



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 05:22 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
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

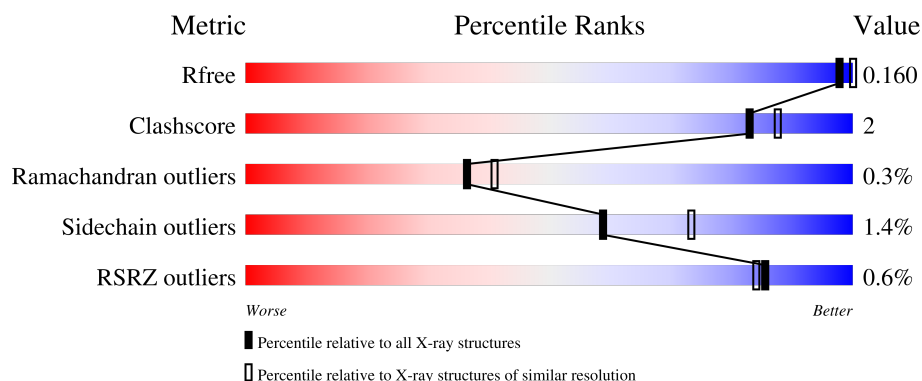
1 Overall quality at a glance

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.






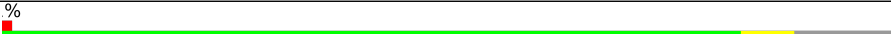

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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 ≥ 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 83% 5% .. 11% </div> </div>
1	B	380	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 2% 83% 6% 11% </div> </div>
1	C	380	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 82% 6% • 11% </div> </div>
1	D	380	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 82% 6% • 11% </div> </div>
1	E	380	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 80% 9% 11% </div> </div>

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

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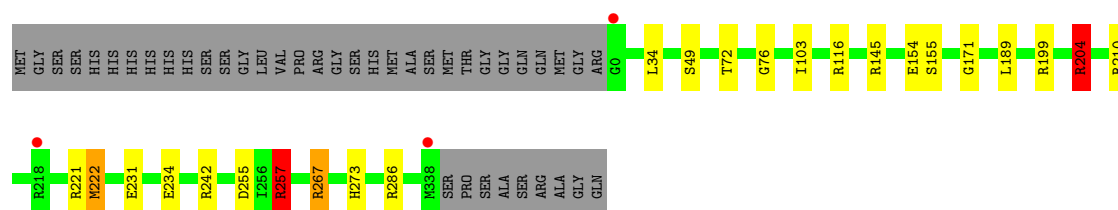
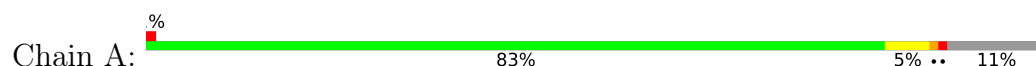
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	160	Total 160	O 160	0	0
3	H	172	Total 172	O 172	0	0
3	I	85	Total 86	O 86	0	1
3	J	133	Total 133	O 133	0	0
3	K	152	Total 153	O 153	0	1
3	L	136	Total 136	O 136	0	0
3	M	159	Total 159	O 159	0	0
3	N	160	Total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

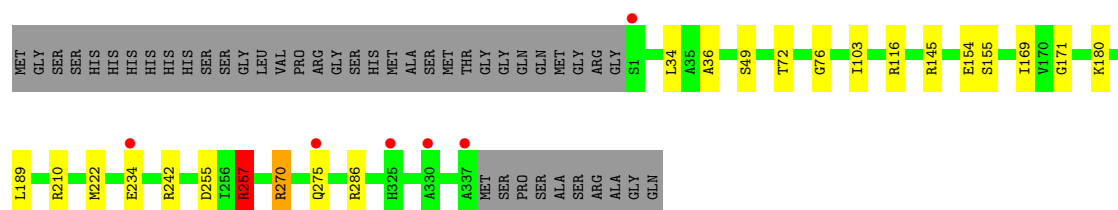
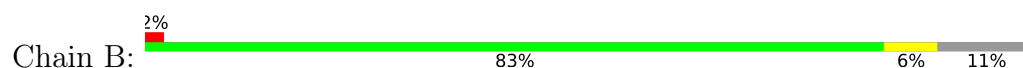
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

