wwPDB X-ray Structure Validation Summary Report (i)

Sep 15, 2023 – 07:37 AM EDT

PDB ID	:	2PNK
Title	:	CRYSTAL STRUCTURE OF AN URONATE ISOMERASE (BH0493) FROM BACILLUS HALODURANS C-125 AT 2.00 A RESOLUTION
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2007-04-24
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

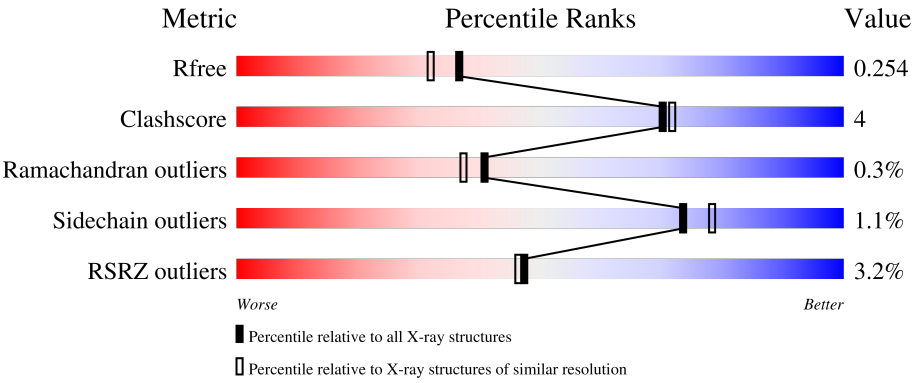
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	428	94% 5%
1	B	428	2% 90% 9%
1	C	428	5% 91% 7%
1	D	428	3% 88% 8%
1	E	428	6% 89% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	428	3% 90% 6%
1	G	428	4% 94% 5%
1	H	428	2% 90% 8%
1	I	428	% 90% 8%
1	J	428	2% 89% 9%
1	K	428	% 93% 6%
1	L	428	6% 92% 7%

