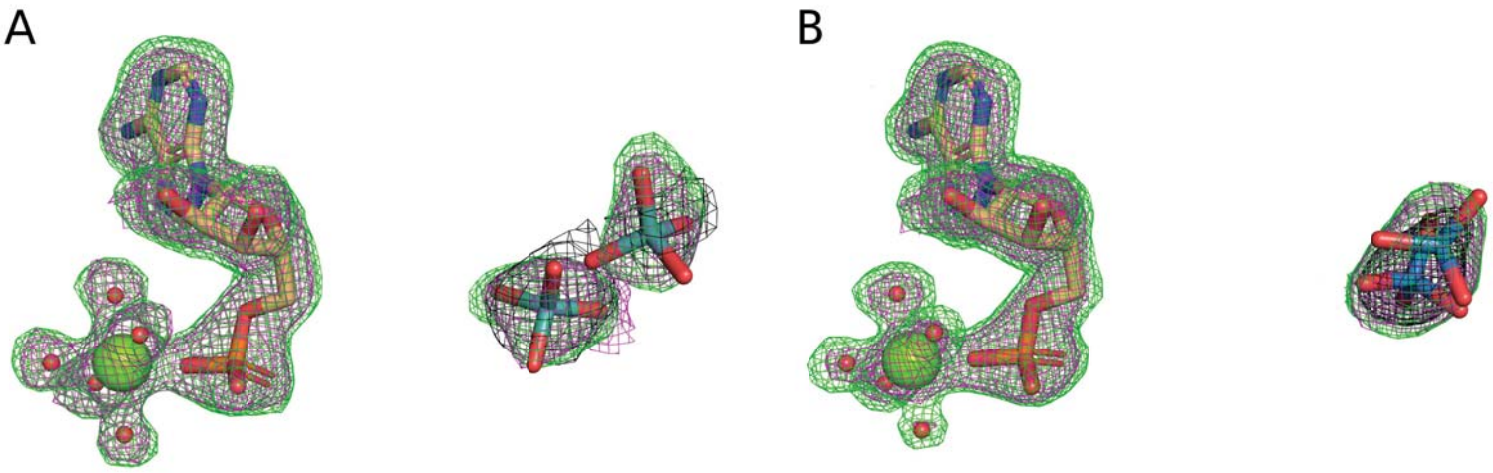


Figure - S1 -

```
Sh       mgerdmvskiliedfnatlhfarvfmkpgkpttflsiphhdnlaiaastttkpkpvlafc       571
Cv       mgdkdfikpllerr--gtvhfgkvkmkpgkpltfakvpvpe---------qgrsllvfg       287
Gp       mgdrdlikpllerq--gvvhfgrvwmkpgkpltfatlelpdgdgpaa----pgrqmlvfg       314
Mn       mgdkdlikpllarq--geihfgrvrmkpgkpltfatlpvaagagapgq--parekvlvfg       334
At       mgdrdfvkplleek--gkvyfskvlmkpgkpltfaeirakptes------mlgktvlafg       321
Ca       mgdrdfvkpllqkk--gtvlfqkvlmkpgkpltfaeilprssdr-------tsskilafg       320
Cs       vgdrdfikpilerq--gtvhfgkvcmkpgkpltfatldgaag--------ssgrglvvfg       306
Kn       mgdkdlvkpllekr--gtvhfgrvlmkpgkpltfasilrakk--------gpgdqllvfg       334
Ad       mgdrdilksilqhyfnatihfgrvnmkpgkpttfatcffqn-----------rkkyllc       402
Hv       mgekdlikkflekf--gdikfgrvnmkpgkpttfatikrgs-----------ittyffa       596
Ml       mgerdlvkqvltadfnatlhfaqvrmkpgkptsfatlsvanr----------hpvlffg       549
Aq       mgekdllkpvlvkdfsanihfgrvfmkpgkpttfatverng-----------klklifa       504
Of       mgekdflkpvledllgatihfgrvfmkpgkpttfattming-----------kkklifa       511
Ta       mgekdylkgvlrgvldatihfgrvfmkpgkpttfatasfng-----------ktklifc       531
La       mgekdllkqvlhvdlqahmhfgrvfmkpgkpttfatvtidd-----------tkklffg       528
Sg       mgekdylkqvldidlhaqihfgrvfmkpglptsfatvdmdg-----------srklifa       623
Rn       mgekdylkqvldidlhaqihfgrvfmkpglpttfatldidg-----------vrkiifa       655
Lp       mgerdwlkpvveqklngkiifgrvmmkpskpttfvalpe--------------gkfmfa       478
Tc       mgesdllkpiierelrgaihfgrvamkpgkpttfatiaatdpn---------eidrllfa       744
Pn       mgasdllkpvieknlngtihfgrvtikpgkpttfatipvvtdag-------s-klkpifa       523
Gpr      mgdldllkpvleqrcgveilfgrvdvkpgkpltvgvlgkdep----------kgrklvfa       526
Lc       mgeadfmkpvleqklgatihfgrvkmkpgkpttfasipdt-------------gklifa       527
Sp       mgeldllkpvleralgatihfgrvllkpgkpttfatipgtdg----------grrklifa       538
Bm       mgeldlmksiieddlkaqlhfgrvnmkpgkpttfatytpens----------eqkklifa       528
Ri       mgefdllkptlersleatihfgrlkmkpgkpttfatiisde-----------ykklifs       428
Sc       mgeldllkptiehslkgtiqfgrvamkpgkpttfatipwhdg----------stklifa       540
Vm       mgeldllkptierslggtihfgrvnmkpgkpttfatvpakndeg-------ervskvifs       569
         :*  * :.  :       : * :: :**. * :.                    :

Sh       lpgnpvscyvtahlfvlpllrkldlrple------------------------------       600
Cv       lpgnpvsslvtfhlavvpclrkmegwqep------------------------------       316
Gp       lpgnpvssfvcfhlvvlpalrkmagwaap------------------------------       343
Mn       lpgnpvssfvcfnlvvlpalrkmsgwgap------------------------------       363
At       lpgnpvsclvcfnifvvptirqlagwtsp------------------------------       350
Ca       lpgnpvscsvcfhlfvvpairhisgwanp------------------------------       349
Cs       lpgnpvssivtfnlvvlpalramagwaep------------------------------       335
Kn       lpgnpvssivtfnlaalpairklagwaep------------------------------       363
Ad       lpgnpvsatvtmnlfalpllkqlckdf-s------------------------------       430
