



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:25 PM UTC

PDB ID : 9HAW / pdb\_00009haw  
Title : F420-dependent glucose-6-phosphate dehydrogenase without ligand  
Authors : Palm, G.J.; Berndt, L.; Lammers, M.  
Deposited on : 2024-11-05  
Resolution : 2.22 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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
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

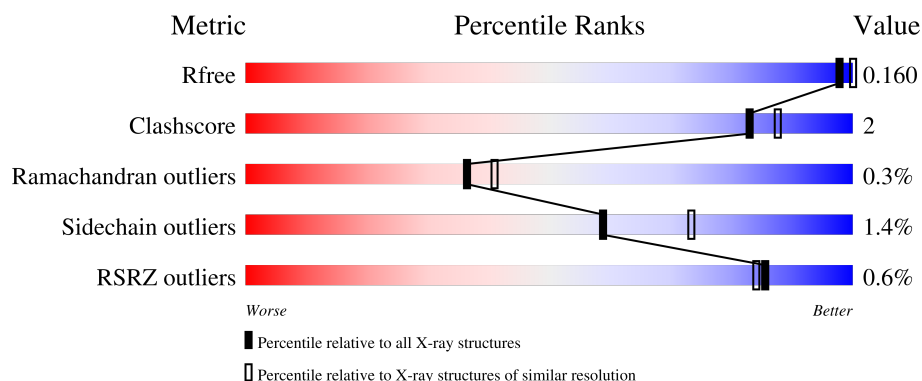
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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  $\geq 3$ , 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	380	
1	B	380	
1	C	380	
1	D	380	
1	E	380	

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Mol	Chain	Length	Quality of chain
1	F	380	 82% 6% • 11%
1	G	380	 83% 5% • 11%
1	H	380	 83% 5% •• 11%
1	I	380	 82% 5% • 11%
1	J	380	 81% 8% 11%
1	K	380	 82% 6% • 11%
1	L	380	 81% 7% 11%
1	M	380	 83% 6% • 11%
1	N	380	 82% 7% • 11%
1	O	380	 83% 5% • 11%
1	P	380	 83% 6% 11%
1	Q	380	 83% 5% 11%
1	R	380	 83% 5% • 11%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 98342 atoms, of which 47516 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 Luciferase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	339	Total	C	H	N	O	S	61	3	0
			5343	1725	2646	482	479	11			
1	B	337	Total	C	H	N	O	S	59	2	0
			5313	1716	2631	481	474	11			
1	C	338	Total	C	H	N	O	S	60	1	0
			5308	1714	2629	480	474	11			
1	D	338	Total	C	H	N	O	S	62	2	0
			5316	1717	2632	481	475	11			
1	E	339	Total	C	H	N	O	S	60	2	0
			5338	1722	2644	485	476	11			
1	F	337	Total	C	H	N	O	S	60	1	0
			5309	1715	2629	480	474	11			
1	G	340	Total	C	H	N	O	S	63	2	0
			5355	1727	2653	486	478	11			
1	H	338	Total	C	H	N	O	S	63	3	0
			5330	1721	2639	482	477	11			
1	I	337	Total	C	H	N	O	S	60	1	0
			5309	1715	2629	480	474	11			
1	J	337	Total	C	H	N	O	S	61	3	0
			5321	1718	2635	481	476	11			
1	K	340	Total	C	H	N	O	S	62	2	0
			5347	1725	2648	486	477	11			
1	L	338	Total	C	H	N	O	S	62	2	0
			5316	1717	2632	481	475	11			
1	M	338	Total	C	H	N	O	S	63	6	0
			5367	1731	2659	486	480	11			
1	N	339	Total	C	H	N	O	S	65	3	0
			5339	1724	2643	483	478	11			
1	Q	339	Total	C	H	N	O	S	61	2	0
			5329	1721	2638	483	476	11			
1	R	338	Total	C	H	N	O	S	60	3	0
			5323	1719	2635	481	477	11			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	O	338	Total	C	H	N	O	S	63	3	0
			5330	1721	2639	482	477	11			
1	P	340	Total	C	H	N	O	S	62	3	0
			5359	1728	2655	487	478	11			

