



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2017 – 09:47 AM EST

PDB ID : 5O5K
Title : X-ray structure of a bacterial adenylyl cyclase soluble domain
Authors : Vercellino, I.; Korkhov, V.M.
Deposited on : unknown
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

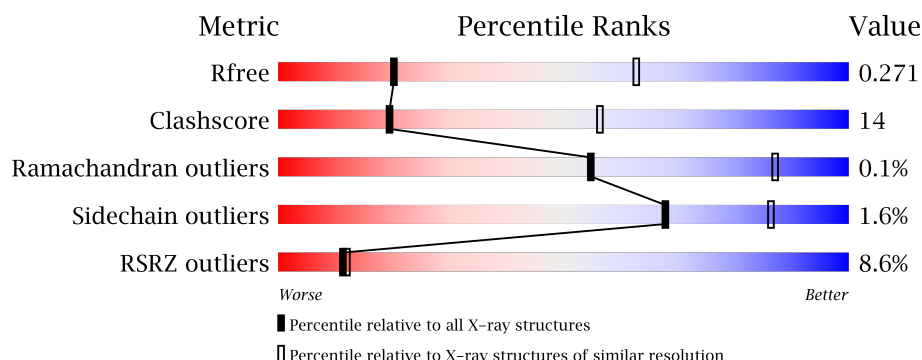
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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 ≥ 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	254	
1	B	254	
1	C	254	
1	D	254	
1	E	254	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	254	
1	G	254	
1	H	254	
1	I	254	
1	J	254	
1	K	254	

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
2	ONM	I	504	-	-	X	-
4	SO4	A	504	-	-	-	X
4	SO4	C	503	-	-	-	X
4	SO4	E	504	-	-	X	-
4	SO4	F	502	-	-	-	X
4	SO4	H	501	-	-	-	X
4	SO4	I	503	-	-	-	X
4	SO4	J	505	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18919 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 Adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	B	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	D	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	C	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	E	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	F	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	I	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	J	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	H	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	G	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	K	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			