Hv       lpgnpvsaivtfylfvlpairklagfskp------------------------------       622
Ml       lpgnpvsafvtanlyvipacrrlggwsap------------------------------       581
Aq       lpgnpvsstvtfqlfvlpalrklaghpnp------------------------------       533
Of       lpgnpvsamvtfnlfvlpalrklagfqhp------------------------------       540
Ta       lpgnpvsavvtchlfvipalrkmagysrp------------------------------       560
La       lpgnpvsaivtcnlyvipalnkmsgypnp------------------------------       557
Sg       lpgnpvsavvtcnlfvipalrkmqgildp------------------------------       652
Rn       lpgnpvsavvtcnlfvvpalrkmqgildp------------------------------       684
Lp       lpgnpasalvafhmfaapairklaghvvnas----------------------------       509
Tc       lpgnpasalvcfyvfvlpslrklagynpttplsmhqqyaergggragmggmgasveddsr       713
Pn       lpgnpasalvcfyifvvpalrrlggwpeks------------------------------       644
Gpr      lpgnpvsaivtfhlfglpalrrlaahpsp------------------------------       555
Lc       lpgnpasatvtfylfvlpalkkiagyaqf------------------------------       556
Sp       lpgnpvsasvtfylfvlpalrkmagysdp------------------------------       567
Bm       lpgnpvsatvtfylfvlpslrkllgysrp------------------------------       557
Ri       lpgnpvsatvtsylfvlpalrkiagydnw------------------------------       457
Sc       lpgnpasamvtfnlfilpslrksagyepa------------------------------       569
Vm       lpgnpasalvtfhlfvlpslhamsgispa------------------------------       598
         *****.*. *   :   *  .
```

```
Sh       -----ewcfpsihvrllhsvklsd-rpdytrarlvwkenseyn--------------qp       639
Cv       -------rlrrlhvrtampikmdperpeyhravahwarpagaepgvc-------------       356
Gp       -------alrrvaarlaaplrldperpeyhrctlqwsppppgspaaaaaaavataaaepp       396
Mn       -------llrrvrvwttsalkldperpeyhraticygrypetagaaaagavaa------a       410
At       -------hplrvrlrlqepiksdpirpefhraiikwkdndgsg-----------------       386
Ca       -------hlprvqarlkhsvktdplrpefhraviswqlndwsg-----------------       385
Cs       -------rlrrvhartqsaikldperpeyhraslswhrtge-s-----------------       370
Kn       -------elrrveaslaqsvkldperpeyhraslhweagk--------------------       396
Ad       -------ipiivktklmssynldp-rpeyarailkwsst----------------------       459
Hv       -------nlqriqarlsfdinldi-rpeyhrvrlnwdtd----------------------       655
Ml       -------rrsvinvklgqeigldp-rpeyhrctlqwpsgi--------------------       613
Aq       -------ssvtikaqlksrvsldp-rpeyqrvvisdwst----------------------       564
Of       -------qltkikvklpqpvdldp-rpeyqrvvlswkpg----------------------       571
Ta       -------qasivkaklgfginlda-rpeyhrtvlswpsq----------------------       591
La       -------rrtvikakissdiqlds-rpeyhrvvlswred----------------------       588
Sg       -------rptiikarlscdvkldp-rpeyhrciltwhhq----------------------       683
Rn       -------rptiikarlscdvkldp-rpeyhrciltwhhq----------------------       715
Lp       -------vddnvahfvgdslaldrgrpefmrgrlvwqkgs--------------------       542
Tc       epmgnpwslpkvtvvlaqsvmtds-rpefhrvvvrae------------------------       840