There are 612 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	initiating methionine	UNP B9L4G2
A	-31	GLY	-	expression tag	UNP B9L4G2
A	-30	SER	-	expression tag	UNP B9L4G2
A	-29	SER	-	expression tag	UNP B9L4G2
A	-28	HIS	-	expression tag	UNP B9L4G2
A	-27	HIS	-	expression tag	UNP B9L4G2
A	-26	HIS	-	expression tag	UNP B9L4G2
A	-25	HIS	-	expression tag	UNP B9L4G2
A	-24	HIS	-	expression tag	UNP B9L4G2
A	-23	HIS	-	expression tag	UNP B9L4G2
A	-22	SER	-	expression tag	UNP B9L4G2
A	-21	SER	-	expression tag	UNP B9L4G2
A	-20	GLY	-	expression tag	UNP B9L4G2
A	-19	LEU	-	expression tag	UNP B9L4G2
A	-18	VAL	-	expression tag	UNP B9L4G2
A	-17	PRO	-	expression tag	UNP B9L4G2
A	-16	ARG	-	expression tag	UNP B9L4G2
A	-15	GLY	-	expression tag	UNP B9L4G2
A	-14	SER	-	expression tag	UNP B9L4G2
A	-13	HIS	-	expression tag	UNP B9L4G2
A	-12	MET	-	expression tag	UNP B9L4G2
A	-11	ALA	-	expression tag	UNP B9L4G2
A	-10	SER	-	expression tag	UNP B9L4G2
A	-9	MET	-	expression tag	UNP B9L4G2
A	-8	THR	-	expression tag	UNP B9L4G2
A	-7	GLY	-	expression tag	UNP B9L4G2
A	-6	GLY	-	expression tag	UNP B9L4G2
A	-5	GLN	-	expression tag	UNP B9L4G2
A	-4	GLN	-	expression tag	UNP B9L4G2
A	-3	MET	-	expression tag	UNP B9L4G2
A	-2	GLY	-	expression tag	UNP B9L4G2
A	-1	ARG	-	expression tag	UNP B9L4G2
A	0	GLY	-	expression tag	UNP B9L4G2
A	1	SER	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-32	MET	-	initiating methionine	UNP B9L4G2
B	-31	GLY	-	expression tag	UNP B9L4G2
B	-30	SER	-	expression tag	UNP B9L4G2
B	-29	SER	-	expression tag	UNP B9L4G2
B	-28	HIS	-	expression tag	UNP B9L4G2
B	-27	HIS	-	expression tag	UNP B9L4G2
B	-26	HIS	-	expression tag	UNP B9L4G2
B	-25	HIS	-	expression tag	UNP B9L4G2
B	-24	HIS	-	expression tag	UNP B9L4G2
B	-23	HIS	-	expression tag	UNP B9L4G2
B	-22	SER	-	expression tag	UNP B9L4G2
B	-21	SER	-	expression tag	UNP B9L4G2
B	-20	GLY	-	expression tag	UNP B9L4G2
B	-19	LEU	-	expression tag	UNP B9L4G2
B	-18	VAL	-	expression tag	UNP B9L4G2
B	-17	PRO	-	expression tag	UNP B9L4G2
B	-16	ARG	-	expression tag	UNP B9L4G2
B	-15	GLY	-	expression tag	UNP B9L4G2
B	-14	SER	-	expression tag	UNP B9L4G2
B	-13	HIS	-	expression tag	UNP B9L4G2
B	-12	MET	-	expression tag	UNP B9L4G2
B	-11	ALA	-	expression tag	UNP B9L4G2
B	-10	SER	-	expression tag	UNP B9L4G2
B	-9	MET	-	expression tag	UNP B9L4G2
B	-8	THR	-	expression tag	UNP B9L4G2
B	-7	GLY	-	expression tag	UNP B9L4G2
B	-6	GLY	-	expression tag	UNP B9L4G2
B	-5	GLN	-	expression tag	UNP B9L4G2
B	-4	GLN	-	expression tag	UNP B9L4G2
B	-3	MET	-	expression tag	UNP B9L4G2
B	-2	GLY	-	expression tag	UNP B9L4G2
B	-1	ARG	-	expression tag	UNP B9L4G2
B	0	GLY	-	expression tag	UNP B9L4G2
B	1	SER	-	expression tag	UNP B9L4G2
C	-32	MET	-	initiating methionine	UNP B9L4G2
C	-31	GLY	-	expression tag	UNP B9L4G2
C	-30	SER	-	expression tag	UNP B9L4G2
C	-29	SER	-	expression tag	UNP B9L4G2
C	-28	HIS	-	expression tag	UNP B9L4G2
C	-27	HIS	-	expression tag	UNP B9L4G2
C	-26	HIS	-	expression tag	UNP B9L4G2
C	-25	HIS	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-24	HIS	-	expression tag	UNP B9L4G2
C	-23	HIS	-	expression tag	UNP B9L4G2
C	-22	SER	-	expression tag	UNP B9L4G2
C	-21	SER	-	expression tag	UNP B9L4G2
C	-20	GLY	-	expression tag	UNP B9L4G2
C	-19	LEU	-	expression tag	UNP B9L4G2
C	-18	VAL	-	expression tag	UNP B9L4G2
C	-17	PRO	-	expression tag	UNP B9L4G2
C	-16	ARG	-	expression tag	UNP B9L4G2
C	-15	GLY	-	expression tag	UNP B9L4G2
C	-14	SER	-	expression tag	UNP B9L4G2
C	-13	HIS	-	expression tag	UNP B9L4G2
C	-12	MET	-	expression tag	UNP B9L4G2
C	-11	ALA	-	expression tag	UNP B9L4G2
C	-10	SER	-	expression tag	UNP B9L4G2
C	-9	MET	-	expression tag	UNP B9L4G2
C	-8	THR	-	expression tag	UNP B9L4G2
C	-7	GLY	-	expression tag	UNP B9L4G2
C	-6	GLY	-	expression tag	UNP B9L4G2
C	-5	GLN	-	expression tag	UNP B9L4G2
C	-4	GLN	-	expression tag	UNP B9L4G2
C	-3	MET	-	expression tag	UNP B9L4G2
C	-2	GLY	-	expression tag	UNP B9L4G2
C	-1	ARG	-	expression tag	UNP B9L4G2
C	0	GLY	-	expression tag	UNP B9L4G2
C	1	SER	-	expression tag	UNP B9L4G2
D	-32	MET	-	initiating methionine	UNP B9L4G2
D	-31	GLY	-	expression tag	UNP B9L4G2
D	-30	SER	-	expression tag	UNP B9L4G2
D	-29	SER	-	expression tag	UNP B9L4G2
D	-28	HIS	-	expression tag	UNP B9L4G2
D	-27	HIS	-	expression tag	UNP B9L4G2
D	-26	HIS	-	expression tag	UNP B9L4G2
D	-25	HIS	-	expression tag	UNP B9L4G2
D	-24	HIS	-	expression tag	UNP B9L4G2
D	-23	HIS	-	expression tag	UNP B9L4G2
D	-22	SER	-	expression tag	UNP B9L4G2
D	-21	SER	-	expression tag	UNP B9L4G2
D	-20	GLY	-	expression tag	UNP B9L4G2
D	-19	LEU	-	expression tag	UNP B9L4G2
D	-18	VAL	-	expression tag	UNP B9L4G2
D	-17	PRO	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	ARG	-	expression tag	UNP B9L4G2
D	-15	GLY	-	expression tag	UNP B9L4G2
D	-14	SER	-	expression tag	UNP B9L4G2
D	-13	HIS	-	expression tag	UNP B9L4G2
D	-12	MET	-	expression tag	UNP B9L4G2
D	-11	ALA	-	expression tag	UNP B9L4G2
D	-10	SER	-	expression tag	UNP B9L4G2
D	-9	MET	-	expression tag	UNP B9L4G2
D	-8	THR	-	expression tag	UNP B9L4G2
D	-7	GLY	-	expression tag	UNP B9L4G2
D	-6	GLY	-	expression tag	UNP B9L4G2
D	-5	GLN	-	expression tag	UNP B9L4G2
D	-4	GLN	-	expression tag	UNP B9L4G2
D	-3	MET	-	expression tag	UNP B9L4G2
D	-2	GLY	-	expression tag	UNP B9L4G2
D	-1	ARG	-	expression tag	UNP B9L4G2
D	0	GLY	-	expression tag	UNP B9L4G2
D	1	SER	-	expression tag	UNP B9L4G2
E	-32	MET	-	initiating methionine	UNP B9L4G2
E	-31	GLY	-	expression tag	UNP B9L4G2
E	-30	SER	-	expression tag	UNP B9L4G2
E	-29	SER	-	expression tag	UNP B9L4G2
E	-28	HIS	-	expression tag	UNP B9L4G2
E	-27	HIS	-	expression tag	UNP B9L4G2
E	-26	HIS	-	expression tag	UNP B9L4G2
E	-25	HIS	-	expression tag	UNP B9L4G2
E	-24	HIS	-	expression tag	UNP B9L4G2
E	-23	HIS	-	expression tag	UNP B9L4G2
E	-22	SER	-	expression tag	UNP B9L4G2
E	-21	SER	-	expression tag	UNP B9L4G2
E	-20	GLY	-	expression tag	UNP B9L4G2
E	-19	LEU	-	expression tag	UNP B9L4G2
E	-18	VAL	-	expression tag	UNP B9L4G2
E	-17	PRO	-	expression tag	UNP B9L4G2
E	-16	ARG	-	expression tag	UNP B9L4G2
E	-15	GLY	-	expression tag	UNP B9L4G2
E	-14	SER	-	expression tag	UNP B9L4G2
E	-13	HIS	-	expression tag	UNP B9L4G2
E	-12	MET	-	expression tag	UNP B9L4G2
E	-11	ALA	-	expression tag	UNP B9L4G2
E	-10	SER	-	expression tag	UNP B9L4G2
E	-9	MET	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	THR	-	expression tag	UNP B9L4G2
E	-7	GLY	-	expression tag	UNP B9L4G2
E	-6	GLY	-	expression tag	UNP B9L4G2
E	-5	GLN	-	expression tag	UNP B9L4G2
E	-4	GLN	-	expression tag	UNP B9L4G2
E	-3	MET	-	expression tag	UNP B9L4G2
E	-2	GLY	-	expression tag	UNP B9L4G2
E	-1	ARG	-	expression tag	UNP B9L4G2
E	0	GLY	-	expression tag	UNP B9L4G2
E	1	SER	-	expression tag	UNP B9L4G2
F	-32	MET	-	initiating methionine	UNP B9L4G2
F	-31	GLY	-	expression tag	UNP B9L4G2
F	-30	SER	-	expression tag	UNP B9L4G2
F	-29	SER	-	expression tag	UNP B9L4G2
F	-28	HIS	-	expression tag	UNP B9L4G2
F	-27	HIS	-	expression tag	UNP B9L4G2
F	-26	HIS	-	expression tag	UNP B9L4G2
F	-25	HIS	-	expression tag	UNP B9L4G2
F	-24	HIS	-	expression tag	UNP B9L4G2
F	-23	HIS	-	expression tag	UNP B9L4G2
F	-22	SER	-	expression tag	UNP B9L4G2
F	-21	SER	-	expression tag	UNP B9L4G2
F	-20	GLY	-	expression tag	UNP B9L4G2
F	-19	LEU	-	expression tag	UNP B9L4G2
F	-18	VAL	-	expression tag	UNP B9L4G2
F	-17	PRO	-	expression tag	UNP B9L4G2
F	-16	ARG	-	expression tag	UNP B9L4G2
F	-15	GLY	-	expression tag	UNP B9L4G2
F	-14	SER	-	expression tag	UNP B9L4G2
F	-13	HIS	-	expression tag	UNP B9L4G2
F	-12	MET	-	expression tag	UNP B9L4G2
F	-11	ALA	-	expression tag	UNP B9L4G2
F	-10	SER	-	expression tag	UNP B9L4G2
F	-9	MET	-	expression tag	UNP B9L4G2
F	-8	THR	-	expression tag	UNP B9L4G2
F	-7	GLY	-	expression tag	UNP B9L4G2
F	-6	GLY	-	expression tag	UNP B9L4G2
F	-5	GLN	-	expression tag	UNP B9L4G2
F	-4	GLN	-	expression tag	UNP B9L4G2
F	-3	MET	-	expression tag	UNP B9L4G2
F	-2	GLY	-	expression tag	UNP B9L4G2
F	-1	ARG	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	expression tag	UNP B9L4G2
F	1	SER	-	expression tag	UNP B9L4G2
G	-32	MET	-	initiating methionine	UNP B9L4G2
G	-31	GLY	-	expression tag	UNP B9L4G2
G	-30	SER	-	expression tag	UNP B9L4G2
G	-29	SER	-	expression tag	UNP B9L4G2
G	-28	HIS	-	expression tag	UNP B9L4G2
G	-27	HIS	-	expression tag	UNP B9L4G2
G	-26	HIS	-	expression tag	UNP B9L4G2
G	-25	HIS	-	expression tag	UNP B9L4G2
G	-24	HIS	-	expression tag	UNP B9L4G2
G	-23	HIS	-	expression tag	UNP B9L4G2
G	-22	SER	-	expression tag	UNP B9L4G2
G	-21	SER	-	expression tag	UNP B9L4G2
G	-20	GLY	-	expression tag	UNP B9L4G2
G	-19	LEU	-	expression tag	UNP B9L4G2
G	-18	VAL	-	expression tag	UNP B9L4G2
G	-17	PRO	-	expression tag	UNP B9L4G2
G	-16	ARG	-	expression tag	UNP B9L4G2
G	-15	GLY	-	expression tag	UNP B9L4G2
G	-14	SER	-	expression tag	UNP B9L4G2
G	-13	HIS	-	expression tag	UNP B9L4G2
G	-12	MET	-	expression tag	UNP B9L4G2
G	-11	ALA	-	expression tag	UNP B9L4G2
G	-10	SER	-	expression tag	UNP B9L4G2
G	-9	MET	-	expression tag	UNP B9L4G2
G	-8	THR	-	expression tag	UNP B9L4G2
G	-7	GLY	-	expression tag	UNP B9L4G2
G	-6	GLY	-	expression tag	UNP B9L4G2
G	-5	GLN	-	expression tag	UNP B9L4G2
G	-4	GLN	-	expression tag	UNP B9L4G2
G	-3	MET	-	expression tag	UNP B9L4G2
G	-2	GLY	-	expression tag	UNP B9L4G2
G	-1	ARG	-	expression tag	UNP B9L4G2
G	0	GLY	-	expression tag	UNP B9L4G2
G	1	SER	-	expression tag	UNP B9L4G2
H	-32	MET	-	initiating methionine	UNP B9L4G2
H	-31	GLY	-	expression tag	UNP B9L4G2
H	-30	SER	-	expression tag	UNP B9L4G2
H	-29	SER	-	expression tag	UNP B9L4G2
H	-28	HIS	-	expression tag	UNP B9L4G2
H	-27	HIS	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-26	HIS	-	expression tag	UNP B9L4G2
H	-25	HIS	-	expression tag	UNP B9L4G2
H	-24	HIS	-	expression tag	UNP B9L4G2
H	-23	HIS	-	expression tag	UNP B9L4G2
H	-22	SER	-	expression tag	UNP B9L4G2
H	-21	SER	-	expression tag	UNP B9L4G2
H	-20	GLY	-	expression tag	UNP B9L4G2
H	-19	LEU	-	expression tag	UNP B9L4G2
H	-18	VAL	-	expression tag	UNP B9L4G2
H	-17	PRO	-	expression tag	UNP B9L4G2
H	-16	ARG	-	expression tag	UNP B9L4G2
H	-15	GLY	-	expression tag	UNP B9L4G2
H	-14	SER	-	expression tag	UNP B9L4G2
H	-13	HIS	-	expression tag	UNP B9L4G2
H	-12	MET	-	expression tag	UNP B9L4G2
H	-11	ALA	-	expression tag	UNP B9L4G2
H	-10	SER	-	expression tag	UNP B9L4G2
H	-9	MET	-	expression tag	UNP B9L4G2
H	-8	THR	-	expression tag	UNP B9L4G2
H	-7	GLY	-	expression tag	UNP B9L4G2
H	-6	GLY	-	expression tag	UNP B9L4G2
H	-5	GLN	-	expression tag	UNP B9L4G2
H	-4	GLN	-	expression tag	UNP B9L4G2
H	-3	MET	-	expression tag	UNP B9L4G2
H	-2	GLY	-	expression tag	UNP B9L4G2
H	-1	ARG	-	expression tag	UNP B9L4G2
H	0	GLY	-	expression tag	UNP B9L4G2
H	1	SER	-	expression tag	UNP B9L4G2
I	-32	MET	-	initiating methionine	UNP B9L4G2
I	-31	GLY	-	expression tag	UNP B9L4G2
I	-30	SER	-	expression tag	UNP B9L4G2
I	-29	SER	-	expression tag	UNP B9L4G2
I	-28	HIS	-	expression tag	UNP B9L4G2
I	-27	HIS	-	expression tag	UNP B9L4G2
I	-26	HIS	-	expression tag	UNP B9L4G2
I	-25	HIS	-	expression tag	UNP B9L4G2
I	-24	HIS	-	expression tag	UNP B9L4G2
I	-23	HIS	-	expression tag	UNP B9L4G2
I	-22	SER	-	expression tag	UNP B9L4G2
I	-21	SER	-	expression tag	UNP B9L4G2
I	-20	GLY	-	expression tag	UNP B9L4G2
I	-19	LEU	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-18	VAL	-	expression tag	UNP B9L4G2
I	-17	PRO	-	expression tag	UNP B9L4G2
I	-16	ARG	-	expression tag	UNP B9L4G2
I	-15	GLY	-	expression tag	UNP B9L4G2
I	-14	SER	-	expression tag	UNP B9L4G2
I	-13	HIS	-	expression tag	UNP B9L4G2
I	-12	MET	-	expression tag	UNP B9L4G2
I	-11	ALA	-	expression tag	UNP B9L4G2
I	-10	SER	-	expression tag	UNP B9L4G2
I	-9	MET	-	expression tag	UNP B9L4G2
I	-8	THR	-	expression tag	UNP B9L4G2
I	-7	GLY	-	expression tag	UNP B9L4G2
I	-6	GLY	-	expression tag	UNP B9L4G2
I	-5	GLN	-	expression tag	UNP B9L4G2
I	-4	GLN	-	expression tag	UNP B9L4G2
I	-3	MET	-	expression tag	UNP B9L4G2
I	-2	GLY	-	expression tag	UNP B9L4G2
I	-1	ARG	-	expression tag	UNP B9L4G2
I	0	GLY	-	expression tag	UNP B9L4G2
I	1	SER	-	expression tag	UNP B9L4G2
J	-32	MET	-	initiating methionine	UNP B9L4G2
J	-31	GLY	-	expression tag	UNP B9L4G2
J	-30	SER	-	expression tag	UNP B9L4G2
J	-29	SER	-	expression tag	UNP B9L4G2
J	-28	HIS	-	expression tag	UNP B9L4G2
J	-27	HIS	-	expression tag	UNP B9L4G2
J	-26	HIS	-	expression tag	UNP B9L4G2
J	-25	HIS	-	expression tag	UNP B9L4G2
J	-24	HIS	-	expression tag	UNP B9L4G2
J	-23	HIS	-	expression tag	UNP B9L4G2
J	-22	SER	-	expression tag	UNP B9L4G2
J	-21	SER	-	expression tag	UNP B9L4G2
J	-20	GLY	-	expression tag	UNP B9L4G2
J	-19	LEU	-	expression tag	UNP B9L4G2
J	-18	VAL	-	expression tag	UNP B9L4G2
J	-17	PRO	-	expression tag	UNP B9L4G2
J	-16	ARG	-	expression tag	UNP B9L4G2
J	-15	GLY	-	expression tag	UNP B9L4G2
J	-14	SER	-	expression tag	UNP B9L4G2
J	-13	HIS	-	expression tag	UNP B9L4G2
J	-12	MET	-	expression tag	UNP B9L4G2
J	-11	ALA	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-10	SER	-	expression tag	UNP B9L4G2
J	-9	MET	-	expression tag	UNP B9L4G2
J	-8	THR	-	expression tag	UNP B9L4G2
J	-7	GLY	-	expression tag	UNP B9L4G2
J	-6	GLY	-	expression tag	UNP B9L4G2
J	-5	GLN	-	expression tag	UNP B9L4G2
J	-4	GLN	-	expression tag	UNP B9L4G2
J	-3	MET	-	expression tag	UNP B9L4G2
J	-2	GLY	-	expression tag	UNP B9L4G2
J	-1	ARG	-	expression tag	UNP B9L4G2
J	0	GLY	-	expression tag	UNP B9L4G2
J	1	SER	-	expression tag	UNP B9L4G2
K	-32	MET	-	initiating methionine	UNP B9L4G2
K	-31	GLY	-	expression tag	UNP B9L4G2
K	-30	SER	-	expression tag	UNP B9L4G2
K	-29	SER	-	expression tag	UNP B9L4G2
K	-28	HIS	-	expression tag	UNP B9L4G2
K	-27	HIS	-	expression tag	UNP B9L4G2
K	-26	HIS	-	expression tag	UNP B9L4G2
K	-25	HIS	-	expression tag	UNP B9L4G2
K	-24	HIS	-	expression tag	UNP B9L4G2
K	-23	HIS	-	expression tag	UNP B9L4G2
K	-22	SER	-	expression tag	UNP B9L4G2
K	-21	SER	-	expression tag	UNP B9L4G2
K	-20	GLY	-	expression tag	UNP B9L4G2
K	-19	LEU	-	expression tag	UNP B9L4G2
K	-18	VAL	-	expression tag	UNP B9L4G2
K	-17	PRO	-	expression tag	UNP B9L4G2
K	-16	ARG	-	expression tag	UNP B9L4G2
K	-15	GLY	-	expression tag	UNP B9L4G2
K	-14	SER	-	expression tag	UNP B9L4G2
K	-13	HIS	-	expression tag	UNP B9L4G2
K	-12	MET	-	expression tag	UNP B9L4G2
K	-11	ALA	-	expression tag	UNP B9L4G2
K	-10	SER	-	expression tag	UNP B9L4G2
K	-9	MET	-	expression tag	UNP B9L4G2
K	-8	THR	-	expression tag	UNP B9L4G2
K	-7	GLY	-	expression tag	UNP B9L4G2
K	-6	GLY	-	expression tag	UNP B9L4G2
K	-5	GLN	-	expression tag	UNP B9L4G2
K	-4	GLN	-	expression tag	UNP B9L4G2
K	-3	MET	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	GLY	-	expression tag	UNP B9L4G2
K	-1	ARG	-	expression tag	UNP B9L4G2
K	0	GLY	-	expression tag	UNP B9L4G2
K	1	SER	-	expression tag	UNP B9L4G2
L	-32	MET	-	initiating methionine	UNP B9L4G2
L	-31	GLY	-	expression tag	UNP B9L4G2
L	-30	SER	-	expression tag	UNP B9L4G2
L	-29	SER	-	expression tag	UNP B9L4G2
L	-28	HIS	-	expression tag	UNP B9L4G2
L	-27	HIS	-	expression tag	UNP B9L4G2
L	-26	HIS	-	expression tag	UNP B9L4G2
L	-25	HIS	-	expression tag	UNP B9L4G2
L	-24	HIS	-	expression tag	UNP B9L4G2
L	-23	HIS	-	expression tag	UNP B9L4G2
L	-22	SER	-	expression tag	UNP B9L4G2
L	-21	SER	-	expression tag	UNP B9L4G2
L	-20	GLY	-	expression tag	UNP B9L4G2
L	-19	LEU	-	expression tag	UNP B9L4G2
L	-18	VAL	-	expression tag	UNP B9L4G2
L	-17	PRO	-	expression tag	UNP B9L4G2
L	-16	ARG	-	expression tag	UNP B9L4G2
L	-15	GLY	-	expression tag	UNP B9L4G2
L	-14	SER	-	expression tag	UNP B9L4G2
L	-13	HIS	-	expression tag	UNP B9L4G2
L	-12	MET	-	expression tag	UNP B9L4G2
L	-11	ALA	-	expression tag	UNP B9L4G2
L	-10	SER	-	expression tag	UNP B9L4G2
L	-9	MET	-	expression tag	UNP B9L4G2
L	-8	THR	-	expression tag	UNP B9L4G2
L	-7	GLY	-	expression tag	UNP B9L4G2
L	-6	GLY	-	expression tag	UNP B9L4G2
L	-5	GLN	-	expression tag	UNP B9L4G2
L	-4	GLN	-	expression tag	UNP B9L4G2
L	-3	MET	-	expression tag	UNP B9L4G2
L	-2	GLY	-	expression tag	UNP B9L4G2
L	-1	ARG	-	expression tag	UNP B9L4G2
L	0	GLY	-	expression tag	UNP B9L4G2
L	1	SER	-	expression tag	UNP B9L4G2
M	-32	MET	-	initiating methionine	UNP B9L4G2
M	-31	GLY	-	expression tag	UNP B9L4G2
M	-30	SER	-	expression tag	UNP B9L4G2
M	-29	SER	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-28	HIS	-	expression tag	UNP B9L4G2
M	-27	HIS	-	expression tag	UNP B9L4G2
M	-26	HIS	-	expression tag	UNP B9L4G2
M	-25	HIS	-	expression tag	UNP B9L4G2
M	-24	HIS	-	expression tag	UNP B9L4G2
M	-23	HIS	-	expression tag	UNP B9L4G2
M	-22	SER	-	expression tag	UNP B9L4G2
M	-21	SER	-	expression tag	UNP B9L4G2
M	-20	GLY	-	expression tag	UNP B9L4G2
M	-19	LEU	-	expression tag	UNP B9L4G2
M	-18	VAL	-	expression tag	UNP B9L4G2
M	-17	PRO	-	expression tag	UNP B9L4G2
M	-16	ARG	-	expression tag	UNP B9L4G2
M	-15	GLY	-	expression tag	UNP B9L4G2
M	-14	SER	-	expression tag	UNP B9L4G2
M	-13	HIS	-	expression tag	UNP B9L4G2
M	-12	MET	-	expression tag	UNP B9L4G2
M	-11	ALA	-	expression tag	UNP B9L4G2
M	-10	SER	-	expression tag	UNP B9L4G2
M	-9	MET	-	expression tag	UNP B9L4G2
M	-8	THR	-	expression tag	UNP B9L4G2
M	-7	GLY	-	expression tag	UNP B9L4G2
M	-6	GLY	-	expression tag	UNP B9L4G2
M	-5	GLN	-	expression tag	UNP B9L4G2
M	-4	GLN	-	expression tag	UNP B9L4G2
M	-3	MET	-	expression tag	UNP B9L4G2
M	-2	GLY	-	expression tag	UNP B9L4G2
M	-1	ARG	-	expression tag	UNP B9L4G2
M	0	GLY	-	expression tag	UNP B9L4G2
M	1	SER	-	expression tag	UNP B9L4G2
N	-32	MET	-	initiating methionine	UNP B9L4G2
N	-31	GLY	-	expression tag	UNP B9L4G2
N	-30	SER	-	expression tag	UNP B9L4G2
N	-29	SER	-	expression tag	UNP B9L4G2
N	-28	HIS	-	expression tag	UNP B9L4G2
N	-27	HIS	-	expression tag	UNP B9L4G2
N	-26	HIS	-	expression tag	UNP B9L4G2
N	-25	HIS	-	expression tag	UNP B9L4G2
N	-24	HIS	-	expression tag	UNP B9L4G2
N	-23	HIS	-	expression tag	UNP B9L4G2
N	-22	SER	-	expression tag	UNP B9L4G2
N	-21	SER	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-20	GLY	-	expression tag	UNP B9L4G2
N	-19	LEU	-	expression tag	UNP B9L4G2
N	-18	VAL	-	expression tag	UNP B9L4G2
N	-17	PRO	-	expression tag	UNP B9L4G2
N	-16	ARG	-	expression tag	UNP B9L4G2
N	-15	GLY	-	expression tag	UNP B9L4G2
N	-14	SER	-	expression tag	UNP B9L4G2
N	-13	HIS	-	expression tag	UNP B9L4G2
N	-12	MET	-	expression tag	UNP B9L4G2
N	-11	ALA	-	expression tag	UNP B9L4G2
N	-10	SER	-	expression tag	UNP B9L4G2
N	-9	MET	-	expression tag	UNP B9L4G2
N	-8	THR	-	expression tag	UNP B9L4G2
N	-7	GLY	-	expression tag	UNP B9L4G2
N	-6	GLY	-	expression tag	UNP B9L4G2
N	-5	GLN	-	expression tag	UNP B9L4G2
N	-4	GLN	-	expression tag	UNP B9L4G2
N	-3	MET	-	expression tag	UNP B9L4G2
N	-2	GLY	-	expression tag	UNP B9L4G2
N	-1	ARG	-	expression tag	UNP B9L4G2
N	0	GLY	-	expression tag	UNP B9L4G2
N	1	SER	-	expression tag	UNP B9L4G2
Q	-32	MET	-	initiating methionine	UNP B9L4G2
Q	-31	GLY	-	expression tag	UNP B9L4G2
Q	-30	SER	-	expression tag	UNP B9L4G2
Q	-29	SER	-	expression tag	UNP B9L4G2
Q	-28	HIS	-	expression tag	UNP B9L4G2
Q	-27	HIS	-	expression tag	UNP B9L4G2
Q	-26	HIS	-	expression tag	UNP B9L4G2
Q	-25	HIS	-	expression tag	UNP B9L4G2
Q	-24	HIS	-	expression tag	UNP B9L4G2
Q	-23	HIS	-	expression tag	UNP B9L4G2
Q	-22	SER	-	expression tag	UNP B9L4G2
Q	-21	SER	-	expression tag	UNP B9L4G2
Q	-20	GLY	-	expression tag	UNP B9L4G2
Q	-19	LEU	-	expression tag	UNP B9L4G2
Q	-18	VAL	-	expression tag	UNP B9L4G2
Q	-17	PRO	-	expression tag	UNP B9L4G2
Q	-16	ARG	-	expression tag	UNP B9L4G2
Q	-15	GLY	-	expression tag	UNP B9L4G2
Q	-14	SER	-	expression tag	UNP B9L4G2
Q	-13	HIS	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-12	MET	-	expression tag	UNP B9L4G2
Q	-11	ALA	-	expression tag	UNP B9L4G2
Q	-10	SER	-	expression tag	UNP B9L4G2
Q	-9	MET	-	expression tag	UNP B9L4G2
Q	-8	THR	-	expression tag	UNP B9L4G2
Q	-7	GLY	-	expression tag	UNP B9L4G2
Q	-6	GLY	-	expression tag	UNP B9L4G2
Q	-5	GLN	-	expression tag	UNP B9L4G2
Q	-4	GLN	-	expression tag	UNP B9L4G2
Q	-3	MET	-	expression tag	UNP B9L4G2
Q	-2	GLY	-	expression tag	UNP B9L4G2
Q	-1	ARG	-	expression tag	UNP B9L4G2
Q	0	GLY	-	expression tag	UNP B9L4G2
Q	1	SER	-	expression tag	UNP B9L4G2
R	-32	MET	-	initiating methionine	UNP B9L4G2
R	-31	GLY	-	expression tag	UNP B9L4G2
R	-30	SER	-	expression tag	UNP B9L4G2
R	-29	SER	-	expression tag	UNP B9L4G2
R	-28	HIS	-	expression tag	UNP B9L4G2
R	-27	HIS	-	expression tag	UNP B9L4G2
R	-26	HIS	-	expression tag	UNP B9L4G2
R	-25	HIS	-	expression tag	UNP B9L4G2
R	-24	HIS	-	expression tag	UNP B9L4G2
R	-23	HIS	-	expression tag	UNP B9L4G2
R	-22	SER	-	expression tag	UNP B9L4G2
R	-21	SER	-	expression tag	UNP B9L4G2
R	-20	GLY	-	expression tag	UNP B9L4G2
R	-19	LEU	-	expression tag	UNP B9L4G2
R	-18	VAL	-	expression tag	UNP B9L4G2
R	-17	PRO	-	expression tag	UNP B9L4G2
R	-16	ARG	-	expression tag	UNP B9L4G2
R	-15	GLY	-	expression tag	UNP B9L4G2
R	-14	SER	-	expression tag	UNP B9L4G2
R	-13	HIS	-	expression tag	UNP B9L4G2
R	-12	MET	-	expression tag	UNP B9L4G2
R	-11	ALA	-	expression tag	UNP B9L4G2
R	-10	SER	-	expression tag	UNP B9L4G2
R	-9	MET	-	expression tag	UNP B9L4G2
R	-8	THR	-	expression tag	UNP B9L4G2
R	-7	GLY	-	expression tag	UNP B9L4G2
R	-6	GLY	-	expression tag	UNP B9L4G2
R	-5	GLN	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-4	GLN	-	expression tag	UNP B9L4G2
R	-3	MET	-	expression tag	UNP B9L4G2
R	-2	GLY	-	expression tag	UNP B9L4G2
R	-1	ARG	-	expression tag	UNP B9L4G2
R	0	GLY	-	expression tag	UNP B9L4G2
R	1	SER	-	expression tag	UNP B9L4G2
O	-32	MET	-	initiating methionine	UNP B9L4G2
O	-31	GLY	-	expression tag	UNP B9L4G2
O	-30	SER	-	expression tag	UNP B9L4G2
O	-29	SER	-	expression tag	UNP B9L4G2
O	-28	HIS	-	expression tag	UNP B9L4G2
O	-27	HIS	-	expression tag	UNP B9L4G2
O	-26	HIS	-	expression tag	UNP B9L4G2
O	-25	HIS	-	expression tag	UNP B9L4G2
O	-24	HIS	-	expression tag	UNP B9L4G2
O	-23	HIS	-	expression tag	UNP B9L4G2
O	-22	SER	-	expression tag	UNP B9L4G2
O	-21	SER	-	expression tag	UNP B9L4G2
O	-20	GLY	-	expression tag	UNP B9L4G2
O	-19	LEU	-	expression tag	UNP B9L4G2
O	-18	VAL	-	expression tag	UNP B9L4G2
O	-17	PRO	-	expression tag	UNP B9L4G2
O	-16	ARG	-	expression tag	UNP B9L4G2
O	-15	GLY	-	expression tag	UNP B9L4G2
O	-14	SER	-	expression tag	UNP B9L4G2
O	-13	HIS	-	expression tag	UNP B9L4G2
O	-12	MET	-	expression tag	UNP B9L4G2
O	-11	ALA	-	expression tag	UNP B9L4G2
O	-10	SER	-	expression tag	UNP B9L4G2
O	-9	MET	-	expression tag	UNP B9L4G2
O	-8	THR	-	expression tag	UNP B9L4G2
O	-7	GLY	-	expression tag	UNP B9L4G2
O	-6	GLY	-	expression tag	UNP B9L4G2
O	-5	GLN	-	expression tag	UNP B9L4G2
O	-4	GLN	-	expression tag	UNP B9L4G2
O	-3	MET	-	expression tag	UNP B9L4G2
O	-2	GLY	-	expression tag	UNP B9L4G2
O	-1	ARG	-	expression tag	UNP B9L4G2
O	0	GLY	-	expression tag	UNP B9L4G2
O	1	SER	-	expression tag	UNP B9L4G2
P	-32	MET	-	initiating methionine	UNP B9L4G2
P	-31	GLY	-	expression tag	UNP B9L4G2

