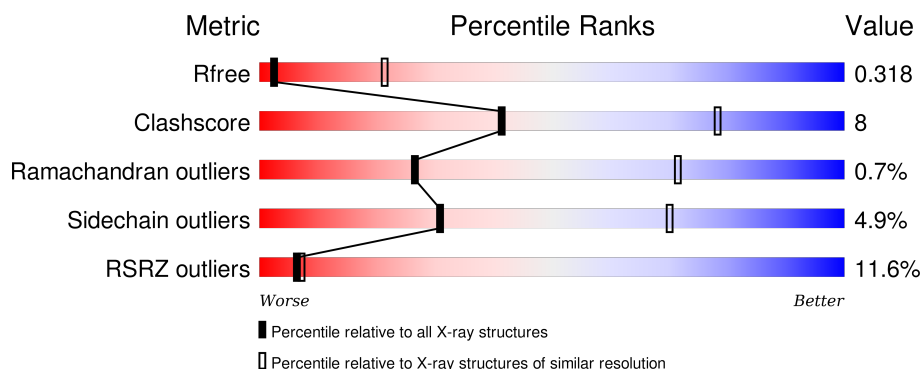
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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 ≥ 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>10%</div> <div>74%</div> <div>21%</div> <div>• •</div> </div>
2	B	305	<div> <div>15%</div> <div>67%</div> <div>19%</div> <div>• 12%</div> </div>
3	G	74	<div> <div>%</div> <div>35%</div> <div>18%</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

2 Entry composition [i](#)

There are 10 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⁺,K⁺-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: F₄Mg).



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

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

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

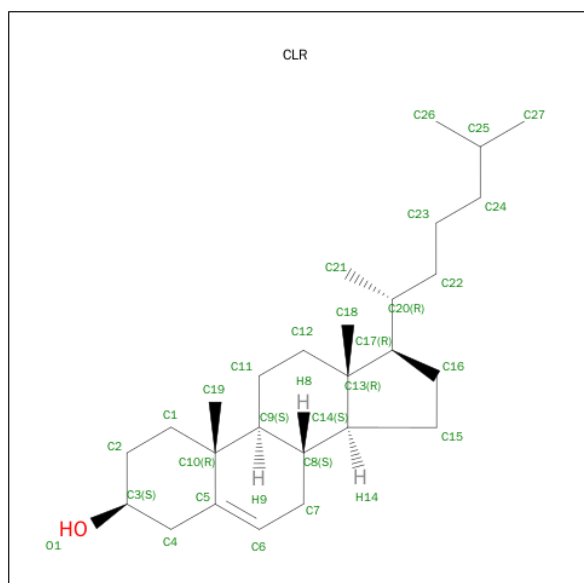
- Molecule 6 is THALLIUM (I) ION (three-letter code: TL) (formula: Tl).

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

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



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

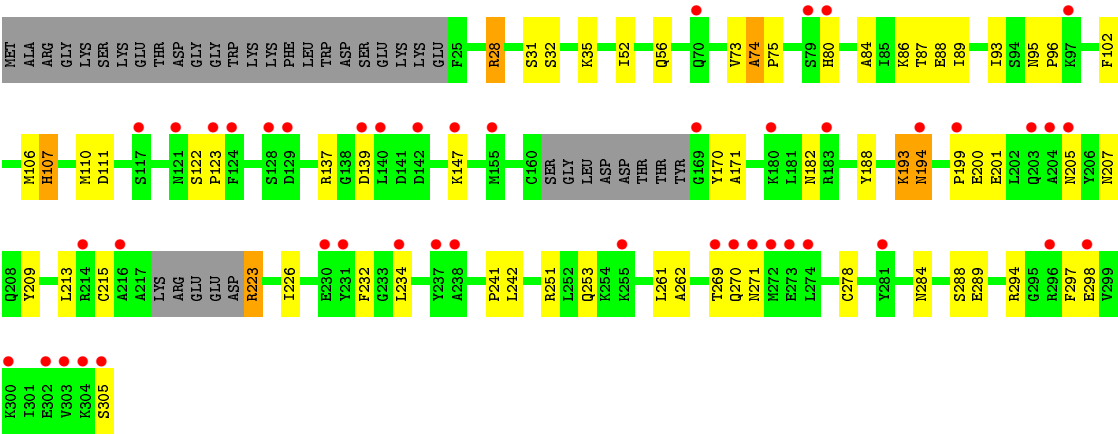
- Molecule 9 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