Pn       ------cqlsrikvqiqdsmrldp-rtefhrvivsag------------------------       583
Gpr      -------hlptvparllhsvptds-rpeymrarlrmirspatg-----------------       590
Lc       -------tnpiipvkiteqvyldp-rpeyhrvrvsvt-----------------------       585
Sp       -------ilpvvraeladtiqldpsrpefhrahiaia--pssg-----------------       601
Bm       -------qlptlkvkishslrldt-rpeyhraiivpt--lv--------------------       588
Ri       -------nlpivqaelsnnisldp-rpeyhratisyd--y--------------------       487
Sc       -------alpkikvilaesvrldp-rpeyhrailhvd------------------------       598
Vm       -------gltkipvtlghefkldpgrpeyhraivtvg------------------------       628
                        :          .  *  :: *
```

```
Sh       svp----cascdmienqmssclasclnsnlllvlppivnd-----gpqelpvdsvvnalv       690
Cv       -----cgelvaastggqissrllslrsanvlleipqasra------sgvlpagtmvsalv       405
Gp       ssplaghelwavstgnqissrllsarsanallelpca---------egtlaagtlvsall       447
Mn       vggadacvwyavstgnqissrllsarsanallevpqa---------sgalaagtevsali       461
At       -----tpgfvaestghqmssrllsmrsanallelpat---------gnvlsagssvsaii       432
Ca       -----yqgfiaestghqissrllsmksanallelpas---------etslpagasvsail       431
Cs       -----agelaaastggqissrllsmrsanallelpav---------qgvlpagslvsall       416
Kn       -------gfiaestgrqissrllsmrsasallelprs---------sgvlpagtkvsalv       440
Ad       -----dilplaystgdqisskllncknanallmlpartte-----k-tilqegdvvqaml       510
Hv       -----dgvplaittgsqcssrllsmrschalvempsneav-------rnltkgslvtall       701
Ml       ---dadvlptawstgsqassrllscqsasgllilparsds-----l-lslpaghvtqcml       664
Aq       ------vpptvestglqrssrllsmrgatglavlppmdeg-----gktgmepgeiidlil       613
Of       -----eaipwaistgsqcssrllsmrtanallvlqprsdn-----l-srigageivdali       620
Ta       -----enlpiasttgsqcssritsmrsanallmlppkqdn-----l-krleigsivdalm       640
La       -----dpvpwasstgsqissrllsmcsanallmlppktke-----q-kemktgdvaeaiv       637
Sg       -----eplpwaqstgnqvssrlmsmrsangllmlppkteq-----y-velrkgevvdvmv       732
Rn       -----eplpwaqstgnqmssrlmsmrsangllmlppkteq-----y-velhkgevvdvmv       764
Lp       -----skwtveaadrhqqssrmasmqganalialpigtad------kptvsnnelvdviv       591
Tc       -----ngqfvaystgsqrssgmhsmatanalvcvparrkdt----piyrieagekveail       891
Pn       -----ssgliarstggqrssrvasmsganglvilpqkrdn-----gptelkegeladail       633
Gpr      ---latvewiaeitgmqrssrvaslaganalvrvsprkerevegkevgrvgegevveavv       647
Lc       ----pkgefvaestggqrssrmlsllqangllqlpaase------dqsqlpsgtqvpcll       635
Sp       ---hqgtrlvaystgsqrssrmvsmrganallkmpagtq------grmevaqgevvdavl       652
Bm       ---gnemtlvasstgvqqssrmlsmrsanallmlpssdd------gktvleegsfvnail       639
Ri       ----tkgkflavstgnqissrllsmcscnallklpgktd------qlkelvkgtmvdail       537
Sc       ----negrlkahstggqrssrigsmqkanallclpsimeln----gktelaagetvdalv       650
Vm       ----engvlsatstggqrssrvgslkganallcmpkg---------agplqkgtkvdall       675
                       * ** : .   .  *  :              :  .     ::
```