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-30	SER	-	expression tag	UNP B9L4G2
P	-29	SER	-	expression tag	UNP B9L4G2
P	-28	HIS	-	expression tag	UNP B9L4G2
P	-27	HIS	-	expression tag	UNP B9L4G2
P	-26	HIS	-	expression tag	UNP B9L4G2
P	-25	HIS	-	expression tag	UNP B9L4G2
P	-24	HIS	-	expression tag	UNP B9L4G2
P	-23	HIS	-	expression tag	UNP B9L4G2
P	-22	SER	-	expression tag	UNP B9L4G2
P	-21	SER	-	expression tag	UNP B9L4G2
P	-20	GLY	-	expression tag	UNP B9L4G2
P	-19	LEU	-	expression tag	UNP B9L4G2
P	-18	VAL	-	expression tag	UNP B9L4G2
P	-17	PRO	-	expression tag	UNP B9L4G2
P	-16	ARG	-	expression tag	UNP B9L4G2
P	-15	GLY	-	expression tag	UNP B9L4G2
P	-14	SER	-	expression tag	UNP B9L4G2
P	-13	HIS	-	expression tag	UNP B9L4G2
P	-12	MET	-	expression tag	UNP B9L4G2
P	-11	ALA	-	expression tag	UNP B9L4G2
P	-10	SER	-	expression tag	UNP B9L4G2
P	-9	MET	-	expression tag	UNP B9L4G2
P	-8	THR	-	expression tag	UNP B9L4G2
P	-7	GLY	-	expression tag	UNP B9L4G2
P	-6	GLY	-	expression tag	UNP B9L4G2
P	-5	GLN	-	expression tag	UNP B9L4G2
P	-4	GLN	-	expression tag	UNP B9L4G2
P	-3	MET	-	expression tag	UNP B9L4G2
P	-2	GLY	-	expression tag	UNP B9L4G2
P	-1	ARG	-	expression tag	UNP B9L4G2
P	0	GLY	-	expression tag	UNP B9L4G2
P	1	SER	-	expression tag	UNP B9L4G2