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	FMT	E	428	-	-	X	-
6	UNL	B	428	-	-	X	-
6	UNL	H	430	-	-	X	-
6	UNL	J	430	-	-	X	-
8	MPD	G	434	-	-	X	-
9	ACT	L	429	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 45764 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 BH0493 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	Se	0	3	0
			3491	2225	600	644	4	18			
1	B	423	Total	C	N	O	S	Se	0	9	0
			3519	2249	606	642	4	18			
1	C	420	Total	C	N	O	S	Se	0	6	0
			3475	2217	597	639	4	18			
1	D	414	Total	C	N	O	S	Se	0	2	0
			3413	2177	586	629	4	17			
1	E	418	Total	C	N	O	S	Se	0	5	0
			3455	2205	596	633	4	17			
1	F	413	Total	C	N	O	S	Se	0	3	0
			3406	2174	588	624	4	16			
1	G	423	Total	C	N	O	S	Se	0	6	0
			3505	2236	605	642	4	18			
1	H	421	Total	C	N	O	S	Se	0	4	0
			3481	2217	602	641	4	17			
1	I	420	Total	C	N	O	S	Se	0	7	0
			3488	2223	604	641	4	16			
1	J	420	Total	C	N	O	S	Se	0	5	1
			3480	2216	602	642	4	16			
1	K	424	Total	C	N	O	S	Se	0	6	0
			3509	2236	609	643	4	17			
1	L	422	Total	C	N	O	S	Se	0	4	0
			3483	2225	601	636	4	17			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q9KFI6
A	1	MSE	MET	modified residue	UNP Q9KFI6
A	25	MSE	MET	modified residue	UNP Q9KFI6
A	56	MSE	MET	modified residue	UNP Q9KFI6
A	69	MSE	MET	modified residue	UNP Q9KFI6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	MSE	MET	modified residue	UNP Q9KFI6
A	215	MSE	MET	modified residue	UNP Q9KFI6
A	220	MSE	MET	modified residue	UNP Q9KFI6
A	257	MSE	MET	modified residue	UNP Q9KFI6
A	258	MSE	MET	modified residue	UNP Q9KFI6
A	281	MSE	MET	modified residue	UNP Q9KFI6
A	300	MSE	MET	modified residue	UNP Q9KFI6
A	320	MSE	MET	modified residue	UNP Q9KFI6
A	328	MSE	MET	modified residue	UNP Q9KFI6
A	337	MSE	MET	modified residue	UNP Q9KFI6
A	340	MSE	MET	modified residue	UNP Q9KFI6
A	342	MSE	MET	modified residue	UNP Q9KFI6
A	344	MSE	MET	modified residue	UNP Q9KFI6
B	0	GLY	-	expression tag	UNP Q9KFI6
B	1	MSE	MET	modified residue	UNP Q9KFI6
B	25	MSE	MET	modified residue	UNP Q9KFI6
B	56	MSE	MET	modified residue	UNP Q9KFI6
B	69	MSE	MET	modified residue	UNP Q9KFI6
B	142	MSE	MET	modified residue	UNP Q9KFI6
B	215	MSE	MET	modified residue	UNP Q9KFI6
B	220	MSE	MET	modified residue	UNP Q9KFI6
B	257	MSE	MET	modified residue	UNP Q9KFI6
B	258	MSE	MET	modified residue	UNP Q9KFI6
B	281	MSE	MET	modified residue	UNP Q9KFI6
B	300	MSE	MET	modified residue	UNP Q9KFI6
B	320	MSE	MET	modified residue	UNP Q9KFI6
B	328	MSE	MET	modified residue	UNP Q9KFI6
B	337	MSE	MET	modified residue	UNP Q9KFI6
B	340	MSE	MET	modified residue	UNP Q9KFI6
B	342	MSE	MET	modified residue	UNP Q9KFI6
B	344	MSE	MET	modified residue	UNP Q9KFI6
C	0	GLY	-	expression tag	UNP Q9KFI6
C	1	MSE	MET	modified residue	UNP Q9KFI6
C	25	MSE	MET	modified residue	UNP Q9KFI6
C	56	MSE	MET	modified residue	UNP Q9KFI6
C	69	MSE	MET	modified residue	UNP Q9KFI6
C	142	MSE	MET	modified residue	UNP Q9KFI6
C	215	MSE	MET	modified residue	UNP Q9KFI6
C	220	MSE	MET	modified residue	UNP Q9KFI6
C	257	MSE	MET	modified residue	UNP Q9KFI6
C	258	MSE	MET	modified residue	UNP Q9KFI6
C	281	MSE	MET	modified residue	UNP Q9KFI6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	300	MSE	MET	modified residue	UNP Q9KFI6
C	320	MSE	MET	modified residue	UNP Q9KFI6
C	328	MSE	MET	modified residue	UNP Q9KFI6
C	337	MSE	MET	modified residue	UNP Q9KFI6
C	340	MSE	MET	modified residue	UNP Q9KFI6
C	342	MSE	MET	modified residue	UNP Q9KFI6
C	344	MSE	MET	modified residue	UNP Q9KFI6
D	0	GLY	-	expression tag	UNP Q9KFI6
D	1	MSE	MET	modified residue	UNP Q9KFI6
D	25	MSE	MET	modified residue	UNP Q9KFI6
D	56	MSE	MET	modified residue	UNP Q9KFI6
D	69	MSE	MET	modified residue	UNP Q9KFI6
D	142	MSE	MET	modified residue	UNP Q9KFI6
D	215	MSE	MET	modified residue	UNP Q9KFI6
D	220	MSE	MET	modified residue	UNP Q9KFI6
D	257	MSE	MET	modified residue	UNP Q9KFI6
D	258	MSE	MET	modified residue	UNP Q9KFI6
D	281	MSE	MET	modified residue	UNP Q9KFI6
D	300	MSE	MET	modified residue	UNP Q9KFI6
D	320	MSE	MET	modified residue	UNP Q9KFI6
D	328	MSE	MET	modified residue	UNP Q9KFI6
D	337	MSE	MET	modified residue	UNP Q9KFI6
D	340	MSE	MET	modified residue	UNP Q9KFI6
D	342	MSE	MET	modified residue	UNP Q9KFI6
D	344	MSE	MET	modified residue	UNP Q9KFI6
E	0	GLY	-	expression tag	UNP Q9KFI6
E	1	MSE	MET	modified residue	UNP Q9KFI6
E	25	MSE	MET	modified residue	UNP Q9KFI6
E	56	MSE	MET	modified residue	UNP Q9KFI6
E	69	MSE	MET	modified residue	UNP Q9KFI6
E	142	MSE	MET	modified residue	UNP Q9KFI6
E	215	MSE	MET	modified residue	UNP Q9KFI6
E	220	MSE	MET	modified residue	UNP Q9KFI6
E	257	MSE	MET	modified residue	UNP Q9KFI6
E	258	MSE	MET	modified residue	UNP Q9KFI6
E	281	MSE	MET	modified residue	UNP Q9KFI6
E	300	MSE	MET	modified residue	UNP Q9KFI6
E	320	MSE	MET	modified residue	UNP Q9KFI6
E	328	MSE	MET	modified residue	UNP Q9KFI6
E	337	MSE	MET	modified residue	UNP Q9KFI6
E	340	MSE	MET	modified residue	UNP Q9KFI6
E	342	MSE	MET	modified residue	UNP Q9KFI6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	344	MSE	MET	modified residue	UNP Q9KFI6
F	0	GLY	-	expression tag	UNP Q9KFI6
F	1	MSE	MET	modified residue	UNP Q9KFI6
F	25	MSE	MET	modified residue	UNP Q9KFI6
F	56	MSE	MET	modified residue	UNP Q9KFI6
F	69	MSE	MET	modified residue	UNP Q9KFI6
F	142	MSE	MET	modified residue	UNP Q9KFI6
F	215	MSE	MET	modified residue	UNP Q9KFI6
F	220	MSE	MET	modified residue	UNP Q9KFI6
F	257	MSE	MET	modified residue	UNP Q9KFI6
F	258	MSE	MET	modified residue	UNP Q9KFI6
F	281	MSE	MET	modified residue	UNP Q9KFI6
F	300	MSE	MET	modified residue	UNP Q9KFI6
F	320	MSE	MET	modified residue	UNP Q9KFI6
F	328	MSE	MET	modified residue	UNP Q9KFI6
F	337	MSE	MET	modified residue	UNP Q9KFI6
F	340	MSE	MET	modified residue	UNP Q9KFI6
F	342	MSE	MET	modified residue	UNP Q9KFI6
F	344	MSE	MET	modified residue	UNP Q9KFI6
G	0	GLY	-	expression tag	UNP Q9KFI6
G	1	MSE	MET	modified residue	UNP Q9KFI6
G	25	MSE	MET	modified residue	UNP Q9KFI6
G	56	MSE	MET	modified residue	UNP Q9KFI6
G	69	MSE	MET	modified residue	UNP Q9KFI6
G	142	MSE	MET	modified residue	UNP Q9KFI6
G	215	MSE	MET	modified residue	UNP Q9KFI6
G	220	MSE	MET	modified residue	UNP Q9KFI6
G	257	MSE	MET	modified residue	UNP Q9KFI6
G	258	MSE	MET	modified residue	UNP Q9KFI6
G	281	MSE	MET	modified residue	UNP Q9KFI6
G	300	MSE	MET	modified residue	UNP Q9KFI6
G	320	MSE	MET	modified residue	UNP Q9KFI6
G	328	MSE	MET	modified residue	UNP Q9KFI6
G	337	MSE	MET	modified residue	UNP Q9KFI6
G	340	MSE	MET	modified residue	UNP Q9KFI6
G	342	MSE	MET	modified residue	UNP Q9KFI6
G	344	MSE	MET	modified residue	UNP Q9KFI6
H	0	GLY	-	expression tag	UNP Q9KFI6
H	1	MSE	MET	modified residue	UNP Q9KFI6
H	25	MSE	MET	modified residue	UNP Q9KFI6
H	56	MSE	MET	modified residue	UNP Q9KFI6
H	69	MSE	MET	modified residue	UNP Q9KFI6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	142	MSE	MET	modified residue	UNP Q9KFI6
H	215	MSE	MET	modified residue	UNP Q9KFI6
H	220	MSE	MET	modified residue	UNP Q9KFI6
H	257	MSE	MET	modified residue	UNP Q9KFI6
H	258	MSE	MET	modified residue	UNP Q9KFI6
H	281	MSE	MET	modified residue	UNP Q9KFI6
H	300	MSE	MET	modified residue	UNP Q9KFI6
H	320	MSE	MET	modified residue	UNP Q9KFI6
H	328	MSE	MET	modified residue	UNP Q9KFI6
H	337	MSE	MET	modified residue	UNP Q9KFI6
H	340	MSE	MET	modified residue	UNP Q9KFI6
H	342	MSE	MET	modified residue	UNP Q9KFI6
H	344	MSE	MET	modified residue	UNP Q9KFI6
I	0	GLY	-	expression tag	UNP Q9KFI6
I	1	MSE	MET	modified residue	UNP Q9KFI6
I	25	MSE	MET	modified residue	UNP Q9KFI6
I	56	MSE	MET	modified residue	UNP Q9KFI6
I	69	MSE	MET	modified residue	UNP Q9KFI6
I	142	MSE	MET	modified residue	UNP Q9KFI6
I	215	MSE	MET	modified residue	UNP Q9KFI6
I	220	MSE	MET	modified residue	UNP Q9KFI6
I	257	MSE	MET	modified residue	UNP Q9KFI6
I	258	MSE	MET	modified residue	UNP Q9KFI6
I	281	MSE	MET	modified residue	UNP Q9KFI6
I	300	MSE	MET	modified residue	UNP Q9KFI6
I	320	MSE	MET	modified residue	UNP Q9KFI6
I	328	MSE	MET	modified residue	UNP Q9KFI6
I	337	MSE	MET	modified residue	UNP Q9KFI6
I	340	MSE	MET	modified residue	UNP Q9KFI6
I	342	MSE	MET	modified residue	UNP Q9KFI6
I	344	MSE	MET	modified residue	UNP Q9KFI6
J	0	GLY	-	expression tag	UNP Q9KFI6
J	1	MSE	MET	modified residue	UNP Q9KFI6
J	25	MSE	MET	modified residue	UNP Q9KFI6
J	56	MSE	MET	modified residue	UNP Q9KFI6
J	69	MSE	MET	modified residue	UNP Q9KFI6
J	142	MSE	MET	modified residue	UNP Q9KFI6
J	215	MSE	MET	modified residue	UNP Q9KFI6
J	220	MSE	MET	modified residue	UNP Q9KFI6
J	257	MSE	MET	modified residue	UNP Q9KFI6
J	258	MSE	MET	modified residue	UNP Q9KFI6
J	281	MSE	MET	modified residue	UNP Q9KFI6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	300	MSE	MET	modified residue	UNP Q9KFI6
J	320	MSE	MET	modified residue	UNP Q9KFI6
J	328	MSE	MET	modified residue	UNP Q9KFI6
J	337	MSE	MET	modified residue	UNP Q9KFI6
J	340	MSE	MET	modified residue	UNP Q9KFI6
J	342	MSE	MET	modified residue	UNP Q9KFI6
J	344	MSE	MET	modified residue	UNP Q9KFI6
K	0	GLY	-	expression tag	UNP Q9KFI6
K	1	MSE	MET	modified residue	UNP Q9KFI6
K	25	MSE	MET	modified residue	UNP Q9KFI6
K	56	MSE	MET	modified residue	UNP Q9KFI6
K	69	MSE	MET	modified residue	UNP Q9KFI6
K	142	MSE	MET	modified residue	UNP Q9KFI6
K	215	MSE	MET	modified residue	UNP Q9KFI6
K	220	MSE	MET	modified residue	UNP Q9KFI6
K	257	MSE	MET	modified residue	UNP Q9KFI6
K	258	MSE	MET	modified residue	UNP Q9KFI6
K	281	MSE	MET	modified residue	UNP Q9KFI6
K	300	MSE	MET	modified residue	UNP Q9KFI6
K	320	MSE	MET	modified residue	UNP Q9KFI6
K	328	MSE	MET	modified residue	UNP Q9KFI6
K	337	MSE	MET	modified residue	UNP Q9KFI6
K	340	MSE	MET	modified residue	UNP Q9KFI6
K	342	MSE	MET	modified residue	UNP Q9KFI6
K	344	MSE	MET	modified residue	UNP Q9KFI6
L	0	GLY	-	expression tag	UNP Q9KFI6
L	1	MSE	MET	modified residue	UNP Q9KFI6
L	25	MSE	MET	modified residue	UNP Q9KFI6
L	56	MSE	MET	modified residue	UNP Q9KFI6
L	69	MSE	MET	modified residue	UNP Q9KFI6
L	142	MSE	MET	modified residue	UNP Q9KFI6
L	215	MSE	MET	modified residue	UNP Q9KFI6
L	220	MSE	MET	modified residue	UNP Q9KFI6
L	257	MSE	MET	modified residue	UNP Q9KFI6
L	258	MSE	MET	modified residue	UNP Q9KFI6
L	281	MSE	MET	modified residue	UNP Q9KFI6
L	300	MSE	MET	modified residue	UNP Q9KFI6
L	320	MSE	MET	modified residue	UNP Q9KFI6
L	328	MSE	MET	modified residue	UNP Q9KFI6
L	337	MSE	MET	modified residue	UNP Q9KFI6
L	340	MSE	MET	modified residue	UNP Q9KFI6
L	342	MSE	MET	modified residue	UNP Q9KFI6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	344	MSE	MET	modified residue	UNP Q9KFI6