Figure -S2-

Phylum (class), species	Species (Abbreviation)	Sequence identifier
Viridiplantae		
Chlorophyta (Chlorophyceae), *G. pectorale* *M. neglectum*	 *G. pectorale* (Gp) *M. neglectum* (Mn)	 KXZ48662.1 XP_013900022.1
Chlorophyta (Trebouxiophyceae), *C. subellipsoidea C-169*, *C. variabilis*	 *C. subellipsoidea C-169* (Cs) *C. variabilis* (Cv)	 XP_005646314.1 XP_005844769.1
Streptophyta (Klebsormidiophyceae) *K. nitens*	 *K. nitens* (Kn)	 GAQ83347.1
Streptophyta (Embryophyta*) *A. thaliana* *C. annuum*	 *A. thaliana* (At) *C. annuum* (Ca)	 Q39054.2 PHT93935.1
Metazoa		
Platyhelminthes (Trematoda), *S. haematobium* Platyhelminthes (Rhabditophora), *M. lignano*	 *S. haematobium* (Sh) *M. lignano* (Ml)	 XP_012798932.1 PAA94425.1
Cnidaria (Hydrozoa), *H. vulgaris* Cnidaria (Anthozoa), *O. faveolata*	*H. vulgaris* (Hv) *O. faveolata* (Of)	XP_004208356.1 XP_020604198.1
Placozoa (Trichoplax), *T. adhaerens*	*T. adhaerens* (Ta)	XP_002117252.1
Porifera (Demospongiae), *A. queenslandica*	 *A. queenslandica* (Aq)	 XP_019855253.1
Protostomia* (Insecta), *A. dorsata* Protostomia* (Lingulata) *L. anatina*	 *A. dorsata* (Ad) *L. anatina* (La)	 XP_006623824.1 XP_013398832.1
Deuterostomia* (Actinopteri), *S. grahami* Deuterostomia* (Mammalia), *R. norvegicus*	 *S. graham* (Sg) *R. norvegicus* (Rn)	 XP_016098340.1 Q03555.3