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total 1	Cl 1	0	0
2	G	1	Total 1	Cl 1	0	0
2	H	1	Total 1	Cl 1	0	0
2	I	1	Total 1	Cl 1	0	0
2	J	1	Total 1	Cl 1	0	0
2	K	1	Total 1	Cl 1	0	0
2	L	1	Total 1	Cl 1	0	0
2	M	1	Total 1	Cl 1	0	0
2	N	1	Total 1	Cl 1	0	0
2	Q	1	Total 1	Cl 1	0	0
2	R	1	Total 1	Cl 1	0	0
2	O	1	Total 1	Cl 1	0	0
2	P	1	Total 1	Cl 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total 132	O 132	0	0
3	B	90	Total 90	O 90	0	0
3	C	133	Total 133	O 133	0	0
3	D	137	Total 137	O 137	0	0
3	E	124	Total 124	O 124	0	0
3	F	73	Total 73	O 73	0	0

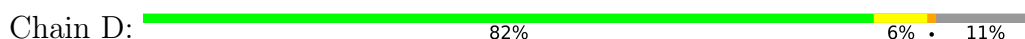
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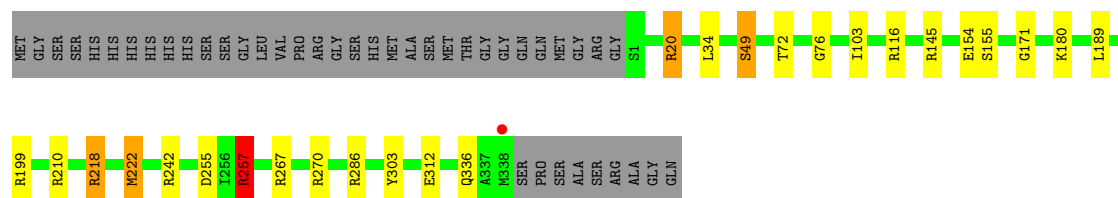
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	160	Total 160	O 160	0	0
3	H	172	Total 172	O 172	0	0
3	I	85	Total 86	O 86	0	1
3	J	133	Total 133	O 133	0	0
3	K	152	Total 153	O 153	0	1
3	L	136	Total 136	O 136	0	0
3	M	159	Total 159	O 159	0	0
3	N	160	Total 160	O 160	0	0
3	Q	112	Total 112	O 112	0	0
3	R	110	Total 110	O 110	0	0
3	O	153	Total 153	O 153	0	0
3	P	151	Total 151	O 151	0	0



