



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:16 AM UTC

PDB ID : 9HAX / pdb\_00009hax  
Title : F420-dependent glucose-6-phosphate dehydrogenase  
Authors : Palm, G.J.; Berndt, L.; Lammers, M.  
Deposited on : 2024-11-05  
Resolution : 2.51 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

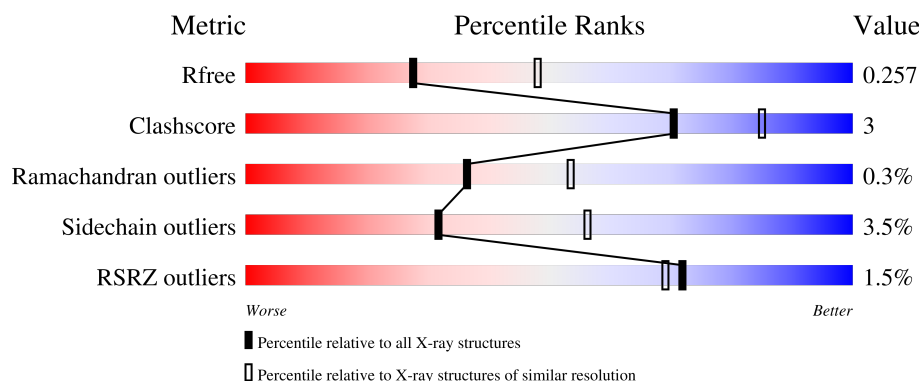
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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.



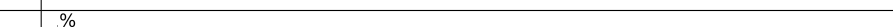

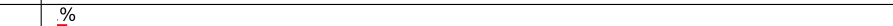



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	<div> <div>%</div> <div>77% 10% • 10%</div> </div>
1	B	380	<div> <div>%</div> <div>78% 9% • 11%</div> </div>
1	C	380	<div> <div>2%</div> <div>81% 8% •• 10%</div> </div>
1	D	380	<div> <div>%</div> <div>80% 7% •• 10%</div> </div>
1	E	380	<div> <div>%</div> <div>79% 8% •• 11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	380	 <div>80%8%11%</div>
1	G	380	 <div>79%8%10%</div>
1	H	380	 <div>78%9%11%</div>
1	I	380	 <div>80%8%11%</div>
1	J	380	 <div>82%6%10%</div>
1	K	380	 <div>78%10%10%</div>
1	L	380	 <div>78%9%10%</div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 64926 atoms, of which 31941 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	341	Total	C	H	N	O	S	59	3	0
			5386	1736	2671	487	479	13			
1	B	337	Total	C	H	N	O	S	59	1	0
			5305	1713	2629	479	472	12			
1	C	341	Total	C	H	N	O	S	59	4	0
			5388	1737	2670	487	481	13			
1	D	341	Total	C	H	N	O	S	59	2	0
			5372	1732	2663	486	478	13			
1	E	337	Total	C	H	N	O	S	59	4	0
			5350	1726	2654	482	476	12			
1	F	340	Total	C	H	N	O	S	59	3	0
			5376	1732	2667	488	477	12			
1	G	341	Total	C	H	N	O	S	59	2	0
			5372	1732	2663	486	478	13			
1	H	339	Total	C	H	N	O	S	59	1	0
			5336	1721	2645	484	474	12			
1	I	339	Total	C	H	N	O	S	59	3	0
			5369	1730	2664	487	476	12			
1	J	341	Total	C	H	N	O	S	59	4	0
			5405	1741	2682	489	480	13			
1	K	341	Total	C	H	N	O	S	59	1	0
			5360	1728	2657	486	476	13			
1	L	341	Total	C	H	N	O	S	59	3	0
			5393	1737	2676	489	478	13			

There are 408 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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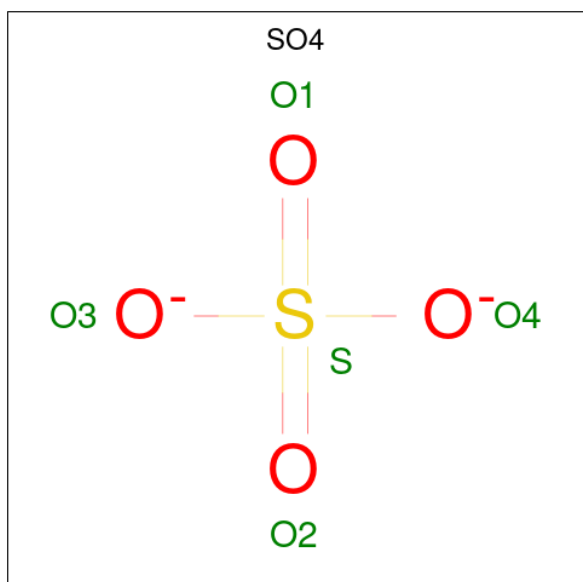
Chain	Residue	Modelled	Actual	Comment	Reference
K	-31	GLY	-	expression tag	UNP B9L4G2
K	-30	SER	-	expression tag	UNP B9L4G2
K	-29	SER	-	expression tag	UNP B9L4G2
K	-28	HIS	-	expression tag	UNP B9L4G2
K	-27	HIS	-	expression tag	UNP B9L4G2
K	-26	HIS	-	expression tag	UNP B9L4G2
K	-25	HIS	-	expression tag	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	1	Total	Cl	0	0
			1	1		
3	C	2	Total	Cl	0	0
			2	2		
3	D	2	Total	Cl	0	0
			2	2		
3	E	2	Total	Cl	0	0
			2	2		
3	F	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total 2	Cl 2	0	0
3	H	2	Total 2	Cl 2	0	0
3	I	1	Total 1	Cl 1	0	0
3	J	2	Total 2	Cl 2	0	0
3	K	1	Total 1	Cl 1	0	0
3	L	1	Total 1	Cl 1	0	0

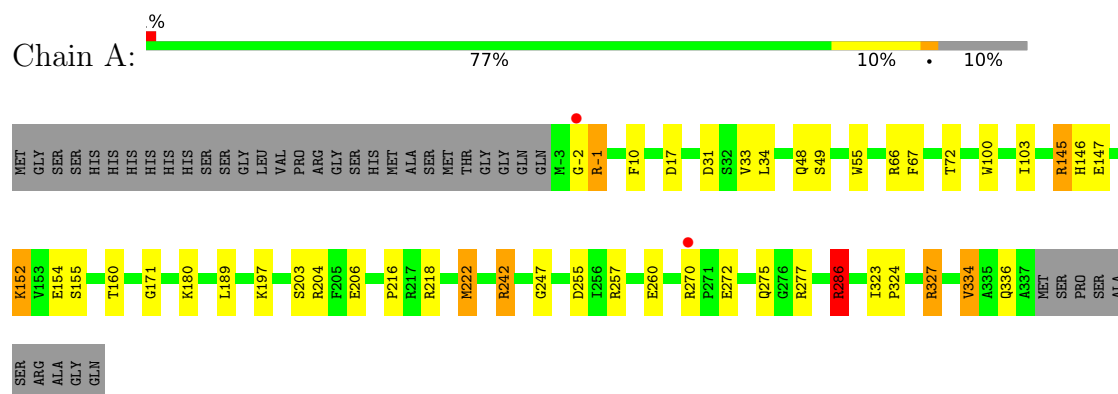
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total 35	O 35	0	0
4	B	29	Total 29	O 29	0	0
4	C	25	Total 25	O 25	0	0
4	D	29	Total 29	O 29	0	0
4	E	19	Total 19	O 19	0	0
4	F	22	Total 22	O 22	0	0
4	G	40	Total 40	O 40	0	0
4	H	25	Total 25	O 25	0	0
4	I	22	Total 22	O 22	0	0
4	J	27	Total 27	O 27	0	0
4	K	23	Total 23	O 23	0	0
4	L	24	Total 24	O 24	0	0

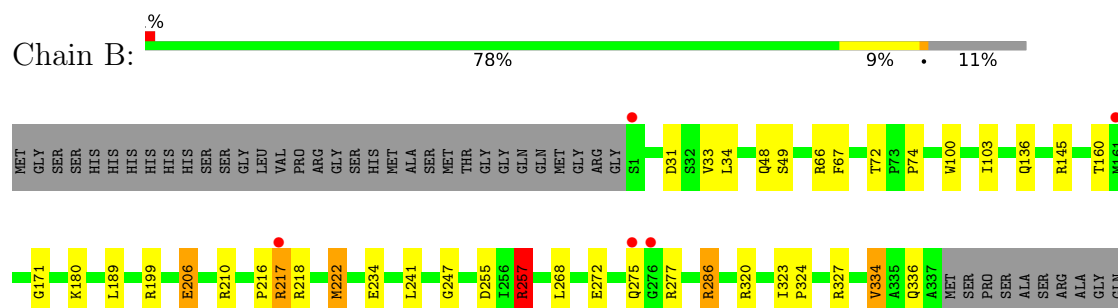
### 3 Residue-property plots [i](#)

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.