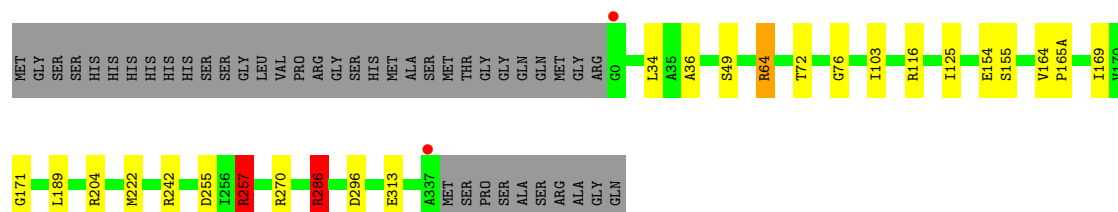
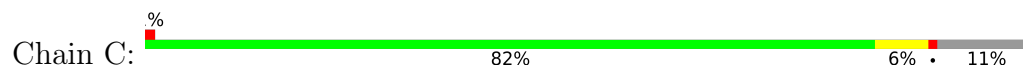
- Molecule 1: Luciferase family protein



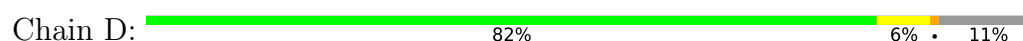
- Molecule 1: Luciferase family protein

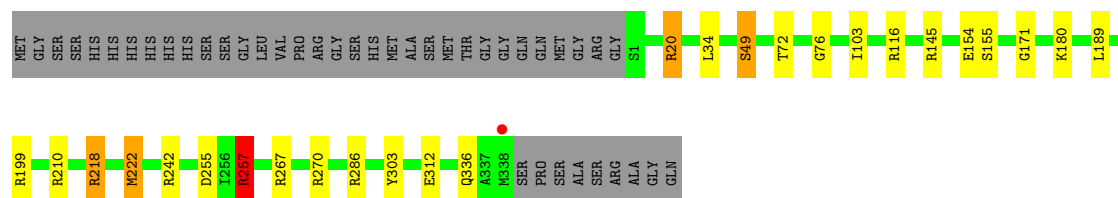


- Molecule 1: Luciferase family protein



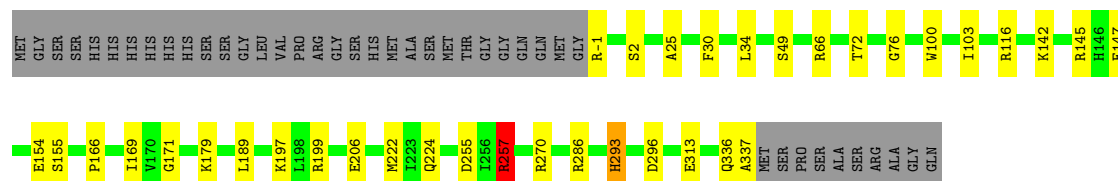
- Molecule 1: Luciferase family protein





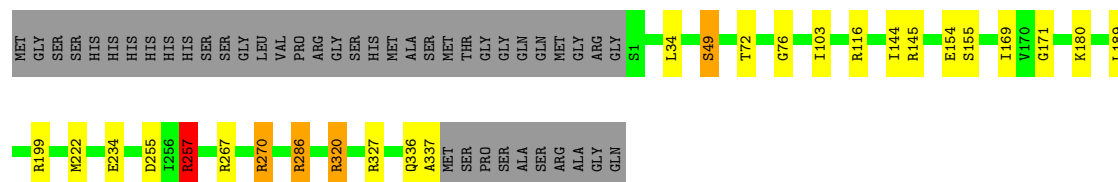
