



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:34 AM GMT

PDB ID : 3EZW  
Title : Crystal Structure of a Hyperactive Escherichia coli Glycerol Kinase Mutant Gly230 → Asp Obtained Using Microfluidic Crystallization Devices  
Authors : Anderson, M.J.; DeLaBarre, B.; Dunten, P.; Brunger, A.T.; Quake, S.R.  
Deposited on : 2008-10-23  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

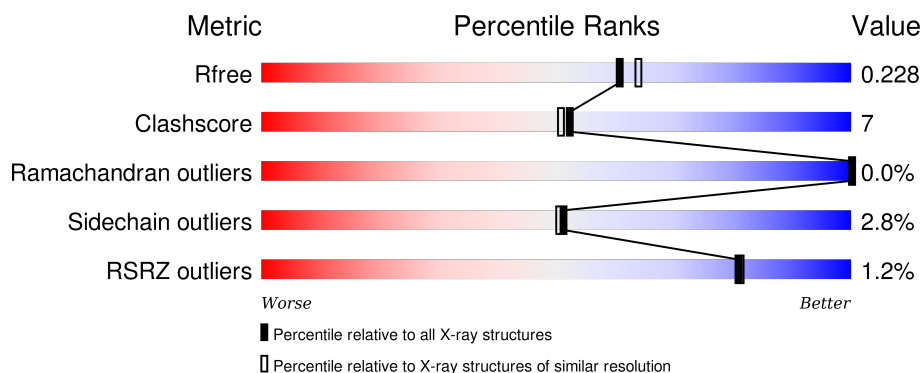
# 1 Overall quality at a glance

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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	526	<div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	B	526	<div> <div> <div>81%</div> <div>13%</div> <div>• 6%</div> </div> </div>
1	C	526	<div> <div> <div>75%</div> <div>17%</div> <div>• 7%</div> </div> </div>
1	D	526	<div> <div> <div>3%</div> <div>71%</div> <div>20%</div> <div>• 8%</div> </div> </div>
1	E	526	<div> <div> <div>2%</div> <div>76%</div> <div>17%</div> <div>• 6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	526	 % 79% 12% • 6%
1	G	526	 % 81% 12% • 5%
1	H	526	 % 77% 16% • 6%

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
5	EDO	E	2643	-	-	-	X
5	EDO	G	2647	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 32916 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	5	0
			3970	2501	698	750	21			
1	B	496	Total	C	N	O	S	0	2	0
			3933	2481	687	746	19			
1	E	492	Total	C	N	O	S	0	2	0
			3908	2464	683	742	19			
1	G	498	Total	C	N	O	S	0	3	0
			3948	2488	689	752	19			
1	C	489	Total	C	N	O	S	0	3	0
			3890	2452	682	735	21			
1	D	482	Total	C	N	O	S	0	1	0
			3818	2409	666	723	20			
1	F	492	Total	C	N	O	S	0	0	0
			3890	2454	680	737	19			
1	H	492	Total	C	N	O	S	0	1	0
			3900	2461	681	739	19			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	ASP	GLY	ENGINEERED	UNP P0A6F3
A	501	GLN	-	EXPRESSION TAG	UNP P0A6F3
A	502	LEU	-	EXPRESSION TAG	UNP P0A6F3
A	503	TYR	-	EXPRESSION TAG	UNP P0A6F3
A	504	THR	-	EXPRESSION TAG	UNP P0A6F3
A	505	ARG	-	EXPRESSION TAG	UNP P0A6F3
A	506	ALA	-	EXPRESSION TAG	UNP P0A6F3
A	507	SER	-	EXPRESSION TAG	UNP P0A6F3
A	508	GLN	-	EXPRESSION TAG	UNP P0A6F3
A	509	PRO	-	EXPRESSION TAG	UNP P0A6F3
A	510	GLU	-	EXPRESSION TAG	UNP P0A6F3
A	511	LEU	-	EXPRESSION TAG	UNP P0A6F3
A	512	ALA	-	EXPRESSION TAG	UNP P0A6F3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	513	PRO	-	EXPRESSION TAG	UNP P0A6F3
A	514	GLU	-	EXPRESSION TAG	UNP P0A6F3
A	515	ASP	-	EXPRESSION TAG	UNP P0A6F3
A	516	PRO	-	EXPRESSION TAG	UNP P0A6F3
A	517	GLU	-	EXPRESSION TAG	UNP P0A6F3
A	518	ASP	-	EXPRESSION TAG	UNP P0A6F3
A	519	LEU	-	EXPRESSION TAG	UNP P0A6F3
A	520	GLU	-	EXPRESSION TAG	UNP P0A6F3
A	521	HIS	-	EXPRESSION TAG	UNP P0A6F3
A	522	HIS	-	EXPRESSION TAG	UNP P0A6F3
A	523	HIS	-	EXPRESSION TAG	UNP P0A6F3
A	524	HIS	-	EXPRESSION TAG	UNP P0A6F3
A	525	HIS	-	EXPRESSION TAG	UNP P0A6F3
A	526	HIS	-	EXPRESSION TAG	UNP P0A6F3
B	230	ASP	GLY	ENGINEERED	UNP P0A6F3
B	501	GLN	-	EXPRESSION TAG	UNP P0A6F3
B	502	LEU	-	EXPRESSION TAG	UNP P0A6F3
B	503	TYR	-	EXPRESSION TAG	UNP P0A6F3
B	504	THR	-	EXPRESSION TAG	UNP P0A6F3
B	505	ARG	-	EXPRESSION TAG	UNP P0A6F3
B	506	ALA	-	EXPRESSION TAG	UNP P0A6F3
B	507	SER	-	EXPRESSION TAG	UNP P0A6F3
B	508	GLN	-	EXPRESSION TAG	UNP P0A6F3
B	509	PRO	-	EXPRESSION TAG	UNP P0A6F3
B	510	GLU	-	EXPRESSION TAG	UNP P0A6F3
B	511	LEU	-	EXPRESSION TAG	UNP P0A6F3
B	512	ALA	-	EXPRESSION TAG	UNP P0A6F3
B	513	PRO	-	EXPRESSION TAG	UNP P0A6F3
B	514	GLU	-	EXPRESSION TAG	UNP P0A6F3
B	515	ASP	-	EXPRESSION TAG	UNP P0A6F3
B	516	PRO	-	EXPRESSION TAG	UNP P0A6F3
B	517	GLU	-	EXPRESSION TAG	UNP P0A6F3
B	518	ASP	-	EXPRESSION TAG	UNP P0A6F3
B	519	LEU	-	EXPRESSION TAG	UNP P0A6F3
B	520	GLU	-	EXPRESSION TAG	UNP P0A6F3
B	521	HIS	-	EXPRESSION TAG	UNP P0A6F3
B	522	HIS	-	EXPRESSION TAG	UNP P0A6F3
B	523	HIS	-	EXPRESSION TAG	UNP P0A6F3
B	524	HIS	-	EXPRESSION TAG	UNP P0A6F3
B	525	HIS	-	EXPRESSION TAG	UNP P0A6F3
B	526	HIS	-	EXPRESSION TAG	UNP P0A6F3
E	230	ASP	GLY	ENGINEERED	UNP P0A6F3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	501	GLN	-	EXPRESSION TAG	UNP P0A6F3
E	502	LEU	-	EXPRESSION TAG	UNP P0A6F3
E	503	TYR	-	EXPRESSION TAG	UNP P0A6F3
E	504	THR	-	EXPRESSION TAG	UNP P0A6F3
E	505	ARG	-	EXPRESSION TAG	UNP P0A6F3
E	506	ALA	-	EXPRESSION TAG	UNP P0A6F3
E	507	SER	-	EXPRESSION TAG	UNP P0A6F3
E	508	GLN	-	EXPRESSION TAG	UNP P0A6F3
E	509	PRO	-	EXPRESSION TAG	UNP P0A6F3
E	510	GLU	-	EXPRESSION TAG	UNP P0A6F3
E	511	LEU	-	EXPRESSION TAG	UNP P0A6F3
E	512	ALA	-	EXPRESSION TAG	UNP P0A6F3
E	513	PRO	-	EXPRESSION TAG	UNP P0A6F3
E	514	GLU	-	EXPRESSION TAG	UNP P0A6F3
E	515	ASP	-	EXPRESSION TAG	UNP P0A6F3
E	516	PRO	-	EXPRESSION TAG	UNP P0A6F3
E	517	GLU	-	EXPRESSION TAG	UNP P0A6F3
E	518	ASP	-	EXPRESSION TAG	UNP P0A6F3
E	519	LEU	-	EXPRESSION TAG	UNP P0A6F3
E	520	GLU	-	EXPRESSION TAG	UNP P0A6F3
E	521	HIS	-	EXPRESSION TAG	UNP P0A6F3
E	522	HIS	-	EXPRESSION TAG	UNP P0A6F3
E	523	HIS	-	EXPRESSION TAG	UNP P0A6F3
E	524	HIS	-	EXPRESSION TAG	UNP P0A6F3
E	525	HIS	-	EXPRESSION TAG	UNP P0A6F3
E	526	HIS	-	EXPRESSION TAG	UNP P0A6F3
G	230	ASP	GLY	ENGINEERED	UNP P0A6F3
G	501	GLN	-	EXPRESSION TAG	UNP P0A6F3
G	502	LEU	-	EXPRESSION TAG	UNP P0A6F3
G	503	TYR	-	EXPRESSION TAG	UNP P0A6F3
G	504	THR	-	EXPRESSION TAG	UNP P0A6F3
G	505	ARG	-	EXPRESSION TAG	UNP P0A6F3
G	506	ALA	-	EXPRESSION TAG	UNP P0A6F3
G	507	SER	-	EXPRESSION TAG	UNP P0A6F3
G	508	GLN	-	EXPRESSION TAG	UNP P0A6F3
G	509	PRO	-	EXPRESSION TAG	UNP P0A6F3
G	510	GLU	-	EXPRESSION TAG	UNP P0A6F3
G	511	LEU	-	EXPRESSION TAG	UNP P0A6F3
G	512	ALA	-	EXPRESSION TAG	UNP P0A6F3
G	513	PRO	-	EXPRESSION TAG	UNP P0A6F3
G	514	GLU	-	EXPRESSION TAG	UNP P0A6F3
G	515	ASP	-	EXPRESSION TAG	UNP P0A6F3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	516	PRO	-	EXPRESSION TAG	UNP P0A6F3
G	517	GLU	-	EXPRESSION TAG	UNP P0A6F3
G	518	ASP	-	EXPRESSION TAG	UNP P0A6F3
G	519	LEU	-	EXPRESSION TAG	UNP P0A6F3
G	520	GLU	-	EXPRESSION TAG	UNP P0A6F3
G	521	HIS	-	EXPRESSION TAG	UNP P0A6F3
G	522	HIS	-	EXPRESSION TAG	UNP P0A6F3
G	523	HIS	-	EXPRESSION TAG	UNP P0A6F3
G	524	HIS	-	EXPRESSION TAG	UNP P0A6F3
G	525	HIS	-	EXPRESSION TAG	UNP P0A6F3
G	526	HIS	-	EXPRESSION TAG	UNP P0A6F3
C	230	ASP	GLY	ENGINEERED	UNP P0A6F3
C	501	GLN	-	EXPRESSION TAG	UNP P0A6F3
C	502	LEU	-	EXPRESSION TAG	UNP P0A6F3
C	503	TYR	-	EXPRESSION TAG	UNP P0A6F3
C	504	THR	-	EXPRESSION TAG	UNP P0A6F3
C	505	ARG	-	EXPRESSION TAG	UNP P0A6F3
C	506	ALA	-	EXPRESSION TAG	UNP P0A6F3
C	507	SER	-	EXPRESSION TAG	UNP P0A6F3
C	508	GLN	-	EXPRESSION TAG	UNP P0A6F3
C	509	PRO	-	EXPRESSION TAG	UNP P0A6F3
C	510	GLU	-	EXPRESSION TAG	UNP P0A6F3
C	511	LEU	-	EXPRESSION TAG	UNP P0A6F3
C	512	ALA	-	EXPRESSION TAG	UNP P0A6F3
C	513	PRO	-	EXPRESSION TAG	UNP P0A6F3
C	514	GLU	-	EXPRESSION TAG	UNP P0A6F3
C	515	ASP	-	EXPRESSION TAG	UNP P0A6F3
C	516	PRO	-	EXPRESSION TAG	UNP P0A6F3
C	517	GLU	-	EXPRESSION TAG	UNP P0A6F3
C	518	ASP	-	EXPRESSION TAG	UNP P0A6F3
C	519	LEU	-	EXPRESSION TAG	UNP P0A6F3
C	520	GLU	-	EXPRESSION TAG	UNP P0A6F3
C	521	HIS	-	EXPRESSION TAG	UNP P0A6F3
C	522	HIS	-	EXPRESSION TAG	UNP P0A6F3
C	523	HIS	-	EXPRESSION TAG	UNP P0A6F3
C	524	HIS	-	EXPRESSION TAG	UNP P0A6F3
C	525	HIS	-	EXPRESSION TAG	UNP P0A6F3
C	526	HIS	-	EXPRESSION TAG	UNP P0A6F3
D	230	ASP	GLY	ENGINEERED	UNP P0A6F3
D	501	GLN	-	EXPRESSION TAG	UNP P0A6F3
D	502	LEU	-	EXPRESSION TAG	UNP P0A6F3
D	503	TYR	-	EXPRESSION TAG	UNP P0A6F3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	504	THR	-	EXPRESSION TAG	UNP P0A6F3
D	505	ARG	-	EXPRESSION TAG	UNP P0A6F3
D	506	ALA	-	EXPRESSION TAG	UNP P0A6F3
D	507	SER	-	EXPRESSION TAG	UNP P0A6F3
D	508	GLN	-	EXPRESSION TAG	UNP P0A6F3
D	509	PRO	-	EXPRESSION TAG	UNP P0A6F3
D	510	GLU	-	EXPRESSION TAG	UNP P0A6F3
D	511	LEU	-	EXPRESSION TAG	UNP P0A6F3
D	512	ALA	-	EXPRESSION TAG	UNP P0A6F3
D	513	PRO	-	EXPRESSION TAG	UNP P0A6F3
D	514	GLU	-	EXPRESSION TAG	UNP P0A6F3
D	515	ASP	-	EXPRESSION TAG	UNP P0A6F3
D	516	PRO	-	EXPRESSION TAG	UNP P0A6F3
D	517	GLU	-	EXPRESSION TAG	UNP P0A6F3
D	518	ASP	-	EXPRESSION TAG	UNP P0A6F3
D	519	LEU	-	EXPRESSION TAG	UNP P0A6F3
D	520	GLU	-	EXPRESSION TAG	UNP P0A6F3
D	521	HIS	-	EXPRESSION TAG	UNP P0A6F3
D	522	HIS	-	EXPRESSION TAG	UNP P0A6F3
D	523	HIS	-	EXPRESSION TAG	UNP P0A6F3
D	524	HIS	-	EXPRESSION TAG	UNP P0A6F3
D	525	HIS	-	EXPRESSION TAG	UNP P0A6F3
D	526	HIS	-	EXPRESSION TAG	UNP P0A6F3
F	230	ASP	GLY	ENGINEERED	UNP P0A6F3
F	501	GLN	-	EXPRESSION TAG	UNP P0A6F3
F	502	LEU	-	EXPRESSION TAG	UNP P0A6F3
F	503	TYR	-	EXPRESSION TAG	UNP P0A6F3
F	504	THR	-	EXPRESSION TAG	UNP P0A6F3
F	505	ARG	-	EXPRESSION TAG	UNP P0A6F3
F	506	ALA	-	EXPRESSION TAG	UNP P0A6F3
F	507	SER	-	EXPRESSION TAG	UNP P0A6F3
F	508	GLN	-	EXPRESSION TAG	UNP P0A6F3
F	509	PRO	-	EXPRESSION TAG	UNP P0A6F3
F	510	GLU	-	EXPRESSION TAG	UNP P0A6F3
F	511	LEU	-	EXPRESSION TAG	UNP P0A6F3
F	512	ALA	-	EXPRESSION TAG	UNP P0A6F3
F	513	PRO	-	EXPRESSION TAG	UNP P0A6F3
F	514	GLU	-	EXPRESSION TAG	UNP P0A6F3
F	515	ASP	-	EXPRESSION TAG	UNP P0A6F3
F	516	PRO	-	EXPRESSION TAG	UNP P0A6F3
F	517	GLU	-	EXPRESSION TAG	UNP P0A6F3
F	518	ASP	-	EXPRESSION TAG	UNP P0A6F3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	519	LEU	-	EXPRESSION TAG	UNP P0A6F3
F	520	GLU	-	EXPRESSION TAG	UNP P0A6F3
F	521	HIS	-	EXPRESSION TAG	UNP P0A6F3
F	522	HIS	-	EXPRESSION TAG	UNP P0A6F3
F	523	HIS	-	EXPRESSION TAG	UNP P0A6F3
F	524	HIS	-	EXPRESSION TAG	UNP P0A6F3
F	525	HIS	-	EXPRESSION TAG	UNP P0A6F3
F	526	HIS	-	EXPRESSION TAG	UNP P0A6F3
H	230	ASP	GLY	ENGINEERED	UNP P0A6F3
H	501	GLN	-	EXPRESSION TAG	UNP P0A6F3
H	502	LEU	-	EXPRESSION TAG	UNP P0A6F3
H	503	TYR	-	EXPRESSION TAG	UNP P0A6F3
H	504	THR	-	EXPRESSION TAG	UNP P0A6F3
H	505	ARG	-	EXPRESSION TAG	UNP P0A6F3
H	506	ALA	-	EXPRESSION TAG	UNP P0A6F3
H	507	SER	-	EXPRESSION TAG	UNP P0A6F3
H	508	GLN	-	EXPRESSION TAG	UNP P0A6F3
H	509	PRO	-	EXPRESSION TAG	UNP P0A6F3
H	510	GLU	-	EXPRESSION TAG	UNP P0A6F3
H	511	LEU	-	EXPRESSION TAG	UNP P0A6F3
H	512	ALA	-	EXPRESSION TAG	UNP P0A6F3
H	513	PRO	-	EXPRESSION TAG	UNP P0A6F3
H	514	GLU	-	EXPRESSION TAG	UNP P0A6F3
H	515	ASP	-	EXPRESSION TAG	UNP P0A6F3
H	516	PRO	-	EXPRESSION TAG	UNP P0A6F3
H	517	GLU	-	EXPRESSION TAG	UNP P0A6F3
H	518	ASP	-	EXPRESSION TAG	UNP P0A6F3
H	519	LEU	-	EXPRESSION TAG	UNP P0A6F3
H	520	GLU	-	EXPRESSION TAG	UNP P0A6F3
H	521	HIS	-	EXPRESSION TAG	UNP P0A6F3
H	522	HIS	-	EXPRESSION TAG	UNP P0A6F3
H	523	HIS	-	EXPRESSION TAG	UNP P0A6F3
H	524	HIS	-	EXPRESSION TAG	UNP P0A6F3
H	525	HIS	-	EXPRESSION TAG	UNP P0A6F3
H	526	HIS	-	EXPRESSION TAG	UNP P0A6F3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		