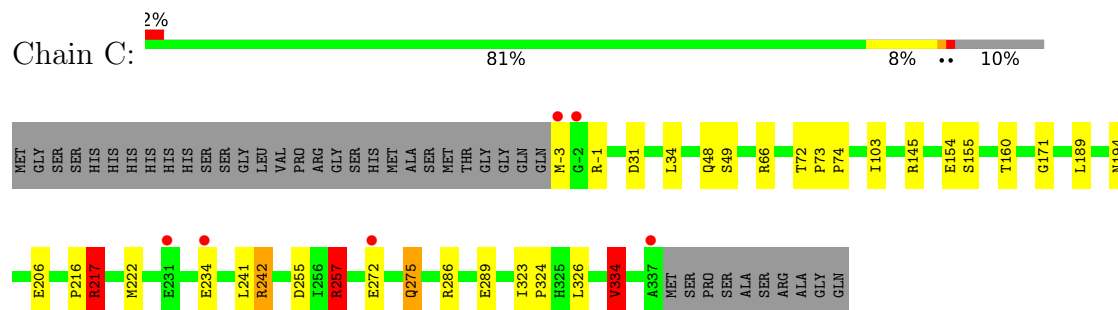
- Molecule 1: Luciferase family protein



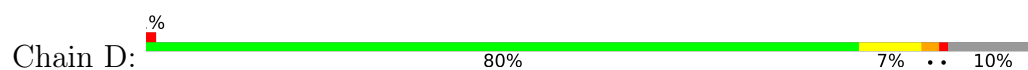
- Molecule 1: Luciferase family protein

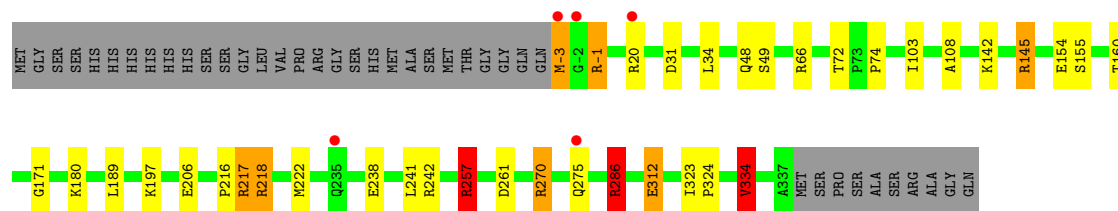


- Molecule 1: Luciferase family protein

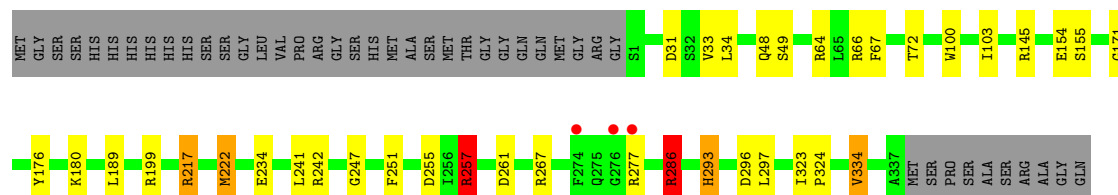
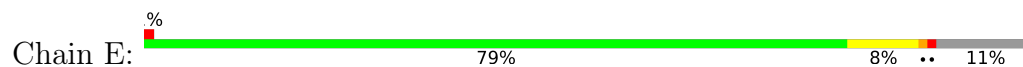


- Molecule 1: Luciferase family protein

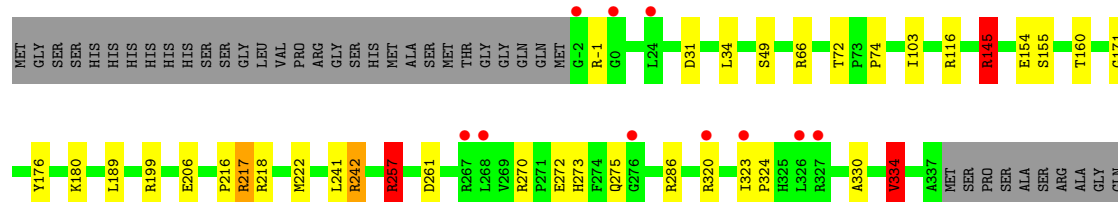
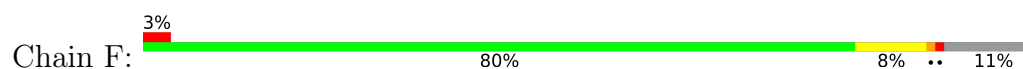




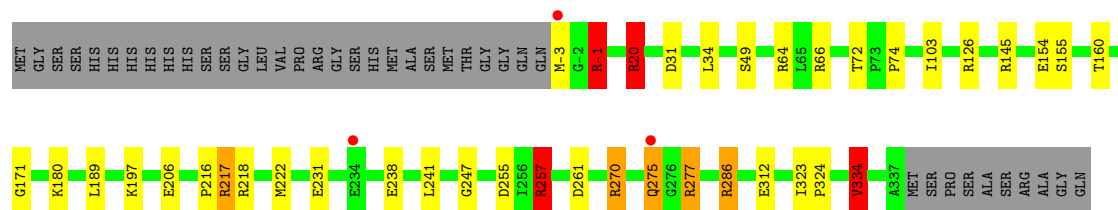
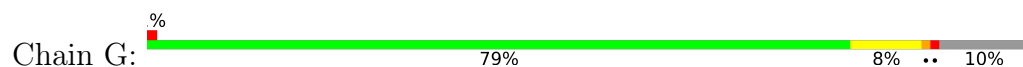
• Molecule 1: Luciferase family protein



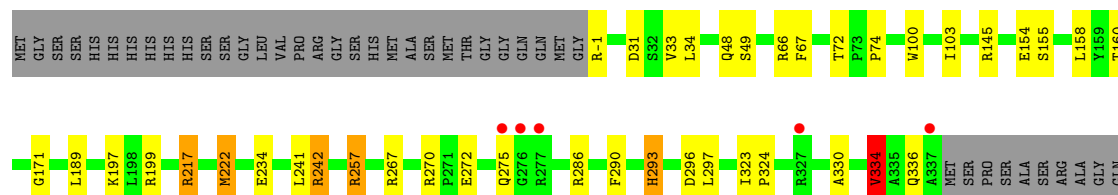
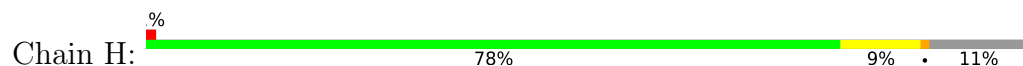
• Molecule 1: Luciferase family protein