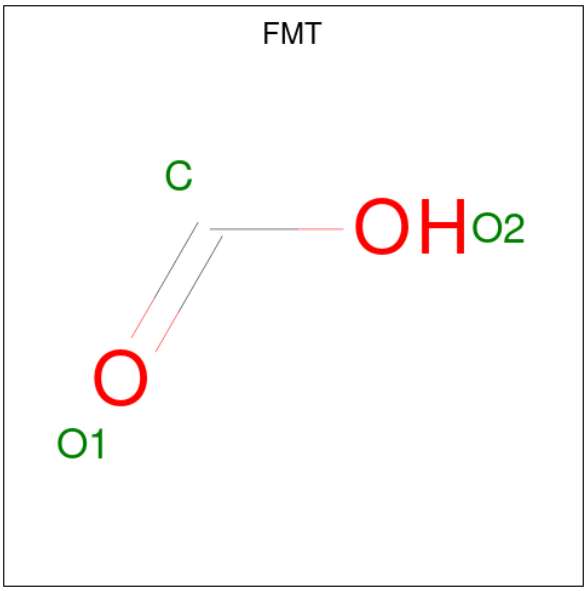
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	J	1	Total Na 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

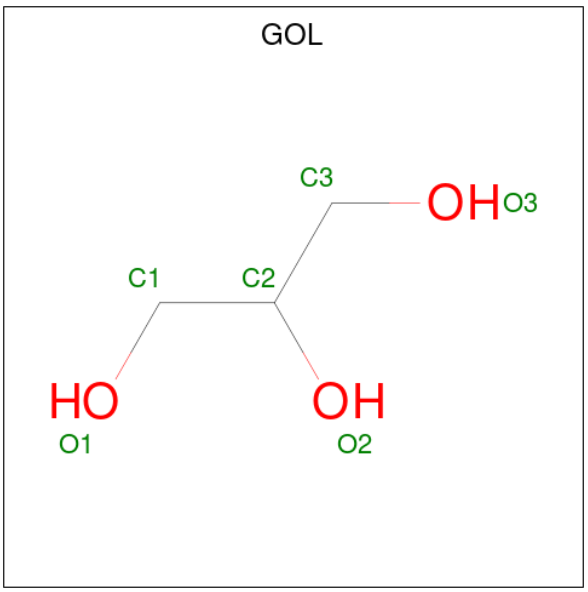
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	G	3	Total Cl 3 3	0	0
3	H	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0
3	L	1	Total Cl 1 1	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			3	1	2			
4	B	1	Total	C	O		0	0
			3	1	2			
4	C	1	Total	C	O		0	0
			3	1	2			
4	D	1	Total	C	O		0	0
			3	1	2			
4	D	1	Total	C	O		0	0
			3	1	2			
4	E	1	Total	C	O		0	0
			3	1	2			
4	F	1	Total	C	O		0	0
			3	1	2			
4	G	1	Total	C	O		0	0
			3	1	2			
4	H	1	Total	C	O		0	0
			3	1	2			
4	I	1	Total	C	O		0	0
			3	1	2			
4	J	1	Total	C	O		0	0
			3	1	2			
4	J	1	Total	C	O		0	0
			3	1	2			
4	K	1	Total	C	O		0	0
			3	1	2			
4	L	1	Total	C	O		0	0
			3	1	2			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0

Continued on next page...

