



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:10 PM UTC

PDB ID : 2PNK / pdb_00002pnk
Title : CRYSTAL STRUCTURE OF AN URONATE ISOMERASE (BH0493) FROM
BACILLUS HALODURANS C-125 AT 2.00 Å RESOLUTION
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2007-04-24
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

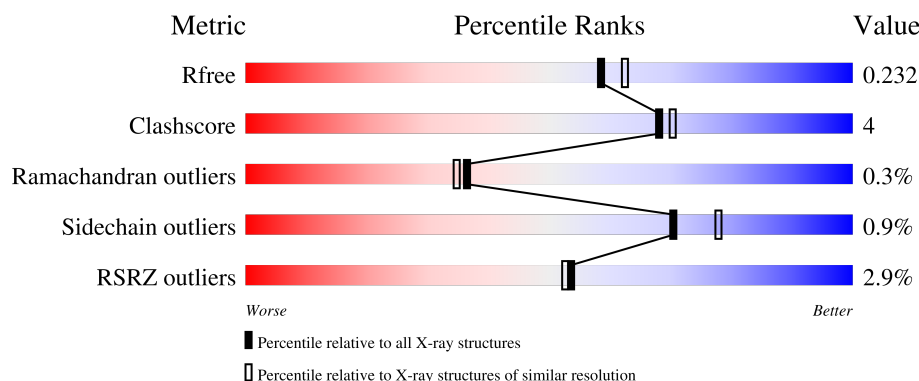
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	428	% 94% 5% .
1	B	428	2% 90% 8% ..
1	C	428	6% 90% 8% .
1	D	428	% 89% 8% .
1	E	428	4% 89% 9% .

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Mol	Chain	Length	Quality of chain
1	F	428	
1	G	428	
1	H	428	
1	I	428	
1	J	428	
1	K	428	
1	L	428	

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
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

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

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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

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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

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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

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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

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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

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

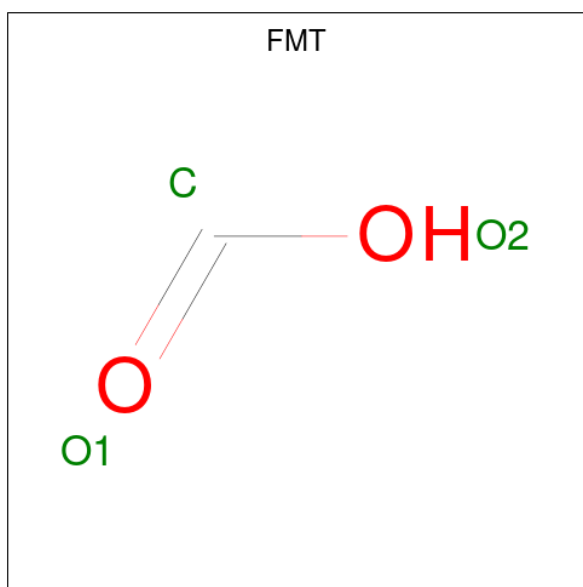
- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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 (CCD ID: CL) (formula: Cl).

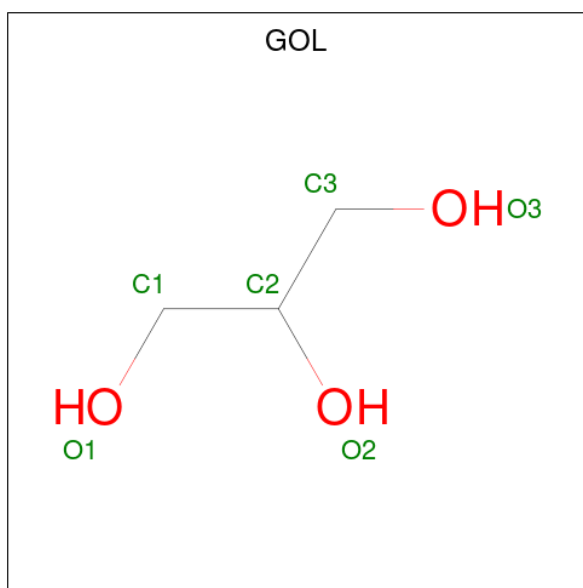
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	G	3	Total Cl 3 3	0	0
3	H	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0
3	L	1	Total Cl 1 1	0	0

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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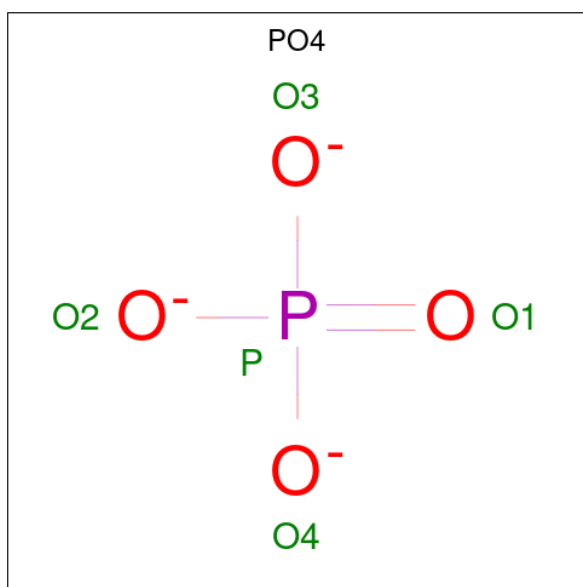
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0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

- Molecule 6 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

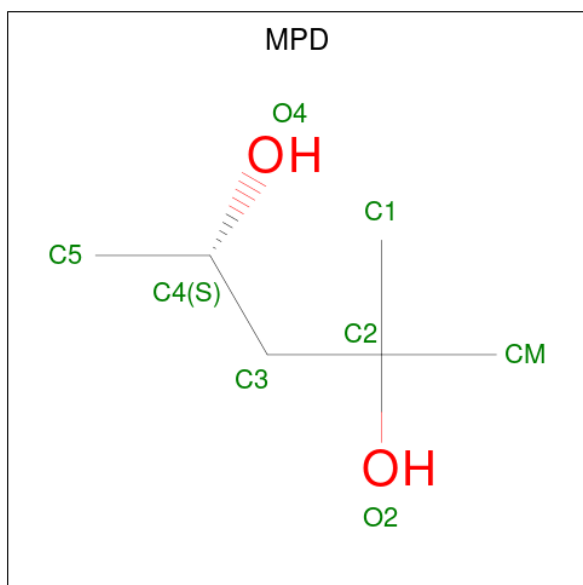
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	As	O	0	0
			16	1	15		
6	H	1	Total	As	O	0	0
			16	1	15		
6	J	1	Total	As	O	0	0
			18	1	17		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



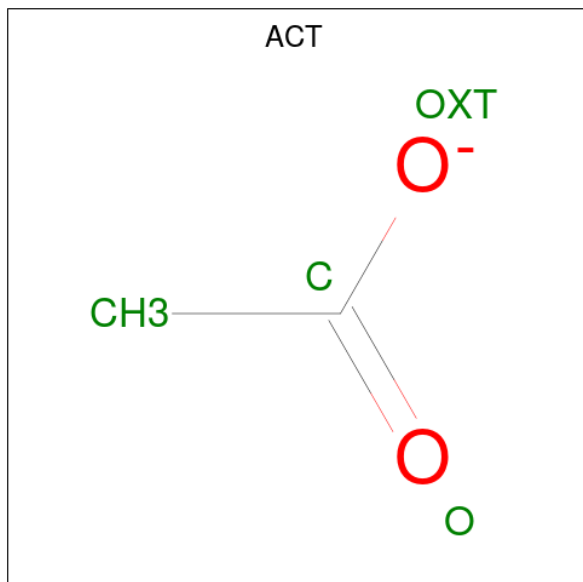
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	P	0	0
			5	4	1		
7	D	1	Total	O	P	0	0
			5	4	1		
7	F	1	Total	O	P	0	0
			5	4	1		
7	K	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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 (CCD ID: 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

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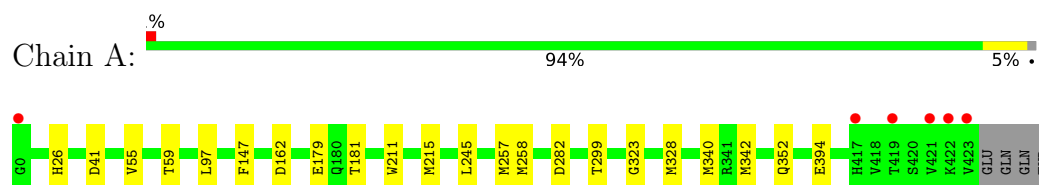
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	292	Total 292	O 292	0	0
10	C	267	Total 267	O 267	0	0
10	D	224	Total 224	O 224	0	0
10	E	179	Total 179	O 179	0	0
10	F	234	Total 234	O 234	0	0
10	G	366	Total 366	O 366	0	0
10	H	371	Total 371	O 371	0	0
10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

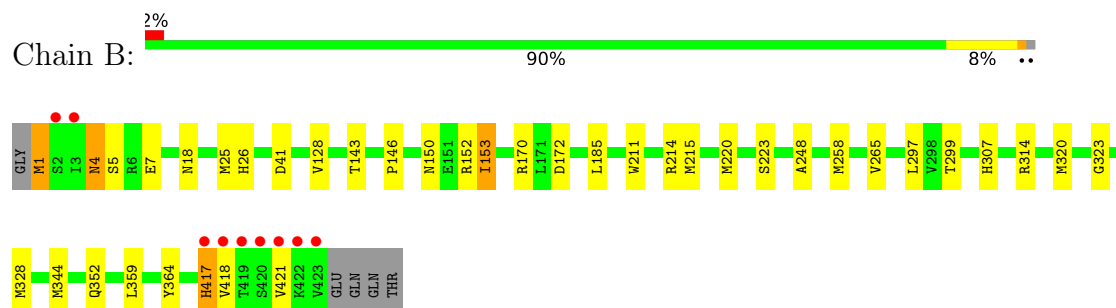
3 Residue-property plots [i](#)

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.