There are 308 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	MET	-	initiating methionine	UNP X8CHM4
A	177	GLY	-	expression tag	UNP X8CHM4
A	178	HIS	-	expression tag	UNP X8CHM4
A	179	HIS	-	expression tag	UNP X8CHM4
A	180	HIS	-	expression tag	UNP X8CHM4
A	181	HIS	-	expression tag	UNP X8CHM4
A	182	HIS	-	expression tag	UNP X8CHM4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	HIS	-	expression tag	UNP X8CHM4
A	184	HIS	-	expression tag	UNP X8CHM4
A	185	HIS	-	expression tag	UNP X8CHM4
A	186	HIS	-	expression tag	UNP X8CHM4
A	187	HIS	-	expression tag	UNP X8CHM4
A	188	SER	-	expression tag	UNP X8CHM4
A	189	SER	-	expression tag	UNP X8CHM4
A	190	GLY	-	expression tag	UNP X8CHM4
A	191	LEU	-	expression tag	UNP X8CHM4
A	192	GLU	-	expression tag	UNP X8CHM4
A	193	VAL	-	expression tag	UNP X8CHM4
A	194	LEU	-	expression tag	UNP X8CHM4
A	195	PHE	-	expression tag	UNP X8CHM4
A	196	GLN	-	expression tag	UNP X8CHM4
A	197	GLY	-	expression tag	UNP X8CHM4
A	198	PRO	-	expression tag	UNP X8CHM4
A	199	SER	-	expression tag	UNP X8CHM4
A	200	GLY	-	expression tag	UNP X8CHM4
A	201	HIS	-	expression tag	UNP X8CHM4
A	202	MET	-	expression tag	UNP X8CHM4
A	342	PRO	ALA	conflict	UNP X8CHM4
B	176	MET	-	initiating methionine	UNP X8CHM4
B	177	GLY	-	expression tag	UNP X8CHM4
B	178	HIS	-	expression tag	UNP X8CHM4
B	179	HIS	-	expression tag	UNP X8CHM4
B	180	HIS	-	expression tag	UNP X8CHM4
B	181	HIS	-	expression tag	UNP X8CHM4
B	182	HIS	-	expression tag	UNP X8CHM4
B	183	HIS	-	expression tag	UNP X8CHM4
B	184	HIS	-	expression tag	UNP X8CHM4
B	185	HIS	-	expression tag	UNP X8CHM4
B	186	HIS	-	expression tag	UNP X8CHM4
B	187	HIS	-	expression tag	UNP X8CHM4
B	188	SER	-	expression tag	UNP X8CHM4
B	189	SER	-	expression tag	UNP X8CHM4
B	190	GLY	-	expression tag	UNP X8CHM4
B	191	LEU	-	expression tag	UNP X8CHM4
B	192	GLU	-	expression tag	UNP X8CHM4
B	193	VAL	-	expression tag	UNP X8CHM4
B	194	LEU	-	expression tag	UNP X8CHM4
B	195	PHE	-	expression tag	UNP X8CHM4
B	196	GLN	-	expression tag	UNP X8CHM4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	197	GLY	-	expression tag	UNP X8CHM4
B	198	PRO	-	expression tag	UNP X8CHM4
B	199	SER	-	expression tag	UNP X8CHM4
B	200	GLY	-	expression tag	UNP X8CHM4
B	201	HIS	-	expression tag	UNP X8CHM4
B	202	MET	-	expression tag	UNP X8CHM4
B	342	PRO	ALA	conflict	UNP X8CHM4
D	176	MET	-	initiating methionine	UNP X8CHM4
D	177	GLY	-	expression tag	UNP X8CHM4
D	178	HIS	-	expression tag	UNP X8CHM4
D	179	HIS	-	expression tag	UNP X8CHM4
D	180	HIS	-	expression tag	UNP X8CHM4
D	181	HIS	-	expression tag	UNP X8CHM4
D	182	HIS	-	expression tag	UNP X8CHM4
D	183	HIS	-	expression tag	UNP X8CHM4
D	184	HIS	-	expression tag	UNP X8CHM4
D	185	HIS	-	expression tag	UNP X8CHM4
D	186	HIS	-	expression tag	UNP X8CHM4
D	187	HIS	-	expression tag	UNP X8CHM4
D	188	SER	-	expression tag	UNP X8CHM4
D	189	SER	-	expression tag	UNP X8CHM4
D	190	GLY	-	expression tag	UNP X8CHM4
D	191	LEU	-	expression tag	UNP X8CHM4
D	192	GLU	-	expression tag	UNP X8CHM4
D	193	VAL	-	expression tag	UNP X8CHM4
D	194	LEU	-	expression tag	UNP X8CHM4
D	195	PHE	-	expression tag	UNP X8CHM4
D	196	GLN	-	expression tag	UNP X8CHM4
D	197	GLY	-	expression tag	UNP X8CHM4
D	198	PRO	-	expression tag	UNP X8CHM4
D	199	SER	-	expression tag	UNP X8CHM4
D	200	GLY	-	expression tag	UNP X8CHM4
D	201	HIS	-	expression tag	UNP X8CHM4
D	202	MET	-	expression tag	UNP X8CHM4
D	342	PRO	ALA	conflict	UNP X8CHM4
C	176	MET	-	initiating methionine	UNP X8CHM4
C	177	GLY	-	expression tag	UNP X8CHM4
C	178	HIS	-	expression tag	UNP X8CHM4
C	179	HIS	-	expression tag	UNP X8CHM4
C	180	HIS	-	expression tag	UNP X8CHM4
C	181	HIS	-	expression tag	UNP X8CHM4
C	182	HIS	-	expression tag	UNP X8CHM4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	183	HIS	-	expression tag	UNP X8CHM4
C	184	HIS	-	expression tag	UNP X8CHM4
C	185	HIS	-	expression tag	UNP X8CHM4
C	186	HIS	-	expression tag	UNP X8CHM4
C	187	HIS	-	expression tag	UNP X8CHM4
C	188	SER	-	expression tag	UNP X8CHM4
C	189	SER	-	expression tag	UNP X8CHM4
C	190	GLY	-	expression tag	UNP X8CHM4
C	191	LEU	-	expression tag	UNP X8CHM4
C	192	GLU	-	expression tag	UNP X8CHM4
C	193	VAL	-	expression tag	UNP X8CHM4
C	194	LEU	-	expression tag	UNP X8CHM4
C	195	PHE	-	expression tag	UNP X8CHM4
C	196	GLN	-	expression tag	UNP X8CHM4
C	197	GLY	-	expression tag	UNP X8CHM4
C	198	PRO	-	expression tag	UNP X8CHM4
C	199	SER	-	expression tag	UNP X8CHM4
C	200	GLY	-	expression tag	UNP X8CHM4
C	201	HIS	-	expression tag	UNP X8CHM4
C	202	MET	-	expression tag	UNP X8CHM4
C	342	PRO	ALA	conflict	UNP X8CHM4
E	176	MET	-	initiating methionine	UNP X8CHM4
E	177	GLY	-	expression tag	UNP X8CHM4
E	178	HIS	-	expression tag	UNP X8CHM4
E	179	HIS	-	expression tag	UNP X8CHM4
E	180	HIS	-	expression tag	UNP X8CHM4
E	181	HIS	-	expression tag	UNP X8CHM4
E	182	HIS	-	expression tag	UNP X8CHM4
E	183	HIS	-	expression tag	UNP X8CHM4
E	184	HIS	-	expression tag	UNP X8CHM4
E	185	HIS	-	expression tag	UNP X8CHM4
E	186	HIS	-	expression tag	UNP X8CHM4
E	187	HIS	-	expression tag	UNP X8CHM4
E	188	SER	-	expression tag	UNP X8CHM4
E	189	SER	-	expression tag	UNP X8CHM4
E	190	GLY	-	expression tag	UNP X8CHM4
E	191	LEU	-	expression tag	UNP X8CHM4
E	192	GLU	-	expression tag	UNP X8CHM4