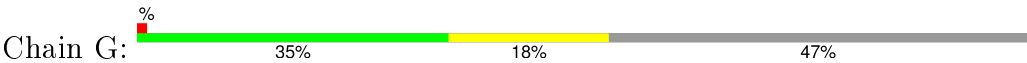
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		

- 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, α , β , γ	220.59Å 50.67Å 163.92Å 90.00° 103.63° 90.00°	Depositor
Resolution (Å)	14.94 – 3.45 38.92 – 3.45	Depositor EDS
% Data completeness (in resolution range)	85.6 (14.94-3.45) 93.8 (38.92-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.308 , 0.305 0.306 , 0.318	Depositor DCC
R_{free} test set	666 reflections (3.11%)	DCC
Wilson B-factor (Å ²)	107.8	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 67.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 23463 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10235	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.36	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

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	125	1
2	B	2174	0	2146	45	0
3	G	305	0	318	10	0
4	A	5	0	0	0	0
5	A	1	0	0	0	0
6	A	3	0	0	0	0
7	A	1	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	10235	0	10247	173	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (173) 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:497:LYS:HE2	1:A:499:SER:HB2	1.68	0.76
1:A:868:SER:O	1:A:872:ILE:HG12	1.86	0.75
1:A:905:GLN:NE2	2:B:182:ASN:HA	2.00	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	0.72
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	1.78	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
2:B:28:ARG:NH1	8:B:3001:CLR:H22	2.12	0.64
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:160:SER:HB3	1:A:741:VAL:HG22	1.80	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	2.00	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	0.61
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:270:GLN:HG2	2:B:271:ASN:ND2	2.16	0.60
2:B:31:SER:O	2:B:35:LYS:HG3	2.01	0.60
1:A:344:LEU:HB3	1:A:361:LEU:HG	1.85	0.59
2:B:84:ALA:HB1	2:B:88:GLU:H	1.67	0.59
1:A:392:TRP:HB3	1:A:588:LEU:HB2	1.84	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
1:A:106:ILE:O	1:A:110:LEU:HB2	2.03	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	0.58

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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
1:A:1016:TRP:HE1	2:B:35:LYS:HE3	1.68	0.57
2:B:193:LYS:HA	2:B:207:ASN:ND2	2.20	0.57
1:A:491:SER:HB3	1:A:493:HIS:NE2	2.19	0.57
2:B:74:ALA:HB3	2:B:75:PRO:CD	2.29	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:818:PRO:HB3	1:A:934:LEU:HD22	1.87	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	1.72	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:596:ARG:HB2	1:A:599:VAL:HG23	1.89	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	0.54
1:A:994:TYR:HA	1:A:997:ILE:HG22	1.89	0.54
1:A:924:ILE:HD12	1:A:983:LEU:HD12	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	0.54
1:A:51:LEU:CD1	1:A:204:ARG:HG3	2.36	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: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:956:PHE:CE1	3:G:38:LEU:HD22	2.44	0.52
1:A:766:ARG:HD2	1:A:832:MET:HE2	1.91	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:161:PHE:HA	1:A:164:MET:HE3	1.92	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
3:G:25:ILE:O	3:G:29:VAL:HG23	2.11	0.51
1:A:788:THR:N	1:A:789:PRO:HD2	2.26	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:826:GLN:HE22	1:A:950:LYS:HE3	1.78	0.49