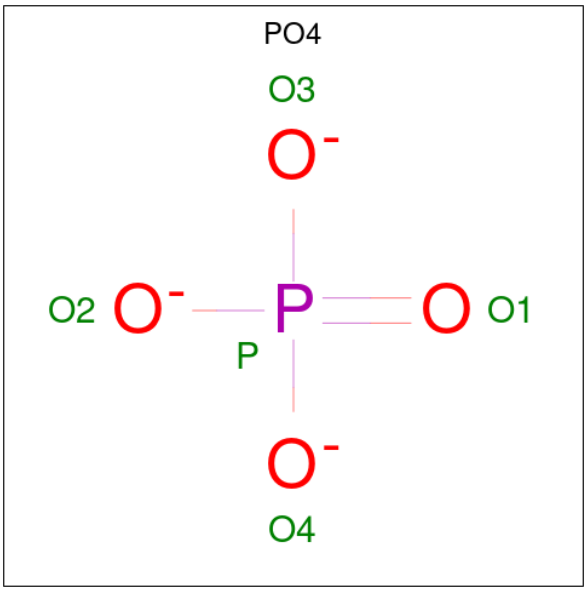
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0
5	J	1	Total C O 6 3 3	0	0
5	J	1	Total C O 6 3 3	0	0
5	K	1	Total C O 6 3 3	0	0
5	K	1	Total C O 6 3 3	0	0
5	K	1	Total C O 6 3 3	0	0
5	K	1	Total C O 6 3 3	0	0
5	L	1	Total C O 6 3 3	0	0
5	L	1	Total C O 6 3 3	0	0

- Molecule 6 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

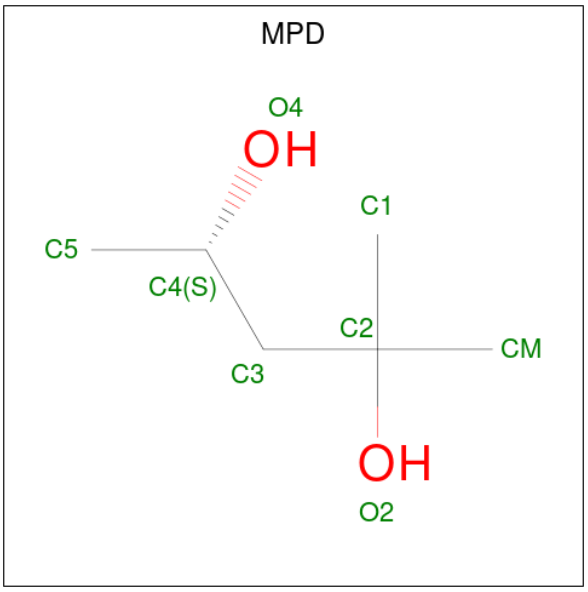
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total As O 16 1 15	0	0
6	H	1	Total As O 16 1 15	0	0
6	J	1	Total As O 18 1 17	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



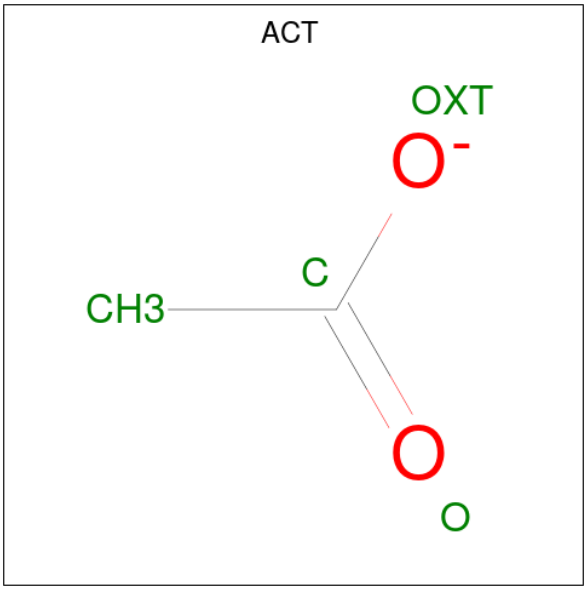
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total O P 5 4 1	0	0
7	D	1	Total O P 5 4 1	0	0
7	F	1	Total O P 5 4 1	0	0
7	K	1	Total O P 5 4 1	0	0

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 8 6 2	0	0
8	G	1	Total C O 8 6 2	0	0
8	G	1	Total C O 8 6 2	0	0
8	K	1	Total C O 8 6 2	0	0
8	K	1	Total C O 8 6 2	0	0
8	L	1	Total C O 8 6 2	0	0

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total C O 4 2 2	0	0
9	I	1	Total C O 4 2 2	0	0
9	L	1	Total C O 4 2 2	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	377	Total O 377 377	0	0

Continued on next page...

Continued from previous page...

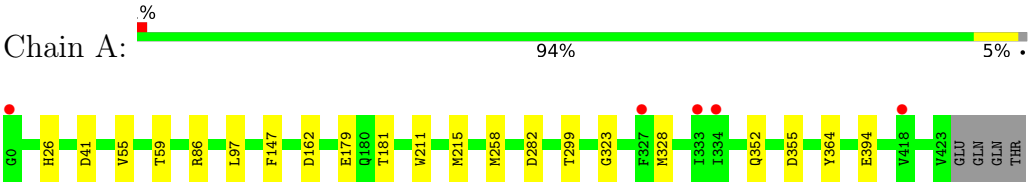
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	292	Total O 292 292	0	0
10	C	267	Total O 267 267	0	0
10	D	224	Total O 224 224	0	0
10	E	179	Total O 179 179	0	0
10	F	234	Total O 234 234	0	0
10	G	366	Total O 366 366	0	0
10	H	371	Total O 371 371	0	0
10	I	262	Total O 262 262	0	0
10	J	405	Total O 405 405	0	0
10	K	407	Total O 407 407	0	0
10	L	348	Total O 348 348	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 (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.

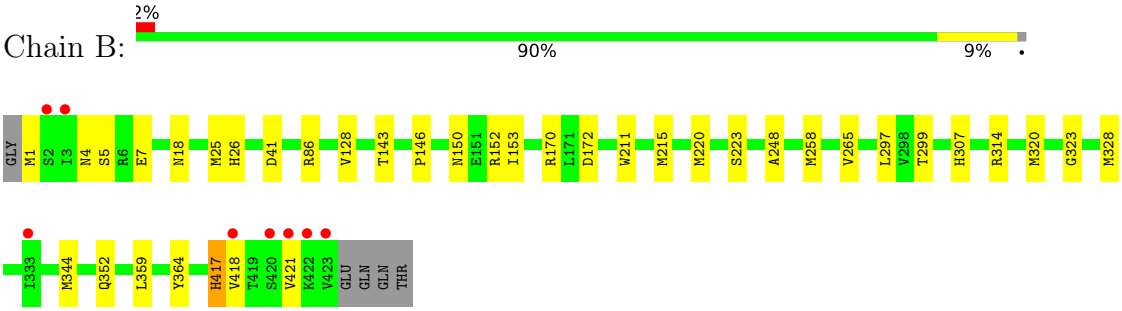
• Molecule 1: BH0493 protein

Chain A:



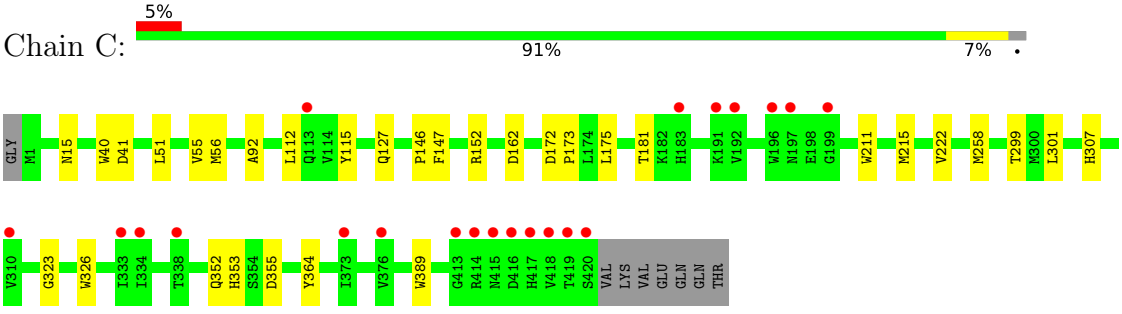
• Molecule 1: BH0493 protein

Chain B:



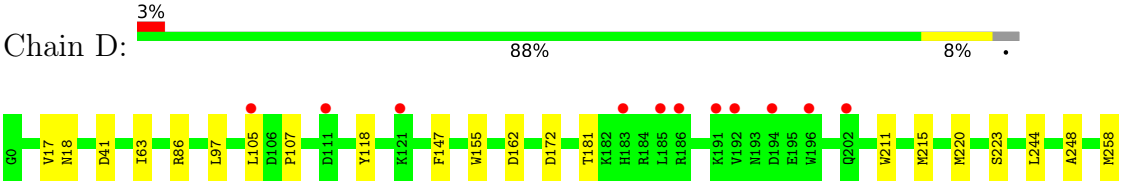
• Molecule 1: BH0493 protein

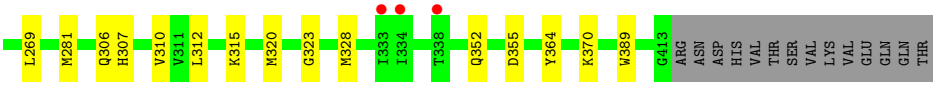
Chain C:



• Molecule 1: BH0493 protein

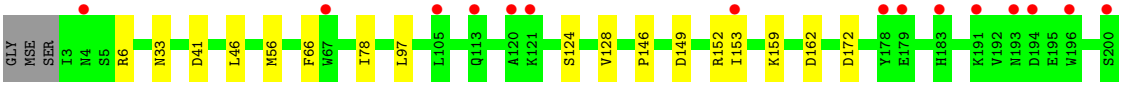
Chain D:

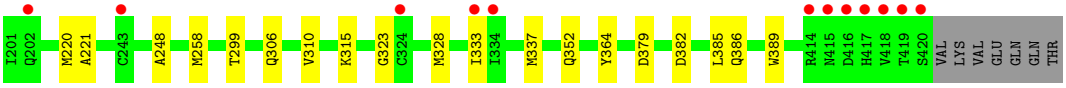




• Molecule 1: BH0493 protein

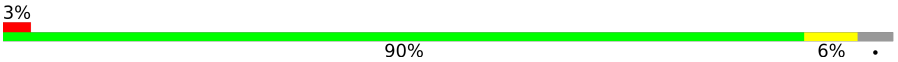
Chain E:

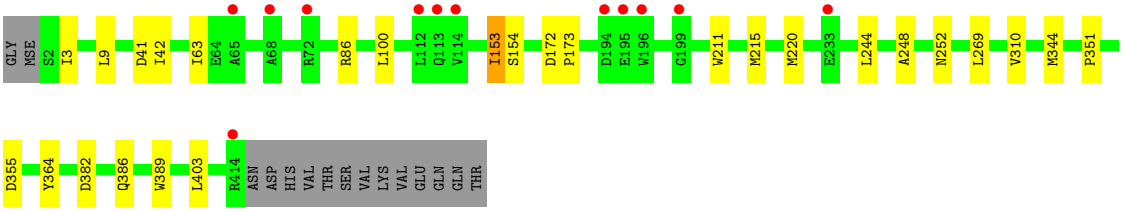




• Molecule 1: BH0493 protein

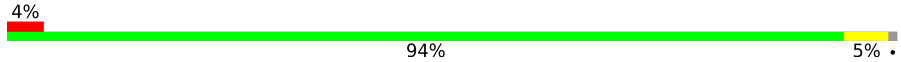
Chain F:

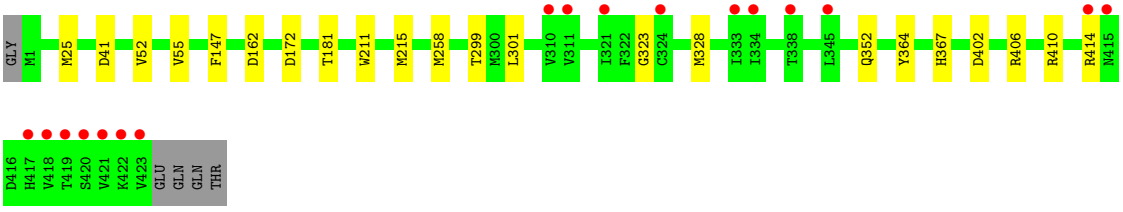




• Molecule 1: BH0493 protein

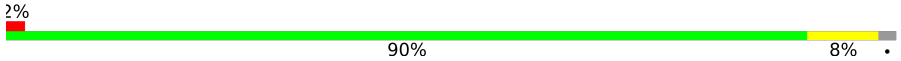
Chain G:

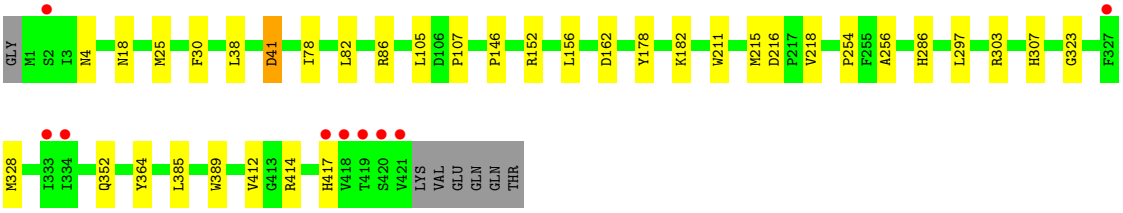




• Molecule 1: BH0493 protein

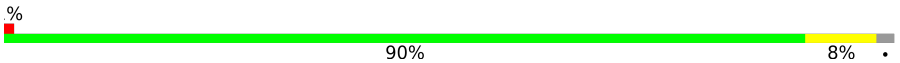
Chain H:

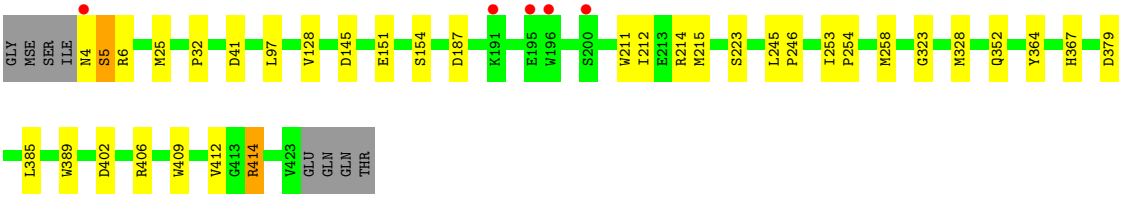




• Molecule 1: BH0493 protein

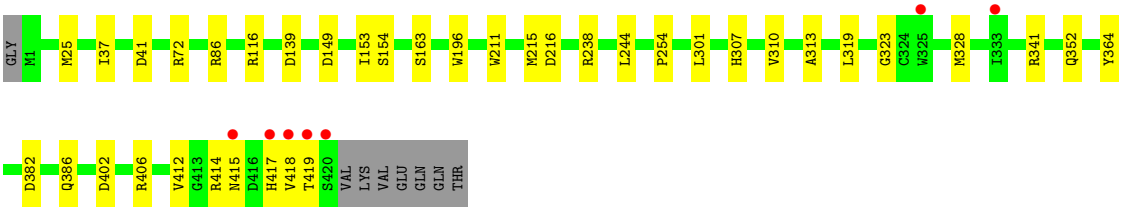
Chain I:





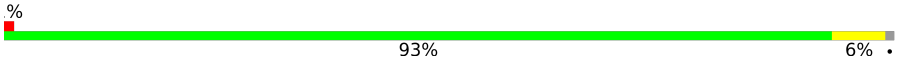
• Molecule 1: BH0493 protein

Chain J:



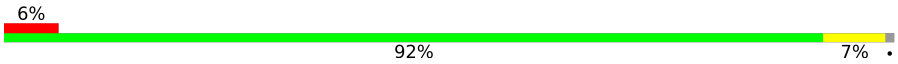
• Molecule 1: BH0493 protein

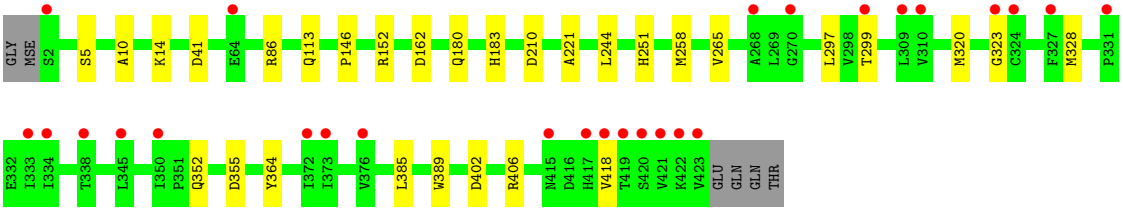
Chain K:



• Molecule 1: BH0493 protein

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	273.72Å 158.56Å 181.24Å 90.00° 116.03° 90.00°	Depositor
Resolution (Å)	48.56 – 2.00 48.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.56-2.00) 93.7 (48.59-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.148 , 0.178 0.173 , 0.254	Depositor DCC
R_{free} test set	1525 reflections (0.35%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	45764	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2462e-03.*

[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: FMT, UNL, ACT, PO4, MPD, GOL, NA, CL

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	0.67	0/3568	0.69	0/4806
1	B	0.60	0/3615	0.69	0/4868
1	C	0.59	0/3561	0.67	0/4799
1	D	0.59	0/3486	0.65	0/4695
1	E	0.57	0/3539	0.63	0/4770
1	F	0.58	0/3483	0.67	0/4694
1	G	0.70	0/3592	0.74	2/4839 (0.0%)
1	H	0.71	0/3562	0.74	2/4800 (0.0%)
1	I	0.64	0/3579	0.69	0/4823
1	J	0.69	0/3564	0.75	0/4801
1	K	0.73	0/3594	0.74	0/4838
1	L	0.73	0/3565	0.76	0/4803
All	All	0.65	0/42708	0.70	4/57536 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	303	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	H	303	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	G	410[A]	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	G	410[B]	ARG	NE-CZ-NH1	5.17	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3491	0	3410	12	0
1	B	3519	0	3462	23	0
1	C	3475	0	3407	17	0
1	D	3413	0	3338	24	0
1	E	3455	0	3375	20	0
1	F	3406	0	3330	14	0
1	G	3505	0	3443	8	0
1	H	3481	0	3403	22	0
1	I	3488	0	3405	21	0
1	J	3480	0	3406	21	0
1	K	3509	0	3432	12	0
1	L	3483	0	3407	19	0
2	A	1	0	0	0	0
2	H	1	0	0	0	0
2	J	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	G	3	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	A	3	0	1	0	0
4	B	3	0	1	1	0
4	C	3	0	1	0	0
4	D	6	0	2	1	0
4	E	3	0	1	2	0
4	F	3	0	1	0	0
4	G	3	0	1	0	0
4	H	3	0	1	0	0
4	I	3	0	1	0	0
4	J	6	0	2	0	0
4	K	3	0	1	1	0
4	L	3	0	1	0	0
5	A	24	0	32	1	0
5	B	6	0	8	0	0
5	D	12	0	16	0	0
5	E	12	0	16	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	6	0	8	0	0
5	H	24	0	32	3	0
5	I	12	0	16	0	0
5	J	12	0	16	0	0
5	K	24	0	32	0	0
5	L	12	0	16	0	0
6	B	16	0	0	27	0
6	H	16	0	0	27	0
6	J	18	0	0	30	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
7	F	5	0	0	0	0
7	K	5	0	0	0	0
8	C	8	0	14	0	0
8	G	16	0	28	6	0
8	K	16	0	28	1	0
8	L	8	0	14	1	0
9	F	4	0	3	0	0
9	I	4	0	3	0	0
9	L	4	0	3	3	0
10	A	377	0	0	2	0
10	B	292	0	0	7	0
10	C	267	0	0	1	0
10	D	224	0	0	3	0
10	E	179	0	0	0	0
10	F	234	0	0	0	0
10	G	366	0	0	2	0
10	H	371	0	0	4	0
10	I	262	0	0	4	0
10	J	405	0	0	3	0
10	K	407	0	0	2	0
10	L	348	0	0	3	0
All	All	45764	0	41117	295	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 295 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)
6:J:430:UNL:O5	6:J:430:UNL:AS	2.14	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:430:UNL:O12	6:J:430:UNL:O2	1.59	1.20
6:J:430:UNL:O12	6:J:430:UNL:O4	1.57	1.16
6:B:428:UNL:O9	6:B:428:UNL:AS	2.26	1.13
6:B:428:UNL:AS	6:B:428:UNL:O1	2.29	1.11

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	425/428 (99%)	420 (99%)	4 (1%)	1 (0%)	47	44
1	B	430/428 (100%)	422 (98%)	7 (2%)	1 (0%)	47	44
1	C	424/428 (99%)	415 (98%)	8 (2%)	1 (0%)	47	44
1	D	414/428 (97%)	409 (99%)	4 (1%)	1 (0%)	47	44
1	E	421/428 (98%)	416 (99%)	4 (1%)	1 (0%)	47	44
1	F	414/428 (97%)	406 (98%)	7 (2%)	1 (0%)	47	44
1	G	427/428 (100%)	419 (98%)	7 (2%)	1 (0%)	47	44
1	H	423/428 (99%)	418 (99%)	4 (1%)	1 (0%)	47	44
1	I	425/428 (99%)	416 (98%)	7 (2%)	2 (0%)	29	23
1	J	423/428 (99%)	419 (99%)	3 (1%)	1 (0%)	47	44
1	K	428/428 (100%)	422 (99%)	5 (1%)	1 (0%)	47	44
1	L	424/428 (99%)	418 (99%)	4 (1%)	2 (0%)	29	23
All	All	5078/5136 (99%)	5000 (98%)	64 (1%)	14 (0%)	41	37