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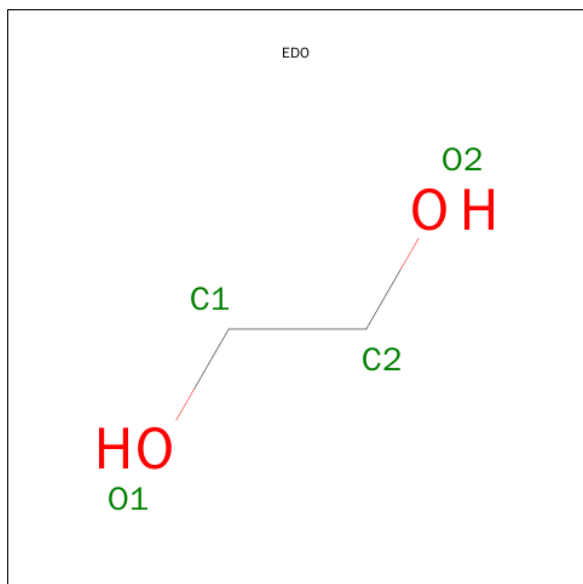
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	214	Total O 214 214	0	0
6	B	237	Total O 237 237	0	0
6	E	209	Total O 209 209	0	0
6	G	218	Total O 218 218	0	0

*Continued on next page...*

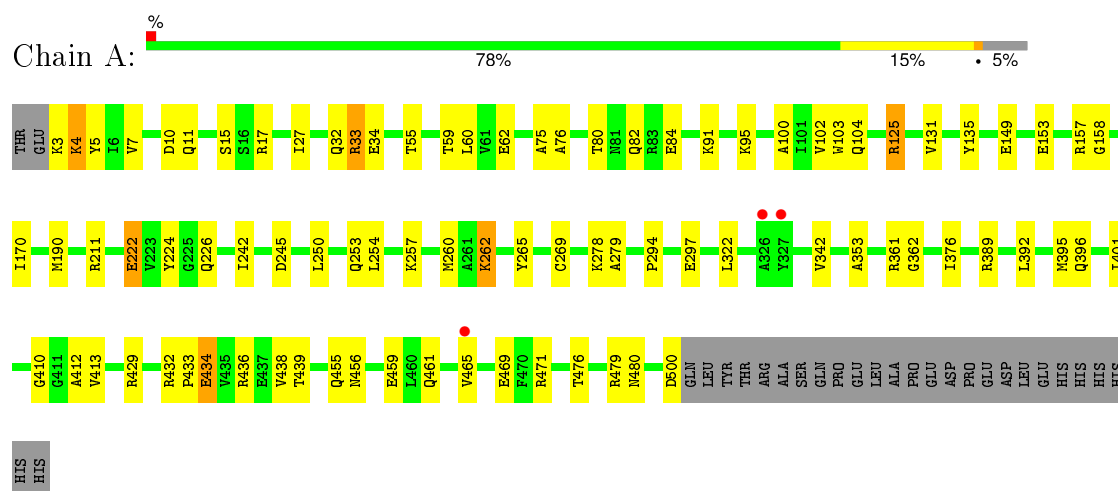
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	157	Total 157	O 157	0	0
6	D	130	Total 130	O 130	0	0
6	F	193	Total 193	O 193	0	0
6	H	168	Total 168	O 168	0	0