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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: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
2:B:87:THR:HB	2:B:298:GLU:O	2.14	0.47
1:A:132:LEU:HD21	1:A:804:THR:HG21	1.96	0.47
1:A:797:ASN:HD22	1:A:887:ARG:HD3	1.79	0.47
1:A:171:VAL:HG12	1:A:191:VAL:HG22	1.97	0.47
1:A:814:THR:HB	1:A:961:GLU:HG3	1.96	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:127:ASN:HB3	1:A:131:TYR:CD1	2.50	0.47
1:A:336:LEU:HD11	1:A:776:ILE:HG12	1.96	0.47
1:A:985:PRO:HD3	3:G:19:LEU:HD11	1.97	0.46
1:A:924:ILE:HD12	1:A:983:LEU:CD1	2.45	0.46
1:A:631:VAL:HG23	1:A:633:ILE:HG12	1.96	0.46
2:B:226:ILE:HG22	2:B:269:THR:HB	1.96	0.46
2:B:215:CYS:HA	2:B:278:CYS:HA	1.96	0.46
2:B:122:SER:HA	2:B:123:PRO:HA	1.76	0.46
1:A:63:LEU:HD22	1:A:189:ASP:HB3	1.96	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:905:GLN:HE21	2:B:182:ASN:HA	1.78	0.45
1:A:303:GLY:HA2	1:A:327:ILE:HG21	1.97	0.45
1:A:475:PRO:HD2	1:A:494:GLU:HB2	1.98	0.45
1:A:209:HIS:HB3	1:A:253:THR:HG22	1.98	0.45
1:A:889:ARG:HD2	1:A:895:ILE:CD1	2.46	0.45
2:B:84:ALA:HB1	2:B:88:GLU:N	2.31	0.45
1:A:631:VAL:CG2	1:A:633:ILE:HG12	2.46	0.45
1:A:676:GLU:H	1:A:676:GLU:CD	2.20	0.45
1:A:847:GLU:H	1:A:847:GLU:CD	2.20	0.45
1:A:722:SER:OG	1:A:723:PRO:HD3	2.17	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:234:LEU:HG	2:B:241:PRO:HG3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:TRP:CH2	2:B:86:LYS:HG2	2.53	0.44
1:A:246:SER:OG	1:A:267:MET:HG3	2.18	0.43
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:956:PHE:CD1	3:G:38:LEU:HD22	2.54	0.43
1:A:790:PHE:O	1:A:794:ILE:HG12	2.19	0.43
2:B:147:LYS:HB2	2:B:253:GLN:HG3	1.99	0.43
1:A:87:PRO:HD2	1:A:90:ILE:HD12	1.99	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
3:G:4:GLU:CD	3:G:5:GLY:H	2.23	0.43
1:A:300:VAL:O	1:A:304:VAL:HG22	2.19	0.42
2:B:74:ALA:CB	2:B:75:PRO:CD	2.92	0.42
1:A:64:THR:HA	1:A:174:ASP:OD1	2.19	0.42
1:A:797:ASN:HB3	1:A:885:GLY:HA2	2.00	0.42
1:A:661:LYS:HA	1:A:661:LYS:HE2	2.00	0.42
1:A:940:ARG:HE	1:A:1023:TYR:HB2	1.84	0.42
1:A:170:LEU:HD21	1:A:177:LYS:HD3	2.00	0.42
2:B:223:ARG:HH11	2:B:223:ARG:HB2	1.84	0.42
2:B:95:ASN:HA	2:B:96:PRO:HD3	1.86	0.42
2:B:188:TYR:O	2:B:284:ASN:ND2	2.53	0.42
1:A:291:PHE:HA	1:A:294:ILE:HD12	2.01	0.42
1:A:291:PHE:HB3	1:A:845:VAL:HB	2.02	0.42
2:B:89:ILE:HG22	2:B:102:PHE:CE2	2.55	0.42
1:A:784:ILE:N	1:A:785:PRO:HD2	2.35	0.42
1:A:378:THR:HA	1:A:382:THR:OG1	2.20	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:367:LEU:HD23	1:A:761:GLY:HA3	2.01	0.42
1:A:502:ARG:HE	1:A:562:GLU:HG2	1.85	0.41
1:A:48:LEU:HD23	1:A:59:LEU:HD11	2.01	0.41
1:A:920:THR:HG21	1:A:981:TYR:O	2.20	0.41
1:A:846:ASN:ND2	1:A:848:ARG:HB2	2.35	0.41
1:A:110:LEU:CD2	1:A:324:LEU:HD12	2.50	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:44:HIS:HB3	1:A:242:ILE:HD11	2.02	0.41
1:A:426:ALA:O	1:A:471:ARG:HD2	2.20	0.41
1:A:342:VAL:HB	1:A:820:ILE:HD12	2.03	0.41
3:G:17:TYR:O	3:G:21:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ASN:N	1:A:540:ASN:HD22	2.18	0.41
1:A:458:LYS:O	1:A:462:LEU:HB2	2.21	0.41
1:A:502:ARG:HG3	1:A:562:GLU:HG2	2.02	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:301:PHE:O	1:A:305:SER:HB2	2.20	0.41
1:A:284:ILE:O	1:A:288:ILE:HG12	2.21	0.41
1:A:702:VAL:HG13	1:A:712:VAL:HG21	2.03	0.41
1:A:900:ASP:OD1	1:A:904:GLN:HB2	2.21	0.40
1:A:831:ILE:O	1:A:834:ARG:HG2	2.22	0.40
1:A:354:LYS:HE2	1:A:760:THR:HB	2.02	0.40
1:A:613:VAL:HG12	1:A:633:ILE:HD12	2.04	0.40
1:A:925:SER:O	1:A:929:VAL:HG22	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:NH2	1:A:648:LEU:O[1_565]	2.07	0.13