- Molecule 1: Luciferase family protein

Chain E: 80% 9% 11%



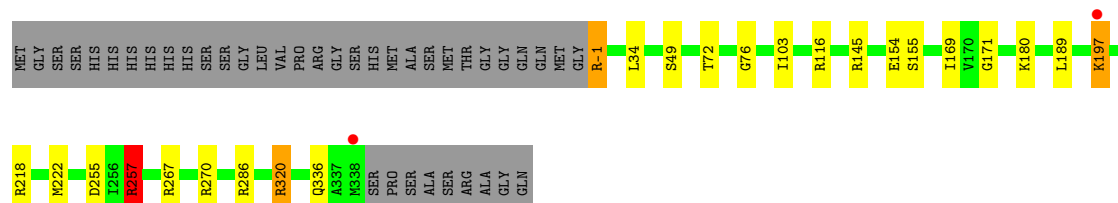
- Molecule 1: Luciferase family protein

Chain F: 82% 6% 11%



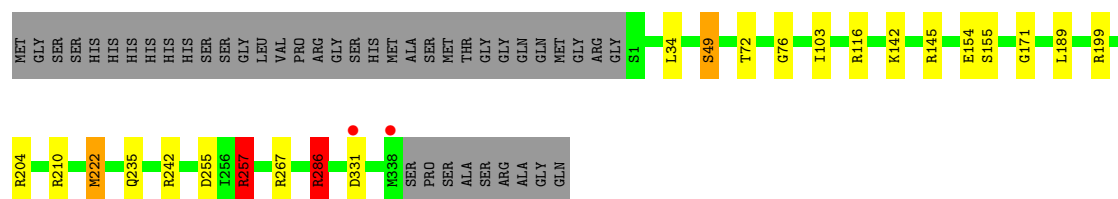
- Molecule 1: Luciferase family protein

Chain G: 83% 5% 11%

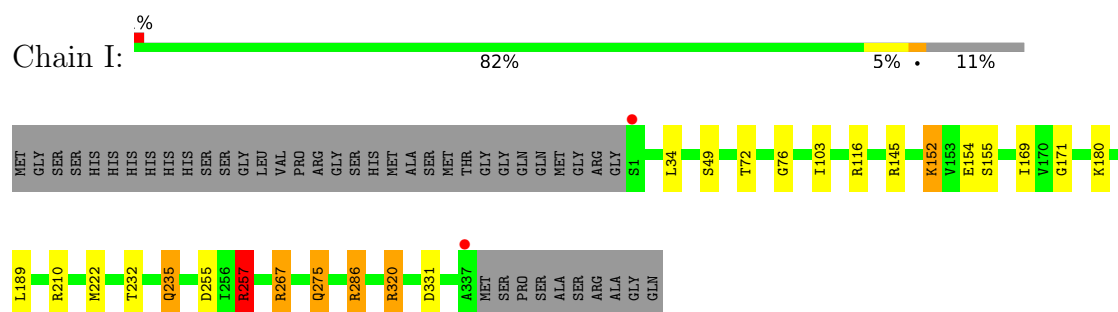


- Molecule 1: Luciferase family protein

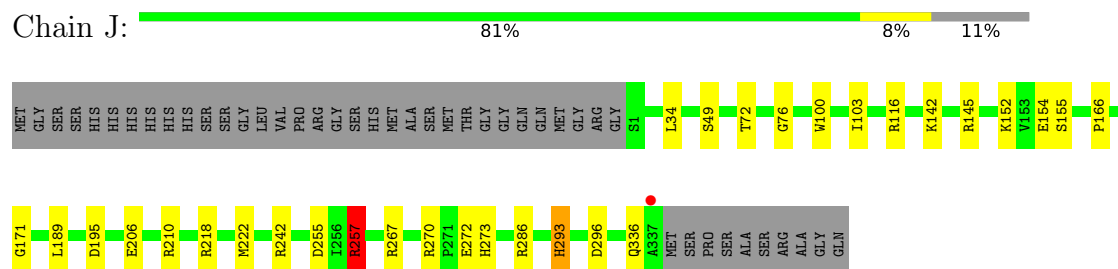