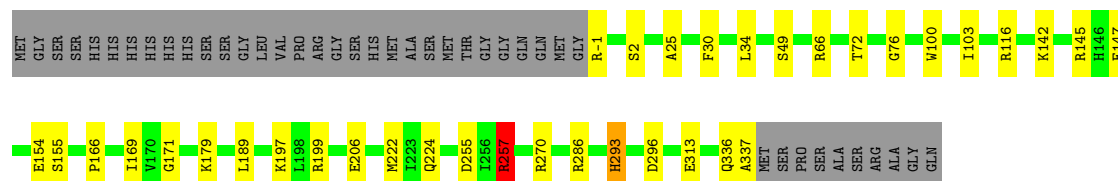
- Molecule 1: Luciferase family protein





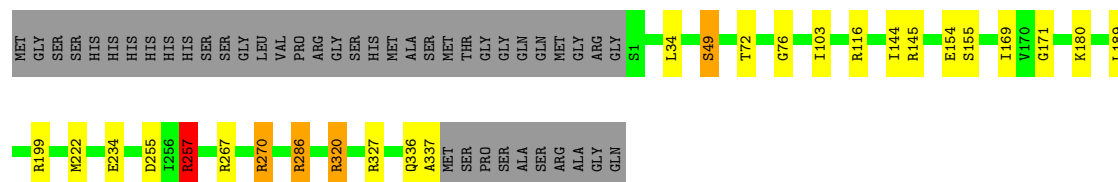
- Molecule 1: Luciferase family protein

Chain E: 80% 9% 11%



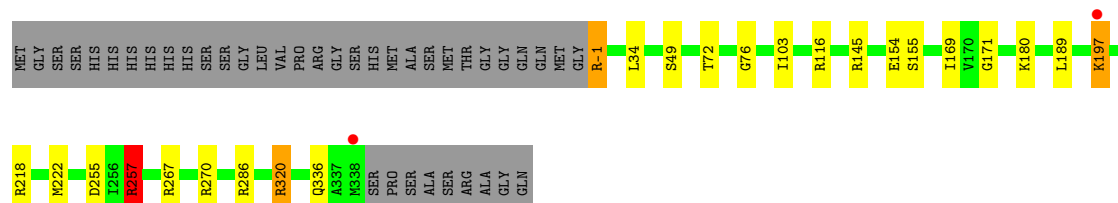
- Molecule 1: Luciferase family protein

Chain F: 82% 6% 11%



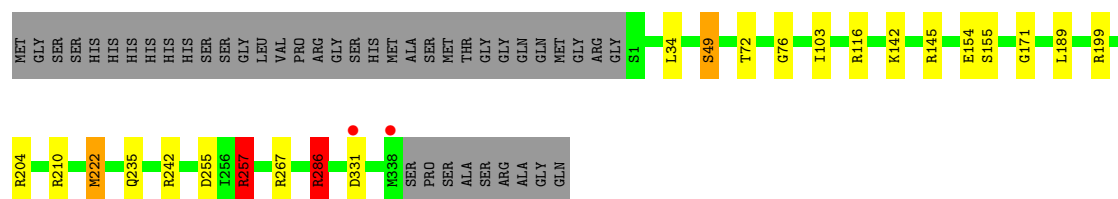
- Molecule 1: Luciferase family protein

Chain G: 83% 5% 11%

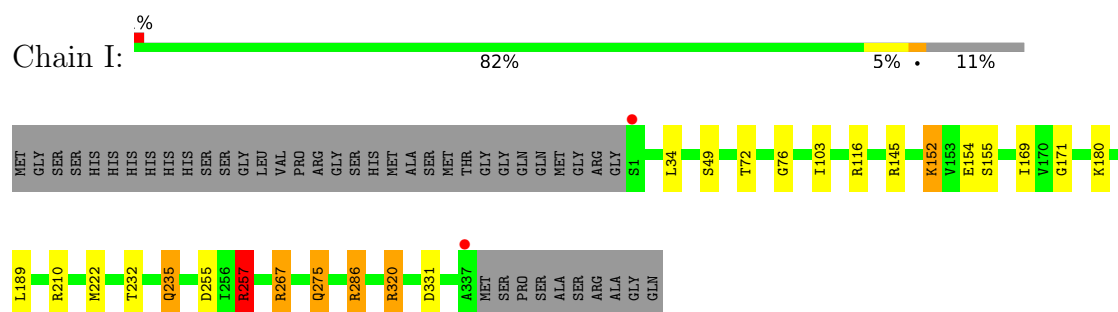


- Molecule 1: Luciferase family protein

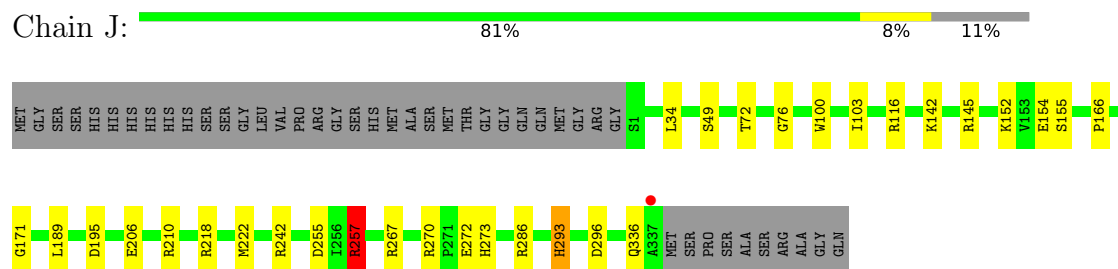
Chain H: 83% 5% 11%



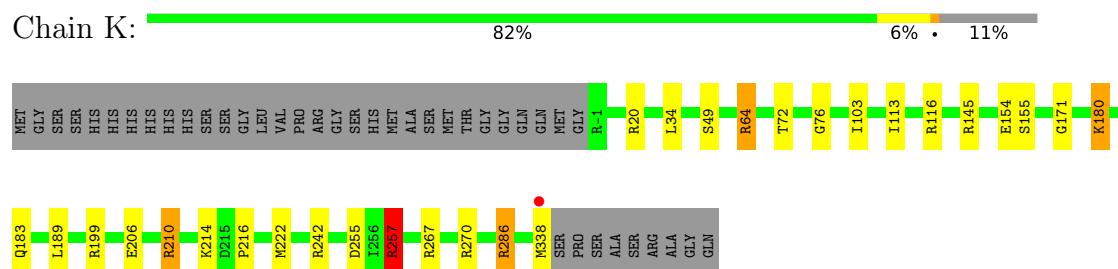
- Molecule 1: Luciferase family protein



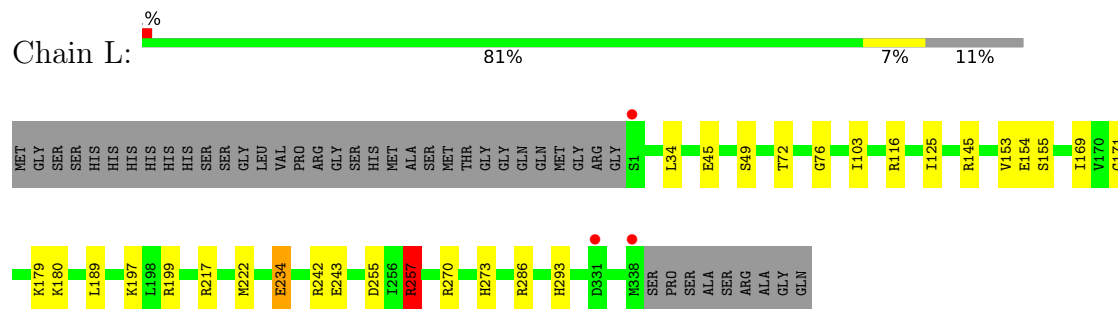
- Molecule 1: Luciferase family protein



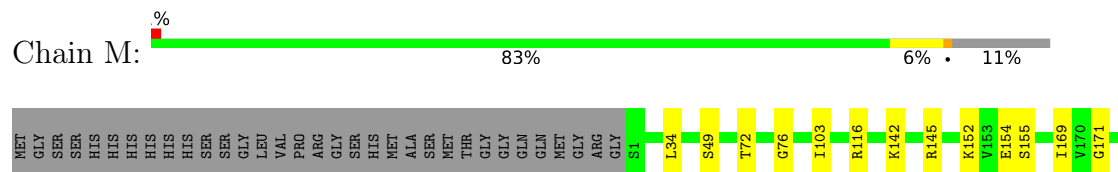
- Molecule 1: Luciferase family protein



- Molecule 1: Luciferase family protein



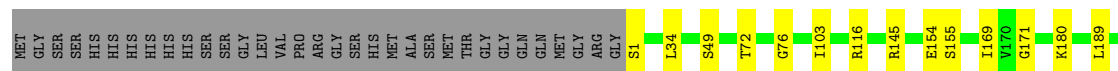
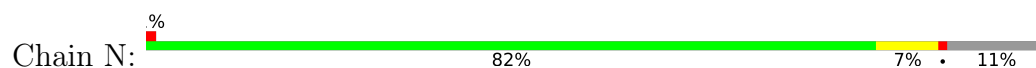
- Molecule 1: Luciferase family protein



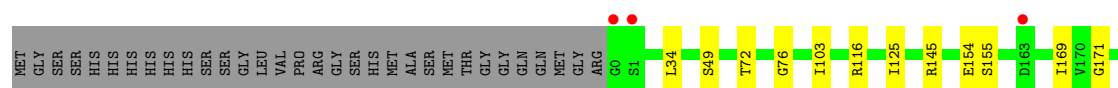
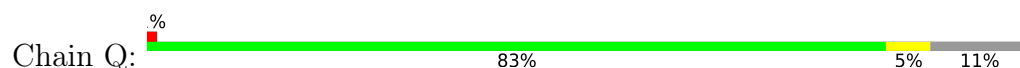




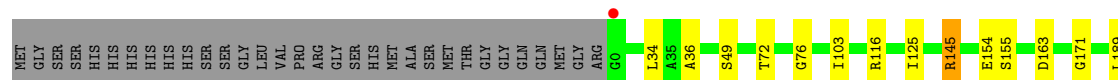
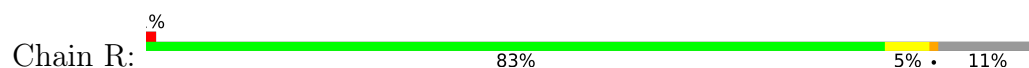
- Molecule 1: Luciferase family protein



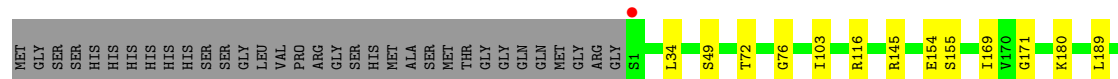
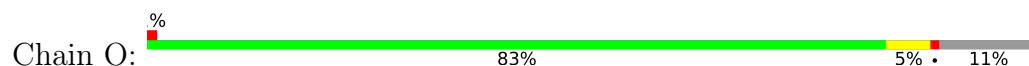
- Molecule 1: Luciferase family protein



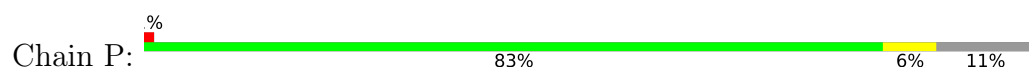
- Molecule 1: Luciferase family protein

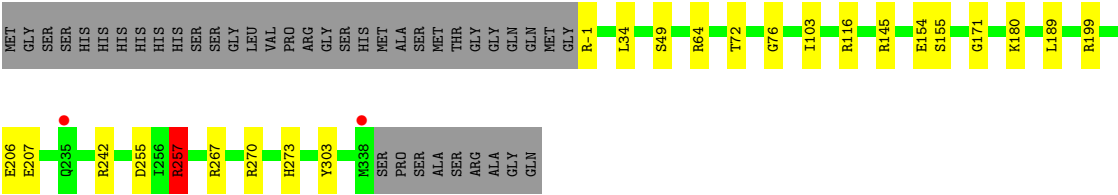


- Molecule 1: Luciferase family protein



- Molecule 1: Luciferase family protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	200.48Å 376.88Å 104.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	177.63 – 2.22 177.63 – 2.45	Depositor EDS
% Data completeness (in resolution range)	90.2 (177.63-2.22) 90.1 (177.63-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.173 , 0.193 0.164 , 0.160	Depositor DCC
$R_{free}$ test set	14228 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 30.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	98342	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.86% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.64	1/2788 (0.0%)	0.98	7/3786 (0.2%)
1	B	0.57	0/2765	0.94	4/3755 (0.1%)
1	C	0.62	0/2762	0.96	5/3751 (0.1%)
1	D	0.64	0/2770	1.00	7/3763 (0.2%)
1	E	0.71	3/2780 (0.1%)	1.03	10/3775 (0.3%)
1	F	0.57	0/2759	0.96	5/3749 (0.1%)
1	G	0.59	0/2785	0.97	6/3783 (0.2%)
1	H	0.64	0/2777	0.98	5/3774 (0.1%)
1	I	0.57	0/2759	0.97	6/3749 (0.2%)
1	J	0.66	1/2772 (0.0%)	0.99	6/3767 (0.2%)
1	K	0.61	0/2785	0.98	6/3782 (0.2%)
1	L	0.64	0/2770	0.95	4/3763 (0.1%)
1	M	0.62	0/2804	0.97	5/3810 (0.1%)
1	N	0.62	0/2782	0.96	4/3781 (0.1%)
1	O	0.61	0/2777	0.95	4/3774 (0.1%)
1	P	0.61	0/2792	0.98	4/3791 (0.1%)
1	Q	0.58	0/2775	0.93	2/3769 (0.1%)
1	R	0.56	0/2777	0.94	3/3772 (0.1%)
All	All	0.62	5/49979 (0.0%)	0.97	93/67894 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	4
1	C	0	5
1	D	0	7
1	E	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	6
1	G	0	5
1	H	0	6
1	I	0	5
1	J	0	3
1	K	0	5
1	L	0	3
1	M	0	3
1	N	0	3
1	O	0	6
1	P	0	4
1	Q	0	4
1	R	0	4
All	All	0	83

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	293	HIS	CG-CD2	-6.40	1.28	1.35
1	E	166	PRO	C-O	-5.64	1.20	1.24
1	E	224	GLN	C-O	-5.45	1.17	1.24
1	A	221	ARG	CZ-NH1	5.42	1.40	1.32
1	J	166	PRO	C-O	-5.07	1.20	1.24