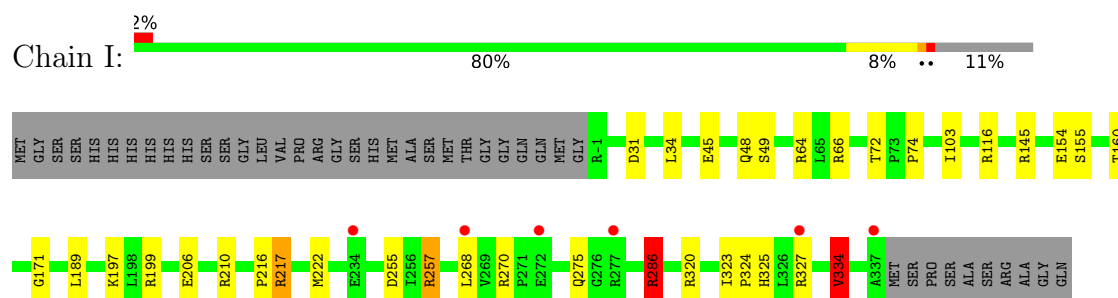
• Molecule 1: Luciferase family protein



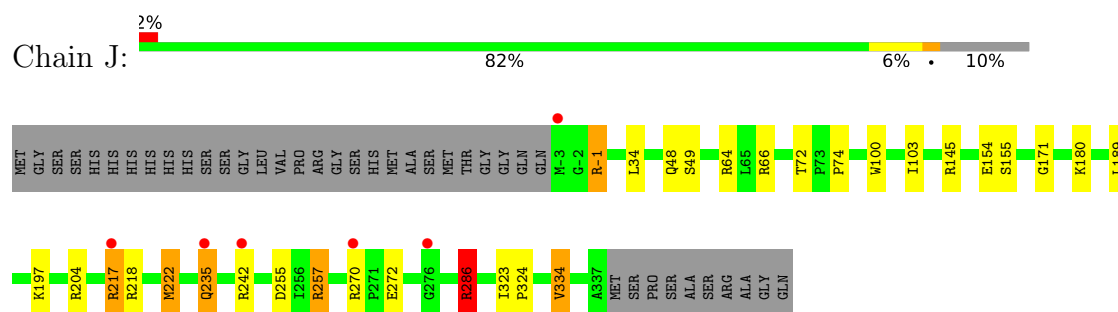
• Molecule 1: Luciferase family protein



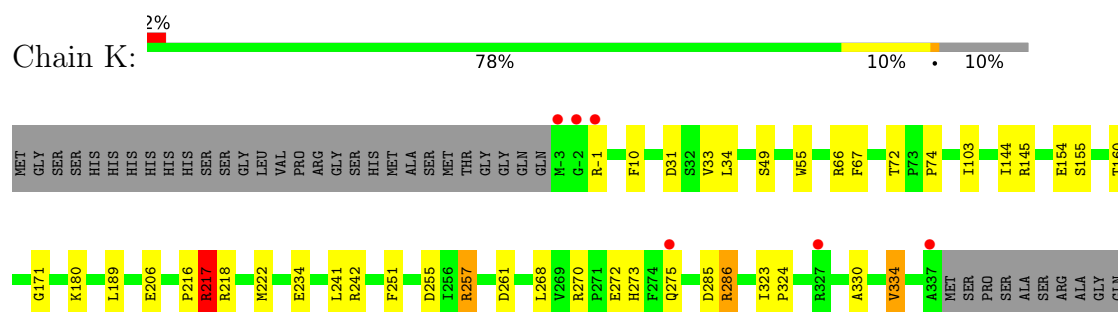
- Molecule 1: Luciferase family protein



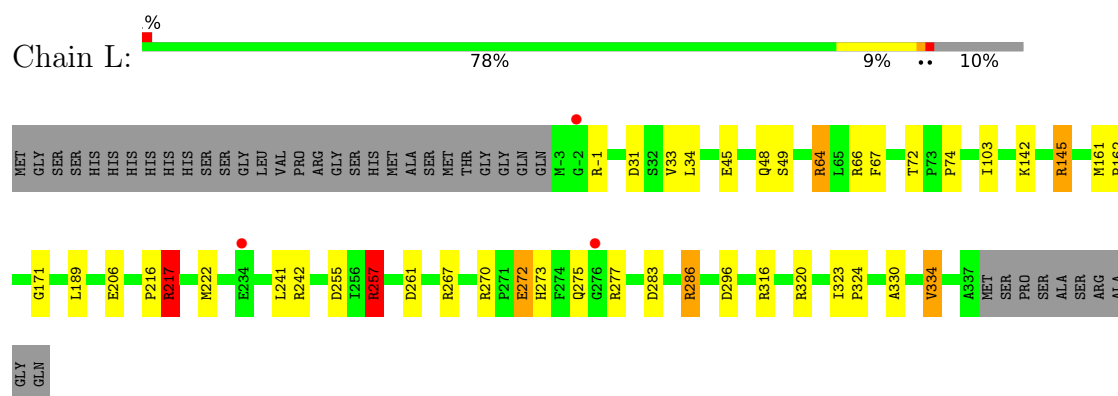
- Molecule 1: Luciferase family protein



- Molecule 1: Luciferase family protein



- Molecule 1: Luciferase family protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.53Å 239.41Å 108.20Å 90.00° 108.59° 90.00°	Depositor
Resolution (Å)	49.23 – 2.51 49.23 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.23-2.51) 98.1 (49.23-2.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.45	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.231 , 0.257 0.231 , 0.257	Depositor DCC
$R_{free}$ test set	8203 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 37.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	64926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% 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: SO4, 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	0.69	1/2805 (0.0%)	1.11	9/3807 (0.2%)
1	B	0.68	0/2760	1.08	9/3749 (0.2%)
1	C	0.66	0/2816	1.08	8/3822 (0.2%)
1	D	0.69	0/2796	1.13	18/3795 (0.5%)
1	E	0.68	0/2789	1.08	6/3788 (0.2%)
1	F	0.63	0/2799	1.07	7/3800 (0.2%)
1	G	0.69	0/2796	1.13	14/3795 (0.4%)
1	H	0.69	0/2775	1.10	10/3768 (0.3%)
1	I	0.64	0/2795	1.08	11/3795 (0.3%)
1	J	0.70	0/2816	1.11	5/3822 (0.1%)
1	K	0.65	0/2787	1.08	8/3783 (0.2%)
1	L	0.67	0/2807	1.09	12/3810 (0.3%)
All	All	0.67	1/33541 (0.0%)	1.09	117/45534 (0.3%)

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	3
1	D	0	5
1	E	0	4
1	F	0	4
1	G	0	5
1	H	0	2
1	I	0	4
1	J	0	5
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	7
All	All	0	51