E	193	VAL	-	expression tag	UNP X8CHM4
E	194	LEU	-	expression tag	UNP X8CHM4
E	195	PHE	-	expression tag	UNP X8CHM4
E	196	GLN	-	expression tag	UNP X8CHM4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	197	GLY	-	expression tag	UNP X8CHM4
E	198	PRO	-	expression tag	UNP X8CHM4
E	199	SER	-	expression tag	UNP X8CHM4
E	200	GLY	-	expression tag	UNP X8CHM4
E	201	HIS	-	expression tag	UNP X8CHM4
E	202	MET	-	expression tag	UNP X8CHM4
E	342	PRO	ALA	conflict	UNP X8CHM4
F	176	MET	-	initiating methionine	UNP X8CHM4
F	177	GLY	-	expression tag	UNP X8CHM4
F	178	HIS	-	expression tag	UNP X8CHM4
F	179	HIS	-	expression tag	UNP X8CHM4
F	180	HIS	-	expression tag	UNP X8CHM4
F	181	HIS	-	expression tag	UNP X8CHM4
F	182	HIS	-	expression tag	UNP X8CHM4
F	183	HIS	-	expression tag	UNP X8CHM4
F	184	HIS	-	expression tag	UNP X8CHM4
F	185	HIS	-	expression tag	UNP X8CHM4
F	186	HIS	-	expression tag	UNP X8CHM4
F	187	HIS	-	expression tag	UNP X8CHM4
F	188	SER	-	expression tag	UNP X8CHM4
F	189	SER	-	expression tag	UNP X8CHM4
F	190	GLY	-	expression tag	UNP X8CHM4
F	191	LEU	-	expression tag	UNP X8CHM4
F	192	GLU	-	expression tag	UNP X8CHM4
F	193	VAL	-	expression tag	UNP X8CHM4
F	194	LEU	-	expression tag	UNP X8CHM4
F	195	PHE	-	expression tag	UNP X8CHM4
F	196	GLN	-	expression tag	UNP X8CHM4
F	197	GLY	-	expression tag	UNP X8CHM4
F	198	PRO	-	expression tag	UNP X8CHM4
F	199	SER	-	expression tag	UNP X8CHM4
F	200	GLY	-	expression tag	UNP X8CHM4
F	201	HIS	-	expression tag	UNP X8CHM4
F	202	MET	-	expression tag	UNP X8CHM4
F	342	PRO	ALA	conflict	UNP X8CHM4
I	176	MET	-	initiating methionine	UNP X8CHM4
I	177	GLY	-	expression tag	UNP X8CHM4
I	178	HIS	-	expression tag	UNP X8CHM4
I	179	HIS	-	expression tag	UNP X8CHM4
I	180	HIS	-	expression tag	UNP X8CHM4
I	181	HIS	-	expression tag	UNP X8CHM4
I	182	HIS	-	expression tag	UNP X8CHM4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	183	HIS	-	expression tag	UNP X8CHM4
I	184	HIS	-	expression tag	UNP X8CHM4
I	185	HIS	-	expression tag	UNP X8CHM4
I	186	HIS	-	expression tag	UNP X8CHM4
I	187	HIS	-	expression tag	UNP X8CHM4
I	188	SER	-	expression tag	UNP X8CHM4
I	189	SER	-	expression tag	UNP X8CHM4
I	190	GLY	-	expression tag	UNP X8CHM4
I	191	LEU	-	expression tag	UNP X8CHM4
I	192	GLU	-	expression tag	UNP X8CHM4
I	193	VAL	-	expression tag	UNP X8CHM4
I	194	LEU	-	expression tag	UNP X8CHM4
I	195	PHE	-	expression tag	UNP X8CHM4
I	196	GLN	-	expression tag	UNP X8CHM4
I	197	GLY	-	expression tag	UNP X8CHM4
I	198	PRO	-	expression tag	UNP X8CHM4
I	199	SER	-	expression tag	UNP X8CHM4
I	200	GLY	-	expression tag	UNP X8CHM4
I	201	HIS	-	expression tag	UNP X8CHM4
I	202	MET	-	expression tag	UNP X8CHM4
I	342	PRO	ALA	conflict	UNP X8CHM4
J	176	MET	-	initiating methionine	UNP X8CHM4
J	177	GLY	-	expression tag	UNP X8CHM4
J	178	HIS	-	expression tag	UNP X8CHM4
J	179	HIS	-	expression tag	UNP X8CHM4
J	180	HIS	-	expression tag	UNP X8CHM4
J	181	HIS	-	expression tag	UNP X8CHM4
J	182	HIS	-	expression tag	UNP X8CHM4
J	183	HIS	-	expression tag	UNP X8CHM4
J	184	HIS	-	expression tag	UNP X8CHM4
J	185	HIS	-	expression tag	UNP X8CHM4
J	186	HIS	-	expression tag	UNP X8CHM4
J	187	HIS	-	expression tag	UNP X8CHM4
J	188	SER	-	expression tag	UNP X8CHM4
J	189	SER	-	expression tag	UNP X8CHM4
J	190	GLY	-	expression tag	UNP X8CHM4
J	191	LEU	-	expression tag	UNP X8CHM4
J	192	GLU	-	expression tag	UNP X8CHM4
J	193	VAL	-	expression tag	UNP X8CHM4
J	194	LEU	-	expression tag	UNP X8CHM4
J	195	PHE	-	expression tag	UNP X8CHM4
J	196	GLN	-	expression tag	UNP X8CHM4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	197	GLY	-	expression tag	UNP X8CHM4
J	198	PRO	-	expression tag	UNP X8CHM4
J	199	SER	-	expression tag	UNP X8CHM4
J	200	GLY	-	expression tag	UNP X8CHM4
J	201	HIS	-	expression tag	UNP X8CHM4
J	202	MET	-	expression tag	UNP X8CHM4
J	342	PRO	ALA	conflict	UNP X8CHM4
H	176	MET	-	initiating methionine	UNP X8CHM4
H	177	GLY	-	expression tag	UNP X8CHM4
H	178	HIS	-	expression tag	UNP X8CHM4
H	179	HIS	-	expression tag	UNP X8CHM4
H	180	HIS	-	expression tag	UNP X8CHM4
H	181	HIS	-	expression tag	UNP X8CHM4
H	182	HIS	-	expression tag	UNP X8CHM4
H	183	HIS	-	expression tag	UNP X8CHM4
H	184	HIS	-	expression tag	UNP X8CHM4
H	185	HIS	-	expression tag	UNP X8CHM4
H	186	HIS	-	expression tag	UNP X8CHM4
H	187	HIS	-	expression tag	UNP X8CHM4
H	188	SER	-	expression tag	UNP X8CHM4
H	189	SER	-	expression tag	UNP X8CHM4
H	190	GLY	-	expression tag	UNP X8CHM4
H	191	LEU	-	expression tag	UNP X8CHM4
H	192	GLU	-	expression tag	UNP X8CHM4
H	193	VAL	-	expression tag	UNP X8CHM4
H	194	LEU	-	expression tag	UNP X8CHM4
H	195	PHE	-	expression tag	UNP X8CHM4
H	196	GLN	-	expression tag	UNP X8CHM4
H	197	GLY	-	expression tag	UNP X8CHM4
H	198	PRO	-	expression tag	UNP X8CHM4
H	199	SER	-	expression tag	UNP X8CHM4
H	200	GLY	-	expression tag	UNP X8CHM4
H	201	HIS	-	expression tag	UNP X8CHM4
H	202	MET	-	expression tag	UNP X8CHM4
H	342	PRO	ALA	conflict	UNP X8CHM4
G	176	MET	-	initiating methionine	UNP X8CHM4
G	177	GLY	-	expression tag	UNP X8CHM4
G	178	HIS	-	expression tag	UNP X8CHM4
G	179	HIS	-	expression tag	UNP X8CHM4
G	180	HIS	-	expression tag	UNP X8CHM4
G	181	HIS	-	expression tag	UNP X8CHM4
G	182	HIS	-	expression tag	UNP X8CHM4