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	179	LYS	CG-CD-CE	9.55	133.26	111.30
1	A	267	ARG	NE-CZ-NH1	-9.48	112.02	121.50
1	H	286	ARG	CG-CD-NE	-8.93	92.36	112.00
1	I	286	ARG	CG-CD-NE	-8.68	92.91	112.00
1	R	286	ARG	CG-CD-NE	-8.63	93.01	112.00
1	E	293	HIS	CB-CG-ND1	-8.62	109.77	122.70
1	I	275	GLN	CA-CB-CG	-8.60	96.91	114.10
1	C	286	ARG	CG-CD-NE	-8.44	93.43	112.00
1	O	286	ARG	CB-CG-CD	8.29	130.38	111.30
1	M	257	ARG	NE-CZ-NH1	-8.15	113.35	121.50
1	D	312	GLU	CB-CG-CD	8.07	126.33	112.60
1	N	145	ARG	NE-CZ-NH2	8.01	126.41	119.20
1	E	293	HIS	CB-CG-CD2	7.92	141.50	131.20
1	M	207	GLU	CB-CG-CD	-7.53	99.80	112.60
1	F	336	GLN	CB-CA-C	-7.43	96.56	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	336	GLN	CB-CA-C	-7.42	96.58	110.16
1	H	257	ARG	NE-CZ-NH1	-7.37	114.13	121.50
1	F	327	ARG	CA-CB-CG	7.27	128.64	114.10
1	I	257	ARG	NE-CZ-NH1	-7.24	114.26	121.50
1	E	336	GLN	N-CA-CB	-7.22	100.36	111.56
1	F	320	ARG	NE-CZ-NH1	-7.13	114.37	121.50
1	A	267	ARG	CD-NE-CZ	-7.10	114.46	124.40
1	G	336	GLN	CB-CA-C	-6.98	97.39	110.16
1	P	257	ARG	NE-CZ-NH1	-6.75	114.75	121.50
1	I	320	ARG	NE-CZ-NH1	-6.67	114.83	121.50
1	P	207	GLU	CB-CG-CD	-6.63	101.33	112.60
1	G	320	ARG	NE-CZ-NH1	-6.49	115.01	121.50
1	L	286	ARG	CB-CG-CD	6.48	126.21	111.30
1	E	257	ARG	NE-CZ-NH2	6.43	124.98	119.20
1	E	336	GLN	CB-CA-C	-6.39	98.74	110.62
1	B	234	GLU	CG-CD-OE1	-6.38	103.72	118.40
1	P	270	ARG	CB-CG-CD	6.30	125.80	111.30
1	A	257	ARG	NE-CZ-NH1	-6.28	115.22	121.50
1	G	257	ARG	NE-CZ-NH1	-6.21	115.29	121.50
1	D	222	MET	CG-SD-CE	6.20	114.55	100.90
1	A	257	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	D	257	ARG	NE-CZ-NH1	-6.20	115.30	121.50
1	J	336	GLN	N-CA-CB	-6.20	100.54	111.39
1	K	286	ARG	CB-CG-CD	6.20	125.55	111.30
1	R	257	ARG	NE-CZ-NH1	-6.20	115.31	121.50
1	G	336	GLN	N-CA-CB	-6.19	100.56	111.39
1	O	257	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	O	257	ARG	NE-CZ-NH2	5.94	124.55	119.20
1	D	336	GLN	N-CA-CB	-5.94	101.00	111.39
1	M	257	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	C	257	ARG	NE-CZ-NH1	-5.90	115.60	121.50
1	G	320	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	K	257	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	K	286	ARG	CA-CB-CG	5.86	125.81	114.10
1	B	257	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	N	234	GLU	CB-CG-CD	5.83	122.51	112.60
1	J	257	ARG	NE-CZ-NH1	-5.77	115.73	121.50
1	N	257	ARG	NE-CZ-NH1	-5.73	115.77	121.50
1	O	218	ARG	CB-CG-CD	5.70	124.42	111.30
1	H	331	ASP	CA-CB-CG	5.65	118.25	112.60
1	M	207	GLU	CA-CB-CG	5.63	125.37	114.10
1	R	257	ARG	NE-CZ-NH2	5.62	124.26	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	257	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	I	257	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	B	257	ARG	NE-CZ-NH1	-5.56	115.94	121.50
1	E	147	GLU	CB-CG-CD	5.54	122.01	112.60
1	A	222	MET	CG-SD-CE	5.50	113.01	100.90
1	E	293	HIS	CA-CB-CG	5.50	119.30	113.80
1	F	336	GLN	N-CA-CB	-5.49	101.78	111.39
1	F	257	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	E	206	GLU	CB-CG-CD	5.46	121.88	112.60
1	J	257	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	Q	257	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	J	206	GLU	CB-CG-CD	5.43	121.84	112.60
1	B	234	GLU	CG-CD-OE2	5.43	130.88	118.40
1	D	257	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	K	222	MET	CG-SD-CE	5.37	112.72	100.90
1	H	222	MET	CG-SD-CE	5.36	112.70	100.90
1	C	296	ASP	CA-CB-CG	5.36	117.96	112.60
1	D	218	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	I	152	LYS	CD-CE-NZ	5.33	128.96	111.90
1	Q	257	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	242	ARG	CG-CD-NE	-5.32	100.29	112.00
1	A	234	GLU	CB-CG-CD	5.32	121.65	112.60
1	E	313	GLU	CB-CG-CD	5.31	121.62	112.60
1	J	210	ARG	CG-CD-NE	-5.26	100.42	112.00
1	N	286	ARG	CB-CG-CD	5.26	123.39	111.30
1	P	206	GLU	CB-CG-CD	5.23	121.49	112.60
1	C	257	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	L	286	ARG	CA-CB-CG	5.21	124.53	114.10
1	C	313	GLU	CB-CG-CD	5.16	121.37	112.60
1	D	20	ARG	CB-CG-CD	5.15	123.14	111.30
1	H	242	ARG	CG-CD-NE	-5.12	100.73	112.00
1	G	197	LYS	CG-CD-CE	5.10	123.02	111.30
1	K	64	ARG	CG-CD-NE	-5.06	100.87	112.00
1	L	234	GLU	CA-CB-CG	5.06	124.22	114.10
1	M	152	LYS	CG-CD-CE	5.03	122.87	111.30
1	K	206	GLU	CB-CG-CD	5.02	121.14	112.60

There are no chirality outliers.

All (83) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	199	ARG	Sidechain
1	A	204	ARG	Sidechain
1	A	210	ARG	Sidechain
1	A	257	ARG	Sidechain
1	A	267	ARG	Sidechain
1	B	145	ARG	Sidechain
1	B	210	ARG	Sidechain
1	B	242	ARG	Sidechain
1	B	257	ARG	Sidechain
1	C	204	ARG	Sidechain
1	C	242	ARG	Sidechain
1	C	257	ARG	Sidechain
1	C	286	ARG	Sidechain
1	C	64	ARG	Sidechain
1	D	145	ARG	Sidechain
1	D	199	ARG	Sidechain
1	D	210	ARG	Sidechain
1	D	242	ARG	Sidechain
1	D	257	ARG	Sidechain
1	D	267	ARG	Sidechain
1	D	270	ARG	Sidechain
1	E	145	ARG	Sidechain
1	E	199	ARG	Sidechain
1	E	257	ARG	Sidechain
1	E	66	ARG	Sidechain
1	F	145	ARG	Sidechain
1	F	199	ARG	Sidechain
1	F	257	ARG	Sidechain
1	F	267	ARG	Sidechain
1	F	270	ARG	Sidechain
1	F	320	ARG	Sidechain
1	G	-1	ARG	Sidechain
1	G	145	ARG	Sidechain
1	G	257	ARG	Sidechain
1	G	286	ARG	Sidechain
1	G	320	ARG	Sidechain
1	H	145	ARG	Sidechain
1	H	199	ARG	Sidechain
1	H	210	ARG	Sidechain
1	H	257	ARG	Sidechain
1	H	267	ARG	Sidechain
1	H	286	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	I	145	ARG	Sidechain
1	I	210	ARG	Sidechain
1	I	257	ARG	Sidechain
1	I	267	ARG	Sidechain
1	I	320	ARG	Sidechain
1	J	145	ARG	Sidechain
1	J	242	ARG	Sidechain
1	J	257	ARG	Sidechain
1	K	145	ARG	Sidechain
1	K	199	ARG	Sidechain
1	K	210	ARG	Sidechain
1	K	242	ARG	Sidechain
1	K	257	ARG	Sidechain
1	L	145	ARG	Sidechain
1	L	242	ARG	Sidechain
1	L	257	ARG	Sidechain
1	M	145	ARG	Sidechain
1	M	242	ARG	Sidechain
1	M	267	ARG	Sidechain
1	N	204	ARG	Sidechain
1	N	257	ARG	Sidechain
1	N	286	ARG	Sidechain
1	O	145	ARG	Sidechain
1	O	218	ARG	Sidechain
1	O	257	ARG	Sidechain
1	O	267	ARG	Sidechain
1	O	270	ARG	Sidechain
1	O	286	ARG	Sidechain
1	P	145	ARG	Sidechain
1	P	199	ARG	Sidechain
1	P	242	ARG	Sidechain
1	P	257	ARG	Sidechain
1	Q	145	ARG	Sidechain
1	Q	257	ARG	Sidechain
1	Q	267	ARG	Sidechain
1	Q	270	ARG	Sidechain
1	R	145	ARG	Sidechain
1	R	210	ARG	Sidechain
1	R	242	ARG	Sidechain
1	R	257	ARG	Sidechain