Fungi		
Chytridiomycota (Chytridiomycetes), *S. Punctatus* (Monoblepharidomycetes), *G. Prolifera JEL478*	*S. punctatus* (Sp) *G. prolifera JEL478* (Gp)	XP_016611223.1 KXS17208.1
Ascomycetes (Taphrinomycetes), *S. complicate NRRL Y-17804* (Sordariomycetes), *V. mali var. pyri*	*S. complicate* (Sc) *Valsa mali var. Pyri* (Vm)	XP_019023185.1 KUI54811.1
Basidiomycota (Agaricomycetes), *P. noxius* (Exobasidiomycetes) *T. controversa*	*P. noxius* (Pn) *T. controversa* (Tc)	PAV21040.1 OAJ32057.1
Mucoromycota (Glomeromycetes), *R. irregularis DAOM 197198w* (Mucoromycotina***), *L. corymbifera*	*R. irregularis DAOM 197198w* (Ri) *L. corymbifera* (Lc)	EXX61118.1 CDH58228.1
Zoopagomycota (Basidiobolomycetes), *B. meristosporus CBS 931.73* (Kickxellales), *L. pennispora*	*B. meristosporus CBS 931.73* (Bm) *L. pennispora* (Lp)	ORY03538.1 ORX67920.1

Table –S1–

	K294A	K294A+Mo	S328A	S328A+Mo	R369A	R369A+Mo
Data collection						
Wavelength (Å)	0.9184	1.000	0.9184	1.000	0.9184	1.000
Space group	I222					
Unit cell parameters						
a (Å)	6.47±0.03	65.22±0.05	66.02±0.03	65.31±0.03	66.03±0.03	65.85±0.03
b (Å)	123.42±0.01	122.13±0.02	123.80±0.02	122.58±0.01	123.97±0.05	123.90±0.01
c (Å)	132.28±0.01	131.68±0.01	123.81±0.03	133.00±0.02	132.68±0.04	131.54±0.02
α≡β≡γ (°)	:= 90	:= 90	:= 90	:= 90	:= 90	:= 90
Resolution (Å)						
$d_{hkl,max} - d_{hkl,min}$	42.79-1.81 (2.09-1.81)	89.55-1.77 (1.94-1.75)	66.41-1.65 (1.84-1.65)	90.14-1.66 (1.76-1.66)	66.34-1.69 (1.85-1.69)	65.77-1.56 (1.73-1.56)
$d_{h00,min}$	2.28	1.95	1.95	1.71	2.00	1.93
$d_{0k0,min}$	2.15	2.23	2.09	1.91	1.98	1.91
$d_{00l,min}$	1.81	1.75	1.65	1.66	1.69	1.56
d_{eff}[a] [d_{opt}]	2.05 [~1.8]	1.96 [~1.79]	1.88 [~1.67]	1.74 [~1.63]	1.86 [~1.69]	1.76 [~1.64]
No. of reflections						
total	145,911 (12,738)	498.081 (25,021)	186,796 (9,532)	707,633 (32,733)	186,276 (8,823)	689,995 (36,058)
unique	32,849 (2,737)	36,842 (1,843)	41,912 (2,096)	53,670 (2,683)	42,230 (2,113)	51,433 (2,572)
Completeness						
spherical	0.663 (0.162)	0.712 (0.150)	0.661 (0.132)	0.830 (0.240)	0.717 (0.177)	0.709 (0.162)
ellipsoidal[b]	0.948 (0.784)	0.954 (0.724)	0.929 (0.762)	0.958 (0.609)	0.892 (0.718)	0.961 (0.841)
Multiplicity	4.4 (4.7)	13.5 (13.6)	4.5 (4.5)	13.2 (12.2)	4.4 (4.2)	13.4 (14.0)
Mean *I/σ(I)*	8.3 (1.9)	12.8 (1.6)	7.0 (1.7)	23.5 (1.3)	16.9 (1.5)	21.1 (1.6)
Wilson B ($Å^2$)	24.9	29.7	20.7	27.9	24.4	26.2
R_{merge}	0.089 (0.665)	0.103 (1.495)	0.119 (0.772)	0.055 (1.757)	0.042 (0.902)	0.055 (1.496)
R_{meas}	0.115 (0.854)	0.111 (1.612)	0.154 (0.991)	0.060 (1.917)	0.054 (1.022)	0.060 (1.544)
R_{pim}	0.072 (0.532)	0.042 (0.599)	0.097 (0.615)	0.023 (0.763)	0.034 (0.665)	0.022 (0.573
CC1/2	0.995 (0.732)	0.998 (0.648)	0.990 (0.675)	1.000 (0.637)	0.999 (0.615)	0.999 (0.738)
Refinement						
No. of reflections used	32,830 (2,735)	36,828 (1,842)	41,907 (2,094)	53,664 (2,682)	42,207 (2,111)	51,431 (2,572)
R_{work} / R_{free}	0.1880 / 0.2150	0.1860 / 0.2150	0.1850 / 0.2150	0.1930 / 0.2180	0.1651 / 0.1979	0.1627 / 0.1874