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ARG	NE-CZ	5.71	1.39	1.33

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	64	ARG	CB-CG-CD	10.15	134.65	111.30
1	J	-1	ARG	CA-CB-CG	9.68	133.46	114.10
1	D	312	GLU	CG-CD-OE1	-8.33	99.23	118.40
1	B	74	PRO	N-CA-CB	-8.17	97.34	102.81
1	G	-1	ARG	CA-CB-CG	7.96	130.03	114.10
1	K	145	ARG	NE-CZ-NH2	7.69	126.12	119.20
1	H	293	HIS	CB-CG-ND1	-7.47	111.50	122.70
1	A	152	LYS	CB-CG-CD	7.38	128.27	111.30
1	G	20	ARG	CG-CD-NE	7.34	128.16	112.00
1	H	293	HIS	CB-CG-CD2	7.30	140.69	131.20
1	A	257	ARG	NE-CZ-NH2	7.03	125.52	119.20
1	D	74	PRO	N-CA-CB	-6.98	98.13	102.81
1	F	74	PRO	N-CA-CB	-6.92	98.17	102.81
1	D	-1	ARG	CB-CG-CD	6.80	126.94	111.30
1	D	257	ARG	NE-CZ-NH1	-6.63	114.87	121.50
1	L	74	PRO	N-CA-CB	-6.60	98.39	102.81
1	J	74	PRO	N-CA-CB	-6.43	98.50	102.81
1	K	74	PRO	N-CA-CB	-6.41	98.52	102.81
1	D	312	GLU	CG-CD-OE2	6.39	133.11	118.40
1	I	74	PRO	N-CA-CB	-6.29	98.60	102.81
1	D	145	ARG	NE-CZ-NH2	6.25	124.82	119.20
1	D	-1	ARG	CG-CD-NE	-6.18	98.41	112.00
1	L	145	ARG	NE-CZ-NH2	-6.11	113.70	119.20
1	I	325	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	H	74	PRO	N-CA-CB	-6.04	98.76	102.81
1	G	217	ARG	CG-CD-NE	6.02	125.24	112.00
1	J	235	GLN	CG-CD-NE2	5.98	125.38	116.40
1	L	286	ARG	CB-CG-CD	5.97	125.03	111.30
1	H	272	GLU	CB-CG-CD	5.94	122.70	112.60
1	G	74	PRO	N-CA-CB	-5.88	98.87	102.81
1	I	257	ARG	NE-CZ-NH1	-5.81	115.69	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	-3	MET	CG-SD-CE	5.79	113.65	100.90
1	C	74	PRO	N-CA-CB	-5.76	98.95	102.81
1	G	-1	ARG	CB-CG-CD	5.75	124.52	111.30
1	L	261	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	336	GLN	O-C-N	-5.71	118.27	123.41
1	C	31	ASP	CA-CB-CG	5.71	118.31	112.60
1	K	31	ASP	CA-CB-CG	5.69	118.29	112.60
1	E	261	ASP	CA-CB-CG	5.67	118.27	112.60
1	L	257	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	F	320	ARG	CD-NE-CZ	5.64	132.29	124.40
1	C	257	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	D	270	ARG	CG-CD-NE	-5.59	99.71	112.00
1	E	293	HIS	CA-CB-CG	5.55	119.36	113.80
1	D	261	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	257	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	B	320	ARG	CD-NE-CZ	5.47	132.06	124.40
1	L	217	ARG	CG-CD-NE	5.47	124.04	112.00
1	C	289	GLU	CG-CD-OE2	5.45	130.94	118.40
1	H	31	ASP	CA-CB-CG	5.45	118.05	112.60
1	I	325	HIS	CB-CG-ND1	5.44	130.85	122.70
1	D	197	LYS	N-CA-CB	-5.43	101.93	110.30
1	K	261	ASP	CA-CB-CG	5.43	118.03	112.60
1	F	261	ASP	CA-CB-CG	5.42	118.02	112.60
1	G	238	GLU	CG-CD-OE2	-5.42	105.93	118.40
1	K	272	GLU	CB-CG-CD	5.40	121.78	112.60
1	B	206	GLU	CB-CG-CD	5.39	121.77	112.60
1	B	31	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	31	ASP	CA-CB-CG	5.37	117.97	112.60
1	D	218	ARG	CB-CG-CD	5.36	123.62	111.30
1	I	31	ASP	CA-CB-CG	5.35	117.95	112.60
1	G	31	ASP	CA-CB-CG	5.35	117.95	112.60
1	G	257	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	C	257	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	H	336	GLN	N-CA-CB	-5.33	102.69	111.69
1	G	261	ASP	CA-CB-CG	5.33	117.92	112.60
1	D	31	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	286	ARG	N-CA-CB	-5.31	102.30	110.16
1	B	136	GLN	OE1-CD-NE2	5.30	127.90	122.60
1	A	336	GLN	N-CA-CB	-5.29	102.75	111.69
1	I	116	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	I	327	ARG	CD-NE-CZ	5.27	131.78	124.40
1	B	336	GLN	N-CA-CB	-5.26	102.80	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	145	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	B	257	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	F	116	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	D	238	GLU	CG-CD-OE1	5.22	130.40	118.40
1	H	257	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	D	334	VAL	N-CA-CB	-5.20	102.19	111.92
1	I	334	VAL	N-CA-CB	-5.18	102.23	111.92
1	J	197	LYS	N-CA-CB	-5.18	102.33	110.30
1	H	242	ARG	CB-CG-CD	5.17	123.19	111.30
1	A	286	ARG	N-CA-CB	-5.16	102.52	110.16
1	F	31	ASP	CA-CB-CG	5.16	117.76	112.60
1	D	238	GLU	CG-CD-OE2	-5.15	106.56	118.40
1	L	64	ARG	CG-CD-NE	5.15	123.33	112.00
1	H	334	VAL	N-CA-CB	-5.15	102.29	111.92
1	E	251	PHE	CA-CB-CG	5.14	118.94	113.80
1	C	242	ARG	CB-CG-CD	5.14	123.12	111.30
1	K	251	PHE	CA-CB-CG	5.14	118.94	113.80
1	G	238	GLU	CG-CD-OE1	5.13	130.20	118.40
1	E	257	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	K	286	ARG	CB-CA-C	5.12	119.55	110.85
1	C	334	VAL	N-CA-CB	-5.12	102.35	111.92
1	B	286	ARG	CB-CA-C	5.10	119.52	110.85
1	L	31	ASP	CA-CB-CG	5.10	117.70	112.60
1	G	257	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	G	334	VAL	N-CA-CB	-5.09	102.39	111.92
1	A	17	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	197	LYS	N-CA-CB	-5.08	102.48	110.30
1	E	31	ASP	CA-CB-CG	5.08	117.68	112.60
1	D	142	LYS	CB-CG-CD	5.07	122.97	111.30
1	G	286	ARG	N-CA-CB	-5.07	102.65	110.16
1	I	320	ARG	CD-NE-CZ	5.07	131.50	124.40
1	C	73	PRO	N-CA-C	5.05	116.87	110.70
1	L	217	ARG	CD-NE-CZ	5.05	131.48	124.40
1	E	286	ARG	CB-CA-C	5.05	119.44	110.85
1	K	285	ASP	CA-CB-CG	5.05	117.65	112.60
1	I	197	LYS	N-CA-CB	-5.04	102.54	110.30
1	L	283	ASP	CA-CB-CG	5.04	117.64	112.60
1	H	197	LYS	N-CA-CB	-5.04	102.55	110.30
1	A	260	GLU	CB-CG-CD	5.02	121.14	112.60
1	L	296	ASP	CA-CB-CG	5.02	117.62	112.60
1	F	334	VAL	N-CA-CB	-5.01	102.55	111.92
1	G	197	LYS	N-CA-CB	-5.01	102.59	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	286	ARG	CB-CA-C	5.01	119.36	110.85
1	L	286	ARG	CB-CA-C	5.00	119.35	110.85