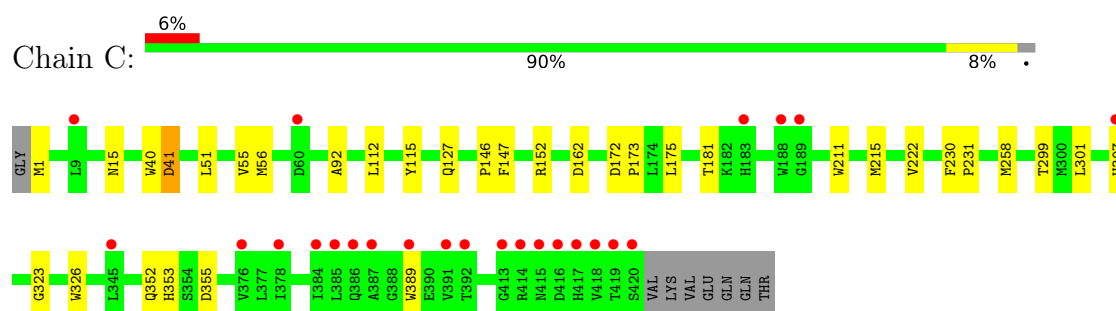
- Molecule 1: BH0493 protein



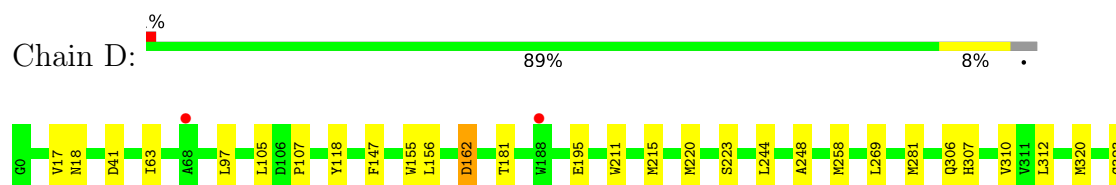
- Molecule 1: BH0493 protein



- Molecule 1: BH0493 protein

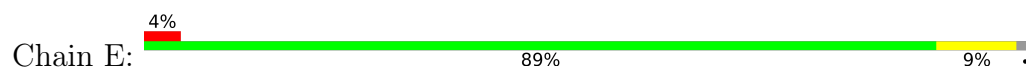


- Molecule 1: BH0493 protein

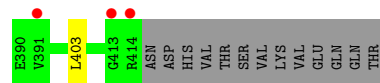
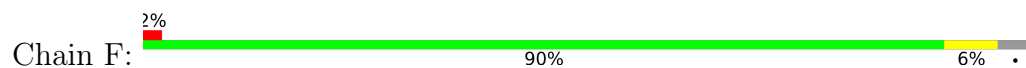




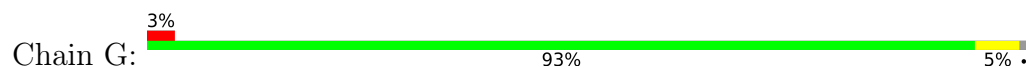
• Molecule 1: BH0493 protein



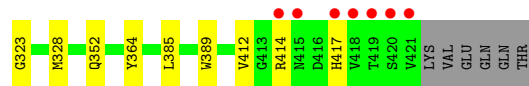
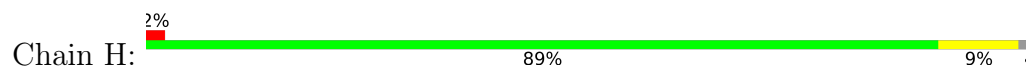
• Molecule 1: BH0493 protein



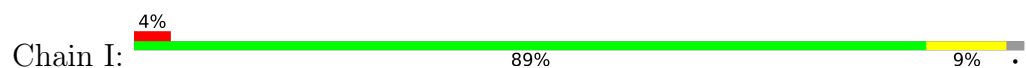
• Molecule 1: BH0493 protein

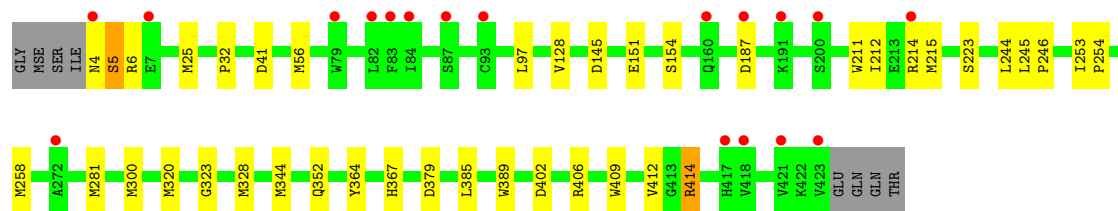


• Molecule 1: BH0493 protein

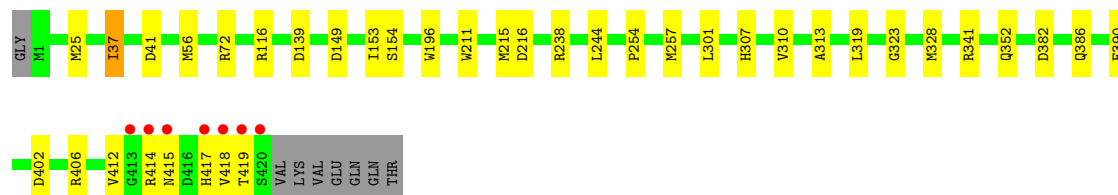
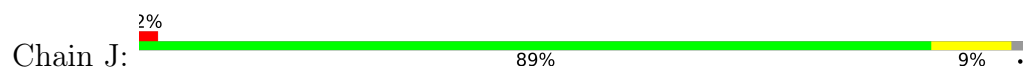


• Molecule 1: BH0493 protein

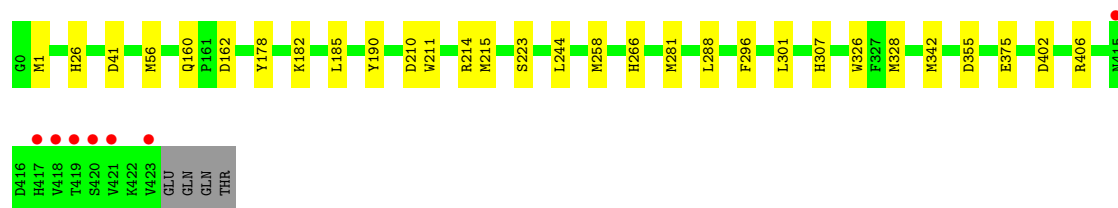




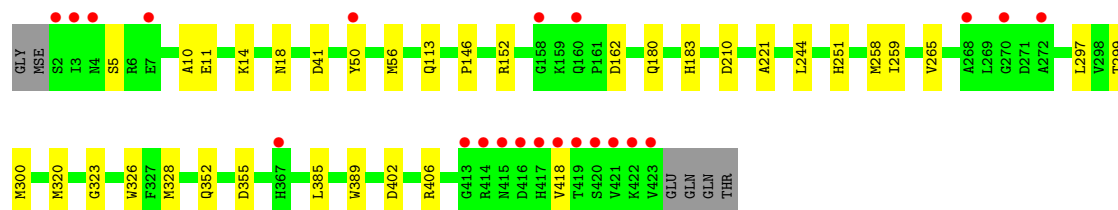
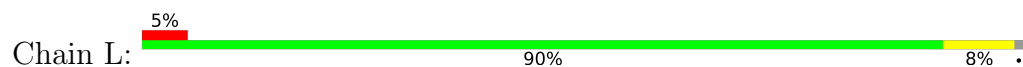
• Molecule 1: BH0493 protein