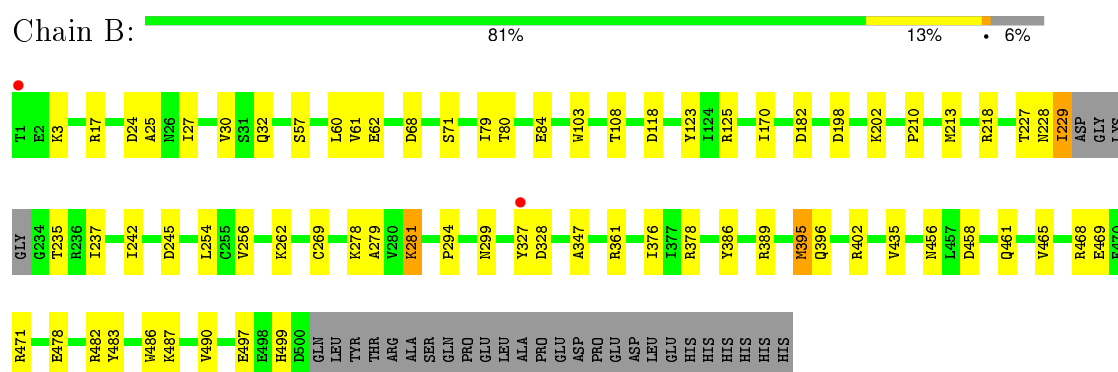
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

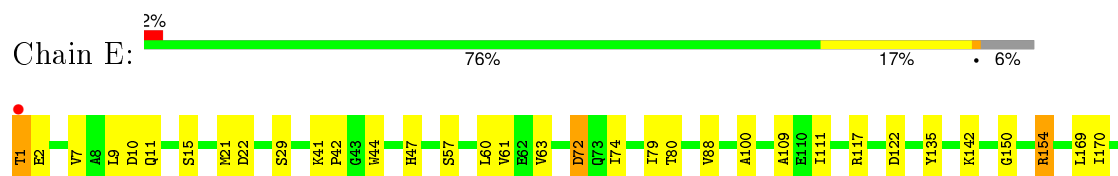
#### • Molecule 1: Glycerol kinase

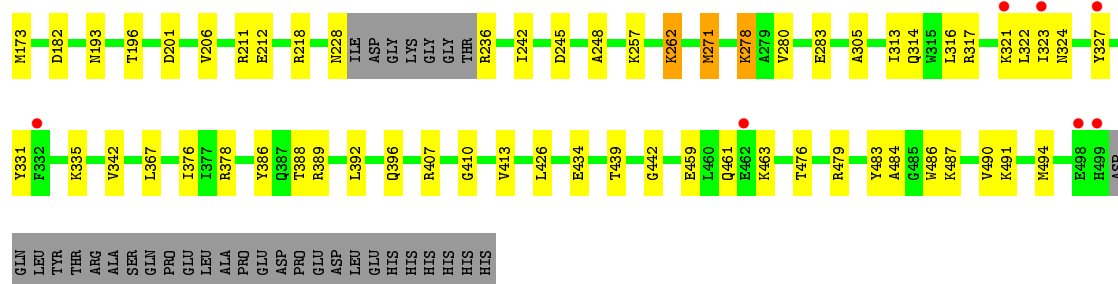


#### • Molecule 1: Glycerol kinase

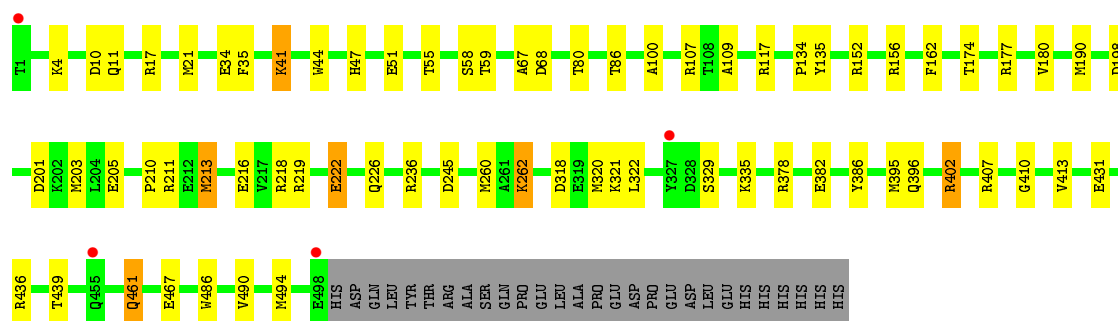
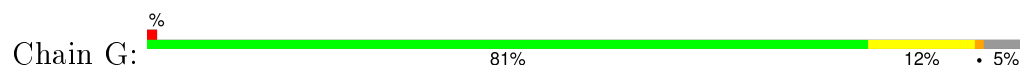


#### • Molecule 1: Glycerol kinase

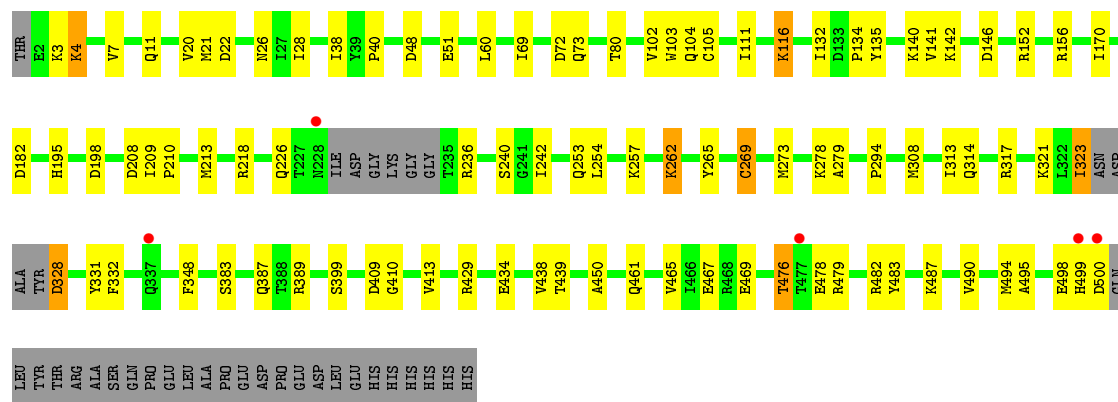
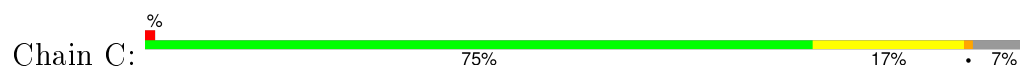




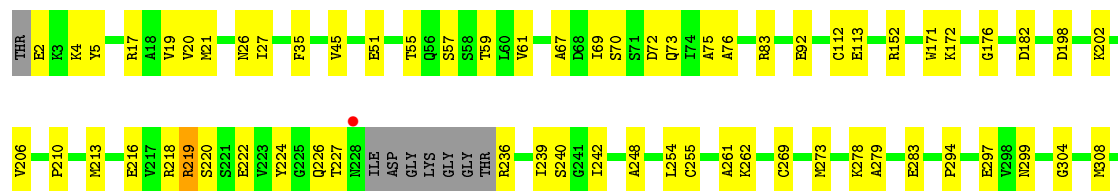
• Molecule 1: Glycerol kinase

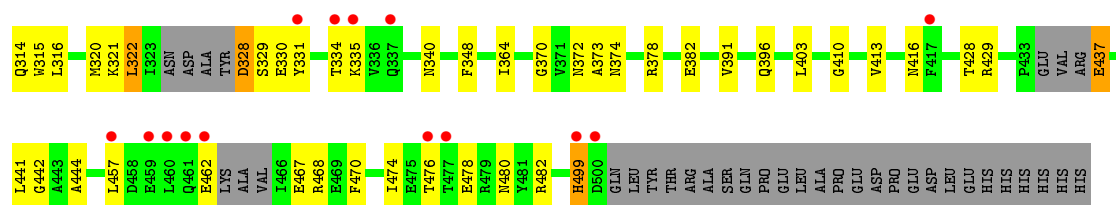


• Molecule 1: Glycerol kinase

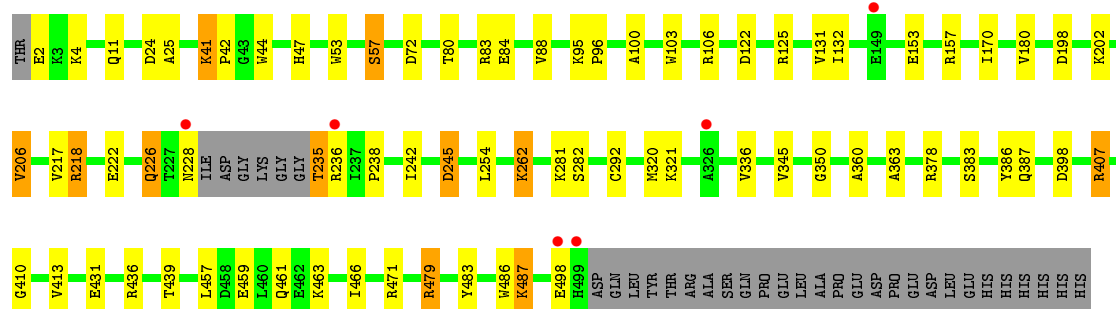
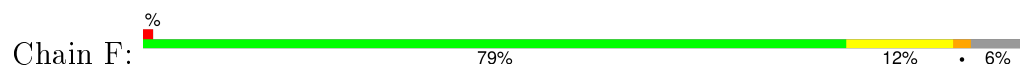


• Molecule 1: Glycerol kinase

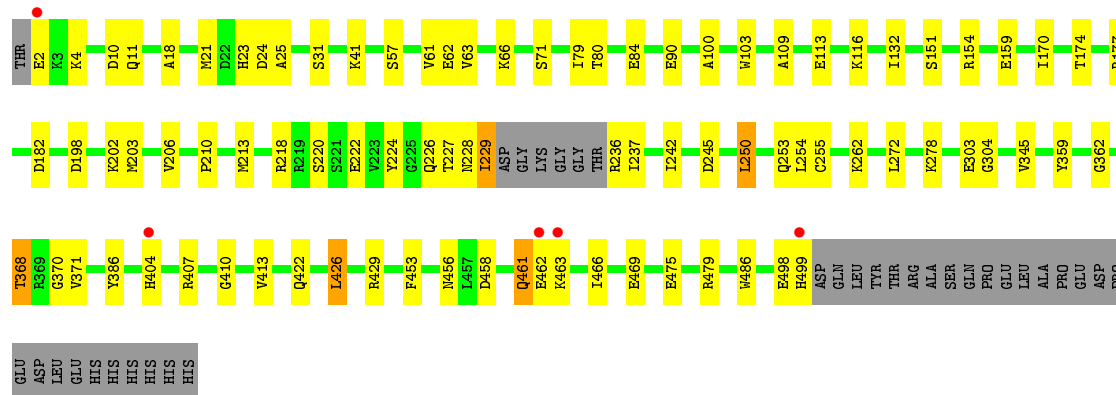
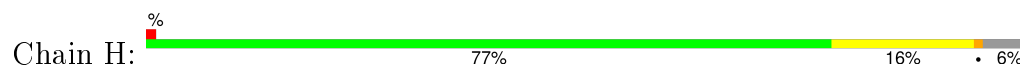