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-1	ARG	Sidechain
1	A	145	ARG	Sidechain
1	A	204	ARG	Sidechain
1	A	242	ARG	Sidechain
1	A	286	ARG	Sidechain
1	A	327	ARG	Sidechain
1	B	145	ARG	Sidechain
1	B	199	ARG	Sidechain
1	B	210	ARG	Sidechain
1	B	257	ARG	Sidechain
1	C	145	ARG	Sidechain
1	C	217	ARG	Sidechain
1	C	257	ARG	Sidechain
1	D	145	ARG	Sidechain
1	D	20	ARG	Sidechain
1	D	242	ARG	Sidechain
1	D	257	ARG	Sidechain
1	D	270	ARG	Sidechain
1	E	242	ARG	Sidechain
1	E	257	ARG	Sidechain
1	E	267	ARG	Sidechain
1	E	286	ARG	Sidechain
1	F	145	ARG	Sidechain
1	F	199	ARG	Sidechain
1	F	242	ARG	Sidechain
1	F	257	ARG	Sidechain
1	G	-1	ARG	Sidechain
1	G	145	ARG	Sidechain
1	G	20	ARG	Sidechain
1	G	257	ARG	Sidechain
1	G	277	ARG	Sidechain
1	H	145	ARG	Sidechain
1	H	267	ARG	Sidechain
1	I	145	ARG	Sidechain
1	I	199	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	I	210	ARG	Sidechain
1	I	286	ARG	Sidechain
1	J	145	ARG	Sidechain
1	J	204	ARG	Sidechain
1	J	217	ARG	Sidechain
1	J	257	ARG	Sidechain
1	J	286	ARG	Sidechain
1	K	217	ARG	Sidechain
1	K	257	ARG	Sidechain
1	L	145	ARG	Sidechain
1	L	217	ARG	Sidechain
1	L	257	ARG	Sidechain
1	L	267	ARG	Sidechain
1	L	316	ARG	Sidechain
1	L	320	ARG	Sidechain
1	L	64	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	2715	2671	2659	26	0
1	B	2676	2629	2617	19	0
1	C	2718	2670	2650	18	0
1	D	2709	2663	2651	15	0
1	E	2696	2654	2642	20	0
1	F	2709	2667	2655	21	0
1	G	2709	2663	2651	18	0
1	H	2691	2645	2633	25	0
1	I	2705	2664	2652	19	0
1	J	2723	2682	2670	20	0
1	K	2703	2657	2644	27	0
1	L	2717	2676	2664	31	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
2	E	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	15	0	0	0	0
2	G	15	0	0	0	0
2	H	15	0	0	0	0
2	I	10	0	0	0	0
2	J	15	0	0	0	0
2	K	15	0	0	0	0
2	L	15	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	1	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	1	0	0	0	0
3	J	2	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	35	0	0	6	0
4	B	29	0	0	1	0
4	C	25	0	0	2	0
4	D	29	0	0	1	0
4	E	19	0	0	0	0
4	F	22	0	0	1	0
4	G	40	0	0	6	0
4	H	25	0	0	1	0
4	I	22	0	0	3	0
4	J	27	0	0	3	0
4	K	23	0	0	4	0
4	L	24	0	0	1	0
All	All	32985	31941	31788	220	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (220) 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:K:270:ARG:NH1	1:L:272[A]:GLU:OE2	1.59	1.34
1:J:235:GLN:HG2	4:J:524:HOH:O	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:161[B]:MET:HE2	1:L:162:PRO:HD2	1.50	0.93
1:K:270:ARG:HG3	4:K:514:HOH:O	1.72	0.88
1:K:270:ARG:CG	4:K:514:HOH:O	2.30	0.79
1:C:217:ARG:HH11	1:C:217:ARG:HB2	1.46	0.78
1:K:217:ARG:HH11	1:K:217:ARG:HB2	1.50	0.77
1:E:217:ARG:HB2	1:E:217:ARG:HH11	1.53	0.74
1:L:277:ARG:HD2	4:L:517:HOH:O	1.87	0.73
1:F:145:ARG:NH2	4:F:501:HOH:O	1.74	0.73
1:G:270:ARG:HD3	1:H:270:ARG:CZ	2.18	0.73
1:F:217:ARG:HH11	1:F:217:ARG:HB2	1.54	0.72
1:H:217:ARG:HH11	1:H:217:ARG:HB2	1.54	0.72
1:K:270:ARG:HD3	1:L:270[B]:ARG:CZ	2.19	0.72
1:I:217:ARG:HH11	1:I:217:ARG:HB2	1.54	0.71
1:B:217:ARG:HH11	1:B:217:ARG:HB2	1.55	0.71
1:E:199:ARG:HG3	1:H:199:ARG:HG3	1.72	0.71
1:G:216:PRO:O	4:G:501:HOH:O	2.09	0.71
1:J:286:ARG:HG2	1:J:286:ARG:HH11	1.56	0.70
1:L:270[B]:ARG:HB2	1:L:270[B]:ARG:NH1	2.08	0.68
1:L:272[B]:GLU:CD	1:L:272[B]:GLU:H	1.99	0.68
1:I:268:LEU:O	1:I:270[B]:ARG:HD2	1.94	0.68
1:J:235:GLN:CG	4:J:524:HOH:O	2.31	0.67
1:D:257:ARG:HD3	1:E:255:ASP:OD2	1.96	0.65
1:C:326:LEU:HB2	4:C:505:HOH:O	1.96	0.64
1:B:327:ARG:NH2	4:B:502:HOH:O	2.31	0.64
1:A:327:ARG:CG	4:A:528:HOH:O	2.47	0.62
1:I:257:ARG:HD3	1:J:255:ASP:OD2	1.99	0.62
1:L:217:ARG:HH11	1:L:217:ARG:HB2	1.63	0.61
1:F:272[B]:GLU:H	1:F:272[B]:GLU:CD	2.06	0.61
1:H:286:ARG:HH11	1:H:286:ARG:HG2	1.66	0.60
1:C:217:ARG:HH11	1:C:217:ARG:CB	2.15	0.60
1:G:126:ARG:NH1	4:G:502:HOH:O	2.33	0.60
1:J:270[B]:ARG:HG3	1:J:270[B]:ARG:HH11	1.65	0.60
1:G:160:THR:OG1	1:L:48:GLN:NE2	2.35	0.59
1:J:286:ARG:HG2	1:J:286:ARG:NH1	2.16	0.59
1:I:255:ASP:OD2	1:J:257:ARG:HD3	2.01	0.59
1:I:217:ARG:HH11	1:I:217:ARG:CB	2.16	0.58
1:D:217:ARG:HB2	1:D:217:ARG:HH11	1.68	0.58
1:F:217:ARG:HH11	1:F:217:ARG:CB	2.17	0.58
1:E:217:ARG:HH11	1:E:217:ARG:CB	2.16	0.58
1:F:286:ARG:HG2	1:F:286:ARG:HH11	1.69	0.58
1:K:270:ARG:CD	1:L:270[B]:ARG:CZ	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:270[B]:ARG:NH2	1:L:273:HIS:HE1	2.03	0.57
1:K:255:ASP:OD2	1:L:257:ARG:HD3	2.05	0.57
1:C:194:ASN:HB2	3:C:405:CL:CL	2.42	0.57
1:B:217:ARG:HH11	1:B:217:ARG:CB	2.18	0.56
1:E:48:GLN:NE2	1:F:160:THR:OG1	2.38	0.56
1:E:296:ASP:OD2	1:H:296:ASP:OD2	2.24	0.54
1:H:217:ARG:HH11	1:H:217:ARG:CB	2.19	0.54
1:B:268:LEU:HD11	4:C:512:HOH:O	2.08	0.54
1:A:147:GLU:CD	4:A:525:HOH:O	2.51	0.53
1:J:255:ASP:HB2	4:J:508:HOH:O	2.08	0.53
1:A:160:THR:OG1	1:B:48:GLN:NE2	2.41	0.53
1:H:160:THR:OG1	1:I:48:GLN:NE2	2.42	0.53
1:G:20:ARG:NH1	4:G:504:HOH:O	2.40	0.53
1:B:206:GLU:HG2	1:B:216:PRO:HB2	1.92	0.52
1:B:255:ASP:CG	1:C:257:ARG:HH21	2.17	0.52
1:K:217:ARG:HH11	1:K:217:ARG:CB	2.21	0.52
1:H:48:GLN:NE2	1:I:160:THR:OG1	2.43	0.51
1:I:45:GLU:HB3	4:I:520:HOH:O	2.10	0.51
1:D:217:ARG:HH11	1:D:217:ARG:CB	2.24	0.51
1:A:72:THR:O	1:A:103:ILE:HA	2.12	0.50
1:K:268:LEU:O	1:L:270[B]:ARG:NH2	2.44	0.50
1:C:171:GLY:HA2	1:C:189:LEU:O	2.12	0.50
1:G:286:ARG:HG2	1:G:286:ARG:HH11	1.76	0.50
1:B:255:ASP:OD2	1:C:257:ARG:HD3	2.12	0.50
1:G:72:THR:O	1:G:103:ILE:HA	2.12	0.50
1:D:171:GLY:HA2	1:D:189:LEU:O	2.12	0.50
1:F:72:THR:O	1:F:103:ILE:HA	2.12	0.49
1:B:257:ARG:HD3	1:C:255:ASP:OD2	2.12	0.49
1:G:255:ASP:OD2	1:H:257:ARG:HD3	2.12	0.49
1:L:72:THR:O	1:L:103:ILE:HA	2.13	0.49
1:H:171:GLY:HA2	1:H:189:LEU:O	2.12	0.49
1:I:64:ARG:HD3	4:I:503:HOH:O	2.13	0.49
1:H:290:PHE:O	1:H:293:HIS:HB3	2.12	0.49
1:K:171:GLY:HA2	1:K:189:LEU:O	2.13	0.49
1:L:171:GLY:HA2	1:L:189:LEU:O	2.13	0.49
1:B:72:THR:O	1:B:103:ILE:HA	2.12	0.49
1:G:206:GLU:HG2	1:G:216:PRO:HB2	1.92	0.49
1:K:257:ARG:HD3	1:L:255:ASP:OD2	2.12	0.49
1:D:72:THR:O	1:D:103:ILE:HA	2.12	0.49
1:K:273:HIS:HE1	1:L:270[B]:ARG:HH21	1.59	0.48
1:C:72:THR:O	1:C:103:ILE:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:ARG:NH1	1:E:286:ARG:HG2	2.28	0.48
1:E:171:GLY:HA2	1:E:189:LEU:O	2.14	0.48
1:F:171:GLY:HA2	1:F:189:LEU:O	2.14	0.48
1:J:72:THR:O	1:J:103:ILE:HA	2.12	0.48
1:J:272[B]:GLU:CD	1:J:272[B]:GLU:H	2.21	0.48
1:I:72:THR:O	1:I:103:ILE:HA	2.14	0.48
1:I:171:GLY:HA2	1:I:189:LEU:O	2.14	0.48
1:H:72:THR:O	1:H:103:ILE:HA	2.14	0.48
1:A:171:GLY:HA2	1:A:189:LEU:O	2.14	0.48
1:K:72:THR:O	1:K:103:ILE:HA	2.15	0.47
1:K:255:ASP:CG	1:L:257:ARG:HH21	2.22	0.47
1:L:270[B]:ARG:HH22	1:L:273:HIS:HE1	1.62	0.47
1:H:100:TRP:CH2	1:H:222:MET:HE1	2.50	0.47
1:G:270:ARG:HD3	1:H:270:ARG:NH2	2.29	0.47
1:A:255:ASP:CG	1:F:257:ARG:HH21	2.23	0.47