• Molecule 1: BH0493 protein



• Molecule 1: BH0493 protein



4 Data and refinement statistics

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 48.56 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.56-2.00) 93.7 (48.56-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.148 , 0.178 0.156 , 0.232	Depositor DCC
R_{free} test set	1525 reflections (0.34%)	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)	0.36 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, PO4, NA, UNL, GOL, ACT, FMT, 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	0.83	3/3568 (0.1%)	0.85	2/4806 (0.0%)
1	B	0.75	0/3615	0.83	0/4868
1	C	0.74	0/3561	0.81	0/4799
1	D	0.72	0/3486	0.82	0/4695
1	E	0.72	1/3539 (0.0%)	0.81	0/4770
1	F	0.72	0/3483	0.81	0/4694
1	G	0.90	4/3592 (0.1%)	0.89	0/4839
1	H	0.91	4/3562 (0.1%)	0.89	1/4800 (0.0%)
1	I	0.83	5/3579 (0.1%)	0.84	0/4823
1	J	0.89	2/3564 (0.1%)	0.87	1/4801 (0.0%)
1	K	0.94	4/3594 (0.1%)	0.91	2/4838 (0.0%)
1	L	0.93	2/3565 (0.1%)	0.90	1/4803 (0.0%)
All	All	0.83	25/42708 (0.1%)	0.85	7/57536 (0.0%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	56	MSE	SE-CE	-9.75	1.66	1.95
1	H	281	MSE	SE-CE	-9.13	1.68	1.95
1	I	56	MSE	SE-CE	-8.74	1.69	1.95
1	H	56	MSE	SE-CE	-8.04	1.71	1.95
1	E	320	MSE	SE-CE	-7.65	1.72	1.95
1	G	257	MSE	SE-CE	-7.31	1.73	1.95
1	L	56	MSE	SE-CE	-7.11	1.74	1.95
1	A	257	MSE	SE-CE	-6.91	1.74	1.95
1	L	300	MSE	SE-CE	-6.86	1.74	1.95
1	J	257	MSE	SE-CE	-6.80	1.75	1.95
1	K	342	MSE	SE-CE	-6.68	1.75	1.95
1	K	281	MSE	SE-CE	-6.46	1.76	1.95
1	I	300	MSE	SE-CE	-6.27	1.76	1.95
1	J	56	MSE	SE-CE	-6.22	1.76	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	320	MSE	SE-CE	-6.18	1.76	1.95
1	I	281	MSE	SE-CE	-6.18	1.76	1.95
1	G	220	MSE	SE-CE	-5.99	1.77	1.95
1	A	340	MSE	SE-CE	-5.64	1.78	1.95
1	I	344	MSE	SE-CE	-5.61	1.78	1.95
1	H	279	ALA	CA-CB	5.43	1.62	1.53
1	G	328	MSE	SE-CE	-5.35	1.79	1.95
1	G	401	ALA	CA-CB	5.17	1.61	1.53
1	A	342	MSE	SE-CE	-5.05	1.80	1.95
1	H	320	MSE	SE-CE	-5.04	1.80	1.95
1	K	1	MSE	SE-CE	5.03	2.10	1.95

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	266	HIS	CA-C-N	6.59	126.09	119.24
1	K	266	HIS	C-N-CA	6.59	126.09	119.24
1	J	37	ILE	CB-CA-C	-6.05	102.78	112.16
1	H	81	GLU	N-CA-C	5.14	116.96	111.36
1	L	259	ILE	N-CA-C	5.13	115.97	108.53
1	A	245	LEU	CA-C-N	5.06	124.50	119.24
1	A	245	LEU	C-N-CA	5.06	124.50	119.24

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	24	0
1	C	3475	0	3407	18	0
1	D	3413	0	3338	25	0
1	E	3455	0	3375	19	0
1	F	3406	0	3330	14	0
1	G	3505	0	3443	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3481	0	3403	22	0
1	I	3488	0	3405	22	0
1	J	3480	0	3406	20	0
1	K	3509	0	3432	13	0
1	L	3483	0	3407	21	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	0	0
4	E	3	0	1	1	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	0	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	0
10	E	179	0	0	0	0
10	F	234	0	0	0	0
10	G	366	0	0	3	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	4	0
All	All	45764	0	41117	302	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.