## 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	2697	2646	2625	11	0
1	B	2682	2631	2617	16	0
1	C	2679	2629	2616	13	0
1	D	2684	2632	2610	8	0
1	E	2694	2644	2624	14	1
1	F	2680	2629	2619	15	0
1	G	2702	2653	2638	14	0
1	H	2691	2639	2617	11	0
1	I	2680	2629	2619	11	0
1	J	2686	2635	2615	16	1
1	K	2699	2648	2626	18	0
1	L	2684	2632	2610	21	0
1	M	2708	2659	2629	16	0
1	N	2696	2643	2619	17	0
1	O	2691	2639	2617	13	0
1	P	2704	2655	2634	11	0
1	Q	2691	2638	2620	16	0
1	R	2688	2635	2615	18	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
3	A	132	0	0	0	0
3	B	90	0	0	2	0
3	C	133	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	137	0	0	1	0
3	E	124	0	0	3	0
3	F	73	0	0	1	0
3	G	160	0	0	1	0
3	H	172	0	0	2	0
3	I	86	0	0	1	0
3	J	133	0	0	2	0
3	K	153	0	0	3	0
3	L	136	0	0	8	0
3	M	159	0	0	1	0
3	N	160	0	0	3	0
3	O	153	0	0	3	0
3	P	151	0	0	2	0
3	Q	112	0	0	7	0
3	R	110	0	0	6	0
All	All	50826	47516	47170	225	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (225) 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:L:243:GLU:OE2	3:L:501:HOH:O	1.96	0.84
1:L:243:GLU:HG2	3:L:501:HOH:O	1.84	0.78
1:R:36:ALA:HB3	3:R:563:HOH:O	1.81	0.78
1:L:217:ARG:HG2	3:L:631:HOH:O	1.85	0.76
1:B:36:ALA:HB3	3:B:416:HOH:O	1.86	0.74
1:Q:197:LYS:HG2	3:Q:588:HOH:O	1.87	0.73
1:N:235:GLN:HG2	3:N:642:HOH:O	1.89	0.72
1:O:217:ARG:HD3	3:O:642:HOH:O	1.89	0.71
1:Q:197:LYS:CG	3:Q:588:HOH:O	2.38	0.70
1:N:265:MET:HE3	3:O:584:HOH:O	1.90	0.70
1:M:270:ARG:CZ	1:R:270:ARG:HD3	2.21	0.70
1:Q:270:ARG:HH22	1:P:273:HIS:CE1	2.10	0.69
1:C:36:ALA:HB3	3:C:519:HOH:O	1.93	0.69
1:G:267:ARG:HD3	3:G:652:HOH:O	1.94	0.68
1:L:243:GLU:CG	3:L:501:HOH:O	2.41	0.66
1:I:232:THR:HG23	1:I:235:GLN:H	1.61	0.64
1:R:197:LYS:HD3	3:R:513:HOH:O	1.98	0.64
1:R:163:ASP:HA	3:R:501:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:270:ARG:HE	1:R:270:ARG:HH11	1.48	0.60
1:N:257:ARG:HD3	1:O:255:ASP:OD2	2.01	0.59
1:Q:197:LYS:CD	3:Q:588:HOH:O	2.50	0.59
1:F:337:ALA:C	3:F:464:HOH:O	2.44	0.59
1:J:270:ARG:NH1	1:K:270:ARG:NH1	2.50	0.59
1:A:255:ASP:OD2	1:F:257:ARG:HD3	2.03	0.58
1:G:270:ARG:HH22	1:L:273:HIS:CE1	2.22	0.58
1:I:331:ASP:HB2	3:I:576:HOH:O	2.04	0.58
1:G:270:ARG:NH1	1:L:270:ARG:NH1	2.51	0.58
1:B:275[B]:GLN:O	1:B:275[B]:GLN:HG3	2.04	0.57
1:J:195:ASP:OD1	1:J:293:HIS:CE1	2.58	0.56
1:E:337:ALA:C	3:E:603:HOH:O	2.47	0.56
1:G:257:ARG:HD3	1:L:255:ASP:OD2	2.06	0.56
1:K:64:ARG:NH1	3:K:501:HOH:O	2.37	0.56
1:H:257:ARG:HD3	1:I:255:ASP:OD2	2.06	0.55
1:M:270:ARG:CZ	1:R:270:ARG:CD	2.84	0.55
1:A:273:HIS:HE2	1:F:270:ARG:HH22	1.53	0.54
1:R:197:LYS:CD	3:R:513:HOH:O	2.53	0.54
1:P:267:ARG:HD2	3:P:627:HOH:O	2.08	0.54
1:N:255:ASP:OD2	1:O:257:ARG:HD3	2.07	0.54
1:Q:197:LYS:HD3	3:Q:588:HOH:O	2.07	0.53
1:J:257:ARG:HD3	1:K:255:ASP:OD2	2.08	0.53
1:K:210:ARG:HH12	1:K:216:PRO:HD2	1.72	0.53
1:M:255:ASP:OD2	1:R:257:ARG:HD3	2.08	0.53
1:B:275[B]:GLN:O	1:B:275[B]:GLN:CG	2.58	0.52
1:M:270:ARG:NH2	1:R:270:ARG:CD	2.72	0.52
1:B:257:ARG:HD3	1:C:255:ASP:OD2	2.09	0.52
1:Q:257:ARG:HD3	1:P:255:ASP:OD2	2.09	0.52
1:M:179:LYS:HE3	1:M:207:GLU:HG3	1.92	0.51
1:H:204:ARG:NH2	3:H:504:HOH:O	2.42	0.51
1:M:270:ARG:NH2	1:R:270:ARG:HD2	2.25	0.51
1:H:255:ASP:OD2	1:I:257:ARG:HD3	2.11	0.51
1:E:25:ALA:HB1	1:E:30:PHE:CD2	2.46	0.50
1:A:257:ARG:HD3	1:F:255:ASP:OD2	2.11	0.50
1:J:142:LYS:CE	3:J:626:HOH:O	2.58	0.50
1:L:293:HIS:HB2	1:O:275:GLN:HE22	1.77	0.49
1:N:204:ARG:HA	1:N:204:ARG:HH11	1.76	0.49
1:B:255:ASP:OD2	1:C:257:ARG:HD3	2.11	0.49
3:D:549:HOH:O	1:E:270:ARG:HD2	2.12	0.48
1:B:270:ARG:CG	1:B:270:ARG:HH11	2.26	0.48
1:R:76:GLY:O	1:R:116:ARG:NH2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ARG:HD3	1:E:255:ASP:OD2	2.13	0.48
1:K:286:ARG:HH11	1:K:286:ARG:HG3	1.78	0.48
1:M:231[A]:GLU:CD	1:M:231[A]:GLU:H	2.22	0.48
1:I:171:GLY:HA2	1:I:189:LEU:O	2.15	0.47
1:A:76:GLY:O	1:A:116:ARG:NH2	2.46	0.47
1:G:255:ASP:OD2	1:L:257:ARG:HD3	2.14	0.47
1:R:171:GLY:HA2	1:R:189:LEU:O	2.14	0.47
1:L:125:ILE:HD11	3:L:598:HOH:O	2.15	0.47
1:O:76:GLY:O	1:O:116:ARG:NH2	2.45	0.47
1:J:171:GLY:HA2	1:J:189:LEU:O	2.15	0.47
1:P:171:GLY:HA2	1:P:189:LEU:O	2.15	0.47
1:B:171:GLY:HA2	1:B:189:LEU:O	2.14	0.47
1:N:171:GLY:HA2	1:N:189:LEU:O	2.14	0.47
1:O:171:GLY:HA2	1:O:189:LEU:O	2.14	0.47
1:D:255:ASP:OD2	1:E:257:ARG:HD3	2.14	0.47
1:L:45:GLU:HB3	3:L:532:HOH:O	2.14	0.47
1:P:76:GLY:O	1:P:116:ARG:NH2	2.47	0.47
1:G:171:GLY:HA2	1:G:189:LEU:O	2.15	0.47
1:Q:255:ASP:OD2	1:P:257:ARG:HD3	2.14	0.47
1:A:171:GLY:HA2	1:A:189:LEU:O	2.16	0.46
1:C:171:GLY:HA2	1:C:189:LEU:O	2.15	0.46
1:D:76:GLY:O	1:D:116:ARG:NH2	2.47	0.46
1:E:76:GLY:O	1:E:116:ARG:NH2	2.46	0.46
1:N:76:GLY:O	1:N:116:ARG:NH2	2.47	0.46
1:H:142:LYS:HE3	3:H:624:HOH:O	2.15	0.46
1:I:76:GLY:O	1:I:116:ARG:NH2	2.46	0.46
1:J:255:ASP:OD2	1:K:257:ARG:HD3	2.15	0.46
1:K:171:GLY:HA2	1:K:189:LEU:O	2.15	0.46
1:M:171:GLY:HA2	1:M:189:LEU:O	2.16	0.46
1:F:171:GLY:HA2	1:F:189:LEU:O	2.15	0.46
1:L:171:GLY:HA2	1:L:189:LEU:O	2.15	0.46
1:Q:76:GLY:O	1:Q:116:ARG:NH2	2.47	0.46
1:Q:171:GLY:HA2	1:Q:189:LEU:O	2.15	0.46
1:H:76:GLY:O	1:H:116:ARG:NH2	2.46	0.46
1:M:142:LYS:HE3	3:M:601:HOH:O	2.15	0.46
1:E:171:GLY:HA2	1:E:189:LEU:O	2.16	0.45
1:D:171:GLY:HA2	1:D:189:LEU:O	2.16	0.45
1:Q:125:ILE:HD11	3:Q:561:HOH:O	2.16	0.45
1:B:270:ARG:HH11	1:B:270:ARG:HG2	1.81	0.45
1:G:76:GLY:O	1:G:116:ARG:NH2	2.46	0.45
1:J:195:ASP:OD1	1:J:293:HIS:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ALA:CB	3:B:416:HOH:O	2.55	0.45
1:F:286:ARG:HH11	1:F:286:ARG:HG2	1.81	0.45
1:R:145:ARG:HD3	3:R:605:HOH:O	2.15	0.45
1:H:171:GLY:HA2	1:H:189:LEU:O	2.16	0.45
1:N:338:MET:N	3:N:501:HOH:O	2.27	0.45
1:K:338:MET:C	3:K:513:HOH:O	2.59	0.45
1:J:76:GLY:O	1:J:116:ARG:NH2	2.45	0.45
1:N:270:ARG:NH1	3:N:503:HOH:O	2.40	0.44
1:E:72:THR:O	1:E:103:ILE:HA	2.18	0.44
1:J:72[B]:THR:O	1:J:103:ILE:HA	2.18	0.44
1:L:199:ARG:HD3	1:N:270:ARG:HD3	1.99	0.44
1:O:154:GLU:O	1:O:155:SER:C	2.60	0.44
1:J:72[A]:THR:O	1:J:103:ILE:HA	2.18	0.44
1:H:72[B]:THR:O	1:H:103:ILE:HA	2.18	0.44
1:Q:154:GLU:O	1:Q:155:SER:C	2.60	0.44
1:H:72[A]:THR:O	1:H:103:ILE:HA	2.18	0.44
1:R:154:GLU:O	1:R:155:SER:C	2.61	0.44
1:O:72[B]:THR:O	1:O:103:ILE:HA	2.18	0.44
1:L:72:THR:O	1:L:103:ILE:HA	2.18	0.44
1:R:336:GLN:O	1:R:337:ALA:C	2.61	0.44
1:C:36:ALA:CB	3:C:519:HOH:O	2.61	0.43
1:J:154:GLU:O	1:J:155:SER:C	2.61	0.43
1:A:72:THR:O	1:A:103:ILE:HA	2.18	0.43
1:C:72:THR:O	1:C:103:ILE:HA	2.19	0.43
1:F:169:ILE:HG21	1:F:222:MET:HE2	2.01	0.43
1:K:76:GLY:O	1:K:116:ARG:NH2	2.46	0.43
1:C:154:GLU:O	1:C:155:SER:C	2.61	0.43
1:I:72[A]:THR:O	1:I:103:ILE:HA	2.19	0.43
1:I:72[B]:THR:O	1:I:103:ILE:HA	2.19	0.43
1:J:273:HIS:CE1	1:K:270:ARG:HH22	2.37	0.43
1:M:154:GLU:O	1:M:155:SER:C	2.61	0.43
1:G:72[A]:THR:O	1:G:103:ILE:HA	2.19	0.43
1:G:72[B]:THR:O	1:G:103:ILE:HA	2.19	0.43
1:H:154:GLU:O	1:H:155:SER:C	2.61	0.43
1:J:142:LYS:HE3	3:J:626:HOH:O	2.19	0.43
1:K:154:GLU:O	1:K:155:SER:C	2.61	0.43
1:M:76:GLY:O	1:M:116:ARG:NH2	2.46	0.43
1:B:76:GLY:O	1:B:116:ARG:NH2	2.46	0.43
1:F:76:GLY:O	1:F:116:ARG:NH2	2.46	0.43
1:J:34:LEU:C	1:J:34:LEU:HD23	2.43	0.43
1:L:154:GLU:O	1:L:155:SER:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:169:ILE:HG21	1:N:222:MET:HE2	2.00	0.43
1:B:154:GLU:O	1:B:155:SER:C	2.61	0.43
1:E:34:LEU:C	1:E:34:LEU:HD23	2.43	0.43
1:N:154:GLU:O	1:N:155:SER:C	2.61	0.43
1:N:72[B]:THR:O	1:N:103:ILE:HA	2.18	0.43
1:P:267:ARG:HD3	3:P:641:HOH:O	2.19	0.43
1:A:154:GLU:O	1:A:155:SER:C	2.61	0.43
1:E:2:SER:HA	3:E:548:HOH:O	2.18	0.43
1:G:154:GLU:O	1:G:155:SER:C	2.61	0.43
1:N:72[A]:THR:O	1:N:103:ILE:HA	2.19	0.43
1:B:72:THR:O	1:B:103:ILE:HA	2.19	0.43
1:F:72[A]:THR:O	1:F:103:ILE:HA	2.19	0.43
1:K:210:ARG:NH1	1:K:216:PRO:HD2	2.34	0.43
1:P:72:THR:O	1:P:103:ILE:HA	2.19	0.43
1:C:34:LEU:C	1:C:34:LEU:HD23	2.44	0.43
1:E:142:LYS:HE3	3:E:531:HOH:O	2.19	0.43
1:E:154:GLU:O	1:E:155:SER:C	2.61	0.43
1:F:154:GLU:O	1:F:155:SER:C	2.61	0.43
1:O:34:LEU:C	1:O:34:LEU:HD23	2.44	0.43
1:P:154:GLU:O	1:P:155:SER:C	2.61	0.43
1:C:169:ILE:HG21	1:C:222:MET:HE2	2.01	0.42
1:I:34:LEU:C	1:I:34:LEU:HD23	2.44	0.42
1:R:34:LEU:C	1:R:34:LEU:HD23	2.44	0.42
1:K:72:THR:O	1:K:103:ILE:HA	2.19	0.42
1:K:214:LYS:HE3	3:K:584:HOH:O	2.18	0.42
1:L:234:GLU:HB2	3:L:596:HOH:O	2.18	0.42
1:M:72[B]:THR:O	1:M:103:ILE:HA	2.19	0.42
1:Q:169:ILE:HG21	1:Q:222:MET:HE2	2.01	0.42
1:B:270:ARG:HH11	1:B:270:ARG:HB3	1.84	0.42
1:Q:72:THR:O	1:Q:103:ILE:HA	2.19	0.42
1:D:72:THR:O	1:D:103:ILE:HA	2.19	0.42
1:F:72[B]:THR:O	1:F:103:ILE:HA	2.19	0.42
1:R:72:THR:O	1:R:103:ILE:HA	2.18	0.42
1:D:154:GLU:O	1:D:155:SER:C	2.61	0.42
1:K:113:ILE:O	1:L:153:VAL:HA	2.19	0.42
1:Q:270:ARG:NH1	3:Q:508:HOH:O	2.51	0.42
1:B:34:LEU:HD23	1:B:34:LEU:C	2.44	0.42
1:G:270:ARG:NH1	1:L:270:ARG:HH11	2.17	0.42
1:M:72[A]:THR:O	1:M:103:ILE:HA	2.19	0.42
1:N:34:LEU:C	1:N:34:LEU:HD23	2.45	0.42
1:C:76:GLY:O	1:C:116:ARG:NH2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:LEU:C	1:G:34:LEU:HD23	2.45	0.42
1:M:34:LEU:C	1:M:34:LEU:HD23	2.44	0.42
1:Q:34:LEU:C	1:Q:34:LEU:HD23	2.45	0.42
1:A:204:ARG:HA	1:A:204:ARG:HD2	1.50	0.42
1:I:154:GLU:O	1:I:155:SER:C	2.60	0.42
1:K:286:ARG:HG3	1:K:286:ARG:NH1	2.33	0.42
1:F:34:LEU:C	1:F:34:LEU:HD23	2.45	0.42
1:O:72[A]:THR:O	1:O:103:ILE:HA	2.19	0.42
1:J:72[B]:THR:CG2	1:J:103:ILE:HG22	2.50	0.42
1:J:100:TRP:CH2	1:J:222:MET:HE1	2.55	0.42
1:D:34:LEU:C	1:D:34:LEU:HD23	2.45	0.41
1:E:100:TRP:CH2	1:E:222:MET:HE1	2.56	0.41
1:G:169:ILE:HG21	1:G:222:MET:HE2	2.03	0.41
1:H:34:LEU:C	1:H:34:LEU:HD23	2.45	0.41
1:K:34:LEU:C	1:K:34:LEU:HD23	2.45	0.41
1:R:125:ILE:HD11	3:R:573:HOH:O	2.20	0.41
1:P:34:LEU:HB2	1:P:303:TYR:CD2	2.55	0.41
1:A:34:LEU:C	1:A:34:LEU:HD23	2.45	0.41
1:L:34:LEU:C	1:L:34:LEU:HD23	2.45	0.41
1:L:76:GLY:O	1:L:116:ARG:NH2	2.47	0.41
1:P:34:LEU:C	1:P:34:LEU:HD23	2.45	0.41
1:Q:316:ARG:HD2	3:Q:608:HOH:O	2.20	0.41
1:F:72[B]:THR:CG2	1:F:103:ILE:HG22	2.50	0.41
1:G:72[B]:THR:CG2	1:G:103:ILE:HG22	2.51	0.41
1:L:169:ILE:HG21	1:L:222:MET:HE2	2.02	0.41
1:E:169:ILE:HG21	1:E:222:MET:HE2	2.03	0.41
1:K:180:LYS:HE3	1:K:183:GLN:OE1	2.21	0.41
1:B:270:ARG:HH21	1:C:270:ARG:NH2	2.19	0.41
3:L:610:HOH:O	1:O:272:GLU:HG2	2.21	0.41
1:M:169:ILE:HG21	1:M:222:MET:HE2	2.03	0.41
1:N:265:MET:CE	3:O:584:HOH:O	2.60	0.41
1:N:337:ALA:C	1:N:339:SER:H	2.29	0.41
1:B:169:ILE:HG21	1:B:222:MET:HE2	2.03	0.40
1:C:125:ILE:HD11	3:C:605:HOH:O	2.19	0.40
1:O:286:ARG:NH1	1:O:286:ARG:HG3	2.36	0.40
1:C:164:VAL:HA	1:C:165(A):PRO:HD3	1.95	0.40
1:F:144:ILE:C	1:F:144:ILE:HD12	2.47	0.40
1:O:169:ILE:HG21	1:O:222:MET:HE2	2.02	0.40
1:A:273:HIS:CE1	1:F:270:ARG:HH22	2.39	0.40
1:D:34:LEU:HB2	1:D:303:TYR:CD2	2.57	0.40
1:H:72[B]:THR:CG2	1:H:103:ILE:HG22	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:169:ILE:HG21	1:I:222:MET:HE2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:ASP:OD2	1:J:296:ASP:OD2[4_455]	2.10	0.10