• Molecule 1: Glycerol kinase



• Molecule 1: Glycerol kinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.12Å 114.26Å 212.62Å 90.00° 91.15° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 44.23 – 2.00	Depositor EDS
% Data completeness (in resolution range)	84.0 (20.00-2.00) 84.0 (44.23-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.11 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, $R_{free}$	0.167 , 0.225 0.172 , 0.228	Depositor DCC
$R_{free}$ test set	5032 reflections (2.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.0	EDS
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 246658 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	32916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, EDO, 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	1.18	7/4050 (0.2%)	1.07	14/5488 (0.3%)
1	B	1.17	7/4012 (0.2%)	1.03	8/5439 (0.1%)
1	C	1.14	3/3967 (0.1%)	1.04	10/5374 (0.2%)
1	D	1.06	5/3893 (0.1%)	1.01	4/5272 (0.1%)
1	E	1.15	5/3987 (0.1%)	1.05	8/5405 (0.1%)
1	F	1.07	3/3969 (0.1%)	1.01	12/5381 (0.2%)
1	G	1.14	4/4027 (0.1%)	1.04	9/5458 (0.2%)
1	H	1.04	3/3979 (0.1%)	0.99	6/5394 (0.1%)
All	All	1.12	37/31884 (0.1%)	1.03	71/43211 (0.2%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	LYS	CE-NZ	8.80	1.71	1.49
1	D	269	CYS	CB-SG	-8.78	1.67	1.82
1	C	314	GLN	CG-CD	7.51	1.68	1.51
1	G	461	GLN	CG-CD	7.02	1.67	1.51
1	B	269	CYS	CB-SG	-6.82	1.70	1.82
1	G	431	GLU	CB-CG	-6.70	1.39	1.52
1	C	314	GLN	CB-CG	6.55	1.70	1.52
1	A	5	TYR	CD2-CE2	-6.47	1.29	1.39
1	F	292	CYS	CB-SG	-6.46	1.71	1.82
1	A	353	ALA	CA-CB	6.44	1.66	1.52
1	B	62	GLU	CD-OE1	-6.21	1.18	1.25
1	A	131	VAL	CB-CG1	-6.08	1.40	1.52
1	A	34	GLU	CB-CG	-6.03	1.40	1.52
1	D	314	GLN	CG-CD	6.00	1.64	1.51
1	G	205	GLU	CG-CD	5.98	1.60	1.51
1	F	88	VAL	CB-CG1	5.98	1.65	1.52
1	H	109	ALA	CA-CB	5.83	1.64	1.52
1	A	434	GLU	CB-CG	5.82	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	497	GLU	CB-CG	-5.73	1.41	1.52
1	D	255	CYS	CB-SG	-5.68	1.72	1.81
1	E	109	ALA	CA-CB	5.67	1.64	1.52
1	G	461	GLN	CB-CG	5.67	1.67	1.52
1	B	57	SER	CB-OG	-5.54	1.35	1.42
1	H	90	GLU	CB-CG	-5.54	1.41	1.52
1	D	45	VAL	CB-CG1	5.50	1.64	1.52
1	E	434	GLU	CG-CD	5.45	1.60	1.51
1	A	135	TYR	CG-CD1	-5.29	1.32	1.39
1	B	281	LYS	CG-CD	5.29	1.70	1.52
1	E	88	VAL	CB-CG1	5.28	1.64	1.52
1	C	105	CYS	CB-SG	5.20	1.91	1.82
1	A	100	ALA	CA-CB	5.18	1.63	1.52
1	E	15	SER	CB-OG	-5.10	1.35	1.42
1	H	100	ALA	CA-CB	5.06	1.63	1.52
1	F	345	VAL	CB-CG2	5.04	1.63	1.52
1	D	113	GLU	CG-CD	5.04	1.59	1.51
1	B	3	LYS	CE-NZ	5.03	1.61	1.49
1	E	283	GLU	CB-CG	-5.00	1.42	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	471	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	D	83	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	E	389	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	B	281	LYS	CD-CE-NZ	8.10	130.32	111.70
1	C	389	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	E	378	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	B	198	ASP	CB-CG-OD1	7.51	125.06	118.30
1	F	198	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	H	10	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	F	83	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	E	122	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	A	125	ARG	NE-CZ-NH1	-6.95	116.83	120.30
1	E	389	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	G	198	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	479	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	B	378	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	F	106	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	395	MET	CG-SD-CE	6.53	110.66	100.20
1	C	198	ASP	CB-CG-OD1	6.46	124.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	250	LEU	CB-CG-CD2	-6.37	100.18	111.00
1	H	203	MET	CG-SD-CE	6.18	110.09	100.20
1	H	10	ASP	CB-CG-OD1	6.11	123.80	118.30
1	G	260	MET	CG-SD-CE	6.06	109.89	100.20
1	C	156	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	G	10	ASP	CB-CG-OD1	6.03	123.73	118.30
1	G	203	MET	CG-SD-CE	6.02	109.83	100.20
1	F	198	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	389	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	G	213	MET	CG-SD-CE	5.98	109.76	100.20
1	H	250	LEU	CB-CG-CD2	-5.90	100.97	111.00
1	A	479	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	F	436	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	E	154	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	F	83	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	F	487	LYS	CD-CE-NZ	5.75	124.93	111.70
1	G	107	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	118	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	10	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	432	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	G	395	MET	CG-SD-CE	5.58	109.14	100.20
1	C	135	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	B	68	ASP	CB-CG-OD1	5.58	123.32	118.30
1	D	198	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	389	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	48	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	211	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	G	219	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	33[A]	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	33[B]	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	F	407	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	H	407	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	H	198	ASP	CB-CG-OD1	5.34	123.11	118.30
1	E	122	ASP	CB-CG-OD1	5.32	123.09	118.30
1	F	471	ARG	CG-CD-NE	-5.27	100.74	111.80
1	A	4	LYS	CB-CG-CD	-5.23	97.99	111.60
1	F	245	ASP	CB-CG-OD1	5.23	123.01	118.30
1	G	156	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	118	ASP	CB-CG-OD1	5.23	123.00	118.30
1	E	10	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	C	152	ARG	NE-CZ-NH1	5.18	122.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	B	395	MET	CG-SD-CE	5.15	108.44	100.20
1	D	112	CYS	CA-CB-SG	-5.12	104.79	114.00
1	E	245	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	409	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	283	GLU	CB-CA-C	-5.08	100.25	110.40
1	C	208	ASP	CB-CG-OD1	5.06	122.85	118.30
1	C	409	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	F	218	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	361	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3970	0	3904	47	0
1	B	3933	0	3870	45	0
1	C	3890	0	3825	63	0
1	D	3818	0	3745	84	0
1	E	3908	0	3837	51	0
1	F	3890	0	3822	45	0
1	G	3948	0	3884	38	0
1	H	3900	0	3831	52	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
2	G	6	0	8	0	0
2	H	6	0	8	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
5	A	8	0	12	0	0
5	B	8	0	12	0	0
5	C	16	0	24	1	0
5	D	8	0	12	0	0
5	E	4	0	6	0	0
5	F	8	0	12	0	0
5	G	16	0	24	0	0
5	H	8	0	12	0	0
6	A	214	0	0	2	0
6	B	237	0	0	2	0
6	C	157	0	0	1	0
6	D	130	0	0	3	0
6	E	209	0	0	1	0
6	F	193	0	0	2	0
6	G	218	0	0	2	0
6	H	168	0	0	0	0
All	All	32916	0	30896	419	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 7.