All (302) 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
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
6:H:430:UNL:O1	6:H:430:UNL:AS	2.28	1.10
6:J:430:UNL:O6	6:J:430:UNL:O15	1.67	1.10
6:H:430:UNL:AS	6:H:430:UNL:O6	2.29	1.10
6:J:430:UNL:AS	6:J:430:UNL:O4	2.29	1.10
6:B:428:UNL:O4	6:B:428:UNL:O5	1.70	1.09
6:J:430:UNL:AS	6:J:430:UNL:O13	2.30	1.09
6:H:430:UNL:O4	6:H:430:UNL:O15	1.69	1.08
6:J:430:UNL:O9	6:J:430:UNL:O14	1.73	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:430:UNL:O4	6:H:430:UNL:O13	1.74	1.05
6:J:430:UNL:AS	6:J:430:UNL:O9	2.36	1.03
6:B:428:UNL:AS	6:B:428:UNL:O10	2.38	1.02
6:B:428:UNL:AS	6:B:428:UNL:O14	2.37	1.02
6:H:430:UNL:O8	6:H:430:UNL:O7	1.77	1.02
6:J:430:UNL:O15	6:J:430:UNL:O8	1.76	1.01
6:B:428:UNL:AS	6:B:428:UNL:O6	2.41	0.99
8:G:434:MPD:H11	8:G:434:MPD:H53	1.43	0.99
6:J:430:UNL:O8	6:J:430:UNL:O16	1.79	0.99
6:J:430:UNL:O6	6:J:430:UNL:O17	1.81	0.99
6:J:430:UNL:AS	6:J:430:UNL:O15	2.41	0.98
6:H:430:UNL:AS	6:H:430:UNL:O12	2.42	0.97
6:H:430:UNL:O12	6:H:430:UNL:O10	1.84	0.96
6:B:428:UNL:O9	6:B:428:UNL:O8	1.84	0.95
6:B:428:UNL:AS	6:B:428:UNL:O4	2.46	0.94
6:J:430:UNL:AS	6:J:430:UNL:O16	2.45	0.94
6:B:428:UNL:O5	6:B:428:UNL:O6	1.84	0.94
6:B:428:UNL:O10	6:B:428:UNL:O15	1.86	0.93
6:H:430:UNL:O5	6:H:430:UNL:O14	1.86	0.93
6:H:430:UNL:AS	6:H:430:UNL:O13	2.46	0.93
6:H:430:UNL:O15	6:H:430:UNL:O5	1.87	0.92
6:H:430:UNL:O6	6:H:430:UNL:O14	1.88	0.91
6:J:430:UNL:O15	6:J:430:UNL:O7	1.89	0.90
6:B:428:UNL:O6	6:B:428:UNL:O13	1.90	0.90
6:J:430:UNL:O13	6:J:430:UNL:O10	1.88	0.89
6:H:430:UNL:O13	6:H:430:UNL:O3	1.92	0.87
6:J:430:UNL:O16	6:J:430:UNL:O11	1.92	0.86
6:H:430:UNL:O1	6:H:430:UNL:O2	1.94	0.86
6:B:428:UNL:O14	6:B:428:UNL:O12	1.93	0.85
6:J:430:UNL:O5	6:J:430:UNL:O17	1.94	0.84
8:G:434:MPD:H53	8:G:434:MPD:C1	2.07	0.84
6:B:428:UNL:O4	6:B:428:UNL:O11	1.94	0.84
6:H:430:UNL:AS	6:H:430:UNL:O8	2.56	0.84
1:B:258[B]:MSE:HG3	1:B:299:THR:HG22	1.58	0.83
1:A:258[B]:MSE:HG3	1:A:299:THR:HG22	1.62	0.82
1:D:18:ASN:HB2	10:D:600:HOH:O	1.78	0.82
6:H:430:UNL:AS	6:H:430:UNL:O15	2.57	0.82
6:B:428:UNL:O6	6:B:428:UNL:O7	1.97	0.81
6:J:430:UNL:O16	6:J:430:UNL:O3	1.97	0.81
6:J:430:UNL:O12	6:J:430:UNL:O3	1.98	0.81
6:B:428:UNL:AS	6:B:428:UNL:O3	2.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:428:UNL:O1	6:B:428:UNL:O2	1.98	0.80
6:H:430:UNL:AS	6:H:430:UNL:O9	2.59	0.80
6:H:430:UNL:O10	6:H:430:UNL:O11	2.01	0.79
8:G:434:MPD:C1	8:G:434:MPD:C5	2.60	0.79
6:J:430:UNL:AS	6:J:430:UNL:O12	2.62	0.78
6:J:430:UNL:O10	6:J:430:UNL:O11	2.01	0.78
6:H:430:UNL:O3	6:H:430:UNL:O2	2.01	0.78
6:B:428:UNL:O15	6:B:428:UNL:O11	2.02	0.77
1:F:211:TRP:CE3	1:F:215:MSE:HE3	2.20	0.77
8:K:435:MPD:H52	8:K:435:MPD:HM1	1.65	0.77
1:H:18:ASN:HB2	10:H:773:HOH:O	1.84	0.76
1:K:160:GLN:OE1	1:K:214[A]:ARG:NH1	2.18	0.76
1:F:211:TRP:CZ3	1:F:215:MSE:HE3	2.22	0.75
6:H:430:UNL:O13	6:H:430:UNL:O9	2.04	0.75
6:B:428:UNL:O10	6:B:428:UNL:O11	2.04	0.74
1:E:221:ALA:HB1	1:E:258[B]:MSE:HE1	1.70	0.74
6:B:428:UNL:O4	6:B:428:UNL:O3	2.06	0.74
6:B:428:UNL:O8	6:B:428:UNL:O7	2.06	0.73
6:J:430:UNL:O5	6:J:430:UNL:O6	2.07	0.72
6:H:430:UNL:O7	6:H:430:UNL:O9	2.08	0.72
1:D:211:TRP:CZ3	1:D:215:MSE:HE3	2.25	0.72
1:G:258[B]:MSE:HG3	1:G:299:THR:HG22	1.72	0.71
1:H:286:HIS:HB2	5:H:435:GOL:H2	1.72	0.71
10:K:791:HOH:O	1:L:265:VAL:HG12	1.89	0.70
6:H:430:UNL:O15	6:H:430:UNL:O11	2.09	0.70
6:J:430:UNL:O13	6:J:430:UNL:O11	2.09	0.70
6:H:430:UNL:O6	6:H:430:UNL:O5	2.08	0.69
6:H:430:UNL:AS	6:H:430:UNL:O3	2.70	0.69
8:G:434:MPD:H52	10:G:593:HOH:O	1.92	0.69
6:J:430:UNL:AS	6:J:430:UNL:O3	2.72	0.68
1:B:7:GLU:O	10:B:589:HOH:O	2.12	0.68
6:H:430:UNL:O8	6:H:430:UNL:O9	2.11	0.67
1:L:258[B]:MSE:CE	9:L:429:ACT:H3	2.25	0.67
1:J:211:TRP:CE3	1:J:215:MSE:HE3	2.31	0.65
1:J:244:LEU:C	1:J:244:LEU:HD23	2.21	0.65
1:L:258[B]:MSE:HE1	9:L:429:ACT:H3	1.79	0.64
1:F:42:ILE:HD13	1:F:100:LEU:HD21	1.80	0.64
1:F:244:LEU:C	1:F:244:LEU:HD23	2.23	0.63
6:H:430:UNL:O12	6:H:430:UNL:O11	2.17	0.63
1:B:150:ASN:O	1:B:153:ILE:HG22	1.99	0.63
6:J:430:UNL:O14	6:J:430:UNL:O7	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:178:TYR:O	1:H:182:LYS:HB2	1.99	0.62
1:H:211:TRP:CE3	1:H:215:MSE:HE3	2.35	0.61
1:B:18[B]:ASN:OD1	10:B:650:HOH:O	2.16	0.61
6:J:430:UNL:AS	6:J:430:UNL:O11	2.78	0.61
1:L:221:ALA:HB1	1:L:258[B]:MSE:HE1	1.83	0.61
6:B:428:UNL:O1	6:B:428:UNL:O3	2.19	0.59
1:L:297:LEU:HD23	1:L:320:MSE:HB3	1.85	0.59
1:C:258[B]:MSE:HG3	1:C:299:THR:HG22	1.85	0.59
6:B:428:UNL:O14	6:B:428:UNL:O13	2.20	0.58
1:A:147:PHE:CE1	1:A:181:THR:CG2	2.87	0.58
1:D:244:LEU:C	1:D:244:LEU:HD23	2.27	0.58
6:H:430:UNL:AS	6:H:430:UNL:O5	2.82	0.58
6:H:430:UNL:O1	6:H:430:UNL:O3	2.22	0.58
1:A:147:PHE:CE1	1:A:181:THR:HG23	2.39	0.57
8:G:434:MPD:C5	8:G:434:MPD:H12	2.34	0.57
1:H:146:PRO:O	1:H:152:ARG:HD3	2.04	0.57
6:J:430:UNL:AS	6:J:430:UNL:O8	2.84	0.56
1:H:216:ASP:OD1	1:H:414:ARG:NH2	2.38	0.56
6:B:428:UNL:O3	6:B:428:UNL:O2	2.23	0.56
1:C:172:ASP:HB2	1:C:173:PRO:HD3	1.87	0.56
1:B:146:PRO:O	1:B:152:ARG:HD3	2.06	0.55
1:G:301:LEU:O	1:G:328:MSE:HE3	2.06	0.55
6:J:430:UNL:O9	6:J:430:UNL:O7	2.23	0.55
1:B:7:GLU:HA	10:J:787:HOH:O	2.07	0.55
1:L:323:GLY:HA2	1:L:352:GLN:HA	1.89	0.55
1:F:220:MSE:CE	1:F:248:ALA:HB2	2.37	0.55
6:J:430:UNL:AS	6:J:430:UNL:O7	2.85	0.54
1:C:175:LEU:HD12	1:C:222:VAL:HG21	1.90	0.54
1:J:254:PRO:HG2	1:J:412:VAL:HG12	1.90	0.54
1:B:323:GLY:HA2	1:B:352:GLN:HA	1.89	0.54
1:I:412:VAL:HG23	1:I:414:ARG:HB2	1.90	0.54
1:D:63:ILE:HD13	1:D:269:LEU:HD23	1.89	0.54
1:B:1:MSE:CE	10:B:703:HOH:O	2.56	0.53
1:B:307:HIS:CD2	1:B:344:MSE:HE1	2.42	0.53
1:D:307:HIS:CE1	1:E:328:MSE:CE	2.91	0.53
1:B:7:GLU:CB	10:B:714:HOH:O	2.55	0.53
1:J:149:ASP:O	1:J:153:ILE:HG12	2.08	0.53
1:D:211:TRP:CE3	1:D:215:MSE:HE3	2.43	0.53
1:H:41:ASP:OD2	5:H:434:GOL:H2	2.09	0.53
1:H:156:LEU:O	10:H:710:HOH:O	2.19	0.53
6:B:428:UNL:AS	6:B:428:UNL:O13	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:211:TRP:CE3	1:K:215:MSE:HE3	2.44	0.52
6:B:428:UNL:AS	6:B:428:UNL:O7	2.87	0.52
6:B:428:UNL:O13	6:B:428:UNL:O12	2.27	0.52
1:E:385:LEU:HD23	1:E:389:TRP:O	2.10	0.52
1:I:32:PRO:HG3	1:I:128:VAL:HG21	1.92	0.52
1:G:147:PHE:CE1	1:G:181:THR:HG23	2.45	0.52
1:K:178:TYR:O	1:K:182:LYS:HB2	2.10	0.52
1:L:258[B]:MSE:HG3	1:L:299:THR:HG22	1.92	0.52
1:H:323:GLY:HA2	1:H:352:GLN:HA	1.92	0.51
1:B:128:VAL:HA	1:B:359:LEU:HD21	1.93	0.51
1:E:258[B]:MSE:HG3	1:E:299:THR:HG22	1.93	0.51
1:E:306:GLN:O	1:E:310:VAL:HG23	2.10	0.51
1:H:218:VAL:HG12	1:H:414:ARG:HD2	1.93	0.51
1:A:26:HIS:CE1	1:A:258[B]:MSE:HE3	2.46	0.51
1:E:46:LEU:O	1:E:78:ILE:HD13	2.10	0.51
1:J:418:VAL:HG23	10:J:729:HOH:O	2.10	0.51
1:D:155:TRP:NE1	1:D:215:MSE:HE2	2.26	0.51
1:K:223:SER:OG	1:K:258:MSE:HE3	2.11	0.51
1:K:307:HIS:CE1	1:L:328:MSE:CE	2.94	0.51
1:B:265:VAL:HG12	10:B:708:HOH:O	2.10	0.50
1:A:211:TRP:CE3	1:A:215:MSE:HE3	2.46	0.50
1:D:397:LYS:NZ	10:D:633:HOH:O	2.43	0.50
1:I:212:ILE:HD13	1:I:253:ILE:HD12	1.93	0.50