1:G:171:GLY:HA2	1:G:189:LEU:O	2.14	0.47
1:K:-1:ARG:HG2	1:K:330:ALA:HB2	1.97	0.47
1:B:171:GLY:HA2	1:B:189:LEU:O	2.15	0.46
4:G:510:HOH:O	1:H:270:ARG:HD3	2.15	0.46
1:J:171:GLY:HA2	1:J:189:LEU:O	2.14	0.46
1:E:72:THR:O	1:E:103:ILE:HA	2.14	0.46
4:G:510:HOH:O	1:H:270:ARG:CD	2.63	0.46
1:F:270[B]:ARG:NH1	1:F:273:HIS:NE2	2.63	0.46
1:A:327:ARG:HD3	4:A:528:HOH:O	2.15	0.46
1:G:231:GLU:HB2	4:G:509:HOH:O	2.15	0.46
1:A:327:ARG:CD	4:A:528:HOH:O	2.63	0.46
1:C:48:GLN:NE2	1:D:160:THR:OG1	2.49	0.46
1:D:206:GLU:HG2	1:D:216:PRO:HB2	1.97	0.46
1:L:270[B]:ARG:HH12	1:L:273:HIS:CE1	2.34	0.46
1:E:100:TRP:CH2	1:E:222:MET:HE1	2.51	0.46
1:H:323:ILE:N	1:H:324:PRO:CD	2.79	0.46
1:L:217:ARG:HH11	1:L:217:ARG:CB	2.29	0.46
1:A:48:GLN:NE2	1:B:160:THR:OG1	2.48	0.45
1:D:108:ALA:HB1	4:D:529:HOH:O	2.16	0.45
1:H:158:LEU:HA	4:H:517:HOH:O	2.15	0.45
1:I:64:ARG:NE	4:I:503:HOH:O	2.49	0.45
1:J:100:TRP:CH2	1:J:222:MET:HE1	2.51	0.45
1:K:206:GLU:HG2	1:K:216:PRO:HB2	1.99	0.45
1:B:217:ARG:HB2	1:B:217:ARG:NH1	2.27	0.45
1:A:327:ARG:HG2	4:A:528:HOH:O	2.13	0.45
1:C:160:THR:OG1	1:D:48:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:TYR:CZ	1:E:180:LYS:HD2	2.52	0.45
1:G:66:ARG:CZ	1:G:334:VAL:HG13	2.47	0.45
1:A:66:ARG:CZ	1:A:334:VAL:HG13	2.47	0.44
1:A:286:ARG:NH1	1:A:286:ARG:HG2	2.31	0.44
1:L:270[B]:ARG:NH1	1:L:273:HIS:CE1	2.85	0.44
1:E:297:LEU:HD23	1:H:297:LEU:HA	2.00	0.44
1:L:206:GLU:HG2	1:L:216:PRO:HB2	2.00	0.44
1:J:66:ARG:CZ	1:J:334:VAL:HG13	2.47	0.44
1:L:66:ARG:CZ	1:L:334:VAL:HG13	2.48	0.44
1:L:-1:ARG:HG2	1:L:330:ALA:HB2	2.00	0.43
1:C:66:ARG:CZ	1:C:334:VAL:HG13	2.48	0.43
1:C:272[B]:GLU:CD	1:C:272[B]:GLU:H	2.26	0.43
1:B:100:TRP:CH2	1:B:222:MET:HE1	2.54	0.43
1:F:66:ARG:CZ	1:F:334:VAL:HG13	2.48	0.43
1:D:323:ILE:N	1:D:324:PRO:CD	2.82	0.43
1:E:323:ILE:N	1:E:324:PRO:CD	2.81	0.43
1:G:323:ILE:N	1:G:324:PRO:CD	2.82	0.43
1:K:144:ILE:HA	4:K:519:HOH:O	2.18	0.43
1:K:323:ILE:N	1:K:324:PRO:CD	2.81	0.43
1:A:100:TRP:CH2	1:A:222:MET:HE1	2.54	0.43
1:B:66:ARG:CZ	1:B:334:VAL:HG13	2.49	0.43
1:K:270:ARG:NH2	1:L:270[A]:ARG:CZ	2.82	0.43
1:B:323:ILE:N	1:B:324:PRO:CD	2.81	0.43
1:F:-1:ARG:HG2	1:F:330:ALA:HB2	2.01	0.43
1:I:323:ILE:N	1:I:324:PRO:CD	2.82	0.43
1:A:255:ASP:OD2	1:F:257:ARG:HD3	2.19	0.43
1:C:206:GLU:HG2	1:C:216:PRO:HB2	2.01	0.43
1:F:323:ILE:N	1:F:324:PRO:CD	2.82	0.43
1:G:275:GLN:HE21	1:G:275:GLN:HB2	1.71	0.43
1:I:66:ARG:CZ	1:I:334:VAL:HG13	2.48	0.43
1:A:323:ILE:N	1:A:324:PRO:CD	2.82	0.42
1:H:-1:ARG:HG2	1:H:330:ALA:HB2	2.01	0.42
1:J:323:ILE:N	1:J:324:PRO:CD	2.82	0.42
1:B:34:LEU:C	1:B:34:LEU:HD23	2.44	0.42
1:A:270:ARG:HD3	1:F:270[B]:ARG:NE	2.34	0.42
1:K:34:LEU:C	1:K:34:LEU:HD23	2.45	0.42
1:A:206:GLU:HG2	1:A:216:PRO:HB2	2.01	0.42
1:I:255:ASP:CG	1:J:257:ARG:HH21	2.27	0.42
1:E:66:ARG:CZ	1:E:334:VAL:HG13	2.50	0.42
1:I:154:GLU:O	1:I:155:SER:C	2.63	0.42
1:K:66:ARG:CZ	1:K:334:VAL:HG13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:HIS:HA	2:A:403:SO4:O1	2.19	0.42
1:E:100:TRP:CZ3	1:E:222:MET:HE1	2.55	0.42
1:F:154:GLU:O	1:F:155:SER:C	2.62	0.42
1:A:-2:GLY:HA3	4:A:505:HOH:O	2.18	0.42
1:E:34:LEU:C	1:E:34:LEU:HD23	2.45	0.42
1:L:34:LEU:C	1:L:34:LEU:HD23	2.44	0.42
1:A:270:ARG:HD3	1:F:270[B]:ARG:CZ	2.50	0.42
1:D:66:ARG:CZ	1:D:334:VAL:HG13	2.49	0.42
1:D:257:ARG:HH21	1:E:255:ASP:CG	2.28	0.42
1:D:286:ARG:HH11	1:D:286:ARG:CG	2.32	0.42
1:E:33:VAL:O	1:E:67:PHE:HA	2.20	0.42
1:I:206:GLU:HG2	1:I:216:PRO:HB2	2.02	0.42
1:F:34:LEU:C	1:F:34:LEU:HD23	2.45	0.42
1:G:34:LEU:C	1:G:34:LEU:HD23	2.45	0.42
1:I:34:LEU:C	1:I:34:LEU:HD23	2.45	0.42
1:C:34:LEU:HD23	1:C:34:LEU:C	2.45	0.41
1:H:100:TRP:CZ3	1:H:222:MET:HE1	2.55	0.41
1:L:323:ILE:N	1:L:324:PRO:CD	2.82	0.41
1:A:34:LEU:C	1:A:34:LEU:HD23	2.44	0.41
1:E:154:GLU:O	1:E:155:SER:C	2.63	0.41
1:H:66:ARG:CZ	1:H:334:VAL:HG13	2.50	0.41
1:D:34:LEU:C	1:D:34:LEU:HD23	2.45	0.41
1:H:34:LEU:HD23	1:H:34:LEU:C	2.45	0.41
1:J:48:GLN:NE2	1:K:160:THR:OG1	2.53	0.41
1:C:323:ILE:N	1:C:324:PRO:CD	2.83	0.41
1:G:154:GLU:O	1:G:155:SER:C	2.63	0.41
1:A:33:VAL:O	1:A:67:PHE:HA	2.21	0.41
1:B:33:VAL:O	1:B:67:PHE:HA	2.21	0.41
1:J:154:GLU:O	1:J:155:SER:C	2.64	0.41
1:K:154:GLU:O	1:K:155:SER:C	2.64	0.41
1:A:247:GLY:O	1:A:277:ARG:NH1	2.54	0.41
1:L:45:GLU:CD	1:L:45:GLU:O	2.64	0.41
1:A:270:ARG:CD	1:F:270[B]:ARG:CZ	2.99	0.40
1:G:247:GLY:O	1:G:277:ARG:HD3	2.21	0.40
1:H:154:GLU:O	1:H:155:SER:C	2.64	0.40
1:J:34:LEU:HD23	1:J:34:LEU:C	2.46	0.40
1:K:270:ARG:HD2	1:L:270[B]:ARG:NH1	2.36	0.40
1:C:154:GLU:O	1:C:155:SER:C	2.64	0.40
1:C:275:GLN:HE21	1:C:275:GLN:HB3	1.73	0.40
1:A:154:GLU:O	1:A:155:SER:C	2.64	0.40
1:D:154:GLU:O	1:D:155:SER:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:VAL:O	1:H:67:PHE:HA	2.21	0.40
1:J:100:TRP:CZ3	1:J:222:MET:HE1	2.57	0.40
1:K:33:VAL:O	1:K:67:PHE:HA	2.22	0.40
1:L:33:VAL:O	1:L:67:PHE:HA	2.21	0.40
1:A:10:PHE:HZ	1:A:55:TRP:CD2	2.40	0.40
1:B:247:GLY:O	1:B:277:ARG:CD	2.70	0.40
1:E:247:GLY:O	1:E:277:ARG:NH1	2.55	0.40
1:F:176:TYR:CZ	1:F:180:LYS:HD2	2.57	0.40
1:F:206:GLU:HG2	1:F:216:PRO:HB2	2.04	0.40
1:I:257:ARG:HH21	1:J:255:ASP:CG	2.30	0.40
1:K:10:PHE:HZ	1:K:55:TRP:CD2	2.40	0.40
1:K:270:ARG:HG2	4:K:514:HOH:O	2.08	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/380 (90%)	333 (97%)	8 (2%)	1 (0%)	36	53
1	B	336/380 (88%)	327 (97%)	8 (2%)	1 (0%)	36	53
1	C	343/380 (90%)	334 (97%)	8 (2%)	1 (0%)	36	53
1	D	341/380 (90%)	332 (97%)	8 (2%)	1 (0%)	36	53
1	E	339/380 (89%)	330 (97%)	8 (2%)	1 (0%)	36	53
1	F	341/380 (90%)	332 (97%)	8 (2%)	1 (0%)	36	53
1	G	341/380 (90%)	331 (97%)	9 (3%)	1 (0%)	36	53
1	H	338/380 (89%)	329 (97%)	8 (2%)	1 (0%)	36	53
1	I	340/380 (90%)	331 (97%)	8 (2%)	1 (0%)	36	53
1	J	343/380 (90%)	334 (97%)	8 (2%)	1 (0%)	36	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	340/380 (90%)	331 (97%)	8 (2%)	1 (0%)	36	53
1	L	342/380 (90%)	333 (97%)	8 (2%)	1 (0%)	36	53
All	All	4086/4560 (90%)	3977 (97%)	97 (2%)	12 (0%)	36	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	D	49	SER
1	E	49	SER
1	F	49	SER
1	H	49	SER
1	I	49	SER
1	J	49	SER
1	B	49	SER
1	C	49	SER
1	G	49	SER
1	K	49	SER
1	L	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	275/302 (91%)	264 (96%)	11 (4%)	28	51
1	B	271/302 (90%)	260 (96%)	11 (4%)	27	50
1	C	276/302 (91%)	265 (96%)	11 (4%)	28	51
1	D	274/302 (91%)	263 (96%)	11 (4%)	28	51
1	E	274/302 (91%)	264 (96%)	10 (4%)	31	55
1	F	274/302 (91%)	266 (97%)	8 (3%)	37	63
1	G	274/302 (91%)	261 (95%)	13 (5%)	23	44
1	H	272/302 (90%)	265 (97%)	7 (3%)	40	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	274/302 (91%)	269 (98%)	5 (2%)	51 75
1	J	276/302 (91%)	268 (97%)	8 (3%)	37 63
1	K	273/302 (90%)	263 (96%)	10 (4%)	30 54
1	L	275/302 (91%)	265 (96%)	10 (4%)	31 55
All	All	3288/3624 (91%)	3173 (96%)	115 (4%)	32 56