Chain H: 83% 5% 11%



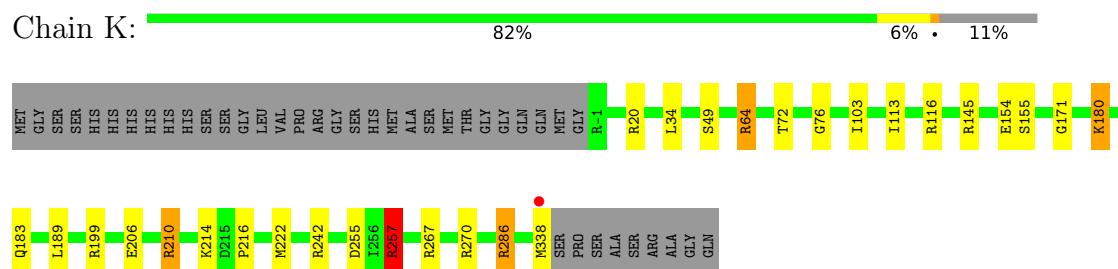
- Molecule 1: Luciferase family protein



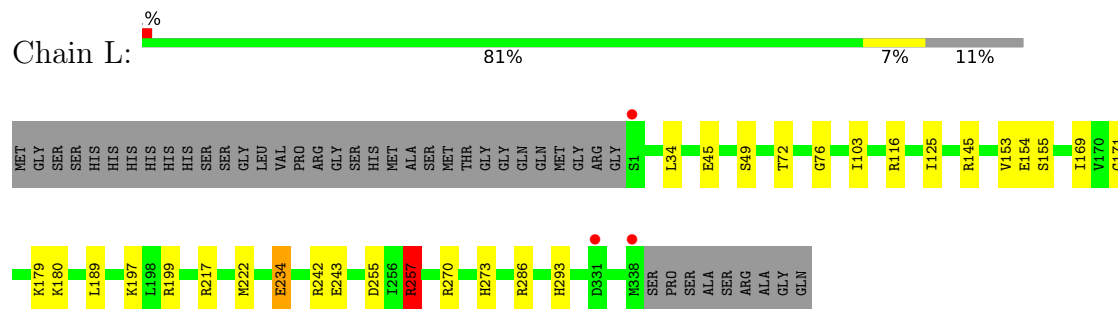
- Molecule 1: Luciferase family protein



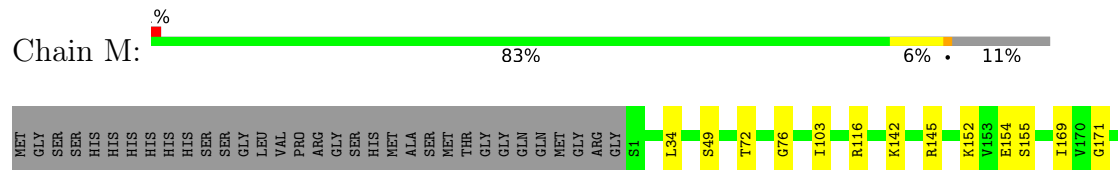
- Molecule 1: Luciferase family protein



- Molecule 1: Luciferase family protein

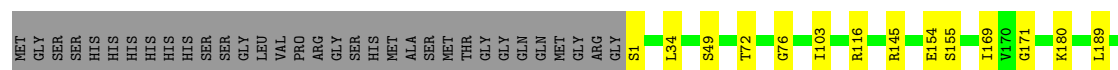
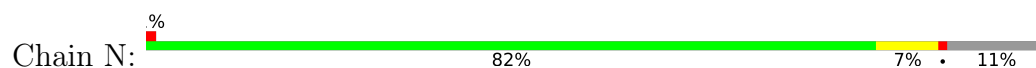