All (419) 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)
1:B:281:LYS:NZ	1:B:281:LYS:CE	1.71	1.51
1:E:317:ARG:O	1:E:321:LYS:HA	1.31	1.25
1:D:21[A]:MET:CE	1:D:441:LEU:HD23	1.79	1.13
1:D:21[A]:MET:HE1	1:D:441:LEU:CD2	1.90	1.00
1:D:70:SER:CB	1:D:72:ASP:OD1	2.10	0.99
1:D:21[A]:MET:HE1	1:D:441:LEU:HD23	0.97	0.96
1:D:70:SER:HB3	1:D:72:ASP:OD1	1.67	0.94
1:D:254:LEU:HD21	1:D:457:LEU:HD22	1.52	0.91
1:D:254:LEU:CD2	1:D:457:LEU:HD22	2.02	0.89
1:F:41:LYS:HB2	1:F:42:PRO:HD2	1.56	0.88
1:H:228:ASN:OD1	1:H:236:ARG:HD3	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:MET:HE2	1:D:348:PHE:HD1	1.40	0.85
1:H:359:TYR:CE2	1:H:499:HIS:HB3	2.12	0.85
1:D:308:MET:CE	1:D:348:PHE:CD1	2.60	0.85
1:D:21[B]:MET:HE1	1:D:444:ALA:HB3	1.57	0.84
1:D:70:SER:HB2	1:D:72:ASP:OD1	1.76	0.84
1:D:308:MET:HE2	1:D:348:PHE:CD1	2.13	0.83
1:D:21[B]:MET:CE	1:D:444:ALA:CB	2.57	0.83
1:A:455:GLN:HB2	1:A:459:GLU:OE2	1.80	0.82
1:C:383:SER:O	1:C:387:GLN:HG3	1.80	0.81
1:D:428:THR:HG22	1:D:429:ARG:N	1.95	0.78
1:C:170:ILE:CD1	1:C:242:ILE:HD11	2.13	0.78
1:H:368:THR:HG23	1:H:370:GLY:H	1.46	0.78
1:D:428:THR:HG22	1:D:429:ARG:O	1.85	0.77
1:F:41:LYS:HB2	1:F:42:PRO:CD	2.15	0.77
1:B:125:ARG:HG2	1:B:281:LYS:HE2	1.66	0.76
1:D:410:GLY:O	1:D:413:VAL:HG22	1.85	0.76
1:B:435:VAL:HG23	1:B:465:VAL:HG21	1.68	0.75
1:D:428:THR:CG2	1:D:429:ARG:N	2.48	0.75
1:E:459:GLU:OE2	1:E:463:LYS:HE2	1.87	0.74
1:B:435:VAL:CG2	1:B:465:VAL:HG21	2.17	0.74
1:E:1:THR:HG23	1:E:2:GLU:N	2.02	0.74
1:D:21[B]:MET:HE2	1:D:444:ALA:CB	2.18	0.73
1:F:202:LYS:O	1:F:206:VAL:HG13	1.89	0.73
1:D:462:GLU:OE1	1:D:462:GLU:HA	1.89	0.73
1:D:21[A]:MET:CE	1:D:441:LEU:CD2	2.58	0.73
1:H:499:HIS:O	1:H:499:HIS:ND1	2.20	0.72
1:D:21[B]:MET:HE1	1:D:444:ALA:CB	2.19	0.72
1:F:483:TYR:CZ	1:F:487:LYS:HE3	2.24	0.72
1:F:153:GLU:HG3	1:F:157:ARG:HH11	1.55	0.71
1:D:308:MET:HE1	1:D:348:PHE:CD1	2.25	0.70
1:D:315:TRP:CH2	1:D:320:MET:HG2	2.26	0.70
1:D:35:PHE:HB2	1:D:51:GLU:HG2	1.73	0.70
1:D:308:MET:CE	1:D:348:PHE:HD1	2.03	0.70
1:H:422:GLN:HE21	1:H:426:LEU:HD22	1.57	0.70
1:C:253:GLN:HG2	1:C:438:VAL:HG11	1.74	0.69
1:F:254:LEU:HD13	1:F:461:GLN:HG2	1.73	0.69
1:C:308:MET:HE2	1:C:348:PHE:HD1	1.58	0.69
1:A:456:ASN:O	1:A:459:GLU:HB2	1.93	0.69
1:C:308:MET:HE2	1:C:348:PHE:CD1	2.27	0.68
1:F:262:LYS:C	1:F:262:LYS:HD2	2.13	0.68
1:D:21[B]:MET:CE	1:D:444:ALA:HB3	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:ILE:HG22	1:E:323:ILE:HD11	1.76	0.68
1:G:226:GLN:NE2	6:G:9166:HOH:O	2.28	0.67
1:D:21[B]:MET:HE2	1:D:444:ALA:HB1	1.77	0.67
1:G:216:GLU:OE2	1:G:218:ARG:NH2	2.27	0.67
1:D:2:GLU:OE1	1:D:4:LYS:HE3	1.95	0.67
1:H:170:ILE:CD1	1:H:242:ILE:HD11	2.25	0.66
1:D:476:THR:O	1:D:480:ASN:HB2	1.95	0.66
1:C:226:GLN:HB3	1:C:236:ARG:HB3	1.78	0.66
1:G:318:ASP:O	1:G:321:LYS:NZ	2.24	0.66
1:H:410:GLY:O	1:H:413:VAL:HG22	1.95	0.66
1:C:328:ASP:O	1:C:331:TYR:HB3	1.97	0.65
1:C:308:MET:CE	1:C:348:PHE:CD1	2.80	0.65
1:B:278:LYS:HE2	1:B:279:ALA:O	1.97	0.64
1:A:429:ARG:HG2	1:A:471:ARG:HG2	1.80	0.64
1:A:429:ARG:HG2	1:A:471:ARG:CG	2.27	0.64
1:A:500:ASP:OD2	6:A:9160:HOH:O	2.15	0.63
1:G:41:LYS:HD3	1:G:44:TRP:CE3	2.33	0.63
1:F:72:ASP:HA	1:F:235:THR:HG21	1.81	0.63
1:C:257:LYS:HE3	1:C:294:PRO:HG3	1.80	0.63
1:B:170:ILE:CD1	1:B:242:ILE:HD11	2.28	0.62
1:C:3:LYS:HD3	1:C:72:ASP:O	1.99	0.62
1:C:278:LYS:HE2	1:C:279:ALA:O	2.00	0.62
1:C:308:MET:CE	1:C:348:PHE:HD1	2.12	0.62
1:A:429:ARG:CG	1:A:471:ARG:HG2	2.29	0.61
1:F:2:GLU:O	6:F:2811:HOH:O	2.16	0.61
1:D:499:HIS:N	1:D:499:HIS:CD2	2.69	0.61
1:C:317:ARG:O	1:C:321:LYS:HG3	2.00	0.61
1:A:278:LYS:HE2	1:A:279:ALA:O	1.99	0.61
1:A:455:GLN:N	1:A:459:GLU:OE2	2.33	0.60
1:D:474:ILE:HD12	1:D:478:GLU:HG2	1.82	0.60
1:H:359:TYR:CZ	1:H:499:HIS:HB3	2.36	0.60
1:F:24:ASP:O	1:F:25:ALA:HB3	2.02	0.60
1:C:257:LYS:HE3	1:C:294:PRO:CG	2.31	0.60
1:H:456:ASN:OD1	1:H:458:ASP:HB2	2.01	0.60
1:B:396:GLN:HE22	1:B:402:ARG:NH2	2.00	0.60
1:F:483:TYR:OH	1:F:487:LYS:HE3	2.02	0.59
1:E:80:THR:HG21	1:E:439:THR:HG22	1.83	0.59
1:A:15:SER:HB2	1:A:33[A]:ARG:O	2.02	0.59
1:A:170:ILE:CD1	1:A:242:ILE:HD11	2.32	0.58
1:B:80:THR:OG1	1:B:245:ASP:HA	2.02	0.58
1:E:41:LYS:HB2	1:E:42:PRO:CD	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LYS:HG3	1:C:132:ILE:HD12	1.83	0.58
1:C:278:LYS:CE	1:C:279:ALA:O	2.52	0.58
1:A:413:VAL:HG22	1:A:436:ARG:HD2	1.86	0.58
1:D:330:GLU:O	1:D:334:THR:HG23	2.03	0.57
1:A:153:GLU:O	1:A:157:ARG:HG3	2.03	0.57
1:H:227:THR:HG23	1:H:229:ILE:CG2	2.34	0.57
1:H:71:SER:HB2	1:H:237:ILE:HD11	1.86	0.57
1:E:22:ASP:C	1:E:22:ASP:OD1	2.40	0.57
1:C:116:LYS:HE2	1:C:132:ILE:HB	1.86	0.57
1:D:428:THR:CG2	1:D:429:ARG:H	2.18	0.56
1:E:305:ALA:O	6:E:2666:HOH:O	2.18	0.56
1:E:111:ILE:HD13	1:E:142:LYS:HD3	1.86	0.56
1:D:21[B]:MET:CE	1:D:441:LEU:HD23	2.34	0.56
1:F:410:GLY:O	1:F:413:VAL:HG22	2.07	0.55
1:A:222:GLU:HG2	1:A:224:TYR:CE2	2.40	0.55
1:B:254:LEU:HD13	1:B:461:GLN:HG2	1.89	0.55
1:E:262:LYS:HA	1:E:407:ARG:O	2.07	0.55
1:B:210:PRO:O	1:B:213:MET:HG2	2.06	0.55
1:A:262:LYS:C	1:A:262:LYS:HD2	2.27	0.55
1:C:273:MET:HE1	1:C:399:SER:CB	2.37	0.55
1:C:262:LYS:HD2	1:C:262:LYS:C	2.27	0.55
1:H:422:GLN:NE2	1:H:426:LEU:HD22	2.22	0.55
1:D:273:MET:CE	1:D:403:LEU:HD21	2.37	0.55
1:G:410:GLY:O	1:G:413:VAL:HG22	2.07	0.55
1:C:195:HIS:ND1	5:C:2653:EDO:H21	2.22	0.54
1:E:41:LYS:HB2	1:E:42:PRO:HD2	1.89	0.54
1:E:1:THR:HG22	1:E:72:ASP:O	2.07	0.54
1:H:218:ARG:NE	1:H:222:GLU:OE2	2.41	0.54
1:C:80:THR:HG21	1:C:439:THR:HG22	1.90	0.54
1:G:80:THR:HG21	1:G:439:THR:HG22	1.89	0.54
1:H:228:ASN:OD1	1:H:236:ARG:CD	2.54	0.54
1:H:229:ILE:HD12	1:H:229:ILE:C	2.27	0.54
1:A:254:LEU:HD12	1:A:461:GLN:NE2	2.23	0.53
1:F:383:SER:O	1:F:387:GLN:HG3	2.06	0.53
1:C:142:LYS:NZ	1:C:146:ASP:OD2	2.42	0.53
1:H:253:GLN:O	1:H:254:LEU:HB2	2.08	0.53
1:E:392:LEU:O	1:E:396[A]:GLN:HG3	2.07	0.53
1:G:35:PHE:HB2	1:G:51:GLU:HG2	1.90	0.53
1:E:170:ILE:CD1	1:E:242:ILE:HD11	2.39	0.53
1:H:2:GLU:O	1:H:4:LYS:HG3	2.09	0.53
1:C:278:LYS:HD3	1:C:279:ALA:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:ILE:CG2	1:E:323:ILE:HD11	2.38	0.52
1:D:17:ARG:NH2	1:D:437:GLU:OE2	2.42	0.52
1:F:53:TRP:O	1:F:57:SER:HB2	2.09	0.52
1:D:328:ASP:O	1:D:331:TYR:HB3	2.09	0.52
1:E:206:VAL:HG22	1:E:206:VAL:O	2.09	0.52
1:B:376:ILE:HD12	1:G:320:MET:SD	2.50	0.52
1:C:434:GLU:OE1	1:C:465:VAL:HG11	2.10	0.52
1:C:495:ALA:HB1	1:C:499:HIS:NE2	2.24	0.52
1:C:22:ASP:OD2	1:C:26:ASN:HB2	2.09	0.52
1:F:170:ILE:CD1	1:F:242:ILE:HD11	2.40	0.52
1:B:27:ILE:HG21	1:B:30:VAL:CG2	2.40	0.52
1:A:342:VAL:HG11	1:A:376:ILE:HD13	1.91	0.52
1:D:372:ASN:OD1	1:D:374:ASN:HB2	2.10	0.51
1:C:4:LYS:HZ2	1:C:73:GLN:HE21	1.58	0.51
1:C:323:ILE:HG22	1:C:332:PHE:CE1	2.46	0.51
1:D:227:THR:HG23	1:D:227:THR:O	2.10	0.51
1:H:31:SER:OG	1:H:63:VAL:HG12	2.10	0.51
1:E:150:GLY:O	1:E:154:ARG:HG3	2.10	0.51
1:C:7:VAL:HG11	1:C:60:LEU:HD13	1.92	0.51
1:D:19:VAL:HG13	1:D:27:ILE:HG23	1.93	0.51
1:E:484:ALA:HA	1:E:487:LYS:HE3	1.93	0.51
1:D:322:LEU:HD13	1:D:373:ALA:HB1	1.93	0.51
1:D:4:LYS:NZ	1:D:73:GLN:HE21	2.09	0.51
1:H:254:LEU:HD13	1:H:461:GLN:HG2	1.93	0.51
1:D:19:VAL:HG11	1:D:27:ILE:HD12	1.92	0.51
1:H:80:THR:OG1	1:H:245:ASP:HA	2.11	0.51
1:A:91:LYS:HE3	1:A:158:GLY:O	2.11	0.51
1:G:47:HIS:HB2	1:G:100:ALA:HB3	1.92	0.50
1:E:228:ASN:OD1	1:E:236:ARG:NE	2.37	0.50
1:A:80:THR:OG1	1:A:245:ASP:HA	2.11	0.50
1:C:182:ASP:HA	1:C:218:ARG:O	2.11	0.50
1:H:24:ASP:O	1:H:25:ALA:HB3	2.10	0.50
1:E:410:GLY:O	1:E:413:VAL:HG22	2.12	0.50
1:F:153:GLU:O	1:F:157:ARG:HG3	2.11	0.50
1:C:483:TYR:CD2	1:C:487:LYS:HE3	2.47	0.50
1:B:396:GLN:HE22	1:B:402:ARG:CZ	2.25	0.50
1:H:429:ARG:HD3	1:H:469:GLU:OE2	2.12	0.49
1:C:498:GLU:C	1:C:500:ASP:H	2.14	0.49
1:C:410:GLY:O	1:C:413:VAL:HG22	2.12	0.49
1:C:102:VAL:HG12	1:C:104:GLN:H	1.77	0.49
1:E:271:MET:HE1	1:E:388:THR:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:404:HIS:CE1	1:H:429:ARG:HH22	2.29	0.49
1:F:336:VAL:O	1:F:378:ARG:NH1	2.45	0.49
1:D:216:GLU:OE2	1:D:218:ARG:NH2	2.45	0.49
1:F:41:LYS:HD3	1:F:44:TRP:CE2	2.48	0.49
1:D:315:TRP:CZ3	1:D:320:MET:HG2	2.47	0.49
1:D:370:GLY:HA3	6:D:2667:HOH:O	2.13	0.49
1:B:17:ARG:NH2	1:B:32:GLN:NE2	2.61	0.49
1:G:262:LYS:HA	1:G:407:ARG:O	2.13	0.49
1:E:483:TYR:CD2	1:E:487:LYS:HE2	2.48	0.49
1:E:201:ASP:OD1	1:E:211:ARG:NH1	2.45	0.49
1:C:429:ARG:NE	1:C:469:GLU:OE2	2.35	0.49
1:A:55:THR:O	1:A:59:THR:HG23	2.13	0.48
1:A:84:GLU:HB2	1:A:103:TRP:HB3	1.95	0.48
1:G:210:PRO:O	1:G:213:MET:HG2	2.13	0.48
1:F:218:ARG:NH1	1:F:222:GLU:OE2	2.41	0.48
1:A:80:THR:HG21	1:A:439:THR:HG22	1.95	0.48
1:D:370:GLY:CA	6:D:2667:HOH:O	2.61	0.48
1:B:456:ASN:OD1	1:B:458:ASP:CG	2.52	0.48
1:C:490:VAL:O	1:C:494:MET:HG3	2.13	0.48
1:H:220:SER:HB3	1:H:242:ILE:O	2.13	0.48
1:F:479:ARG:NH1	6:F:2723:HOH:O	2.46	0.48
1:F:41:LYS:HD3	1:F:44:TRP:CD2	2.49	0.48
1:C:170:ILE:HD13	1:C:242:ILE:HD11	1.94	0.48
1:H:210:PRO:O	1:H:213:MET:HG2	2.14	0.48
1:G:216:GLU:CD	1:G:218:ARG:NH2	2.67	0.47
1:D:220:SER:HB3	1:D:242:ILE:O	2.13	0.47
1:B:456:ASN:OD1	1:B:458:ASP:HB2	2.14	0.47
1:E:317:ARG:O	1:E:321:LYS:CA	2.27	0.47
1:F:262:LYS:HA	1:F:407:ARG:O	2.14	0.47
1:H:174:THR:O	1:H:177:ARG:HG3	2.15	0.47
1:F:153:GLU:HG3	1:F:157:ARG:NH1	2.26	0.47
1:A:33[A]:ARG:HG2	1:A:55:THR:HG22	1.95	0.47
1:D:171:TRP:CE2	1:D:176:GLY:HA2	2.50	0.47
1:E:182:ASP:HA	1:E:218:ARG:O	2.14	0.47
1:H:250:LEU:HG	1:H:255:CYS:HB2	1.97	0.47
1:H:359:TYR:CZ	1:H:499:HIS:CB	2.98	0.47
1:B:435:VAL:HG23	1:B:465:VAL:CG2	2.41	0.47
1:A:429:ARG:HG2	1:A:471:ARG:HG3	1.97	0.47
1:A:410:GLY:O	1:A:413:VAL:HG22	2.15	0.47