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ARG
1	A	152	LYS
1	A	180	LYS
1	A	203	SER
1	A	218	ARG
1	A	222	MET
1	A	242	ARG
1	A	272	GLU
1	A	275	GLN
1	A	286	ARG
1	A	334	VAL
1	B	180	LYS
1	B	217	ARG
1	B	218	ARG
1	B	222	MET
1	B	234	GLU
1	B	241	LEU
1	B	257	ARG
1	B	272	GLU
1	B	275	GLN
1	B	286	ARG
1	B	334	VAL
1	C	-3	MET
1	C	-1	ARG
1	C	217	ARG
1	C	222	MET
1	C	234	GLU
1	C	241	LEU
1	C	242	ARG
1	C	257	ARG
1	C	275	GLN
1	C	286	ARG

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Mol	Chain	Res	Type
1	C	334	VAL
1	D	-3	MET
1	D	-1	ARG
1	D	180	LYS
1	D	217	ARG
1	D	218	ARG
1	D	222	MET
1	D	241	LEU
1	D	275	GLN
1	D	286	ARG
1	D	312	GLU
1	D	334	VAL
1	E	64	ARG
1	E	145	ARG
1	E	217	ARG
1	E	222	MET
1	E	234	GLU
1	E	241	LEU
1	E	257	ARG
1	E	286	ARG
1	E	293	HIS
1	E	334	VAL
1	F	217	ARG
1	F	218	ARG
1	F	222	MET
1	F	241	LEU
1	F	242	ARG
1	F	257	ARG
1	F	275	GLN
1	F	334	VAL
1	G	-3	MET
1	G	-1	ARG
1	G	64	ARG
1	G	180	LYS
1	G	217	ARG
1	G	218	ARG
1	G	222	MET
1	G	241	LEU
1	G	257	ARG
1	G	270	ARG
1	G	275	GLN
1	G	312	GLU