- Molecule 1: Luciferase family protein

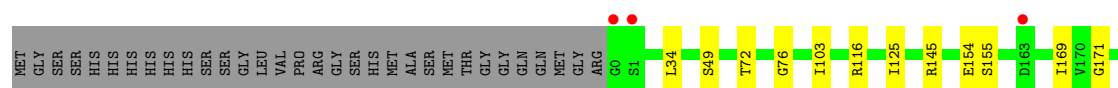
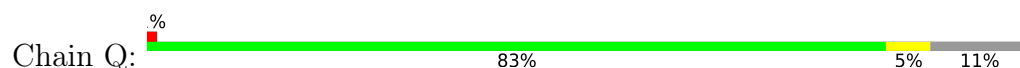




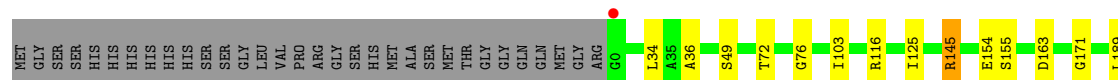
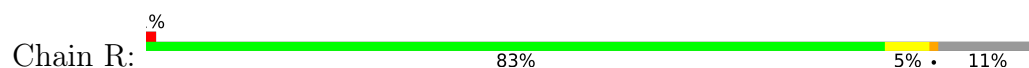
- Molecule 1: Luciferase family protein



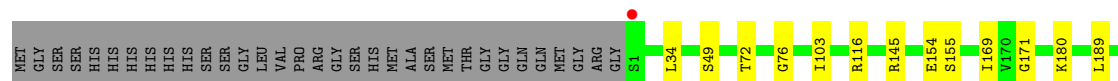
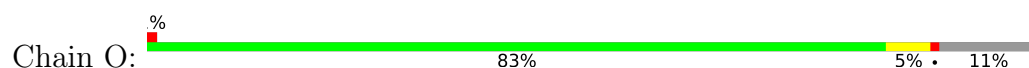
- Molecule 1: Luciferase family protein



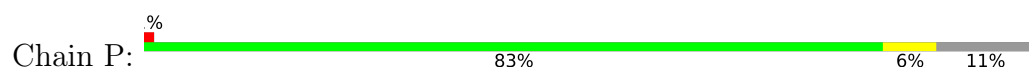
- Molecule 1: Luciferase family protein

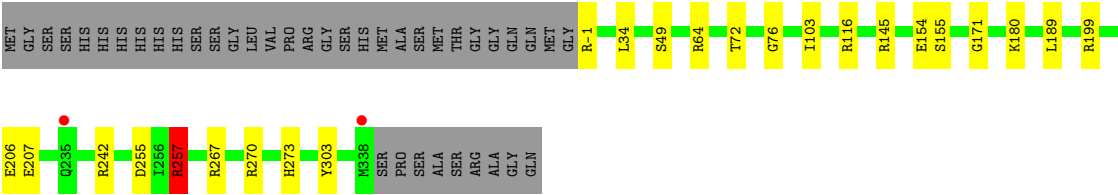


- Molecule 1: Luciferase family protein



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	39.4	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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

The worst 5 of 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

There are no chirality outliers.

5 of 83 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ARG	Sidechain
1	A	199	ARG	Sidechain
1	A	204	ARG	Sidechain
1	A	210	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

The worst 5 of 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

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

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	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
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

5 of 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

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Mol	Chain	Res	Type
1	E	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
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

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	286	ARG

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Mol	Chain	Res	Type
1	Q	286	ARG
1	O	257	ARG
1	G	180	LYS
1	G	-1	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	235	GLN
1	O	235	GLN
1	P	336	GLN
1	O	275	GLN
1	O	224	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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%)

The worst 5 of 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

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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.