No. of non-hydrogen atoms						
total	3,411	3,421	3,601	3,428	3,580	3,572
in protein	3,139	3,153	3,153	3,154	3,163	3,165
in ligands	7	18	22	19	21	22
in ordered solvent	265	250	426	255	396	385
Atomic B-factors (Å^2)						
Average	35.1	40.5	29.3	36.8	33.8	35-3
Protein/Ligands/Solvent	34.9/39.0/38.0	40.1/45.5/44.8	28.1/45.8/37.5	36.3/52.6/40.8	32.7/53.3/41.4	34.4/40.7/42.8
No. of amino acid residues						
total / ordered	470/419	470/419	470/419	470 / 418	470 / 418	470/423
RMSD from ideal						
bonds (Å)	0.014	0.013	0.014	0.014	0.014	0.014
angles (°)	1.69	1.69	1.65	1.69	1.67	1.68
Ramachandran (%)						
favored	98.05	98.78	97.80	98.04	98.53	98.56
allowed	1.71	0.98	1.71	1.47	1.22	0.96
outliers	0.24	0.24	0.49	0.49	0.24	0.48

Table –S2–

Preliminary Full wwPDB X-ray Structure Validation Report (i)

Apr 13, 2018 – 04:03 PM BST

Deposition ID : D_1200009690
PDB ID : *(not yet assigned)*

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

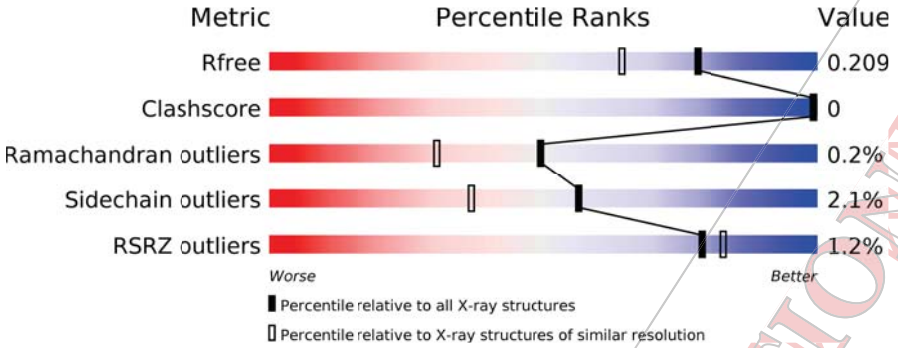
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031021
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031021

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

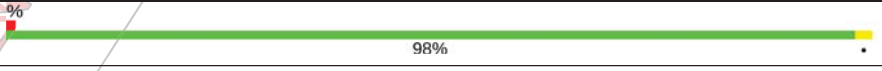
The reported resolution of this entry is 1.71 Å.