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	41	ASP
1	C	41	ASP
1	D	41	ASP
1	E	41	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	382/370 (103%)	378 (99%)	4 (1%)	76	81
1	B	386/370 (104%)	381 (99%)	5 (1%)	69	74
1	C	382/370 (103%)	379 (99%)	3 (1%)	81	86
1	D	374/370 (101%)	369 (99%)	5 (1%)	69	74
1	E	377/370 (102%)	374 (99%)	3 (1%)	81	86
1	F	372/370 (100%)	367 (99%)	5 (1%)	69	74
1	G	385/370 (104%)	380 (99%)	5 (1%)	69	74
1	H	382/370 (103%)	378 (99%)	4 (1%)	76	81
1	I	382/370 (103%)	379 (99%)	3 (1%)	81	86
1	J	383/370 (104%)	379 (99%)	4 (1%)	76	81
1	K	382/370 (103%)	379 (99%)	3 (1%)	81	86
1	L	379/370 (102%)	375 (99%)	4 (1%)	73	78
All	All	4566/4440 (103%)	4518 (99%)	48 (1%)	73	78

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	367	HIS
1	I	364	TYR
1	G	414	ARG
1	H	364	TYR
1	J	37	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	251	HIS
1	F	28	HIS
1	C	28	HIS
1	B	386	GLN
1	E	307	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 65 ligands modelled in this entry, 11 are monoatomic and 3 are unknown - leaving 51 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	$\#\|Z\| > 2$
5	GOL	H	435	-	5,5,5	0.29	0	5,5,5	0.25	0
5	GOL	I	430	-	5,5,5	0.54	0	5,5,5	0.81	0
4	FMT	D	431	-	2,2,2	0.66	0	1,1,1	0.43	0
4	FMT	C	429	-	2,2,2	1.09	0	1,1,1	0.73	0
4	FMT	I	429	-	2,2,2	1.04	0	1,1,1	0.87	0
5	GOL	J	433	-	5,5,5	0.49	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FMT	F	430	-	2,2,2	0.83	0	1,1,1	0.62	0
4	FMT	H	431	-	2,2,2	0.58	0	1,1,1	0.68	0
9	ACT	I	428	-	3,3,3	0.75	0	3,3,3	1.52	0
4	FMT	L	430	-	2,2,2	1.10	0	1,1,1	0.73	0
5	GOL	H	434	-	5,5,5	0.42	0	5,5,5	0.85	0
5	GOL	B	430	-	5,5,5	0.42	0	5,5,5	0.23	0
8	MPD	G	433	-	7,7,7	0.35	0	9,10,10	0.32	0
4	FMT	J	431	-	2,2,2	0.77	0	1,1,1	0.81	0
5	GOL	J	434	-	5,5,5	0.39	0	5,5,5	0.87	0
5	GOL	A	433	-	5,5,5	0.39	0	5,5,5	0.51	0
5	GOL	H	432	-	5,5,5	0.64	0	5,5,5	0.41	0
7	PO4	K	428	-	4,4,4	0.76	0	6,6,6	0.64	0
8	MPD	K	435	-	7,7,7	0.34	0	9,10,10	0.72	0
5	GOL	K	430	-	5,5,5	0.59	0	5,5,5	0.52	0
4	FMT	D	430	-	2,2,2	0.75	0	1,1,1	0.57	0
5	GOL	E	429	-	5,5,5	0.34	0	5,5,5	0.27	0
4	FMT	A	430	-	2,2,2	1.03	0	1,1,1	0.74	0
5	GOL	L	431	-	5,5,5	0.52	0	5,5,5	0.41	0
5	GOL	K	433	-	5,5,5	0.37	0	5,5,5	0.36	0
8	MPD	G	434	-	7,7,7	0.36	0	9,10,10	0.64	0
5	GOL	H	433	-	5,5,5	0.37	0	5,5,5	0.47	0
5	GOL	A	432	-	5,5,5	0.35	0	5,5,5	0.29	0
5	GOL	D	432	-	5,5,5	0.44	0	5,5,5	0.14	0
5	GOL	L	432	-	5,5,5	0.40	0	5,5,5	0.56	0
7	PO4	F	428	-	4,4,4	0.74	0	6,6,6	0.66	0
4	FMT	E	428	-	2,2,2	0.96	0	1,1,1	0.56	0
5	GOL	G	432	-	5,5,5	0.65	0	5,5,5	0.41	0
5	GOL	K	432	-	5,5,5	0.49	0	5,5,5	0.35	0
8	MPD	C	430	-	7,7,7	0.35	0	9,10,10	0.59	0
8	MPD	K	434	-	7,7,7	0.29	0	9,10,10	0.47	0
5	GOL	E	430	-	5,5,5	0.43	0	5,5,5	0.28	0
9	ACT	F	429	-	3,3,3	0.71	0	3,3,3	1.54	0
4	FMT	B	429	-	2,2,2	0.97	0	1,1,1	0.39	0
9	ACT	L	429	-	3,3,3	1.09	0	3,3,3	0.78	0
5	GOL	A	431	-	5,5,5	0.43	0	5,5,5	0.54	0
5	GOL	D	433	-	5,5,5	0.34	0	5,5,5	0.34	0
8	MPD	L	433	-	7,7,7	0.33	0	9,10,10	0.63	0
5	GOL	K	431	-	5,5,5	0.45	0	5,5,5	0.41	0
4	FMT	K	429	-	2,2,2	0.92	0	1,1,1	0.65	0
5	GOL	I	431	-	5,5,5	0.49	0	5,5,5	0.52	0
7	PO4	D	429	-	4,4,4	0.88	0	6,6,6	0.42	0
5	GOL	A	434	-	5,5,5	0.42	0	5,5,5	0.42	0
4	FMT	J	432	-	2,2,2	0.58	0	1,1,1	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FMT	G	431	-	2,2,2	0.78	0	1,1,1	0.70	0
7	PO4	C	428	-	4,4,4	0.70	0	6,6,6	0.68	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
5	GOL	H	435	-	-	4/4/4/4	-
5	GOL	I	430	-	-	2/4/4/4	-
5	GOL	J	433	-	-	2/4/4/4	-
5	GOL	H	434	-	-	2/4/4/4	-
5	GOL	B	430	-	-	2/4/4/4	-
8	MPD	G	433	-	-	1/5/5/5	-
5	GOL	J	434	-	-	0/4/4/4	-
5	GOL	A	433	-	-	2/4/4/4	-
5	GOL	H	432	-	-	2/4/4/4	-
8	MPD	K	435	-	-	3/5/5/5	-
5	GOL	K	430	-	-	1/4/4/4	-
5	GOL	E	429	-	-	0/4/4/4	-
5	GOL	L	431	-	-	4/4/4/4	-
5	GOL	K	433	-	-	2/4/4/4	-
8	MPD	G	434	-	-	4/5/5/5	-
5	GOL	H	433	-	-	4/4/4/4	-
5	GOL	A	432	-	-	4/4/4/4	-
5	GOL	D	432	-	-	1/4/4/4	-
5	GOL	L	432	-	-	2/4/4/4	-
5	GOL	G	432	-	-	2/4/4/4	-
5	GOL	K	432	-	-	0/4/4/4	-
8	MPD	C	430	-	-	1/5/5/5	-
8	MPD	K	434	-	-	0/5/5/5	-
5	GOL	E	430	-	-	0/4/4/4	-
5	GOL	A	431	-	-	4/4/4/4	-
5	GOL	D	433	-	-	2/4/4/4	-
8	MPD	L	433	-	-	0/5/5/5	-
5	GOL	K	431	-	-	2/4/4/4	-
5	GOL	I	431	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	434	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	431	GOL	O1-C1-C2-C3
5	A	431	GOL	C1-C2-C3-O3
5	A	431	GOL	O2-C2-C3-O3
5	A	432	GOL	C1-C2-C3-O3
5	A	433	GOL	O1-C1-C2-C3