## 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	340/380 (90%)	331 (97%)	8 (2%)	1 (0%)	36	41
1	B	337/380 (89%)	329 (98%)	7 (2%)	1 (0%)	36	41
1	C	337/380 (89%)	327 (97%)	9 (3%)	1 (0%)	36	41
1	D	338/380 (89%)	328 (97%)	9 (3%)	1 (0%)	36	41
1	E	339/380 (89%)	331 (98%)	7 (2%)	1 (0%)	36	41
1	F	336/380 (88%)	329 (98%)	6 (2%)	1 (0%)	36	41
1	G	340/380 (90%)	332 (98%)	7 (2%)	1 (0%)	36	41
1	H	339/380 (89%)	330 (97%)	8 (2%)	1 (0%)	36	41
1	I	336/380 (88%)	328 (98%)	7 (2%)	1 (0%)	36	41
1	J	338/380 (89%)	330 (98%)	7 (2%)	1 (0%)	36	41
1	K	340/380 (90%)	332 (98%)	7 (2%)	1 (0%)	36	41
1	L	338/380 (89%)	331 (98%)	6 (2%)	1 (0%)	36	41
1	M	342/380 (90%)	333 (97%)	8 (2%)	1 (0%)	36	41
1	N	340/380 (90%)	330 (97%)	9 (3%)	1 (0%)	36	41
1	O	339/380 (89%)	331 (98%)	7 (2%)	1 (0%)	36	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	341/380 (90%)	333 (98%)	7 (2%)	1 (0%)	36	41
1	Q	339/380 (89%)	331 (98%)	7 (2%)	1 (0%)	36	41
1	R	339/380 (89%)	331 (98%)	7 (2%)	1 (0%)	36	41
All	All	6098/6840 (89%)	5947 (98%)	133 (2%)	18 (0%)	36	41

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	B	49	SER
1	C	49	SER
1	D	49	SER
1	E	49	SER
1	F	49	SER
1	G	49	SER
1	H	49	SER
1	I	49	SER
1	J	49	SER
1	K	49	SER
1	L	49	SER
1	M	49	SER
1	N	49	SER
1	Q	49	SER
1	R	49	SER
1	O	49	SER
1	P	49	SER

### 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	273/302 (90%)	270 (99%)	3 (1%)	65	78
1	B	271/302 (90%)	268 (99%)	3 (1%)	65	78
1	C	271/302 (90%)	269 (99%)	2 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	272/302 (90%)	266 (98%)	6 (2%)	45	59
1	E	273/302 (90%)	268 (98%)	5 (2%)	51	66
1	F	271/302 (90%)	267 (98%)	4 (2%)	57	71
1	G	273/302 (90%)	269 (98%)	4 (2%)	57	71
1	H	273/302 (90%)	269 (98%)	4 (2%)	57	71
1	I	271/302 (90%)	265 (98%)	6 (2%)	45	59
1	J	273/302 (90%)	267 (98%)	6 (2%)	45	59
1	K	273/302 (90%)	269 (98%)	4 (2%)	57	71
1	L	272/302 (90%)	269 (99%)	3 (1%)	65	78
1	M	276/302 (91%)	274 (99%)	2 (1%)	76	86
1	N	273/302 (90%)	267 (98%)	6 (2%)	45	59
1	O	273/302 (90%)	268 (98%)	5 (2%)	51	66
1	P	273/302 (90%)	270 (99%)	3 (1%)	65	78
1	Q	271/302 (90%)	269 (99%)	2 (1%)	76	86
1	R	273/302 (90%)	271 (99%)	2 (1%)	76	86
All	All	4905/5436 (90%)	4835 (99%)	70 (1%)	59	73

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	ARG
1	A	222	MET
1	A	286	ARG
1	B	180	LYS
1	B	270	ARG
1	B	286	ARG
1	C	64	ARG
1	C	286	ARG
1	D	20	ARG
1	D	49	SER
1	D	180	LYS
1	D	218	ARG
1	D	222	MET
1	D	286	ARG
1	E	-1	ARG
1	E	197	LYS
1	E	257	ARG

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Mol	Chain	Res	Type
1	E	286	ARG
1	E	293	HIS
1	F	49	SER
1	F	180	LYS
1	F	234	GLU
1	F	286	ARG
1	G	-1	ARG
1	G	180	LYS
1	G	197	LYS
1	G	218	ARG
1	H	49	SER
1	H	222	MET
1	H	235	GLN
1	H	286	ARG
1	I	152	LYS
1	I	180	LYS
1	I	235	GLN
1	I	267	ARG
1	I	275	GLN
1	I	286	ARG
1	J	152	LYS
1	J	218	ARG
1	J	267	ARG
1	J	272	GLU
1	J	286	ARG
1	J	293	HIS
1	K	20	ARG
1	K	180	LYS
1	K	257	ARG
1	K	267	ARG
1	L	179	LYS
1	L	180	LYS
1	L	197	LYS
1	M	235	GLN
1	M	257	ARG
1	N	1	SER
1	N	180	LYS
1	N	197	LYS
1	N	204	ARG
1	N	267	ARG
1	N	286	ARG
1	Q	180	LYS

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Mol	Chain	Res	Type
1	Q	286	ARG
1	R	218	ARG
1	R	286	ARG
1	O	180	LYS
1	O	197	LYS
1	O	218	ARG
1	O	257	ARG
1	O	267	ARG
1	P	-1	ARG
1	P	64	ARG
1	P	180	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	GLN
1	B	235	GLN
1	C	23	GLN
1	D	224	GLN
1	D	235	GLN
1	E	224	GLN
1	G	235	GLN
1	H	224	GLN
1	I	235	GLN
1	J	293	HIS
1	K	224	GLN
1	L	336	GLN
1	M	224	GLN
1	M	336	GLN
1	N	235	GLN
1	Q	239	ASN
1	O	224	GLN
1	O	235	GLN
1	O	275	GLN
1	P	224	GLN
1	P	336	GLN

### 5.3.3 RNA ⓘ

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 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 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	339/380 (89%)	-0.39	3 (0%) 81 79	24, 38, 62, 90	3 (0%)
1	B	337/380 (88%)	-0.14	6 (1%) 67 65	29, 47, 77, 104	1 (0%)
1	C	338/380 (88%)	-0.36	2 (0%) 85 84	23, 41, 64, 107	1 (0%)
1	D	338/380 (88%)	-0.37	1 (0%) 90 89	17, 40, 64, 90	1 (0%)
1	E	339/380 (89%)	-0.19	0 100 100	21, 46, 70, 117	1 (0%)
1	F	337/380 (88%)	-0.11	0 100 100	21, 52, 81, 100	1 (0%)
1	G	340/380 (89%)	-0.50	2 (0%) 85 84	16, 36, 66, 111	2 (0%)
1	H	338/380 (88%)	-0.57	2 (0%) 85 84	15, 35, 57, 88	2 (0%)
1	I	337/380 (88%)	-0.11	2 (0%) 85 84	21, 50, 79, 101	1 (0%)
1	J	337/380 (88%)	-0.31	1 (0%) 90 89	20, 44, 68, 95	2 (0%)
1	K	340/380 (89%)	-0.58	1 (0%) 90 89	15, 35, 60, 108	1 (0%)
1	L	338/380 (88%)	-0.42	3 (0%) 81 79	16, 35, 60, 85	1 (0%)
1	M	338/380 (88%)	-0.60	2 (0%) 85 84	15, 34, 57, 89	4 (1%)
1	N	339/380 (89%)	-0.50	2 (0%) 85 84	16, 35, 60, 89	2 (0%)
1	O	338/380 (88%)	-0.43	2 (0%) 85 84	16, 39, 65, 90	2 (0%)
1	P	340/380 (89%)	-0.52	2 (0%) 85 84	21, 36, 60, 103	2 (0%)
1	Q	339/380 (89%)	-0.23	4 (1%) 76 75	27, 45, 73, 102	1 (0%)
1	R	338/380 (88%)	-0.19	3 (0%) 81 79	23, 47, 77, 105	2 (0%)
All	All	6090/6840 (89%)	-0.36	38 (0%) 85 84	15, 41, 70, 117	30 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	338	MET	9.0
1	L	338	MET	8.6
1	C	0	GLY	7.4

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Mol	Chain	Res	Type	RSRZ
1	M	338	MET	6.6
1	P	338	MET	6.5
1	D	338	MET	5.6
1	G	338	MET	5.4
1	A	338	MET	5.1
1	N	339	SER	4.7
1	K	338	MET	4.5
1	Q	338	MET	4.3
1	R	337	ALA	4.3
1	N	338	MET	4.2
1	H	338	MET	3.9
1	A	0	GLY	3.7
1	C	337	ALA	3.5
1	Q	163	ASP	3.2
1	B	1	SER	3.1
1	O	1	SER	3.1
1	R	0	GLY	3.0
1	M	331	ASP	2.9
1	B	337	ALA	2.9
1	L	1	SER	2.8
1	I	337	ALA	2.7
1	R	331[A]	ASP	2.6
1	I	1	SER	2.6
1	B	330	ALA	2.6
1	H	331	ASP	2.5
1	B	275[A]	GLN	2.5
1	P	235[A]	GLN	2.4
1	Q	0	GLY	2.4
1	Q	1	SER	2.4
1	B	325	HIS	2.2
1	G	197	LYS	2.2
1	J	337	ALA	2.2
1	B	234	GLU	2.1
1	L	331	ASP	2.1
1	A	218	ARG	2.1

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

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



### 6.3 Carbohydrates [i](#)

There are no 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	K	401	1/1	0.87	0.17	83,83,83,83	0
2	CL	L	401	1/1	0.87	0.23	80,80,80,80	0
2	CL	E	401	1/1	0.88	0.21	89,89,89,89	0
2	CL	H	401	1/1	0.89	0.15	80,80,80,80	0
2	CL	J	401	1/1	0.89	0.16	94,94,94,94	0
2	CL	C	401	1/1	0.92	0.14	78,78,78,78	0
2	CL	P	401	1/1	0.92	0.15	71,71,71,71	0
2	CL	M	401	1/1	0.93	0.13	67,67,67,67	0
2	CL	A	401	1/1	0.93	0.11	73,73,73,73	0
2	CL	I	401	1/1	0.94	0.12	84,84,84,84	0
2	CL	Q	401	1/1	0.95	0.13	83,83,83,83	0
2	CL	R	401	1/1	0.95	0.11	82,82,82,82	0
2	CL	D	401	1/1	0.95	0.09	84,84,84,84	0
2	CL	N	401	1/1	0.96	0.13	75,75,75,75	0
2	CL	O	401	1/1	0.96	0.10	77,77,77,77	0
2	CL	G	401	1/1	0.96	0.09	76,76,76,76	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.