1:D:364:ILE:O	1:F:363:ALA:HA	2.15	0.47
1:B:327:TYR:HA	6:B:2876:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:VAL:HG21	1:H:61:VAL:HG21	1.97	0.47
1:F:320:MET:O	1:F:321:LYS:C	2.52	0.47
1:G:378:ARG:O	1:G:382:GLU:HG3	2.15	0.47
1:F:431:GLU:HB3	1:F:466:ILE:HD12	1.96	0.47
1:H:202:LYS:O	1:H:206:VAL:HG23	2.14	0.47
1:A:27[B]:ILE:N	1:A:27[B]:ILE:HD13	2.30	0.47
1:G:190:MET:O	1:G:190:MET:HG2	2.15	0.47
1:H:224:TYR:CE1	1:H:242:ILE:HG13	2.50	0.47
1:A:17:ARG:HG2	1:A:32:GLN:HG3	1.97	0.47
1:F:226:GLN:HG3	1:F:238:PRO:HA	1.97	0.47
1:B:79:ILE:O	1:B:242:ILE:HA	2.16	0.46
1:C:170:ILE:CD1	1:C:242:ILE:CD1	2.90	0.46
1:G:174:THR:O	1:G:177:ARG:HG3	2.15	0.46
1:F:84:GLU:HB2	1:F:103:TRP:HB3	1.98	0.46
1:B:61:VAL:HG21	1:E:61:VAL:HG21	1.98	0.46
1:H:272:LEU:HG	1:H:303:GLU:HB2	1.97	0.46
1:B:456:ASN:OD1	1:B:458:ASP:CB	2.62	0.46
1:E:490:VAL:O	1:E:494:MET:HG3	2.15	0.46
1:G:436:ARG:NH2	1:G:467:GLU:OE1	2.48	0.46
1:F:483:TYR:OH	1:F:487:LYS:CE	2.64	0.46
1:H:170:ILE:HD11	1:H:242:ILE:HD11	1.95	0.46
1:B:396:GLN:NE2	1:B:402:ARG:NH2	2.63	0.46
1:E:79:ILE:O	1:E:242:ILE:HA	2.16	0.46
1:B:71:SER:HB2	1:B:237:ILE:HD11	1.96	0.46
1:E:476:THR:O	1:E:479:ARG:HG2	2.15	0.46
1:E:324:ASN:OD1	1:E:327:TYR:HB2	2.15	0.46
1:D:320:MET:O	1:D:321:LYS:HB2	2.15	0.46
1:E:29:SER:HB3	1:E:63:VAL:HG22	1.98	0.46
1:D:416:ASN:OD1	1:D:470:PHE:HZ	1.98	0.46
1:H:368:THR:HG23	1:H:370:GLY:N	2.24	0.46
1:E:271:MET:HE2	1:E:271:MET:HB2	1.59	0.46
1:E:7:VAL:HG23	1:E:74:ILE:HD12	1.96	0.46
1:C:210:PRO:O	1:C:213:MET:HG2	2.16	0.46
1:F:262:LYS:O	1:F:262:LYS:HD2	2.16	0.46
1:A:433:PRO:HA	1:A:465:VAL:O	2.15	0.46
1:E:331:TYR:HE2	1:E:335:LYS:HZ1	1.62	0.46
1:B:84:GLU:HB2	1:B:103:TRP:HB3	1.97	0.46
1:D:378:ARG:O	1:D:382:GLU:HG3	2.16	0.46
1:D:4:LYS:HG3	1:D:5:TYR:CE2	2.51	0.46
1:H:345:VAL:O	1:H:362:GLY:HA2	2.16	0.46
1:H:170:ILE:CD1	1:H:242:ILE:CD1	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ALA:O	1:D:76:ALA:HB2	2.16	0.46
1:B:347:ALA:O	1:B:361:ARG:HA	2.16	0.46
1:B:108:THR:HA	6:B:2692:HOH:O	2.16	0.45
1:D:210:PRO:O	1:D:213:MET:HG2	2.17	0.45
1:H:498:GLU:HA	1:H:498:GLU:OE1	2.17	0.45
1:G:117:ARG:HB3	1:G:117:ARG:HE	1.49	0.45
1:C:22:ASP:C	1:C:22:ASP:OD1	2.55	0.45
1:G:386:TYR:HB3	1:G:486:TRP:CD2	2.51	0.45
1:F:72:ASP:CA	1:F:235:THR:HG21	2.45	0.45
1:D:222:GLU:O	1:D:240:SER:HA	2.16	0.45
1:D:20:VAL:HG11	1:D:69:ILE:HD13	1.98	0.45
1:C:111:ILE:HG13	6:C:2767:HOH:O	2.16	0.45
1:E:9:LEU:HD21	1:E:60:LEU:HD13	1.99	0.45
1:G:201:ASP:OD1	1:G:211:ARG:NH1	2.41	0.45
1:C:141:VAL:CG1	1:C:209:ILE:HD12	2.46	0.45
1:C:111:ILE:HD13	1:C:142:LYS:HD3	1.99	0.45
1:D:227:THR:CG2	1:D:227:THR:O	2.64	0.45
1:D:224:TYR:CE1	1:D:242:ILE:HG13	2.51	0.45
1:F:282:SER:OG	1:F:398:ASP:OD2	2.23	0.45
1:D:396:GLN:HE21	1:D:396:GLN:HB3	1.67	0.45
1:G:109:ALA:HA	1:G:134:PRO:HG3	1.98	0.45
1:G:218:ARG:HD2	1:G:222:GLU:OE2	2.17	0.45
1:A:294:PRO:HD2	1:A:297:GLU:OE2	2.17	0.45
1:G:67:ALA:O	1:G:68:ASP:HB3	2.17	0.45
1:D:35:PHE:HB3	1:D:55:THR:HG21	1.99	0.44
1:A:95:LYS:HB2	1:A:95:LYS:HE3	1.76	0.44
1:A:253:GLN:HG2	1:A:438:VAL:HG11	1.99	0.44
1:A:102:VAL:HG12	1:A:104:GLN:H	1.82	0.44
1:D:478:GLU:OE2	1:D:482:ARG:CZ	2.65	0.44
1:G:34[B]:GLU:HG2	6:G:9012:HOH:O	2.17	0.44
1:H:23:HIS:HA	1:H:453:PHE:CE2	2.52	0.44
1:A:455:GLN:CB	1:A:459:GLU:OE2	2.57	0.44
1:A:265:TYR:HB3	1:A:412:ALA:HB3	2.00	0.44
1:C:20:VAL:HG11	1:C:69:ILE:HD13	2.00	0.44
1:G:318:ASP:O	1:G:321:LYS:CE	2.64	0.44
1:G:490:VAL:O	1:G:494:MET:HG3	2.18	0.44
1:A:190:MET:O	1:A:190:MET:HG2	2.18	0.44
1:B:486:TRP:O	1:B:490:VAL:HG23	2.16	0.44
1:F:122:ASP:OD1	1:F:281:LYS:NZ	2.49	0.44
1:G:262:LYS:HD2	1:G:262:LYS:C	2.38	0.44
1:F:459:GLU:HG2	1:F:463:LYS:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ARG:HB3	6:D:2696:HOH:O	2.17	0.44
1:H:368:THR:HG22	1:H:371:VAL:HG23	1.99	0.44
1:E:41:LYS:HD2	1:E:44:TRP:CE2	2.53	0.44
1:F:180:VAL:CG2	1:F:218:ARG:HG3	2.47	0.44
1:E:248:ALA:O	1:E:442:GLY:HA3	2.18	0.44
1:F:80:THR:HG21	1:F:439:THR:HG22	2.00	0.44
1:D:294:PRO:HD2	1:D:297:GLU:OE2	2.18	0.44
1:D:55:THR:O	1:D:59:THR:HG23	2.17	0.44
1:C:4:LYS:NZ	1:C:73:GLN:HE21	2.15	0.44
1:D:202:LYS:O	1:D:206:VAL:HG13	2.18	0.44
1:A:429:ARG:HD2	1:A:469:GLU:CD	2.38	0.43
1:F:217:VAL:C	1:F:218:ARG:HG2	2.37	0.43
1:E:47:HIS:HB2	1:E:100:ALA:HB3	2.00	0.43
1:D:261:ALA:HB2	1:D:273:MET:HB2	1.99	0.43
1:B:27:ILE:HG21	1:B:30:VAL:HG23	1.99	0.43
1:H:154:ARG:O	1:H:159:GLU:HB2	2.18	0.43
1:C:38:ILE:HG22	1:C:40:PRO:HD3	2.00	0.43
1:C:308:MET:HE1	1:C:348:PHE:CD1	2.54	0.43
1:C:226:GLN:HE21	1:C:236:ARG:HB3	1.82	0.43
1:B:468:ARG:HG3	1:B:469:GLU:N	2.32	0.43
1:D:21[B]:MET:HE3	1:D:441:LEU:HD23	1.94	0.43
1:H:475:GLU:OE1	1:H:475:GLU:HA	2.19	0.43
1:D:429:ARG:HA	1:D:470:PHE:O	2.19	0.43
1:A:476:THR:O	1:A:480:ASN:HB2	2.19	0.43
1:B:256:VAL:HB	1:B:294:PRO:HG3	1.99	0.43
1:A:257:LYS:HB3	1:A:260:MET:SD	2.58	0.43
1:E:342:VAL:HG11	1:E:376:ILE:CD1	2.48	0.43
1:C:278:LYS:CD	1:C:279:ALA:O	2.67	0.43
1:F:350:GLY:HA2	1:F:360:ALA:O	2.19	0.43
1:D:248:ALA:O	1:D:442:GLY:HA3	2.19	0.43
1:B:24:ASP:O	1:B:25:ALA:HB3	2.19	0.43
1:C:265:TYR:CD2	1:C:269[A]:CYS:SG	3.12	0.43
1:B:478:GLU:HG2	1:B:482:ARG:HD2	2.00	0.43
1:A:75:ALA:O	1:A:76:ALA:HB2	2.19	0.43
1:E:193:ASN:HB3	1:E:196:THR:OG1	2.18	0.43
1:E:7:VAL:CG2	1:E:74:ILE:HD12	2.49	0.43
1:B:386:TYR:HB3	1:B:486:TRP:CD2	2.53	0.43
1:A:362:GLY:HA3	1:E:367:LEU:HB2	2.00	0.43
1:C:498:GLU:C	1:C:500:ASP:N	2.72	0.42
1:G:35:PHE:HB3	1:G:55:THR:HG21	2.00	0.42
1:C:313:ILE:N	1:C:313:ILE:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:CG2	1:B:30:VAL:HG23	2.48	0.42
1:B:483:TYR:CZ	1:B:487:LYS:HE3	2.55	0.42
1:A:82:GLN:HG3	1:A:82:GLN:O	2.19	0.42
1:D:467:GLU:O	1:D:468:ARG:HB2	2.19	0.42
1:C:273:MET:HE1	1:C:399:SER:HB2	2.00	0.42
1:H:84:GLU:HB2	1:H:103:TRP:HB3	2.02	0.42
1:D:21[B]:MET:HE1	1:D:441:LEU:HA	2.02	0.42
1:C:28:ILE:N	1:C:28:ILE:HD13	2.34	0.42
1:B:123:TYR:CZ	1:B:202:LYS:HD3	2.55	0.42
1:E:278:LYS:HE2	1:E:280:VAL:HG22	2.02	0.42
1:F:47:HIS:HB2	1:F:100:ALA:HB3	2.01	0.42
1:A:125:ARG:HH11	1:A:125:ARG:HD2	1.62	0.42
1:A:469:GLU:O	6:A:9183:HOH:O	2.22	0.42
1:G:80:THR:OG1	1:G:245:ASP:HA	2.20	0.42
1:D:478:GLU:O	1:D:482:ARG:HG3	2.20	0.42
1:C:434:GLU:HG2	1:C:467:GLU:HB2	2.00	0.42
1:D:21[B]:MET:HA	1:D:26:ASN:O	2.19	0.42
1:H:466:ILE:HD13	1:H:466:ILE:HA	1.78	0.42
1:A:33[B]:ARG:HB2	1:A:59:THR:CG2	2.49	0.42
1:H:303:GLU:CG	1:H:304:GLY:N	2.83	0.42
1:C:102:VAL:HG12	1:C:103:TRP:N	2.34	0.41
1:E:342:VAL:HG11	1:E:376:ILE:HD13	2.01	0.41
1:D:304:GLY:HA3	1:D:391:VAL:CG1	2.50	0.41
1:G:17:ARG:HH11	1:G:17:ARG:HD3	1.69	0.41
1:F:80:THR:OG1	1:F:245:ASP:HA	2.20	0.41
1:F:386:TYR:HB3	1:F:486:TRP:CD2	2.55	0.41
1:C:134:PRO:O	1:C:140:LYS:HE2	2.19	0.41
1:B:182:ASP:HA	1:B:218:ARG:O	2.20	0.41
1:E:316:LEU:O	1:E:322:LEU:N	2.53	0.41
1:G:396:GLN:OE1	1:G:402:ARG:HD2	2.20	0.41
1:G:322:LEU:HD23	1:G:322:LEU:HA	1.93	0.41
1:C:257:LYS:HE3	1:C:294:PRO:HG2	2.00	0.41
1:H:18:ALA:HB3	1:H:63:VAL:CG1	2.50	0.41
1:D:67:ALA:HB3	1:D:69:ILE:HD12	2.03	0.41
1:D:316:LEU:HD23	1:D:316:LEU:HA	1.62	0.41
1:C:476:THR:OG1	1:C:479:ARG:NH2	2.54	0.41
1:G:180:VAL:CG2	1:G:218:ARG:HG3	2.51	0.41
1:B:396:GLN:NE2	1:B:402:ARG:CZ	2.84	0.41
1:E:392:LEU:HD23	1:E:426:LEU:HD22	2.03	0.41
1:H:18:ALA:HB3	1:H:63:VAL:HG11	2.02	0.41
1:D:172:LYS:HA	1:D:172:LYS:HD2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:116:LYS:HG3	1:H:132:ILE:HG21	2.03	0.41
1:A:7:VAL:HG11	1:A:60:LEU:HD13	2.02	0.41
1:B:227:THR:HG23	1:B:227:THR:O	2.21	0.41
1:G:386:TYR:HB3	1:G:486:TRP:CE2	2.56	0.41
1:C:240:SER:HB2	1:C:450:ALA:HB3	2.02	0.41
1:D:278:LYS:HG2	1:D:279:ALA:N	2.35	0.41
1:E:257:LYS:NZ	1:E:461:GLN:HE22	2.18	0.41
1:D:227:THR:HB	1:D:239:ILE:HD11	2.03	0.41
1:E:271:MET:CE	1:E:388:THR:HG23	2.51	0.41
1:F:125:ARG:HG2	1:F:281:LYS:HE2	2.03	0.41
1:D:226:GLN:NE2	1:D:236:ARG:HE	2.19	0.41
1:A:392:LEU:O	1:A:396:GLN:HG3	2.20	0.41
1:B:499:HIS:CD2	1:B:499:HIS:N	2.89	0.41
1:G:86:THR:HG23	1:G:162:PHE:HE1	1.86	0.41
1:E:386:TYR:HB3	1:E:486:TRP:CD2	2.55	0.41
1:A:401:ILE:HD13	1:A:401:ILE:HG21	1.87	0.41
1:D:21[B]:MET:CG	1:D:27:ILE:HD13	2.51	0.41
1:H:62:GLU:O	1:H:66:LYS:HG2	2.21	0.41
1:H:182:ASP:HA	1:H:218:ARG:O	2.21	0.40
1:C:21[A]:MET:HA	1:C:26:ASN:O	2.20	0.40
1:B:17:ARG:CZ	1:B:32:GLN:NE2	2.85	0.40
1:G:211:ARG:HH11	1:G:211:ARG:HD2	1.63	0.40
1:A:62:GLU:HB2	1:G:58:SER:HB3	2.02	0.40
1:B:60:LEU:HD21	1:B:229:ILE:HG13	2.02	0.40
1:E:313:ILE:CG2	1:E:323:ILE:CD1	2.99	0.40
1:H:79:ILE:HD13	1:H:170:ILE:HG13	2.02	0.40
1:G:55:THR:O	1:G:59:THR:HG23	2.20	0.40
1:B:328:ASP:C	1:B:328:ASP:OD1	2.60	0.40
1:C:478:GLU:O	1:C:482:ARG:HG3	2.21	0.40
1:G:318:ASP:C	1:G:321:LYS:HD3	2.42	0.40
1:H:113:GLU:OE2	1:H:116:LYS:HD2	2.21	0.40
1:C:254:LEU:CD1	1:C:461:GLN:HA	2.52	0.40
1:H:386:TYR:HB3	1:H:486:TRP:CD2	2.56	0.40
1:B:471:ARG:HH11	1:B:471:ARG:HD3	1.75	0.40
1:F:457:LEU:O	1:F:461:GLN:HG3	2.22	0.40
1:B:483:TYR:O	1:B:486:TRP:HB3	2.22	0.40
1:F:131:VAL:HG12	1:F:132:ILE:N	2.35	0.40
1:E:169:LEU:O	1:E:173:MET:HG3	2.21	0.40
1:F:95:LYS:HA	1:F:96:PRO:HD3	1.99	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	501/526 (95%)	487 (97%)	14 (3%)	0	100	100
1	B	494/526 (94%)	485 (98%)	9 (2%)	0	100	100
1	C	486/526 (92%)	475 (98%)	11 (2%)	0	100	100
1	D	473/526 (90%)	460 (97%)	13 (3%)	0	100	100
1	E	490/526 (93%)	475 (97%)	15 (3%)	0	100	100
1	F	488/526 (93%)	482 (99%)	6 (1%)	0	100	100
1	G	499/526 (95%)	485 (97%)	13 (3%)	1 (0%)	52	48
1	H	489/526 (93%)	479 (98%)	10 (2%)	0	100	100
All	All	3920/4208 (93%)	3828 (98%)	91 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	222	GLU