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	435	GOL	2	0
5	H	434	GOL	1	0
8	K	435	MPD	1	0
4	D	430	FMT	1	0
8	G	434	MPD	6	0
4	E	428	FMT	2	0
4	B	429	FMT	1	0
9	L	429	ACT	3	0
8	L	433	MPD	1	0
4	K	429	FMT	1	0
5	A	434	GOL	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, 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	407/428 (95%)	-0.26	5 (1%)	79	78	18, 23, 38, 67	0
1	B	406/428 (94%)	-0.13	8 (1%)	65	63	17, 23, 39, 79	0
1	C	403/428 (94%)	0.26	21 (5%)	27	26	17, 23, 34, 93	0
1	D	397/428 (92%)	0.05	14 (3%)	44	43	17, 23, 34, 44	0
1	E	402/428 (93%)	0.33	27 (6%)	17	17	17, 23, 36, 90	0
1	F	397/428 (92%)	-0.07	12 (3%)	50	49	17, 23, 34, 48	0
1	G	406/428 (94%)	-0.10	17 (4%)	36	35	17, 23, 37, 110	0
1	H	404/428 (94%)	-0.23	9 (2%)	62	60	18, 23, 37, 74	0
1	I	404/428 (94%)	-0.20	5 (1%)	79	78	16, 23, 37, 55	0
1	J	403/428 (94%)	-0.11	7 (1%)	70	68	17, 22, 36, 93	0
1	K	407/428 (95%)	-0.17	4 (0%)	82	81	16, 23, 36, 86	0
1	L	406/428 (94%)	0.31	27 (6%)	17	17	16, 23, 40, 113	0
All	All	4842/5136 (94%)	-0.03	156 (3%)	47	46	16, 23, 37, 113	0

The worst 5 of 156 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	418	VAL	14.7
1	E	419	THR	11.2
1	L	418	VAL	11.2
1	L	423	VAL	11.1
1	L	421	VAL	11.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	GOL	K	431	6/6	0.55	0.34	55,67,68,69	0
4	FMT	D	431	3/3	0.57	0.27	69,69,70,70	0
9	ACT	I	428	4/4	0.65	0.24	67,69,69,70	0
9	ACT	L	429	4/4	0.73	0.27	38,44,44,45	0
5	GOL	A	434	6/6	0.74	0.28	62,69,72,80	0
5	GOL	A	433	6/6	0.77	0.22	61,64,65,67	0
9	ACT	F	429	4/4	0.77	0.23	65,67,67,67	0
3	CL	H	429	1/1	0.81	0.24	72,72,72,72	0
5	GOL	A	431	6/6	0.81	0.26	42,55,62,65	0
5	GOL	L	432	6/6	0.83	0.16	48,56,60,60	0
5	GOL	I	430	6/6	0.83	0.19	50,53,56,60	0
5	GOL	E	430	6/6	0.84	0.14	52,66,71,75	0
5	GOL	L	431	6/6	0.84	0.18	43,52,60,60	0
5	GOL	H	435	6/6	0.85	0.23	59,65,68,70	0
5	GOL	D	433	6/6	0.85	0.23	66,69,71,71	0
5	GOL	K	433	6/6	0.86	0.23	58,65,66,66	0
5	GOL	H	433	6/6	0.87	0.14	45,58,62,62	0
5	GOL	E	429	6/6	0.87	0.18	60,61,63,64	0
5	GOL	D	432	6/6	0.88	0.20	57,58,62,63	0
5	GOL	J	433	6/6	0.88	0.14	33,41,46,47	0
8	MPD	L	433	8/8	0.88	0.16	49,54,56,57	0
5	GOL	J	434	6/6	0.89	0.14	48,49,54,58	0
5	GOL	K	430	6/6	0.89	0.15	29,36,48,48	0
3	CL	G	428	1/1	0.89	0.23	71,71,71,71	0
8	MPD	G	434	8/8	0.89	0.14	35,45,51,56	0
8	MPD	K	435	8/8	0.90	0.14	29,51,59,61	0
5	GOL	H	434	6/6	0.90	0.30	33,53,59,62	0
5	GOL	K	432	6/6	0.90	0.12	55,56,58,61	0
7	PO4	D	429	5/5	0.90	0.21	86,87,92,92	0
4	FMT	J	432	3/3	0.90	0.16	39,39,43,44	0
5	GOL	H	432	6/6	0.91	0.14	30,38,46,52	0
5	GOL	A	432	6/6	0.91	0.15	38,40,49,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	G	430	1/1	0.92	0.11	53,53,53,53	0
7	PO4	C	428	5/5	0.92	0.21	73,76,79,83	0
5	GOL	I	431	6/6	0.92	0.11	42,51,59,59	0
8	MPD	C	430	8/8	0.92	0.16	57,61,64,64	0
5	GOL	G	432	6/6	0.92	0.12	31,39,51,54	0
8	MPD	K	434	8/8	0.93	0.13	25,31,33,35	0
4	FMT	L	430	3/3	0.93	0.09	13,13,17,22	0
5	GOL	B	430	6/6	0.94	0.11	47,54,57,58	0
4	FMT	K	429	3/3	0.94	0.08	18,18,18,25	0
7	PO4	K	428	5/5	0.94	0.24	54,59,66,71	0
3	CL	L	428	1/1	0.94	0.14	56,56,56,56	0
8	MPD	G	433	8/8	0.94	0.14	34,44,49,50	0
4	FMT	A	430	3/3	0.94	0.13	22,22,24,28	0
4	FMT	F	430	3/3	0.95	0.08	30,30,31,39	0
7	PO4	F	428	5/5	0.95	0.13	79,86,89,90	0
4	FMT	J	431	3/3	0.95	0.09	14,14,17,26	0
4	FMT	D	430	3/3	0.96	0.08	28,28,33,39	0
4	FMT	C	429	3/3	0.96	0.08	18,18,21,31	0
4	FMT	E	428	3/3	0.96	0.08	22,22,29,38	0
4	FMT	I	429	3/3	0.97	0.07	22,22,23,32	0
4	FMT	B	429	3/3	0.97	0.08	21,21,26,29	0
2	NA	A	428	1/1	0.97	0.12	31,31,31,31	0
3	CL	J	429	1/1	0.97	0.07	11,11,11,11	0
6	UNL	J	430	18/-	0.97	0.15	10,18,27,30	0
4	FMT	H	431	3/3	0.97	0.07	26,26,28,35	0
6	UNL	B	428	16/-	0.98	0.18	15,24,32,33	0
3	CL	A	429	1/1	0.98	0.05	17,17,17,17	0
4	FMT	G	431	3/3	0.98	0.05	15,15,17,27	0
2	NA	H	428	1/1	0.98	0.04	20,20,20,20	0
2	NA	J	428	1/1	0.98	0.07	17,17,17,17	0
3	CL	D	428	1/1	0.99	0.03	24,24,24,24	0
6	UNL	H	430	16/-	0.99	0.15	10,18,27,31	0
3	CL	G	429	1/1	1.00	0.02	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.