Continued on next page...

Continued from previous page...

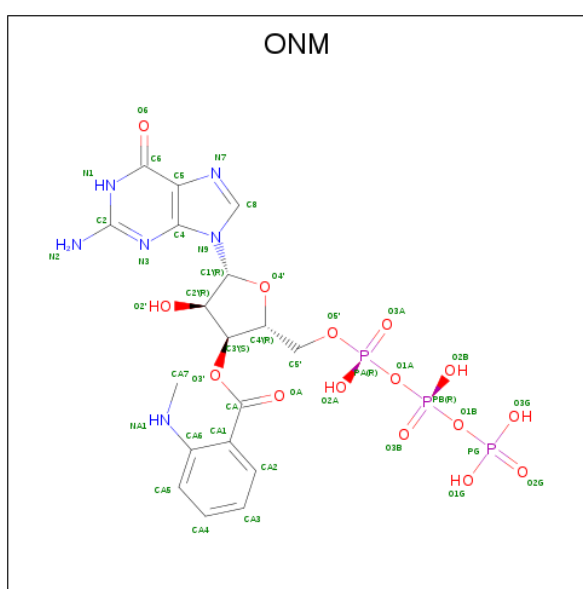
Chain	Residue	Modelled	Actual	Comment	Reference
G	183	HIS	-	expression tag	UNP X8CHM4
G	184	HIS	-	expression tag	UNP X8CHM4
G	185	HIS	-	expression tag	UNP X8CHM4
G	186	HIS	-	expression tag	UNP X8CHM4
G	187	HIS	-	expression tag	UNP X8CHM4
G	188	SER	-	expression tag	UNP X8CHM4
G	189	SER	-	expression tag	UNP X8CHM4
G	190	GLY	-	expression tag	UNP X8CHM4
G	191	LEU	-	expression tag	UNP X8CHM4
G	192	GLU	-	expression tag	UNP X8CHM4
G	193	VAL	-	expression tag	UNP X8CHM4
G	194	LEU	-	expression tag	UNP X8CHM4
G	195	PHE	-	expression tag	UNP X8CHM4
G	196	GLN	-	expression tag	UNP X8CHM4
G	197	GLY	-	expression tag	UNP X8CHM4
G	198	PRO	-	expression tag	UNP X8CHM4
G	199	SER	-	expression tag	UNP X8CHM4
G	200	GLY	-	expression tag	UNP X8CHM4
G	201	HIS	-	expression tag	UNP X8CHM4
G	202	MET	-	expression tag	UNP X8CHM4
G	342	PRO	ALA	conflict	UNP X8CHM4
K	176	MET	-	initiating methionine	UNP X8CHM4
K	177	GLY	-	expression tag	UNP X8CHM4
K	178	HIS	-	expression tag	UNP X8CHM4
K	179	HIS	-	expression tag	UNP X8CHM4
K	180	HIS	-	expression tag	UNP X8CHM4
K	181	HIS	-	expression tag	UNP X8CHM4
K	182	HIS	-	expression tag	UNP X8CHM4
K	183	HIS	-	expression tag	UNP X8CHM4
K	184	HIS	-	expression tag	UNP X8CHM4
K	185	HIS	-	expression tag	UNP X8CHM4
K	186	HIS	-	expression tag	UNP X8CHM4
K	187	HIS	-	expression tag	UNP X8CHM4
K	188	SER	-	expression tag	UNP X8CHM4
K	189	SER	-	expression tag	UNP X8CHM4
K	190	GLY	-	expression tag	UNP X8CHM4
K	191	LEU	-	expression tag	UNP X8CHM4
K	192	GLU	-	expression tag	UNP X8CHM4
K	193	VAL	-	expression tag	UNP X8CHM4
K	194	LEU	-	expression tag	UNP X8CHM4
K	195	PHE	-	expression tag	UNP X8CHM4
K	196	GLN	-	expression tag	UNP X8CHM4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	197	GLY	-	expression tag	UNP X8CHM4
K	198	PRO	-	expression tag	UNP X8CHM4
K	199	SER	-	expression tag	UNP X8CHM4
K	200	GLY	-	expression tag	UNP X8CHM4
K	201	HIS	-	expression tag	UNP X8CHM4
K	202	MET	-	expression tag	UNP X8CHM4
K	342	PRO	ALA	conflict	UNP X8CHM4

- Molecule 2 is 3'-O-(N-METHYLANTHRANILOYL)-GUANOSINE-5'-TRIPHOSPHATE (three-letter code: ONM) (formula: C₁₈H₂₃N₆O₁₅P₃).



Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	J	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	H	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	G	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	K	1	Total	C	N	O	P	0	0
			42	18	6	15	3		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total	Mn	0	0
			2	2		
3	J	2	Total	Mn	0	0
			2	2		
3	D	2	Total	Mn	0	0
			2	2		
3	K	2	Total	Mn	0	0
			2	2		
3	E	2	Total	Mn	0	0
			2	2		
3	H	2	Total	Mn	0	0
			2	2		
3	B	2	Total	Mn	0	0
			2	2		
3	I	2	Total	Mn	0	0
			2	2		
3	C	2	Total	Mn	0	0
			2	2		
3	A	2	Total	Mn	0	0
			2	2		
3	F	2	Total	Mn	0	0
			2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

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 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.

[illegible]

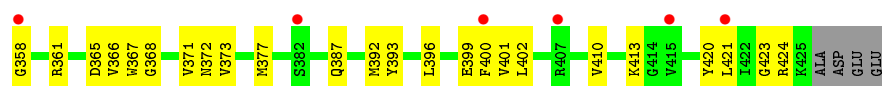
Chain B:

Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.25). The x-axis lists amino acids. A bar at the top shows the overall conservation: 62% (green), 22% (yellow), and 15% (grey).