### 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	415/436 (95%)	405 (98%)	10 (2%)	57	58
1	B	412/436 (94%)	406 (98%)	6 (2%)	72	75
1	C	408/436 (94%)	398 (98%)	10 (2%)	55	55
1	D	400/436 (92%)	386 (96%)	14 (4%)	43	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	409/436 (94%)	396 (97%)	13 (3%)	46	44
1	F	407/436 (93%)	395 (97%)	12 (3%)	50	49
1	G	413/436 (95%)	401 (97%)	12 (3%)	50	49
1	H	408/436 (94%)	393 (96%)	15 (4%)	41	38
All	All	3272/3488 (94%)	3180 (97%)	92 (3%)	51	50

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	LYS
1	A	11	GLN
1	A	149	GLU
1	A	222	GLU
1	A	226	GLN
1	A	262	LYS
1	A	269[A]	CYS
1	A	269[B]	CYS
1	A	434	GLU
1	B	228	ASN
1	B	229	ILE
1	B	235	THR
1	B	262	LYS
1	B	299	ASN
1	B	395	MET
1	E	1	THR
1	E	11	GLN
1	E	21	MET
1	E	57	SER
1	E	72	ASP
1	E	117	ARG
1	E	135	TYR
1	E	212	GLU
1	E	262	LYS
1	E	271	MET
1	E	278	LYS
1	E	314	GLN
1	E	491	LYS
1	G	4	LYS
1	G	11	GLN
1	G	21	MET

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Mol	Chain	Res	Type
1	G	41	LYS
1	G	135	TYR
1	G	152	ARG
1	G	236	ARG
1	G	262	LYS
1	G	329	SER
1	G	335	LYS
1	G	402	ARG
1	G	461	GLN
1	C	4	LYS
1	C	11	GLN
1	C	51	GLU
1	C	116	LYS
1	C	262	LYS
1	C	269[A]	CYS
1	C	269[B]	CYS
1	C	323	ILE
1	C	328	ASP
1	C	476	THR
1	D	57	SER
1	D	92	GLU
1	D	152	ARG
1	D	182	ASP
1	D	219	ARG
1	D	262	LYS
1	D	299	ASN
1	D	322	LEU
1	D	328	ASP
1	D	329	SER
1	D	335	LYS
1	D	340	ASN
1	D	437	GLU
1	D	499	HIS
1	F	4	LYS
1	F	11	GLN
1	F	41	LYS
1	F	57	SER
1	F	206	VAL
1	F	226	GLN
1	F	228	ASN
1	F	235	THR
1	F	236	ARG