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%)	34	77
2	B	262/305 (86%)	223 (85%)	35 (13%)	4 (2%)	13	54
3	G	37/74 (50%)	33 (89%)	4 (11%)	0	100	100
All	All	1289/1407 (92%)	1198 (93%)	82 (6%)	9 (1%)	26	71

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
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%)	29	68
2	B	234/266 (88%)	224 (96%)	10 (4%)	35	74
3	G	32/62 (52%)	32 (100%)	0	100	100
All	All	1106/1197 (92%)	1052 (95%)	54 (5%)	31	70

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 (22) 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	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 10 ligands modelled in this entry, 5 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	0.44	0	48,48,48	1.06	4 (8%)
9	NAG	B	4001	9,2	14,14,15	0.49	0	15,19,21	0.93	1 (6%)
9	NAG	B	4002	9	14,14,15	0.63	0	15,19,21	1.43	1 (6%)
9	NAG	B	4021	2	14,14,15	0.58	0	15,19,21	1.08	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
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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	3001	CLR	C4-C5-C6	-2.19	116.99	120.60
8	B	3001	CLR	C4-C5-C10	2.26	119.69	116.41
9	B	4021	NAG	C1-O5-C5	2.45	115.74	112.14
9	B	4001	NAG	C1-O5-C5	2.48	115.78	112.14
8	B	3001	CLR	C1-C2-C3	2.51	113.75	110.41
8	B	3001	CLR	C15-C14-C13	3.10	107.46	103.83
9	B	4002	NAG	C2-N2-C7	4.17	128.52	123.11