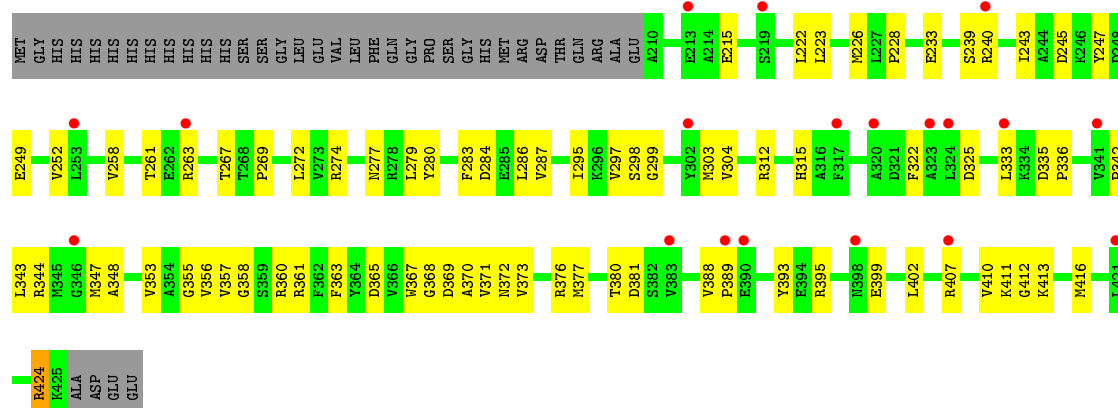
Position	Amino Acid	Information Content (bits)
1	Met	0.00
2	Gly	0.00
3	His	0.00
4	His	0.00
5	His	0.00
6	His	0.00
7	His	0.00
8	His	0.00
9	His	0.00
10	His	0.00
11	His	0.00
12	His	0.00
13	His	0.00
14	His	0.00
15	His	0.00
16	His	0.00
17	His	0.00
18	His	0.00
19	His	0.00
20	His	0.00
21	His	0.00
22	His	0.00
23	His	0.00
24	His	0.00
25	His	0.00
26	His	0.00
27	His	0.00
28	His	0.00
29	His	0.00
30	His	0.00

Chain D:

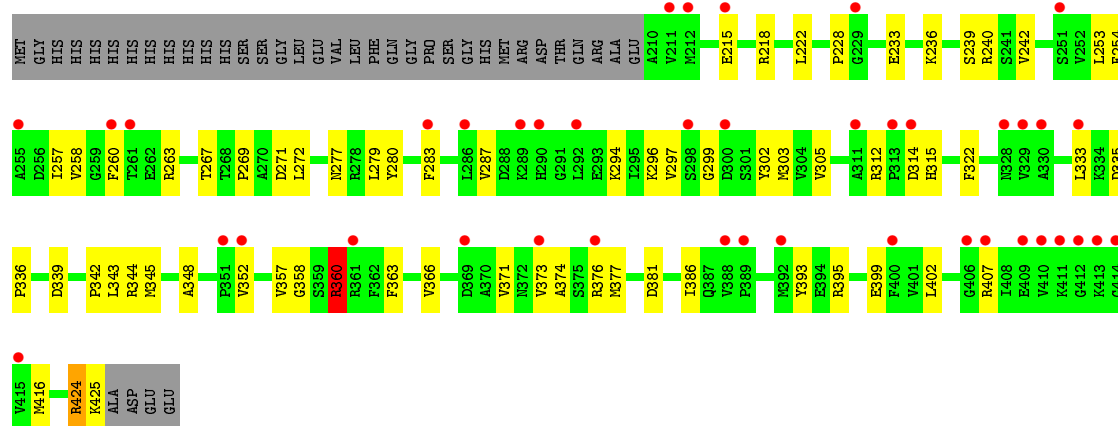
Label	Color
GLY	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
SER	Green
SER	Green
GLY	Green
LEU	Green
GLU	Green
VAL	Green
LEU	Green
PHE	Green
GLN	Green
GLY	Green
PRO	Green
SER	Green
GLY	Green
HIS	Green
MET	Green
ARG	Green
ASP	Green
THR	Green
GLN	Green
ARG	Green
ALA	Green
ALA	Green
GLU	Green
A210	Yellow
V211	Yellow
V212	Yellow
V216	Yellow
A221	Yellow
L222	Yellow
L223	Yellow
A224	Yellow
V225	Yellow
V226	Yellow
R234	Yellow
L235	Yellow
L243	Yellow
A244	Yellow
D245	Yellow
V246	Yellow
V247	Yellow
D248	Yellow
E249	Yellow
V252	Yellow
T252	Yellow
V254	Yellow
A255	Yellow
F260	Yellow
T261	Yellow
E262	Yellow
R263	Yellow
A264	Yellow
T267	Yellow
T268	Yellow
D271	Yellow
L272	Yellow
V273	Yellow
L276	Orange
L279	Orange
Y280	Orange
F283	Orange
L286	Orange
V287	Orange
K294	Orange
I295	Orange
K296	Orange
V297	Orange
D300	Orange
S301	Orange
L319	Orange
F322	Orange
R325	Orange
D325	Orange
L333	Orange
K334	Orange
D335	Orange
P336	Orange
P342	Orange
I343	Orange
R344	Orange
V353	Orange
A354	Orange
G355	Orange
Y364	Orange
D365	Orange
V366	Orange
W367	Orange
V371	Orange
W372	Orange
V373	Orange
A374	Orange
M377	Orange
E378	Orange
D381	Orange
V387	Orange
Q388	Orange
M392	Orange
Y393	Orange
E394	Orange
R395	Orange
L396	Orange
E399	Orange
F400	Orange
V401	Orange
L402	Orange
E409	Orange
V410	Orange
K411	Orange
G412	Orange
K413	Orange
G414	Orange
G415	Orange
M416	Orange
R417	Orange
T418	Orange
W419	Orange
Y420	Orange
L421	Orange
I422	Orange
G423	Orange
R424	Orange
K425	Orange
ALA	Orange
ASP	Orange
GLU	Orange
GLU	Orange