1:L:50:TYR:HH	1:L:326:TRP:CD1	2.30	0.50
1:I:211:TRP:CE3	1:I:215:MSE:HE3	2.45	0.50
1:J:301:LEU:O	1:J:328:MSE:HE3	2.12	0.50
1:J:307:HIS:CE1	1:K:328:MSE:CE	2.94	0.50
1:E:258[A]:MSE:HG2	1:E:299:THR:HG22	1.94	0.49
1:L:210:ASP:HB3	8:L:433:MPD:HM3	1.94	0.48
1:C:146:PRO:O	1:C:152:ARG:HD3	2.13	0.48
1:E:315:LYS:HZ3	4:E:428:FMT:C	2.27	0.48
1:C:15:ASN:HB3	10:C:595:HOH:O	2.13	0.48
1:D:223:SER:OG	1:D:258:MSE:HE3	2.14	0.48
1:F:382:ASP:O	1:F:386:GLN:HG2	2.13	0.48
1:E:323:GLY:HA2	1:E:352:GLN:HA	1.96	0.47
1:B:143:THR:CG2	1:B:170:ARG:HD2	2.44	0.47
1:I:214:ARG:NH2	10:I:654:HOH:O	2.46	0.47
1:D:389:TRP:HB2	1:E:97:LEU:HD13	1.96	0.47
1:B:328:MSE:HE2	1:B:328:MSE:HA	1.97	0.47
1:I:323:GLY:HA2	1:I:352:GLN:HA	1.96	0.47
1:I:385:LEU:HD23	1:I:389:TRP:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:244:LEU:HD23	1:L:244:LEU:C	2.39	0.47
1:L:258[B]:MSE:HE3	9:L:429:ACT:H3	1.96	0.47
1:A:394:GLU:HG3	10:A:804:HOH:O	2.15	0.47
1:E:146:PRO:O	1:E:152:ARG:HD3	2.15	0.47
1:L:113[A]:GLN:HG2	10:L:616:HOH:O	2.13	0.47
8:G:434:MPD:H52	8:G:434:MPD:H12	1.97	0.47
1:A:179:GLU:HG3	10:A:733:HOH:O	2.15	0.46
1:D:17:VAL:HG12	1:D:370:LYS:HD3	1.97	0.46
1:D:63:ILE:HG22	10:D:620:HOH:O	2.14	0.46
1:I:145:ASP:N	1:I:151[B]:GLU:OE1	2.46	0.46
1:H:286:HIS:HB2	5:H:435:GOL:C2	2.43	0.46
1:B:211:TRP:CE3	1:B:215:MSE:HE3	2.50	0.46
1:C:301:LEU:HD11	1:C:326:TRP:HB3	1.97	0.46
1:K:190:TYR:OH	1:K:210:ASP:OD2	2.29	0.46
1:H:30:PHE:O	1:H:38:LEU:HD13	2.15	0.46
1:L:251:HIS:HE1	10:L:744:HOH:O	1.97	0.46
1:F:63:ILE:HD13	1:F:269:LEU:HD23	1.97	0.46
1:A:328:MSE:CE	1:C:307:HIS:CE1	2.99	0.46
1:B:418:VAL:HG23	10:B:722:HOH:O	2.14	0.46
6:B:428:UNL:AS	6:B:428:UNL:O11	2.93	0.46
1:B:220:MSE:CE	1:B:248:ALA:HB2	2.46	0.46
1:B:417:HIS:O	1:B:421:VAL:HG23	2.15	0.46
1:L:418:VAL:HG23	10:L:768:HOH:O	2.15	0.45
1:B:172:ASP:OD2	1:B:223:SER:HB2	2.16	0.45
1:J:139:ASP:OD1	1:J:417:HIS:HB3	2.16	0.45
1:E:333:ILE:HG22	1:E:337:MSE:SE	2.66	0.45
1:C:112:LEU:HA	1:C:115:TYR:CD2	2.51	0.45
1:D:328:MSE:HE2	1:D:328:MSE:HA	1.98	0.45
1:E:149:ASP:O	1:E:153:ILE:HG13	2.16	0.45
1:I:6:ARG:NH2	1:I:379:ASP:OD1	2.49	0.45
1:D:323:GLY:HA2	1:D:352:GLN:HA	1.99	0.45
1:G:295:LYS:NZ	10:G:747:HOH:O	2.50	0.45
1:I:254:PRO:HG2	1:I:412:VAL:HG12	1.96	0.45
1:J:216:ASP:OD1	1:J:414:ARG:NH2	2.49	0.45
1:L:402:ASP:HA	1:L:406:ARG:HB2	1.97	0.45
1:F:3:ILE:HG21	1:F:9:LEU:HD13	1.99	0.45
1:K:375[B]:GLU:OE1	10:K:584:HOH:O	2.21	0.45
1:D:281:MSE:HE3	1:D:312:LEU:HD22	1.99	0.44
1:H:385:LEU:HD23	1:H:389:TRP:O	2.16	0.44
1:E:33:ASN:O	1:E:159:LYS:HE3	2.17	0.44
1:C:147:PHE:CE1	1:C:181:THR:CG2	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:MSE:HE1	1:E:66:PHE:HB2	1.99	0.44
1:L:180:GLN:O	1:L:183[B]:HIS:ND1	2.50	0.44
1:A:282:ASP:HB3	5:A:434:GOL:H11	2.00	0.44
1:J:313:ALA:HA	1:J:319:LEU:HD23	2.00	0.44
1:I:244:LEU:C	1:I:244:LEU:HD23	2.43	0.44
1:C:211:TRP:CE3	1:C:215:MSE:HE3	2.53	0.44
1:D:147:PHE:CE1	1:D:181:THR:HG23	2.53	0.43
1:F:172:ASP:HB2	1:F:173:PRO:HD3	1.99	0.43
1:G:40:TRP:O	1:G:41:ASP:CG	2.62	0.43
1:H:4:ASN:HB2	10:H:611:HOH:O	2.16	0.43
1:J:402:ASP:HA	1:J:406:ARG:HB2	1.99	0.43
1:K:402:ASP:HA	1:K:406:ARG:HB2	1.99	0.43
1:G:323:GLY:HA2	1:G:352:GLN:HA	2.00	0.43
1:I:25:MSE:HG3	10:I:446:HOH:O	2.17	0.43
1:I:409:TRP:HE3	1:I:414:ARG:HB3	1.84	0.43
1:D:147:PHE:CE1	1:D:181:THR:CG2	3.02	0.43
1:H:307:HIS:CE1	1:I:328:MSE:CE	3.02	0.43
1:I:367[A]:HIS:CE1	10:I:667:HOH:O	2.71	0.43
1:D:105:LEU:O	1:D:107:PRO:HD3	2.18	0.43
1:E:382:ASP:O	1:E:386[A]:GLN:HG2	2.19	0.43
1:G:52:VAL:O	1:G:55:VAL:HG12	2.19	0.43
1:I:402:ASP:HA	1:I:406:ARG:HB2	2.00	0.43
1:J:310:VAL:HG22	1:J:341:ARG:HG2	2.01	0.43
1:D:63:ILE:CD1	1:D:269:LEU:HD23	2.48	0.43
1:I:245:LEU:HB2	1:I:246:PRO:HD3	2.00	0.43
1:D:306:GLN:O	1:D:310:VAL:HG23	2.19	0.43
1:J:323:GLY:HA2	1:J:352:GLN:HA	2.00	0.43
1:D:220:MSE:CE	1:D:248:ALA:HB2	2.49	0.43
1:K:244:LEU:C	1:K:244:LEU:HD23	2.43	0.43
1:A:97:LEU:HD13	1:C:389:TRP:HB2	2.01	0.42
1:F:153:ILE:HG22	1:F:154:SER:N	2.34	0.42
1:H:328:MSE:HA	1:H:328:MSE:HE2	2.02	0.42
1:B:297:LEU:HD23	1:B:320:MSE:HB3	2.02	0.42
1:D:97:LEU:HD13	1:F:389:TRP:HB2	2.01	0.42
1:G:25:MSE:HG3	10:G:438:HOH:O	2.19	0.42
1:I:4:ASN:O	1:I:5:SER:CB	2.68	0.42
1:C:323:GLY:HA3	1:C:353:HIS:ND1	2.34	0.42
1:H:254:PRO:HG2	1:H:412:VAL:HG12	2.01	0.42
1:H:256:ALA:HA	1:H:297:LEU:O	2.20	0.42
1:J:382:ASP:O	1:J:386:GLN:HG2	2.20	0.42
1:C:323:GLY:HA2	1:C:352:GLN:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:402:ASP:HA	1:G:406:ARG:HB2	2.02	0.41
1:I:154[A]:SER:OG	10:I:545:HOH:O	2.21	0.41
1:J:72:ARG:HD3	1:J:116:ARG:CZ	2.50	0.41
1:K:26:HIS:CD2	1:K:355:ASP:OD1	2.73	0.41
1:K:288:LEU:HD23	1:K:296:PHE:CD1	2.56	0.41
1:H:78:ILE:HG23	1:H:82:LEU:HD12	2.01	0.41
1:I:223:SER:OG	1:I:258:MSE:HE3	2.20	0.41
1:J:25:MSE:HG3	10:J:464:HOH:O	2.20	0.41
1:K:301:LEU:HD11	1:K:326:TRP:HB3	2.02	0.41
1:J:211:TRP:CZ3	1:J:215:MSE:HE3	2.55	0.41
1:J:244:LEU:HD23	1:J:244:LEU:O	2.20	0.41
1:A:323:GLY:HA2	1:A:352:GLN:HA	2.03	0.41
1:B:314:ARG:HH21	4:B:429:FMT:C	2.33	0.41
1:L:18:ASN:CG	10:L:758:HOH:O	2.63	0.41
1:B:25:MSE:HG3	10:B:454:HOH:O	2.21	0.41
1:C:51:LEU:HD21	1:C:92:ALA:CB	2.50	0.41
1:D:105:LEU:HD21	1:D:118:TYR:HB2	2.02	0.41
1:A:55:VAL:O	1:A:59:THR:HG22	2.20	0.41
1:E:220:MSE:CE	1:E:248:ALA:HB2	2.51	0.41
1:F:310:VAL:HG11	1:F:344:MSE:HE3	2.03	0.41
1:J:196:TRP:CD1	1:J:238:ARG:HD2	2.56	0.41
1:L:146:PRO:O	1:L:152:ARG:HD3	2.21	0.41
1:C:230:PHE:HA	1:C:231:PRO:C	2.46	0.41
1:H:105:LEU:O	1:H:107:PRO:HD3	2.21	0.41
1:H:389:TRP:HB2	1:I:97:LEU:HD13	2.03	0.41
1:B:4:ASN:HD22	1:B:4:ASN:C	2.29	0.40
1:J:415:ASN:HB3	1:J:419:THR:HB	2.03	0.40
1:D:162:ASP:OD1	1:D:162:ASP:C	2.64	0.40
1:E:124:SER:O	1:E:128:VAL:HG23	2.21	0.40
1:F:244:LEU:HD23	1:F:244:LEU:O	2.20	0.40
1:H:25:MSE:HG3	10:H:440:HOH:O	2.21	0.40
6:J:430:UNL:O5	6:J:430:UNL:O4	2.38	0.40
1:L:385:LEU:HD23	1:L:389:TRP:O	2.21	0.40
1:B:26:HIS:CE1	1:B:258[B]:MSE:HE3	2.56	0.40
1:C:40:TRP:CE3	1:C:127:GLN:HG2	2.57	0.40
1:C:51:LEU:HD21	1:C:92:ALA:HB1	2.02	0.40
1:E:6:ARG:NH2	1:E:379:ASP:OD1	2.55	0.40
1:C:55:VAL:HG13	1:C:56:MSE:HE2	2.04	0.40
1:D:320:MSE:HE1	10:D:535:HOH:O	2.21	0.40
1:F:351:PRO:HD2	1:F:403:LEU:O	2.21	0.40
1:G:211:TRP:CE3	1:G:215:MSE:HE3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:10:ALA:O	1:L:14:LYS:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	425/428 (99%)	420 (99%)	4 (1%)	1 (0%)	43	42
1	B	430/428 (100%)	422 (98%)	7 (2%)	1 (0%)	43	42
1	C	424/428 (99%)	415 (98%)	8 (2%)	1 (0%)	43	42
1	D	414/428 (97%)	409 (99%)	4 (1%)	1 (0%)	43	42
1	E	421/428 (98%)	416 (99%)	4 (1%)	1 (0%)	43	42
1	F	414/428 (97%)	406 (98%)	7 (2%)	1 (0%)	43	42
1	G	427/428 (100%)	419 (98%)	7 (2%)	1 (0%)	43	42
1	H	423/428 (99%)	418 (99%)	4 (1%)	1 (0%)	43	42
1	I	425/428 (99%)	416 (98%)	7 (2%)	2 (0%)	24	21
1	J	423/428 (99%)	419 (99%)	3 (1%)	1 (0%)	43	42
1	K	428/428 (100%)	422 (99%)	5 (1%)	1 (0%)	43	42
1	L	424/428 (99%)	418 (99%)	4 (1%)	2 (0%)	24	21
All	All	5078/5136 (99%)	5000 (98%)	64 (1%)	14 (0%)	36	35