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Mol	Chain	Res	Type
1	G	334	VAL
1	H	217	ARG
1	H	222	MET
1	H	234	GLU
1	H	241	LEU
1	H	242	ARG
1	H	275	GLN
1	H	334	VAL
1	I	217	ARG
1	I	222	MET
1	I	275	GLN
1	I	286	ARG
1	I	334	VAL
1	J	-1	ARG
1	J	180	LYS
1	J	217	ARG
1	J	218	ARG
1	J	222	MET
1	J	242	ARG
1	J	286	ARG
1	J	334	VAL
1	K	180	LYS
1	K	217	ARG
1	K	218	ARG
1	K	222	MET
1	K	234	GLU
1	K	241	LEU
1	K	242	ARG
1	K	275	GLN
1	K	286	ARG
1	K	334	VAL
1	L	142	LYS
1	L	217	ARG
1	L	222	MET
1	L	241	LEU
1	L	242	ARG
1	L	272[A]	GLU
1	L	272[B]	GLU
1	L	275	GLN
1	L	286	ARG
1	L	334	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	275	GLN
1	B	48	GLN
1	B	275	GLN
1	C	48	GLN
1	C	258	ASN
1	C	275	GLN
1	D	48	GLN
1	D	258	ASN
1	D	275	GLN
1	E	48	GLN
1	E	275	GLN
1	F	48	GLN
1	F	275	GLN
1	G	239	ASN
1	G	275	GLN
1	H	48	GLN
1	H	235	GLN
1	H	258	ASN
1	H	275	GLN
1	I	48	GLN
1	I	275	GLN
1	J	48	GLN
1	J	258	ASN
1	K	48	GLN
1	K	258	ASN
1	K	275	GLN
1	L	48	GLN
1	L	258	ASN
1	L	273	HIS
1	L	275	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 19 are monoatomic - leaving 35 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	K	401	-	4,4,4	0.27	0	6,6,6	0.24	0
2	SO4	D	403	-	4,4,4	0.22	0	6,6,6	0.29	0
2	SO4	F	401	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	E	403	-	4,4,4	0.35	0	6,6,6	0.42	0
2	SO4	I	401	-	4,4,4	0.28	0	6,6,6	0.10	0
2	SO4	A	402	-	4,4,4	0.34	0	6,6,6	0.25	0
2	SO4	K	403	-	4,4,4	0.25	0	6,6,6	0.25	0
2	SO4	G	401	-	4,4,4	0.28	0	6,6,6	0.14	0
2	SO4	E	402	-	4,4,4	0.28	0	6,6,6	0.18	0
2	SO4	L	401	-	4,4,4	0.33	0	6,6,6	0.26	0
2	SO4	G	402	-	4,4,4	0.24	0	6,6,6	0.18	0
2	SO4	F	402	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	A	401	-	4,4,4	0.35	0	6,6,6	0.17	0
2	SO4	C	402	-	4,4,4	0.26	0	6,6,6	0.23	0
2	SO4	A	403	-	4,4,4	0.28	0	6,6,6	0.20	0
2	SO4	H	402	-	4,4,4	0.33	0	6,6,6	0.18	0
2	SO4	J	402	-	4,4,4	0.22	0	6,6,6	0.21	0
2	SO4	B	402	-	4,4,4	0.31	0	6,6,6	0.25	0
2	SO4	J	401	-	4,4,4	0.29	0	6,6,6	0.20	0
2	SO4	L	402	-	4,4,4	0.33	0	6,6,6	0.17	0
2	SO4	E	401	-	4,4,4	0.28	0	6,6,6	0.12	0
2	SO4	J	403	-	4,4,4	0.19	0	6,6,6	0.20	0
2	SO4	K	402	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	D	402	-	4,4,4	0.32	0	6,6,6	0.13	0
2	SO4	G	403	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	B	401	-	4,4,4	0.24	0	6,6,6	0.17	0
2	SO4	H	401	-	4,4,4	0.29	0	6,6,6	0.11	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	F	403	-	4,4,4	0.32	0	6,6,6	0.12	0
2	SO4	L	403	-	4,4,4	0.25	0	6,6,6	0.21	0
2	SO4	B	403	-	4,4,4	0.30	0	6,6,6	0.23	0
2	SO4	D	401	-	4,4,4	0.31	0	6,6,6	0.16	0
2	SO4	C	403	-	4,4,4	0.27	0	6,6,6	0.17	0
2	SO4	I	402	-	4,4,4	0.32	0	6,6,6	0.18	0
2	SO4	H	403	-	4,4,4	0.21	0	6,6,6	0.27	0
2	SO4	C	401	-	4,4,4	0.25	0	6,6,6	0.25	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	341/380 (89%)	-0.11	2 (0%) 85 84	20, 31, 54, 86	3 (0%)
1	B	337/380 (88%)	-0.10	5 (1%) 72 69	19, 32, 59, 92	1 (0%)
1	C	341/380 (89%)	0.13	6 (1%) 67 64	19, 37, 67, 84	3 (0%)
1	D	341/380 (89%)	-0.06	5 (1%) 72 69	20, 32, 62, 90	2 (0%)
1	E	337/380 (88%)	0.09	3 (0%) 81 79	24, 39, 63, 93	4 (1%)
1	F	340/380 (89%)	0.36	10 (2%) 53 50	22, 44, 73, 103	3 (0%)
1	G	341/380 (89%)	-0.11	3 (0%) 81 79	18, 31, 61, 86	2 (0%)
1	H	339/380 (89%)	0.09	5 (1%) 72 69	23, 38, 61, 103	1 (0%)
1	I	339/380 (89%)	0.19	6 (1%) 67 64	20, 42, 69, 88	3 (0%)
1	J	341/380 (89%)	-0.06	6 (1%) 67 64	17, 31, 55, 87	4 (1%)
1	K	341/380 (89%)	0.07	6 (1%) 67 64	20, 37, 64, 91	1 (0%)
1	L	341/380 (89%)	-0.04	3 (0%) 81 79	18, 33, 61, 88	3 (0%)
All	All	4079/4560 (89%)	0.04	60 (1%) 72 69	17, 35, 65, 103	30 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	276	GLY	4.0
1	F	-2	GLY	3.9
1	H	275	GLN	3.9
1	G	-3	MET	3.8
1	I	337	ALA	3.8
1	A	-2	GLY	3.8
1	E	276	GLY	3.5
1	D	-3	MET	3.4
1	F	320	ARG	3.3
1	F	323	ILE	3.3
1	L	234	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	327	ARG	3.1
1	I	272[A]	GLU	3.0
1	L	-2	GLY	3.0
1	F	276	GLY	2.9
1	J	-3	MET	2.8
1	H	327	ARG	2.8
1	B	276	GLY	2.8
1	F	326	LEU	2.8
1	B	1	SER	2.7
1	K	-3	MET	2.6
1	G	275	GLN	2.6
1	D	275	GLN	2.6
1	J	235	GLN	2.6
1	C	337	ALA	2.6
1	C	234	GLU	2.6
1	B	161[A]	MET	2.5
1	D	235	GLN	2.5
1	H	337	ALA	2.5
1	D	20	ARG	2.5
1	G	234	GLU	2.4
1	L	276	GLY	2.4
1	K	327	ARG	2.4
1	C	-3	MET	2.4
1	I	234	GLU	2.4
1	B	217	ARG	2.4
1	H	277	ARG	2.4
1	I	277	ARG	2.3
1	E	277	ARG	2.3
1	K	-2	GLY	2.3
1	B	275	GLN	2.3
1	F	267	ARG	2.3
1	J	217	ARG	2.3
1	K	-1	ARG	2.2
1	K	275	GLN	2.2
1	F	0	GLY	2.2
1	F	268	LEU	2.2
1	C	-2	GLY	2.2
1	I	268	LEU	2.2
1	C	231	GLU	2.2
1	A	270	ARG	2.1
1	I	327	ARG	2.1
1	J	270[A]	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	-2	GLY	2.1
1	J	242	ARG	2.1
1	J	276	GLY	2.1
1	E	274	PHE	2.0
1	C	272[A]	GLU	2.0
1	F	24	LEU	2.0
1	K	337	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å <sup>2</sup> )	Q<0.9
2	SO4	F	401	5/5	0.34	0.16	95,108,113,117	0
2	SO4	E	401	5/5	0.52	0.17	94,102,105,114	0
2	SO4	H	401	5/5	0.59	0.13	108,117,129,130	0
2	SO4	B	401	5/5	0.62	0.14	86,95,100,105	0
2	SO4	K	401	5/5	0.75	0.14	79,80,85,92	0
2	SO4	G	403	5/5	0.76	0.15	85,101,111,116	0
2	SO4	I	401	5/5	0.77	0.16	91,99,114,128	0
2	SO4	J	403	5/5	0.77	0.16	68,90,104,109	0
2	SO4	H	402	5/5	0.77	0.14	78,85,93,94	0
2	SO4	K	403	5/5	0.78	0.15	85,97,107,121	0
2	SO4	L	402	5/5	0.79	0.16	80,85,90,92	0
2	SO4	H	403	5/5	0.80	0.17	63,81,95,97	0
2	SO4	E	402	5/5	0.81	0.16	68,81,91,97	0
3	CL	F	404	1/1	0.81	0.16	74,74,74,74	0
2	SO4	E	403	5/5	0.82	0.15	59,64,79,87	0
2	SO4	L	401	5/5	0.82	0.14	69,82,87,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	401	5/5	0.82	0.12	74,80,88,106	0
2	SO4	L	403	5/5	0.82	0.13	79,89,96,97	0
2	SO4	D	403	5/5	0.82	0.16	70,79,88,102	0
2	SO4	F	403	5/5	0.83	0.16	63,71,88,96	0
2	SO4	C	403	5/5	0.84	0.12	89,96,99,107	0
2	SO4	F	402	5/5	0.84	0.17	69,82,87,87	0
2	SO4	D	401	5/5	0.84	0.16	71,78,90,104	0
2	SO4	K	402	5/5	0.85	0.14	89,99,101,101	0
3	CL	A	405	1/1	0.85	0.12	55,55,55,55	0
2	SO4	D	402	5/5	0.85	0.22	72,81,85,103	0
2	SO4	G	401	5/5	0.86	0.13	64,72,77,79	0
3	CL	C	405	1/1	0.87	0.12	70,70,70,70	0
2	SO4	B	403	5/5	0.87	0.12	62,72,73,84	0
3	CL	I	403	1/1	0.87	0.14	67,67,67,67	0
3	CL	J	404	1/1	0.87	0.13	53,53,53,53	0
2	SO4	G	402	5/5	0.88	0.18	69,76,78,84	0
3	CL	J	405	1/1	0.88	0.10	61,61,61,61	0
2	SO4	J	401	5/5	0.89	0.14	59,66,73,82	0
2	SO4	I	402	5/5	0.90	0.12	72,74,82,82	0
2	SO4	C	402	5/5	0.90	0.17	62,70,75,76	0
2	SO4	A	403	5/5	0.90	0.12	59,65,71,73	0
3	CL	H	405	1/1	0.91	0.10	57,57,57,57	0
2	SO4	A	401	5/5	0.91	0.09	59,66,70,73	0
3	CL	D	405	1/1	0.91	0.07	48,48,48,48	0
2	SO4	J	402	5/5	0.91	0.13	67,70,71,76	0
2	SO4	B	402	5/5	0.92	0.10	56,60,70,78	0
3	CL	H	404	1/1	0.92	0.13	63,63,63,63	0
3	CL	K	404	1/1	0.92	0.10	50,50,50,50	0
2	SO4	A	402	5/5	0.93	0.13	62,64,66,75	0
3	CL	G	404	1/1	0.94	0.09	48,48,48,48	0
3	CL	G	405	1/1	0.94	0.07	48,48,48,48	0
3	CL	C	404	1/1	0.94	0.07	49,49,49,49	0
3	CL	B	404	1/1	0.94	0.08	56,56,56,56	0
3	CL	E	405	1/1	0.95	0.07	51,51,51,51	0
3	CL	D	404	1/1	0.95	0.08	43,43,43,43	0
3	CL	A	404	1/1	0.96	0.06	40,40,40,40	0
3	CL	E	404	1/1	0.97	0.08	60,60,60,60	0
3	CL	L	404	1/1	0.97	0.08	42,42,42,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.