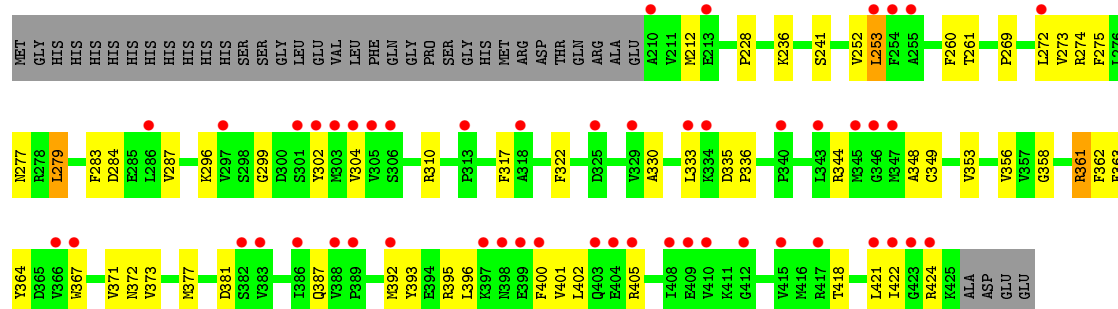
• Molecule 1: Adenylate cyclase



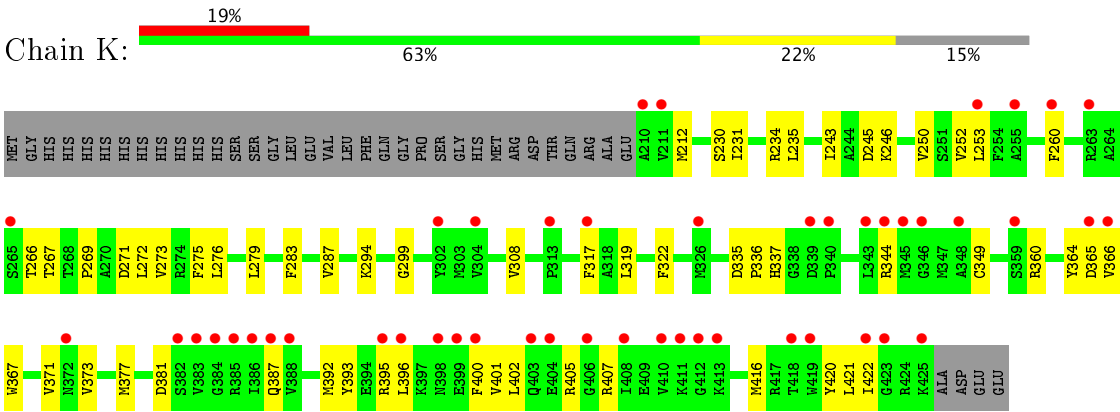
• Molecule 1: Adenylate cyclase



• Molecule 1: Adenylate cyclase



● Molecule 1: Adenylate cyclase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.42Å 85.69Å 318.01Å 90.00° 103.77° 90.00°	Depositor
Resolution (Å)	47.30 – 3.40 47.30 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.30-3.40) 98.4 (47.30-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.245 , 0.266 0.252 , 0.271	Depositor DCC
R_{free} test set	2002 reflections (4.01%)	DCC
Wilson B-factor (Å ²)	106.7	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 109.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18919	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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, 0.333 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: MN, SO4, ONM

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	0.80	1/1701 (0.1%)	1.02	6/2297 (0.3%)
1	B	0.76	0/1701	0.97	7/2297 (0.3%)
1	C	0.77	1/1701 (0.1%)	1.00	5/2297 (0.2%)
1	D	0.69	0/1701	0.93	10/2297 (0.4%)
1	E	0.51	0/1701	0.72	2/2297 (0.1%)
1	F	0.48	0/1701	0.74	1/2297 (0.0%)
1	G	0.42	0/1701	0.64	2/2297 (0.1%)
1	H	0.46	0/1701	0.70	1/2297 (0.0%)
1	I	0.45	0/1701	0.70	1/2297 (0.0%)
1	J	0.46	0/1701	0.70	1/2297 (0.0%)
1	K	0.38	0/1701	0.60	0/2297
All	All	0.58	2/18711 (0.0%)	0.81	36/25267 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	252	VAL	CB-CG1	-6.61	1.39	1.52
1	A	353	VAL	CB-CG2	-5.42	1.41	1.52

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	360	ARG	NE-CZ-NH1	-11.26	114.67	120.30
1	J	360	ARG	NE-CZ-NH1	-10.59	115.00	120.30
1	A	272	LEU	CB-CG-CD2	-10.52	93.11	111.00
1	D	279	LEU	CA-CB-CG	8.80	135.54	115.30
1	D	279	LEU	CB-CG-CD2	-8.60	96.38	111.00

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	1670	0	1670	53	0
1	B	1670	0	1670	44	0
1	C	1670	0	1670	48	0
1	D	1670	0	1670	58	0
1	E	1670	0	1670	40	0
1	F	1670	0	1670	47	0
1	G	1670	0	1670	52	0
1	H	1670	0	1670	54	0
1	I	1670	0	1670	74	0
1	J	1670	0	1670	87	0
1	K	1670	0	1670	42	1
2	A	42	0	19	2	0
2	B	42	0	19	1	0
2	C	42	0	19	1	0
2	D	42	0	19	2	0
2	E	42	0	19	3	0
2	F	42	0	19	6	0
2	G	42	0	19	5	0
2	H	42	0	19	6	0
2	I	42	0	19	21	0
2	J	42	0	19	13	0
2	K	42	0	19	5	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	1	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
4	D	5	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	10	0	0	3	0
4	F	5	0	0	0	0
4	H	5	0	0	1	0
4	I	5	0	0	0	0
4	J	10	0	0	0	0
All	All	18919	0	18579	540	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 14.

The worst 5 of 540 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:H:504:ONM:C4'	2:H:504:ONM:O4'	1.65	1.22
2:K:501:ONM:C4'	2:K:501:ONM:O4'	1.65	1.21
2:I:504:ONM:C4'	2:I:504:ONM:O4'	1.64	1.18
2:A:501:ONM:O4'	2:A:501:ONM:C4'	1.63	1.16
2:J:501:ONM:O4'	2:J:501:ONM:C4'	1.64	1.15

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:K:294:LYS:NZ	1:K:360:ARG:O[2_759]	2.16	0.04