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}	111664	4894 (1.74-1.70)
Clashscore	122126	5296 (1.74-1.70)
Ramachandran outliers	120053	5219 (1.74-1.70)
Sidechain outliers	120020	5219 (1.74-1.70)
RSRZ outliers	108989	4804 (1.74-1.70)

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 <=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	418	

2 Entry composition

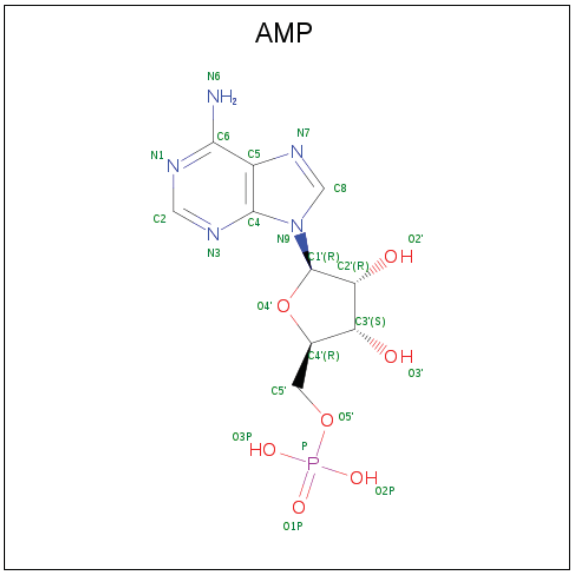
There are 6 unique types of molecules in this entry. The entry contains 6829 atoms, of which 3249 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	418	6356	1991	3216	537	599	13	3216	9	0

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

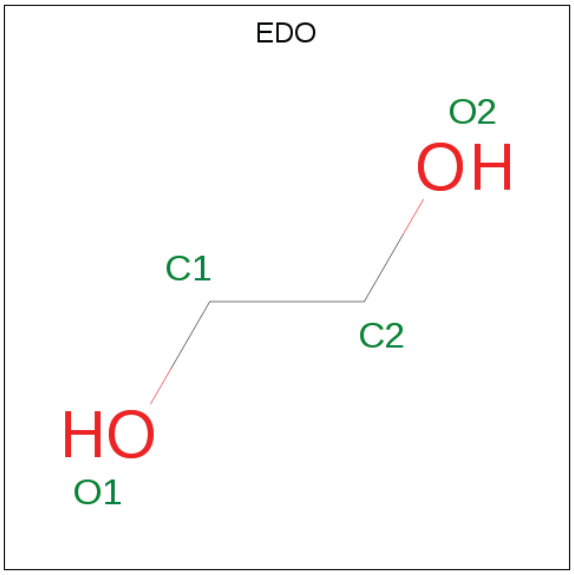


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	B	1	35	10	12	5	7	1	12	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

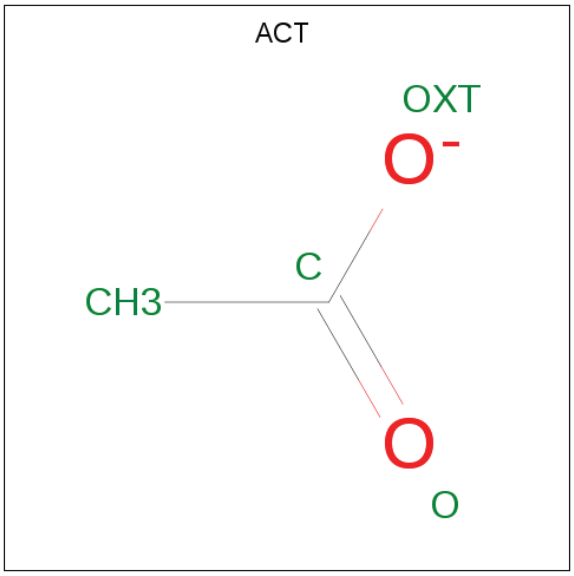
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	C	1	1	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	6	0
			10	2	6	2		
4	D	1	Total	C	H	O	6	0
			10	2	6	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	H	O	3	0
			7	2	3	2		
5	F	1	Total	C	H	O	3	0
			7	2	3	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C H O 7 2 3 2	3	0

- Molecule 6 is water.