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	B	41	ASP
1	C	41	ASP

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Mol	Chain	Res	Type
1	D	41	ASP
1	E	41	ASP
1	F	41	ASP
1	G	41	ASP
1	H	41	ASP
1	I	5	SER
1	I	41	ASP
1	J	41	ASP
1	K	41	ASP
1	L	5	SER
1	L	41	ASP

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	382/370 (103%)	381 (100%)	1 (0%)	86	91
1	B	386/370 (104%)	378 (98%)	8 (2%)	47	52
1	C	382/370 (103%)	378 (99%)	4 (1%)	68	75
1	D	374/370 (101%)	371 (99%)	3 (1%)	73	80
1	E	377/370 (102%)	374 (99%)	3 (1%)	73	80
1	F	372/370 (100%)	368 (99%)	4 (1%)	65	73
1	G	385/370 (104%)	383 (100%)	2 (0%)	81	87
1	H	382/370 (103%)	379 (99%)	3 (1%)	73	80
1	I	382/370 (103%)	379 (99%)	3 (1%)	73	80
1	J	383/370 (104%)	380 (99%)	3 (1%)	73	80
1	K	382/370 (103%)	380 (100%)	2 (0%)	81	87
1	L	379/370 (102%)	376 (99%)	3 (1%)	73	80
All	All	4566/4440 (103%)	4527 (99%)	39 (1%)	70	78