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	214/254 (84%)	211 (99%)	2 (1%)	1 (0%)	32	71
1	B	214/254 (84%)	211 (99%)	3 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	214/254 (84%)	211 (99%)	3 (1%)	0	100	100
1	D	214/254 (84%)	213 (100%)	1 (0%)	0	100	100
1	E	214/254 (84%)	211 (99%)	3 (1%)	0	100	100
1	F	214/254 (84%)	208 (97%)	6 (3%)	0	100	100
1	G	214/254 (84%)	209 (98%)	4 (2%)	1 (0%)	32	71
1	H	214/254 (84%)	210 (98%)	4 (2%)	0	100	100
1	I	214/254 (84%)	212 (99%)	2 (1%)	0	100	100
1	J	214/254 (84%)	206 (96%)	8 (4%)	0	100	100
1	K	214/254 (84%)	210 (98%)	4 (2%)	0	100	100
All	All	2354/2794 (84%)	2312 (98%)	40 (2%)	2 (0%)	55	87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	361	ARG
1	A	299	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	175/207 (84%)	173 (99%)	2 (1%)	78	90
1	B	175/207 (84%)	174 (99%)	1 (1%)	89	95
1	C	175/207 (84%)	172 (98%)	3 (2%)	66	86
1	D	175/207 (84%)	171 (98%)	4 (2%)	56	82
1	E	175/207 (84%)	171 (98%)	4 (2%)	56	82
1	F	175/207 (84%)	172 (98%)	3 (2%)	66	86
1	G	175/207 (84%)	172 (98%)	3 (2%)	66	86
1	H	175/207 (84%)	171 (98%)	4 (2%)	56	82
1	I	175/207 (84%)	173 (99%)	2 (1%)	78	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	175/207 (84%)	172 (98%)	3 (2%)	66	86
1	K	175/207 (84%)	173 (99%)	2 (1%)	78	90
All	All	1925/2277 (84%)	1894 (98%)	31 (2%)	68	86

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	225	ASN
1	I	212	MET
1	G	424	ARG
1	F	395	ARG
1	I	392	MET

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

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 46 ligands modelled in this entry, 22 are monoatomic - leaving 24 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	ONM	A	501	3	38,45,45	4.03	16 (42%)	43,69,69	2.97	13 (30%)
4	SO4	A	504	-	4,4,4	0.29	0	6,6,6	0.15	0
4	SO4	A	505	-	4,4,4	1.27	0	6,6,6	1.25	1 (16%)
2	ONM	B	501	3	38,45,45	3.90	17 (44%)	43,69,69	2.93	10 (23%)
4	SO4	B	502	-	4,4,4	0.18	0	6,6,6	0.14	0
2	ONM	C	501	3	38,45,45	3.84	18 (47%)	43,69,69	2.63	12 (27%)
4	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.22	0
4	SO4	C	503	-	4,4,4	0.22	0	6,6,6	0.18	0
2	ONM	D	501	3	38,45,45	3.92	17 (44%)	43,69,69	3.08	8 (18%)
4	SO4	D	504	-	4,4,4	1.41	0	6,6,6	0.70	0
2	ONM	E	501	3	38,45,45	4.26	20 (52%)	43,69,69	2.91	11 (25%)
4	SO4	E	504	-	4,4,4	0.25	0	6,6,6	0.33	0
4	SO4	E	505	-	4,4,4	1.22	0	6,6,6	0.46	0
2	ONM	F	501	3	38,45,45	4.22	19 (50%)	43,69,69	2.67	13 (30%)
4	SO4	F	502	-	4,4,4	0.29	0	6,6,6	0.24	0
2	ONM	G	501	3	38,45,45	4.83	18 (47%)	43,69,69	3.36	16 (37%)
4	SO4	H	501	-	4,4,4	0.28	0	6,6,6	0.14	0
2	ONM	H	504	3	38,45,45	4.48	17 (44%)	43,69,69	3.34	19 (44%)
4	SO4	I	503	-	4,4,4	0.26	0	6,6,6	0.21	0
2	ONM	I	504	3	38,45,45	4.64	20 (52%)	43,69,69	3.07	17 (39%)
2	ONM	J	501	3	38,45,45	4.54	18 (47%)	43,69,69	2.93	14 (32%)
4	SO4	J	502	-	4,4,4	0.35	0	6,6,6	0.50	0
4	SO4	J	505	-	4,4,4	0.51	0	6,6,6	0.19	0
2	ONM	K	501	3	38,45,45	4.85	20 (52%)	43,69,69	3.38	14 (32%)

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	ONM	A	501	3	-	0/28/48/48	0/4/4/4
4	SO4	A	504	-	-	0/0/0/0	0/0/0/0
4	SO4	A	505	-	-	0/0/0/0	0/0/0/0
2	ONM	B	501	3	-	0/28/48/48	0/4/4/4
4	SO4	B	502	-	-	0/0/0/0	0/0/0/0
2	ONM	C	501	3	-	0/28/48/48	0/4/4/4
4	SO4	C	502	-	-	0/0/0/0	0/0/0/0
4	SO4	C	503	-	-	0/0/0/0	0/0/0/0
2	ONM	D	501	3	-	0/28/48/48	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	D	504	-	-	0/0/0/0	0/0/0/0
2	ONM	E	501	3	-	0/28/48/48	0/4/4/4
4	SO4	E	504	-	-	0/0/0/0	0/0/0/0
4	SO4	E	505	-	-	0/0/0/0	0/0/0/0
2	ONM	F	501	3	-	0/28/48/48	0/4/4/4
4	SO4	F	502	-	-	0/0/0/0	0/0/0/0
2	ONM	G	501	3	-	0/28/48/48	0/4/4/4
4	SO4	H	501	-	-	0/0/0/0	0/0/0/0
2	ONM	H	504	3	-	0/28/48/48	0/4/4/4
4	SO4	I	503	-	-	0/0/0/0	0/0/0/0
2	ONM	I	504	3	-	0/28/48/48	0/4/4/4
2	ONM	J	501	3	-	0/28/48/48	0/4/4/4
4	SO4	J	502	-	-	0/0/0/0	0/0/0/0
4	SO4	J	505	-	-	0/0/0/0	0/0/0/0
2	ONM	K	501	3	-	0/28/48/48	0/4/4/4

The worst 5 of 200 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	ONM	C2'-C1'	-12.56	1.33	1.53
2	D	501	ONM	C2'-C1'	-12.32	1.34	1.53
2	C	501	ONM	C2'-C1'	-10.84	1.36	1.53
2	K	501	ONM	C2'-C1'	-10.83	1.36	1.53
2	A	501	ONM	C2'-C1'	-10.69	1.36	1.53