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Mol	Chain	Res	Type
1	F	262	LYS
1	F	479	ARG
1	F	498	GLU
1	H	11	GLN
1	H	21	MET
1	H	41	LYS
1	H	57	SER
1	H	151	SER
1	H	226	GLN
1	H	229	ILE
1	H	262	LYS
1	H	278	LYS
1	H	368	THR
1	H	426	LEU
1	H	461	GLN
1	H	462	GLU
1	H	463	LYS
1	H	479	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	B	32	GLN
1	B	226	GLN
1	B	396	GLN
1	E	73	GLN
1	E	104	GLN
1	E	461	GLN
1	G	226	GLN
1	C	26	ASN
1	C	73	GLN
1	C	226	GLN
1	D	73	GLN
1	D	175	GLN
1	D	226	GLN
1	D	340	ASN
1	D	396	GLN
1	D	499	HIS
1	F	228	ASN
1	F	461	GLN
1	F	499	HIS

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Mol	Chain	Res	Type
1	H	26	ASN
1	H	404	HIS
1	H	461	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 9 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GOL	A	2647	-	5,5,5	0.32	0	5,5,5	1.24	0
5	EDO	A	2650	-	3,3,3	0.44	0	2,2,2	0.23	0
5	EDO	A	2651	-	3,3,3	0.58	0	2,2,2	0.80	0
2	GOL	B	2648	-	5,5,5	0.31	0	5,5,5	0.85	0
5	EDO	B	2650	-	3,3,3	0.40	0	2,2,2	0.23	0
5	EDO	B	2651	-	3,3,3	0.68	0	2,2,2	0.55	0
2	GOL	C	2649	-	5,5,5	0.81	0	5,5,5	0.51	0
5	EDO	C	2651	-	3,3,3	0.56	0	2,2,2	0.44	0
5	EDO	C	2652	-	3,3,3	0.27	0	2,2,2	0.38	0
5	EDO	C	2653	-	3,3,3	0.32	0	2,2,2	0.78	0
5	EDO	C	2654	-	3,3,3	0.32	0	2,2,2	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	D	2640	-	5,5,5	0.51	0	5,5,5	0.67	0
5	EDO	D	2642	-	3,3,3	0.53	0	2,2,2	0.64	0
5	EDO	D	2643	-	3,3,3	0.67	0	2,2,2	0.32	0
2	GOL	E	2641	-	5,5,5	0.70	0	5,5,5	0.81	0
5	EDO	E	2643	-	3,3,3	0.54	0	2,2,2	0.82	0
2	GOL	F	2642	-	5,5,5	0.59	0	5,5,5	0.53	0
5	EDO	F	2644	-	3,3,3	0.30	0	2,2,2	1.13	0
5	EDO	F	2645	-	3,3,3	0.59	0	2,2,2	0.32	0
2	GOL	G	2643	-	5,5,5	0.66	0	5,5,5	0.62	0
5	EDO	G	2645	-	3,3,3	0.40	0	2,2,2	0.18	0
5	EDO	G	2646	-	3,3,3	0.36	0	2,2,2	0.72	0
5	EDO	G	2647	-	3,3,3	0.34	0	2,2,2	0.68	0
5	EDO	G	2648	-	3,3,3	0.53	0	2,2,2	0.57	0
2	GOL	H	2644	-	5,5,5	0.57	0	5,5,5	0.39	0
5	EDO	H	2646	-	3,3,3	0.40	0	2,2,2	0.50	0
5	EDO	H	2647	-	3,3,3	0.58	0	2,2,2	0.52	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
2	GOL	A	2647	-	-	0/4/4/4	0/0/0/0
5	EDO	A	2650	-	-	0/1/1/1	0/0/0/0
5	EDO	A	2651	-	-	0/1/1/1	0/0/0/0
2	GOL	B	2648	-	-	0/4/4/4	0/0/0/0
5	EDO	B	2650	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2651	-	-	0/1/1/1	0/0/0/0
2	GOL	C	2649	-	-	0/4/4/4	0/0/0/0
5	EDO	C	2651	-	-	0/1/1/1	0/0/0/0
5	EDO	C	2652	-	-	0/1/1/1	0/0/0/0
5	EDO	C	2653	-	-	0/1/1/1	0/0/0/0
5	EDO	C	2654	-	-	0/1/1/1	0/0/0/0
2	GOL	D	2640	-	-	0/4/4/4	0/0/0/0
5	EDO	D	2642	-	-	0/1/1/1	0/0/0/0
5	EDO	D	2643	-	-	0/1/1/1	0/0/0/0
2	GOL	E	2641	-	-	0/4/4/4	0/0/0/0
5	EDO	E	2643	-	-	0/1/1/1	0/0/0/0
2	GOL	F	2642	-	-	0/4/4/4	0/0/0/0
5	EDO	F	2644	-	-	0/1/1/1	0/0/0/0
5	EDO	F	2645	-	-	0/1/1/1	0/0/0/0
2	GOL	G	2643	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	G	2645	-	-	0/1/1/1	0/0/0/0
5	EDO	G	2646	-	-	0/1/1/1	0/0/0/0
5	EDO	G	2647	-	-	0/1/1/1	0/0/0/0
5	EDO	G	2648	-	-	0/1/1/1	0/0/0/0
2	GOL	H	2644	-	-	0/4/4/4	0/0/0/0
5	EDO	H	2646	-	-	0/1/1/1	0/0/0/0
5	EDO	H	2647	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2653	EDO	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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	498/526 (94%)	-0.33	3 (0%) 90 90	17, 24, 44, 57	0
1	B	496/526 (94%)	-0.32	2 (0%) 93 93	17, 24, 42, 57	0
1	C	489/526 (92%)	-0.27	5 (1%) 84 84	17, 28, 47, 71	0
1	D	482/526 (91%)	-0.13	15 (3%) 52 53	19, 31, 56, 71	0
1	E	492/526 (93%)	-0.35	8 (1%) 74 75	16, 25, 45, 61	0
1	F	492/526 (93%)	-0.28	6 (1%) 81 81	19, 28, 45, 66	0
1	G	498/526 (94%)	-0.37	4 (0%) 87 88	17, 26, 42, 56	0
1	H	492/526 (93%)	-0.26	5 (1%) 84 84	21, 30, 48, 66	0
All	All	3939/4208 (93%)	-0.29	48 (1%) 81 81	16, 27, 47, 71	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	500	ASP	5.8
1	C	499	HIS	5.3
1	D	499	HIS	4.6
1	D	331	TYR	4.5
1	B	1	THR	4.3
1	H	499	HIS	3.8
1	G	1	THR	3.5
1	H	2	GLU	3.4
1	A	327	TYR	3.3
1	F	499	HIS	3.3
1	E	499	HIS	3.2
1	D	228	ASN	3.1
1	G	327	TYR	3.0
1	A	326	ALA	3.0
1	D	460	LEU	3.0
1	E	321	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	417	PHE	2.9
1	H	404	HIS	2.9
1	E	323	ILE	2.9
1	F	228	ASN	2.8
1	C	477	THR	2.7
1	G	455	GLN	2.7
1	A	465	VAL	2.6
1	D	457	LEU	2.5
1	F	236	ARG	2.5
1	C	500	ASP	2.5
1	D	477	THR	2.4
1	H	463	LYS	2.4
1	C	337	GLN	2.4
1	D	337	GLN	2.3
1	E	462	GLU	2.2
1	D	461	GLN	2.2
1	D	334	THR	2.2
1	E	327	TYR	2.2
1	D	462	GLU	2.1
1	H	462	GLU	2.1
1	F	498	GLU	2.1
1	F	326	ALA	2.1
1	F	149	GLU	2.1
1	G	498	GLU	2.1
1	E	332	PHE	2.1
1	D	476	THR	2.0
1	E	498	GLU	2.0
1	D	459	GLU	2.0
1	B	327	TYR	2.0
1	E	1	THR	2.0
1	C	228	ASN	2.0
1	D	335	LYS	2.0

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	G	2647	4/4	0.97	0.14	2.71	30,31,31,33	0
5	EDO	E	2643	4/4	0.98	0.13	2.02	23,27,27,28	0
5	EDO	C	2653	4/4	0.95	0.15	1.91	33,35,40,44	0
5	EDO	D	2642	4/4	0.95	0.12	1.59	33,35,35,35	0
5	EDO	G	2646	4/4	0.98	0.16	1.42	31,33,33,34	0
5	EDO	B	2651	4/4	0.96	0.10	1.29	26,27,28,28	0
5	EDO	D	2643	4/4	0.96	0.15	1.19	27,31,33,37	0
2	GOL	A	2647	6/6	0.98	0.13	1.14	14,17,24,27	0
5	EDO	C	2652	4/4	0.98	0.12	1.12	34,35,36,37	0
2	GOL	F	2642	6/6	0.98	0.12	0.95	20,25,27,29	0
5	EDO	H	2646	4/4	0.98	0.14	0.67	25,26,29,32	0
5	EDO	H	2647	4/4	0.95	0.11	0.53	28,33,33,35	0
5	EDO	A	2651	4/4	0.96	0.12	0.50	22,24,25,26	0
2	GOL	H	2644	6/6	0.98	0.13	0.32	21,22,26,30	0
5	EDO	F	2645	4/4	0.97	0.10	0.30	24,27,31,33	0
2	GOL	E	2641	6/6	0.98	0.09	0.26	16,20,22,22	0
5	EDO	G	2648	4/4	0.95	0.10	-0.04	29,38,40,45	0
5	EDO	C	2651	4/4	0.96	0.10	-0.20	24,31,32,33	0
5	EDO	B	2650	4/4	0.97	0.11	-0.25	28,28,28,30	0
2	GOL	G	2643	6/6	0.98	0.11	-0.43	19,20,20,21	0
5	EDO	A	2650	4/4	0.98	0.09	-0.54	33,34,34,35	0
2	GOL	D	2640	6/6	0.97	0.09	-0.75	18,22,26,31	0
2	GOL	C	2649	6/6	0.99	0.09	-0.92	18,19,25,28	0
5	EDO	G	2645	4/4	0.99	0.08	-0.96	22,23,24,29	0
3	CL	A	2648	1/1	0.99	0.08	-1.11	23,23,23,23	0
5	EDO	C	2654	4/4	0.98	0.08	-1.20	24,25,29,31	0
2	GOL	B	2648	6/6	0.98	0.09	-1.55	16,17,22,28	0
3	CL	E	2642	1/1	0.96	0.07	-1.70	34,34,34,34	0
5	EDO	F	2644	4/4	0.99	0.07	-1.92	24,25,28,29	0
3	CL	G	2644	1/1	1.00	0.06	-2.13	28,28,28,28	0
3	CL	D	2641	1/1	0.98	0.06	-2.24	37,37,37,37	0
4	MG	A	2649	1/1	0.87	0.11	-	52,52,52,52	0
3	CL	B	2649	1/1	0.99	0.07	-	33,33,33,33	0
3	CL	H	2645	1/1	0.99	0.05	-	39,39,39,39	0
3	CL	C	2650	1/1	0.99	0.07	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	F	2643	1/1	0.99	0.08	-	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.