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASP
1	B	1	MSE
1	B	4	ASN
1	B	5	SER
1	B	153	ILE
1	B	185	LEU
1	B	214	ARG
1	B	364	TYR
1	B	417	HIS
1	C	1	MSE
1	C	41	ASP
1	C	162	ASP
1	C	355	ASP
1	D	156	LEU
1	D	162	ASP
1	D	195	GLU
1	E	162	ASP
1	E	214	ARG
1	E	364	TYR
1	F	153	ILE
1	F	252	ASN
1	F	331	PRO
1	F	364	TYR
1	G	162	ASP
1	G	414	ARG
1	H	41	ASP
1	H	364	TYR
1	H	417	HIS
1	I	187	ASP
1	I	364	TYR
1	I	414	ARG
1	J	37	ILE
1	J	154	SER
1	J	390	GLU
1	K	162	ASP
1	K	185	LEU
1	L	11	GLU
1	L	162	ASP
1	L	355	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	HIS
1	B	20	GLN
1	B	26	HIS
1	B	193	ASN
1	B	386	GLN
1	C	28	HIS
1	C	180	GLN
1	C	183	HIS
1	D	251	HIS
1	D	286	HIS
1	E	18	ASN
1	E	286	HIS
1	F	74	GLN
1	G	202	GLN
1	H	180	GLN
1	H	193	ASN
1	I	160	GLN
1	J	160	GLN
1	K	251	HIS
1	L	286	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 oligosaccharides 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	I	430	-	5,5,5	0.55	0	5,5,5	0.88	0
4	FMT	B	429	-	2,2,2	0.99	0	1,1,1	0.38	0
4	FMT	H	431	-	2,2,2	0.60	0	1,1,1	0.68	0
8	MPD	K	435	-	7,7,7	0.35	0	9,10,10	0.69	0
5	GOL	D	433	-	5,5,5	0.34	0	5,5,5	0.37	0
5	GOL	A	434	-	5,5,5	0.43	0	5,5,5	0.42	0
4	FMT	D	431	-	2,2,2	0.68	0	1,1,1	0.43	0
8	MPD	G	434	-	7,7,7	0.37	0	9,10,10	0.64	0
9	ACT	F	429	-	3,3,3	0.75	0	3,3,3	1.54	0
5	GOL	J	433	-	5,5,5	0.50	0	5,5,5	0.26	0
7	PO4	C	428	-	4,4,4	0.74	0	6,6,6	0.72	0
4	FMT	E	428	-	2,2,2	0.98	0	1,1,1	0.56	0
4	FMT	J	431	-	2,2,2	0.80	0	1,1,1	0.82	0
4	FMT	G	431	-	2,2,2	0.80	0	1,1,1	0.70	0
5	GOL	K	430	-	5,5,5	0.61	0	5,5,5	0.58	0
5	GOL	K	431	-	5,5,5	0.47	0	5,5,5	0.42	0
4	FMT	J	432	-	2,2,2	0.59	0	1,1,1	0.41	0
9	ACT	I	428	-	3,3,3	0.80	0	3,3,3	1.52	0
4	FMT	K	429	-	2,2,2	0.94	0	1,1,1	0.65	0
5	GOL	B	430	-	5,5,5	0.43	0	5,5,5	0.25	0
5	GOL	A	432	-	5,5,5	0.35	0	5,5,5	0.30	0
5	GOL	H	434	-	5,5,5	0.44	0	5,5,5	0.88	0
5	GOL	K	432	-	5,5,5	0.50	0	5,5,5	0.40	0
4	FMT	I	429	-	2,2,2	1.07	0	1,1,1	0.87	0
5	GOL	A	431	-	5,5,5	0.45	0	5,5,5	0.56	0
7	PO4	D	429	-	4,4,4	0.93	0	6,6,6	0.44	0
7	PO4	F	428	-	4,4,4	0.79	0	6,6,6	0.70	0
5	GOL	H	432	-	5,5,5	0.65	0	5,5,5	0.47	0
8	MPD	K	434	-	7,7,7	0.33	0	9,10,10	0.44	0
5	GOL	J	434	-	5,5,5	0.39	0	5,5,5	0.93	0
5	GOL	D	432	-	5,5,5	0.45	0	5,5,5	0.14	0
7	PO4	K	428	-	4,4,4	0.81	0	6,6,6	0.67	0
5	GOL	I	431	-	5,5,5	0.51	0	5,5,5	0.56	0
5	GOL	L	431	-	5,5,5	0.53	0	5,5,5	0.43	0
5	GOL	L	432	-	5,5,5	0.41	0	5,5,5	0.61	0
4	FMT	C	429	-	2,2,2	1.12	0	1,1,1	0.74	0
8	MPD	C	430	-	7,7,7	0.35	0	9,10,10	0.58	0
5	GOL	A	433	-	5,5,5	0.39	0	5,5,5	0.54	0
5	GOL	E	430	-	5,5,5	0.45	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MPD	L	433	-	7,7,7	0.32	0	9,10,10	0.61	0
5	GOL	G	432	-	5,5,5	0.66	0	5,5,5	0.44	0
5	GOL	K	433	-	5,5,5	0.39	0	5,5,5	0.38	0
4	FMT	A	430	-	2,2,2	1.06	0	1,1,1	0.75	0
4	FMT	F	430	-	2,2,2	0.86	0	1,1,1	0.62	0
4	FMT	L	430	-	2,2,2	1.13	0	1,1,1	0.73	0
5	GOL	H	435	-	5,5,5	0.30	0	5,5,5	0.27	0
8	MPD	G	433	-	7,7,7	0.36	0	9,10,10	0.34	0
4	FMT	D	430	-	2,2,2	0.77	0	1,1,1	0.57	0
9	ACT	L	429	-	3,3,3	1.16	0	3,3,3	0.78	0
5	GOL	E	429	-	5,5,5	0.35	0	5,5,5	0.30	0
5	GOL	H	433	-	5,5,5	0.38	0	5,5,5	0.51	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	I	430	-	-	2/4/4/4	-
8	MPD	K	435	-	-	4/5/5/5	-
5	GOL	D	433	-	-	2/4/4/4	-
5	GOL	A	434	-	-	2/4/4/4	-
8	MPD	G	434	-	-	4/5/5/5	-
5	GOL	J	433	-	-	2/4/4/4	-
5	GOL	K	430	-	-	1/4/4/4	-
5	GOL	K	431	-	-	2/4/4/4	-
5	GOL	B	430	-	-	1/4/4/4	-
5	GOL	H	434	-	-	2/4/4/4	-
5	GOL	A	432	-	-	4/4/4/4	-
5	GOL	K	432	-	-	0/4/4/4	-
5	GOL	A	431	-	-	4/4/4/4	-
5	GOL	H	432	-	-	2/4/4/4	-
8	MPD	K	434	-	-	0/5/5/5	-
5	GOL	J	434	-	-	0/4/4/4	-
5	GOL	D	432	-	-	1/4/4/4	-
5	GOL	I	431	-	-	2/4/4/4	-
5	GOL	L	431	-	-	4/4/4/4	-
5	GOL	L	432	-	-	1/4/4/4	-
8	MPD	C	430	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	433	-	-	2/4/4/4	-
5	GOL	E	430	-	-	0/4/4/4	-
8	MPD	L	433	-	-	0/5/5/5	-
5	GOL	G	432	-	-	2/4/4/4	-
5	GOL	K	433	-	-	1/4/4/4	-
5	GOL	H	435	-	-	4/4/4/4	-
8	MPD	G	433	-	-	2/5/5/5	-
5	GOL	E	429	-	-	0/4/4/4	-
5	GOL	H	433	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (56) 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
5	A	434	GOL	O1-C1-C2-C3
5	G	432	GOL	C1-C2-C3-O3
5	H	435	GOL	C1-C2-C3-O3
5	I	431	GOL	O1-C1-C2-C3
5	K	431	GOL	C1-C2-C3-O3
5	L	431	GOL	O1-C1-C2-C3
5	L	431	GOL	C1-C2-C3-O3
8	G	434	MPD	C1-C2-C3-C4
8	G	434	MPD	C2-C3-C4-C5
8	K	435	MPD	O2-C2-C3-C4
8	K	435	MPD	CM-C2-C3-C4
5	A	434	GOL	O1-C1-C2-O2
5	A	432	GOL	O1-C1-C2-C3
5	D	433	GOL	O1-C1-C2-C3
5	H	433	GOL	O1-C1-C2-C3
5	H	433	GOL	C1-C2-C3-O3
5	H	434	GOL	O1-C1-C2-C3
5	J	433	GOL	C1-C2-C3-O3
5	A	431	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	432	GOL	O2-C2-C3-O3
5	D	433	GOL	O1-C1-C2-O2
5	H	435	GOL	O2-C2-C3-O3
5	I	431	GOL	O1-C1-C2-O2
5	K	431	GOL	O2-C2-C3-O3
5	A	432	GOL	O1-C1-C2-O2
5	A	433	GOL	O1-C1-C2-O2
5	G	432	GOL	O2-C2-C3-O3
5	H	433	GOL	O2-C2-C3-O3
5	J	433	GOL	O2-C2-C3-O3
5	L	431	GOL	O1-C1-C2-O2
5	L	431	GOL	O2-C2-C3-O3
5	H	432	GOL	O2-C2-C3-O3
5	H	434	GOL	O1-C1-C2-O2
5	I	430	GOL	O1-C1-C2-O2
5	K	433	GOL	O1-C1-C2-O2
5	D	432	GOL	O2-C2-C3-O3
5	H	433	GOL	O1-C1-C2-O2
5	H	432	GOL	C1-C2-C3-O3
8	C	430	MPD	C1-C2-C3-C4
8	G	434	MPD	CM-C2-C3-C4
8	K	435	MPD	C2-C3-C4-C5
5	I	430	GOL	O1-C1-C2-C3
5	B	430	GOL	O1-C1-C2-O2
5	K	430	GOL	O2-C2-C3-O3
5	H	435	GOL	O1-C1-C2-C3
5	L	432	GOL	O2-C2-C3-O3
8	G	433	MPD	O2-C2-C3-C4
8	G	434	MPD	O2-C2-C3-C4
5	H	435	GOL	O1-C1-C2-O2
8	G	433	MPD	C1-C2-C3-C4
8	K	435	MPD	C1-C2-C3-C4