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, 95th 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 ²)	Q<0.9
1	A	992/1028 (96%)	0.69	105 (10%) 8 8	112, 134, 175, 200	0
2	B	268/305 (87%)	0.88	45 (16%) 2 2	133, 183, 208, 218	0
3	G	39/74 (52%)	0.31	1 (2%) 59 52	129, 138, 181, 185	0
All	All	1299/1407 (92%)	0.71	151 (11%) 6 7	112, 139, 196, 218	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	579	PRO	8.3
1	A	260	TYR	7.3
1	A	578	PHE	6.6
1	A	580	THR	5.7
1	A	183	GLU	5.7
1	A	571	PHE	5.4
2	B	123	PRO	5.4
1	A	880	PRO	5.2
1	A	530	LEU	5.2
1	A	57	THR	5.2
1	A	585	PHE	5.1
1	A	534	MET	5.0
1	A	41	MET	4.9
2	B	214	ARG	4.9
1	A	563	ASP	4.9
1	A	503	TYR	4.8
1	A	79	SER	4.8
1	A	894	TRP	4.5
1	A	72	LEU	4.4
1	A	78	ASN	4.3
2	B	199	PRO	4.2
1	A	567	GLU	4.1
1	A	815	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	274	LEU	4.0
1	A	573	ALA	4.0
1	A	504	LEU	3.9
1	A	42	ASP	3.9
2	B	298	GLU	3.9
2	B	121	ASN	3.8
2	B	80	HIS	3.8
1	A	171	VAL	3.7
1	A	521	ILE	3.7
1	A	312	ILE	3.7
2	B	273	GLU	3.6
1	A	185	VAL	3.6
2	B	272	MET	3.6
2	B	271	ASN	3.6
2	B	270	GLN	3.6
1	A	562	GLU	3.6
1	A	86	THR	3.5
2	B	79	SER	3.5
1	A	55	TYR	3.5
1	A	660	ALA	3.5
2	B	269	THR	3.4
1	A	80	LEU	3.4
1	A	186	VAL	3.3
1	A	90	ILE	3.3
1	A	317	TRP	3.3
2	B	180	LYS	3.2
1	A	565	TYR	3.2
2	B	155	MET	3.1
1	A	883	LEU	3.1
2	B	305	SER	3.0
1	A	492	ILE	3.0
1	A	556	CYS	3.0
1	A	182	ALA	2.9
1	A	814	THR	2.9
2	B	238	ALA	2.9
2	B	230	GLU	2.9
1	A	91	LYS	2.9
1	A	514	ILE	2.9
1	A	779	THR	2.8
1	A	878	PHE	2.8
2	B	142	ASP	2.8
1	A	574	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	529	PRO	2.7
2	B	194	ASN	2.7
1	A	77	PRO	2.7
1	A	220	GLY	2.7
1	A	517	ARG	2.7
2	B	231	TYR	2.7
1	A	557	HIS	2.7
1	A	505	LEU	2.7
1	A	538	PHE	2.6
2	B	129	ASP	2.6
1	A	335	GLY	2.6
1	A	533	ASP	2.6
1	A	434	GLN	2.6
1	A	566	ASN	2.6
1	A	82	PRO	2.6
1	A	576	PRO	2.6
1	A	99	GLY	2.6
1	A	587	GLY	2.6
1	A	930	GLN	2.6
1	A	586	VAL	2.6
2	B	303	VAL	2.5
2	B	147	LYS	2.5
2	B	205	ASN	2.5
2	B	216	ALA	2.5
3	G	16	TYR	2.5
2	B	281	TYR	2.5
1	A	94	ARG	2.5
1	A	255	ARG	2.5
2	B	128	SER	2.5
1	A	173	ARG	2.4
2	B	139	ASP	2.4
2	B	117	SER	2.4
1	A	558	PHE	2.4
1	A	98	GLY	2.4
1	A	378	THR	2.4
1	A	967	PHE	2.4
1	A	184	PHE	2.4
1	A	781	THR	2.4
2	B	183	ARG	2.3
2	B	255	LYS	2.3
1	A	778	TYR	2.3
1	A	771	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	51	LEU	2.3
2	B	304	LYS	2.3
1	A	427	LEU	2.3
1	A	518	CYS	2.3
1	A	84	PRO	2.3
2	B	140	LEU	2.3
1	A	527	GLU	2.2
1	A	896	SER	2.2
1	A	572	ASP	2.2
1	A	476	LYS	2.2
2	B	237	TYR	2.2
2	B	97	LYS	2.2
1	A	813	GLY	2.2
1	A	577	ASN	2.2
2	B	234	LEU	2.2
1	A	879	LEU	2.2
1	A	569	TYR	2.2
1	A	536	GLU	2.2
1	A	76	GLY	2.2
1	A	493	HIS	2.2
2	B	302	GLU	2.2
1	A	568	GLY	2.2
1	A	126	ALA	2.1
1	A	36	LYS	2.1
2	B	169	GLY	2.1
1	A	1021	THR	2.1
1	A	555	PHE	2.1
2	B	296	ARG	2.1
2	B	70	GLN	2.1
2	B	124	PHE	2.1
1	A	777	ALA	2.1
1	A	83	PRO	2.1
1	A	564	LYS	2.1
2	B	300	LYS	2.1
2	B	204	ALA	2.1
1	A	515	LEU	2.1
1	A	189	ASP	2.1
1	A	798	VAL	2.0
1	A	75	ASP	2.0
2	B	203	GLN	2.0
1	A	87	PRO	2.0
1	A	826	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	785	PRO	2.0
1	A	675	THR	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](#)

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, 95th 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 ²)	Q<0.9
4	MF4	A	2001	5/5	0.88	0.50	2.29	117,119,120,121	0
5	MG	A	2002	1/1	0.81	0.50	2.13	114,114,114,114	0
8	CLR	B	3001	28/28	0.83	0.31	1.32	176,176,176,177	0
6	TL	A	2003	1/1	0.94	0.06	-2.92	135,135,135,135	0
6	TL	A	2006[B]	1/1	0.93	0.04	-3.81	130,130,130,130	1
7	K	A	2005[A]	1/1	0.93	0.04	-3.81	130,130,130,130	1
6	TL	A	2004	1/1	0.97	0.12	-3.96	135,135,135,135	0
9	NAG	B	4001	14/15	0.82	0.38	-	190,193,194,195	0
9	NAG	B	4021	14/15	0.69	0.50	-	196,197,197,197	0
9	NAG	B	4002	14/15	0.43	0.44	-	197,197,198,198	0

6.5 Other polymers [i](#)

There are no such residues in this entry.