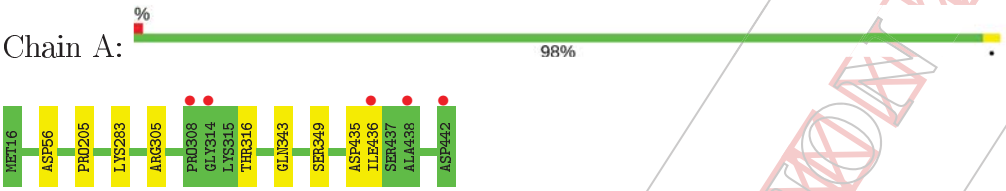
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	S	396	Total O 396 396	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand 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 (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.

- Molecule 1:

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	66.03Å 123.97Å 132.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.07 – 1.71 90.58 – 1.71	Depositor EDS
% Data completeness (in resolution range)	71.6 (25.07-1.71) 71.7 (90.58-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 1.71Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.173 , 0.199 0.174 , 0.209	Depositor DCC
R_{free} test set	2123 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6829	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: AMP, MG, ACT, EDO, CSX

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	0.49	0/3213	0.62	0/4368

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	3140	3216	3191	0	1
2	B	23	12	12	0	0
3	C	1	0	0	0	0
4	D	8	12	12	1	0
5	F	12	9	9	0	0
6	S	396	0	0	1	0
All	All	3580	3249	3224	1	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 0.

All (1) 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)
4:D:2:EDO:H22	6:S:67:HOH:O	2.16	0.45

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:436:ILE:CB	1:A:436:ILE:CB[3_655]	1.24	0.96

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	420/418 (100%)	414 (99%)	5 (1%)	1 (0%)	49 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	435	ASP

5.3.2 Protein sidechains (i)

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	344/343 (100%)	337 (98%)	7 (2%)	58 39

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
1	A	205	PRO
1	A	283	LYS
1	A	305	ARG
1	A	316	THR
1	A	343	GLN
1	A	349	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	CSX	A	154	1	3,6,7	1.27	0	1,6,8	1.74	0

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
1	CSX	A	154	1	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AMP	B	1	3	22,25,25	0.95	1 (4%)	23,38,38	1.70	2 (8%)
4	EDO	D	1	-	3,3,3	0.56	0	2,2,2	0.23	0
4	EDO	D	2	-	3,3,3	0.25	0	2,2,2	0.39	0
5	ACT	F	1	-	1,3,3	1.14	0	0,3,3	0.00	-
5	ACT	F	2	-	1,3,3	1.57	0	0,3,3	0.00	-
5	ACT	F	3	-	1,3,3	1.66	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	B	1	3	-	0/6/26/26	0/3/3/3
4	EDO	D	1	-	-	0/1/1/1	0/0/0/0
4	EDO	D	2	-	-	0/1/1/1	0/0/0/0
5	ACT	F	1	-	-	0/0/0/0	0/0/0/0
5	ACT	F	2	-	-	0/0/0/0	0/0/0/0
5	ACT	F	3	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	AMP	C5-C4	2.65	1.46	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	AMP	N3-C2-N1	-6.85	123.00	128.86
2	B	1	AMP	O3P-P-O2P	2.03	115.63	107.59

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
4	D	2	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	129:ASP	C	134:SER	N	6.68
1	A	308:PRO	C	314:GLY	N	5.18

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^{th} 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	417/418 (99%)	-0.38	5 (1%) 79 83	18, 30, 52, 90	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	436	ILE	3.0
1	A	314	GLY	2.9
1	A	308	PRO	2.6
1	A	438	ALA	2.2
1	A	442	ASP	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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^{th} 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^2)	Q<0.9
1	CSX	A	154	7/?	0.91	0.09	28,30,43,47	6

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. The B-factors column lists the minimum,

median, 95^{th} 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^2)	Q<0.9
5	ACT	F	2	4/?	0.58	0.27	67,67,68,69	3
5	ACT	F	3	4/?	0.79	0.12	62,62,64,66	3
5	ACT	F	1	4/?	0.79	0.21	62,63,64,65	3
4	EDO	D	2	4/?	0.95	0.12	41,42,44,44	6
4	EDO	D	1	4/?	0.95	0.08	29,34,38,38	6
2	AMP	B	1	23/?	0.99	0.07	17,22,27,33	12
3	MG	C	1	1/?	0.99	0.07	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.