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	429	FMT	1	0
8	K	435	MPD	1	0
5	A	434	GOL	1	0
8	G	434	MPD	6	0
4	E	428	FMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	434	GOL	1	0
8	L	433	MPD	1	0
5	H	435	GOL	2	0
9	L	429	ACT	3	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	407/428 (95%)	-0.27	6 (1%) 72 71	14, 23, 38, 67	2 (0%)
1	B	406/428 (94%)	0.00	9 (2%) 62 61	12, 23, 39, 79	8 (1%)
1	C	403/428 (94%)	0.69	24 (5%) 27 26	13, 23, 34, 93	5 (1%)
1	D	397/428 (92%)	0.19	3 (0%) 82 82	14, 23, 34, 44	2 (0%)
1	E	402/428 (93%)	0.35	16 (3%) 42 41	12, 23, 36, 90	4 (0%)
1	F	397/428 (92%)	0.43	10 (2%) 58 58	13, 23, 34, 48	3 (0%)
1	G	406/428 (94%)	-0.21	12 (2%) 52 51	13, 23, 37, 110	5 (1%)
1	H	404/428 (94%)	-0.02	8 (1%) 65 64	13, 23, 37, 74	4 (0%)
1	I	404/428 (94%)	0.50	18 (4%) 38 37	13, 23, 37, 55	7 (1%)
1	J	403/428 (94%)	-0.13	7 (1%) 69 68	12, 22, 36, 93	5 (1%)
1	K	407/428 (95%)	-0.13	7 (1%) 69 68	11, 22, 36, 86	6 (1%)
1	L	406/428 (94%)	0.14	22 (5%) 31 30	14, 23, 40, 113	3 (0%)
All	All	4842/5136 (94%)	0.13	142 (2%) 53 52	11, 23, 37, 113	54 (1%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	418	VAL	6.9
1	C	418	VAL	6.8
1	G	419	THR	6.6
1	J	417	HIS	6.0
1	G	421	VAL	5.9
1	L	419	THR	5.9
1	L	423	VAL	5.8
1	C	419	THR	5.8
1	H	418	VAL	5.7
1	L	421	VAL	5.6
1	J	418	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	L	417	HIS	5.4
1	E	418	VAL	5.3
1	J	420	SER	5.3
1	G	418	VAL	5.2
1	C	417	HIS	5.2
1	B	423	VAL	4.9
1	I	421	VAL	4.9
1	C	420	SER	4.8
1	G	417	HIS	4.7
1	K	418	VAL	4.6
1	K	419	THR	4.6
1	L	413	GLY	4.4
1	B	418	VAL	4.4
1	K	423	VAL	4.3
1	G	422	LYS	4.2
1	E	420	SER	4.1
1	H	417	HIS	4.1
1	J	415	ASN	4.0
1	G	423	VAL	4.0
1	K	421	VAL	3.9
1	I	423	VAL	3.8
1	E	417	HIS	3.7
1	L	270	GLY	3.7
1	C	385	LEU	3.6
1	L	420	SER	3.6
1	L	422	LYS	3.5
1	B	3	ILE	3.5
1	E	4	ASN	3.5
1	L	414	ARG	3.5
1	G	420	SER	3.5
1	C	416	ASP	3.5
1	A	421	VAL	3.5
1	C	387	ALA	3.4
1	L	415	ASN	3.4
1	G	413	GLY	3.4
1	B	422	LYS	3.4
1	J	419	THR	3.3
1	B	421	VAL	3.3
1	E	419	THR	3.3
1	B	420	SER	3.3
1	I	83	PHE	3.3
1	E	3	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	414	ARG	3.2
1	L	7	GLU	3.2
1	C	413	GLY	3.2
1	J	414	ARG	3.1
1	E	385	LEU	3.0
1	K	417	HIS	3.0
1	I	191	LYS	3.0
1	I	87	SER	3.0
1	C	415	ASN	3.0
1	E	153	ILE	3.0
1	E	415	ASN	2.9
1	C	391	VAL	2.9
1	L	416	ASP	2.9
1	B	417	HIS	2.9
1	H	421	VAL	2.9
1	C	188	TRP	2.9
1	I	417	HIS	2.9
1	C	376	VAL	2.8
1	G	414	ARG	2.8
1	G	415	ASN	2.8
1	E	5	SER	2.8
1	E	150	ASN	2.7
1	L	272	ALA	2.7
1	K	415	ASN	2.7
1	L	2	SER	2.7
1	A	423	VAL	2.7
1	I	187	ASP	2.7
1	B	2	SER	2.7
1	H	214	ARG	2.7
1	L	4	ASN	2.6
1	H	414	ARG	2.6
1	F	68	ALA	2.5
1	H	419	THR	2.5
1	I	200	SER	2.5
1	C	9	LEU	2.5
1	C	378	ILE	2.5
1	A	422	LYS	2.5
1	F	378	ILE	2.5
1	L	160	GLN	2.5
1	I	418	VAL	2.4
1	F	414	ARG	2.4
1	C	189	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	386[A]	GLN	2.4
1	F	413	GLY	2.4
1	E	378	ILE	2.4
1	A	0	GLY	2.3
1	C	384	ILE	2.3
1	A	417	HIS	2.3
1	C	183	HIS	2.3
1	D	68	ALA	2.3
1	J	413	GLY	2.3
1	L	3	ILE	2.3
1	I	272	ALA	2.3
1	D	188	TRP	2.3
1	K	420	SER	2.3
1	L	367	HIS	2.3
1	L	268	ALA	2.3
1	G	270	GLY	2.2
1	I	84	ILE	2.2
1	F	391	VAL	2.2
1	G	416	ASP	2.2
1	E	120	ALA	2.2
1	C	386	GLN	2.2
1	I	82	LEU	2.2
1	H	420	SER	2.2
1	A	419	THR	2.2
1	L	158	GLY	2.1
1	F	65	ALA	2.1
1	C	60	ASP	2.1
1	F	9	LEU	2.1
1	I	4	ASN	2.1
1	C	389	TRP	2.1
1	E	67	TRP	2.1
1	F	16	ALA	2.1
1	I	79	TRP	2.1
1	F	374	ALA	2.1
1	C	345	LEU	2.0
1	H	415	ASN	2.0
1	I	93	CYS	2.0
1	I	160	GLN	2.0
1	E	266	HIS	2.0
1	B	419	THR	2.0
1	D	378	ILE	2.0
1	I	7	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	377	LEU	2.0
1	I	214	ARG	2.0
1	C	307	HIS	2.0
1	C	392	THR	2.0
1	L	50	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
9	ACT	I	428	4/4	0.62	0.25	67,69,69,70	0
4	FMT	D	431	3/3	0.67	0.27	69,69,70,70	0
5	GOL	D	433	6/6	0.70	0.18	66,69,71,71	0
5	GOL	D	432	6/6	0.72	0.17	57,58,62,63	0
5	GOL	A	434	6/6	0.74	0.18	62,69,72,80	0
5	GOL	L	432	6/6	0.76	0.16	48,56,60,60	0
7	PO4	C	428	5/5	0.77	0.22	73,76,79,83	0
9	ACT	F	429	4/4	0.77	0.17	65,67,67,67	0
5	GOL	K	431	6/6	0.77	0.19	55,67,68,69	0
9	ACT	L	429	4/4	0.78	0.23	38,44,44,45	0
4	FMT	J	432	3/3	0.80	0.19	39,39,43,44	0
5	GOL	K	432	6/6	0.81	0.16	55,56,58,61	0
5	GOL	E	430	6/6	0.81	0.20	52,66,71,75	0
5	GOL	H	435	6/6	0.82	0.21	59,65,68,70	0
5	GOL	K	433	6/6	0.82	0.16	58,65,66,66	0
8	MPD	K	435	8/8	0.82	0.19	29,51,59,61	0
5	GOL	A	431	6/6	0.83	0.18	42,55,62,65	0
8	MPD	G	434	8/8	0.83	0.17	35,45,51,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	I	430	6/6	0.83	0.18	50,53,56,60	0
8	MPD	C	430	8/8	0.84	0.18	57,61,64,64	0
5	GOL	J	434	6/6	0.85	0.16	48,49,54,58	0
5	GOL	L	431	6/6	0.85	0.15	43,52,60,60	0
5	GOL	K	430	6/6	0.85	0.17	29,36,48,48	0
3	CL	H	429	1/1	0.85	0.14	72,72,72,72	0
5	GOL	H	433	6/6	0.85	0.16	45,58,62,62	0
8	MPD	L	433	8/8	0.86	0.16	49,54,56,57	0
7	PO4	D	429	5/5	0.86	0.15	86,87,92,92	0
7	PO4	F	428	5/5	0.87	0.18	79,86,89,90	0
5	GOL	I	431	6/6	0.87	0.13	42,51,59,59	0
5	GOL	E	429	6/6	0.88	0.16	60,61,63,64	0
5	GOL	A	433	6/6	0.88	0.18	61,64,65,67	0
5	GOL	G	432	6/6	0.88	0.14	31,39,51,54	0
5	GOL	B	430	6/6	0.88	0.14	47,54,57,58	0
5	GOL	H	434	6/6	0.88	0.13	33,53,59,62	0
7	PO4	K	428	5/5	0.89	0.10	54,59,66,71	0
3	CL	G	430	1/1	0.90	0.15	53,53,53,53	0
5	GOL	H	432	6/6	0.91	0.12	30,38,46,52	0
3	CL	G	428	1/1	0.91	0.13	71,71,71,71	0
5	GOL	A	432	6/6	0.91	0.11	38,40,49,55	0
8	MPD	G	433	8/8	0.92	0.11	34,44,49,50	0
8	MPD	K	434	8/8	0.93	0.09	25,31,33,35	0
3	CL	L	428	1/1	0.93	0.11	56,56,56,56	0
5	GOL	J	433	6/6	0.93	0.11	33,41,46,47	0
4	FMT	H	431	3/3	0.94	0.11	26,26,28,35	0
4	FMT	A	430	3/3	0.94	0.12	22,22,24,28	0
4	FMT	L	430	3/3	0.94	0.12	13,13,17,22	0
4	FMT	E	428	3/3	0.94	0.11	22,22,29,38	0
4	FMT	F	430	3/3	0.94	0.13	30,30,31,39	0
4	FMT	D	430	3/3	0.95	0.12	28,28,33,39	0
4	FMT	B	429	3/3	0.96	0.09	21,21,26,29	0
4	FMT	J	431	3/3	0.97	0.11	14,14,17,26	0
2	NA	H	428	1/1	0.97	0.12	20,20,20,20	0
4	FMT	G	431	3/3	0.97	0.11	15,15,17,27	0
2	NA	A	428	1/1	0.97	0.07	31,31,31,31	0
4	FMT	K	429	3/3	0.98	0.10	18,18,18,25	0
4	FMT	C	429	3/3	0.98	0.07	18,18,21,31	0
6	UNL	B	428	16/-	0.98	0.07	15,24,32,33	0
6	UNL	H	430	16/-	0.98	0.07	10,18,27,31	0
6	UNL	J	430	18/-	0.98	0.07	10,18,27,30	0
4	FMT	I	429	3/3	0.98	0.08	22,22,23,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	D	428	1/1	0.99	0.12	24,24,24,24	0
2	NA	J	428	1/1	0.99	0.10	17,17,17,17	0
3	CL	G	429	1/1	0.99	0.10	14,14,14,14	0
3	CL	J	429	1/1	1.00	0.11	11,11,11,11	0
3	CL	A	429	1/1	1.00	0.15	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.