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	501	ONM	C4'-O4'-C1'	-12.65	96.30	109.77
2	G	501	ONM	C4'-O4'-C1'	-12.47	96.50	109.77
2	E	501	ONM	C4'-O4'-C1'	-11.68	97.33	109.77
2	I	504	ONM	C4'-O4'-C1'	-10.33	98.77	109.77
2	D	501	ONM	C4'-O4'-C1'	-9.53	99.62	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ONM	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	ONM	1	0
2	C	501	ONM	1	0
2	D	501	ONM	2	0
4	D	504	SO4	1	0
2	E	501	ONM	3	0
4	E	504	SO4	2	0
4	E	505	SO4	1	0
2	F	501	ONM	6	0
2	G	501	ONM	5	0
4	H	501	SO4	1	0
2	H	504	ONM	6	0
2	I	504	ONM	21	0
2	J	501	ONM	13	0
2	K	501	ONM	5	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	216/254 (85%)	-0.34	0 100 100	40, 72, 142, 305	0
1	B	216/254 (85%)	-0.30	1 (0%) 90 88	37, 81, 156, 301	0
1	C	216/254 (85%)	-0.34	0 100 100	33, 73, 139, 263	0
1	D	216/254 (85%)	-0.21	1 (0%) 90 88	46, 88, 173, 318	0
1	E	216/254 (85%)	0.05	6 (2%) 53 50	60, 128, 229, 357	0
1	F	216/254 (85%)	0.42	20 (9%) 9 10	82, 151, 262, 417	0
1	G	216/254 (85%)	1.10	50 (23%) 1 1	91, 199, 305, 396	0
1	H	216/254 (85%)	1.17	41 (18%) 1 2	104, 186, 308, 402	0
1	I	216/254 (85%)	0.56	18 (8%) 12 13	101, 163, 268, 448	0
1	J	216/254 (85%)	0.54	19 (8%) 11 11	105, 187, 281, 372	0
1	K	216/254 (85%)	1.10	48 (22%) 1 1	131, 212, 317, 380	0
All	All	2376/2794 (85%)	0.34	204 (8%) 11 12	33, 143, 271, 448	0

The worst 5 of 204 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	412	GLY	8.4
1	K	412	GLY	7.0
1	K	313	PRO	6.6
1	H	407	ARG	6.4
1	I	213	GLU	6.4

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, 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	SO4	C	503	5/5	0.66	0.49	6.11	216,219,220,220	0
4	SO4	I	503	5/5	0.55	0.52	4.36	258,260,262,263	0
4	SO4	F	502	5/5	0.70	0.41	3.05	236,238,238,240	0
4	SO4	A	504	5/5	0.87	0.29	2.23	177,180,181,182	0
4	SO4	J	505	5/5	0.55	0.46	1.91	253,258,261,262	0
4	SO4	C	502	5/5	0.96	0.25	1.78	119,125,129,129	0
4	SO4	H	501	5/5	0.52	0.49	1.54	263,265,267,267	0
2	ONM	C	501	42/42	0.97	0.21	0.78	67,76,88,91	0
2	ONM	F	501	42/42	0.94	0.22	0.48	127,135,141,142	0
2	ONM	J	501	42/42	0.91	0.29	0.44	148,156,169,172	0
3	MN	C	504	1/1	0.97	0.18	0.42	68,68,68,68	0
4	SO4	A	505	5/5	0.89	0.21	0.28	135,135,136,137	0
2	ONM	I	504	42/42	0.92	0.29	0.25	163,168,193,200	0
4	SO4	J	502	5/5	0.83	0.28	-0.05	179,184,188,188	0
2	ONM	D	501	42/42	0.96	0.19	-0.17	49,62,86,92	0
2	ONM	B	501	42/42	0.97	0.17	-0.23	70,80,91,94	0
2	ONM	E	501	42/42	0.92	0.22	-0.26	123,130,153,159	0
2	ONM	A	501	42/42	0.96	0.18	-0.47	59,68,91,97	0
2	ONM	G	501	42/42	0.86	0.27	-0.57	167,175,200,207	0
4	SO4	E	505	5/5	0.95	0.20	-0.61	123,123,123,124	0
2	ONM	K	501	42/42	0.80	0.28	-0.76	164,174,200,206	0
2	ONM	H	504	42/42	0.88	0.28	-0.85	140,149,160,163	0
4	SO4	D	504	5/5	0.96	0.20	-0.89	121,121,121,122	0
3	MN	D	502	1/1	0.92	0.14	-0.97	79,79,79,79	0
3	MN	J	503	1/1	0.96	0.15	-1.09	137,137,137,137	0
3	MN	B	503	1/1	0.98	0.14	-1.17	88,88,88,88	0
3	MN	A	502	1/1	0.99	0.14	-1.26	67,67,67,67	0
3	MN	E	502	1/1	0.96	0.15	-1.70	127,127,127,127	0
3	MN	F	503	1/1	0.92	0.17	-	136,136,136,136	0
3	MN	G	502	1/1	0.97	0.10	-	157,157,157,157	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MN	D	503	1/1	0.94	0.30	-	111,111,111,111	0
3	MN	K	502	1/1	0.93	0.06	-	209,209,209,209	0
3	MN	F	504	1/1	0.94	0.33	-	164,164,164,164	0
3	MN	G	503	1/1	0.87	0.27	-	213,213,213,213	0
3	MN	E	503	1/1	0.90	0.18	-	146,146,146,146	0
3	MN	A	503	1/1	0.98	0.17	-	101,101,101,101	0
4	SO4	B	502	5/5	0.96	0.24	-	117,122,127,127	0
3	MN	I	502	1/1	0.98	0.36	-	236,236,236,236	0
3	MN	H	502	1/1	0.88	0.19	-	146,146,146,146	0
3	MN	I	501	1/1	0.96	0.23	-	126,126,126,126	0
3	MN	H	503	1/1	0.85	0.27	-	182,182,182,182	0
3	MN	B	504	1/1	0.99	0.19	-	150,150,150,150	0
3	MN	J	504	1/1	0.90	0.26	-	175,175,175,175	0
3	MN	C	505	1/1	0.92	0.31	-	146,146,146,146	0
4	SO4	E	504	5/5	0.82	0.43	-	203,209,213,215	0
3	MN	K	503	1/1	0.88	0.30	-	258,258,258,258	0

6.5 Other polymers [i](#)

There are no such residues in this entry.