



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:08 PM UTC

PDB ID : 4HNK / pdb_00004hnk
Title : Crystal structure of an Enzyme
Authors : El Bakkouri, M.; Calmettes, C.; Wernimont, A.K.; Houry, W.A.; Hui, R.;
Structural Genomics Consortium (SGC)
Deposited on : 2012-10-19
Resolution : 2.90 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
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

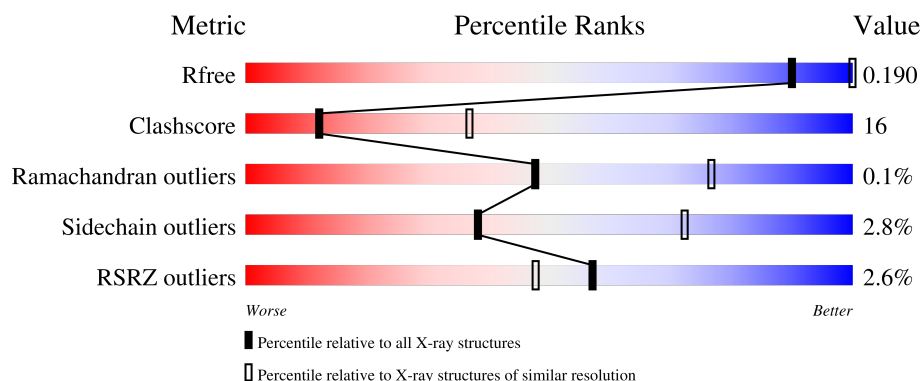
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	219	6% 54% 21% 5% 18%
1	B	219	0% 53% 18% 0% 26%
1	C	219	2% 56% 18% 0% 24%
1	D	219	2% 57% 16% 0% 26%
1	E	219	3% 58% 20% 0% 18%

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Mol	Chain	Length	Quality of chain
1	F	219	
1	G	219	
1	H	219	
1	I	219	
1	J	219	
1	K	219	
1	L	219	
1	M	219	
1	N	219	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	301	-	-	X	-
2	GOL	I	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18940 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1444	930	234	276	4			
1	B	162	Total	C	N	O	S	0	0	0
			1295	834	210	247	4			
1	C	166	Total	C	N	O	S	0	0	0
			1330	855	217	254	4			
1	D	162	Total	C	N	O	S	0	0	0
			1297	835	211	247	4			
1	E	179	Total	C	N	O	S	0	0	0
			1439	927	233	275	4			
1	F	166	Total	C	N	O	S	0	1	0
			1338	859	219	256	4			
1	G	170	Total	C	N	O	S	0	0	0
			1365	876	223	262	4			
1	H	179	Total	C	N	O	S	0	0	0
			1439	927	233	275	4			
1	I	165	Total	C	N	O	S	0	0	0
			1322	850	215	253	4			
1	J	166	Total	C	N	O	S	0	0	0
			1330	854	217	255	4			
1	K	161	Total	C	N	O	S	0	0	0
			1285	830	207	244	4			
1	L	176	Total	C	N	O	S	0	0	0
			1412	910	229	269	4			
1	M	156	Total	C	N	O	S	0	0	0
			1243	804	200	236	3			
1	N	165	Total	C	N	O	S	0	0	0
			1319	848	215	252	4			

There are 322 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP Q8IL98

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP Q8IL98
A	28	SER	-	expression tag	UNP Q8IL98
A	29	SER	-	expression tag	UNP Q8IL98
A	30	HIS	-	expression tag	UNP Q8IL98
A	31	HIS	-	expression tag	UNP Q8IL98
A	32	HIS	-	expression tag	UNP Q8IL98
A	33	HIS	-	expression tag	UNP Q8IL98
A	34	HIS	-	expression tag	UNP Q8IL98
A	35	HIS	-	expression tag	UNP Q8IL98
A	36	SER	-	expression tag	UNP Q8IL98
A	37	SER	-	expression tag	UNP Q8IL98
A	38	GLY	-	expression tag	UNP Q8IL98
A	39	ARG	-	expression tag	UNP Q8IL98
A	40	GLU	-	expression tag	UNP Q8IL98
A	41	ASN	-	expression tag	UNP Q8IL98
A	42	LEU	-	expression tag	UNP Q8IL98
A	43	TYR	-	expression tag	UNP Q8IL98
A	44	PHE	-	expression tag	UNP Q8IL98
A	45	GLN	-	expression tag	UNP Q8IL98
A	46	GLY	-	expression tag	UNP Q8IL98
A	47	HIS	-	expression tag	UNP Q8IL98
A	48	MET	-	expression tag	UNP Q8IL98
B	26	MET	-	expression tag	UNP Q8IL98
B	27	GLY	-	expression tag	UNP Q8IL98
B	28	SER	-	expression tag	UNP Q8IL98
B	29	SER	-	expression tag	UNP Q8IL98
B	30	HIS	-	expression tag	UNP Q8IL98
B	31	HIS	-	expression tag	UNP Q8IL98
B	32	HIS	-	expression tag	UNP Q8IL98
B	33	HIS	-	expression tag	UNP Q8IL98
B	34	HIS	-	expression tag	UNP Q8IL98
B	35	HIS	-	expression tag	UNP Q8IL98
B	36	SER	-	expression tag	UNP Q8IL98
B	37	SER	-	expression tag	UNP Q8IL98
B	38	GLY	-	expression tag	UNP Q8IL98
B	39	ARG	-	expression tag	UNP Q8IL98
B	40	GLU	-	expression tag	UNP Q8IL98
B	41	ASN	-	expression tag	UNP Q8IL98
B	42	LEU	-	expression tag	UNP Q8IL98
B	43	TYR	-	expression tag	UNP Q8IL98
B	44	PHE	-	expression tag	UNP Q8IL98
B	45	GLN	-	expression tag	UNP Q8IL98

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Chain	Residue	Modelled	Actual	Comment	Reference
B	46	GLY	-	expression tag	UNP Q8IL98
B	47	HIS	-	expression tag	UNP Q8IL98
B	48	MET	-	expression tag	UNP Q8IL98
C	26	MET	-	expression tag	UNP Q8IL98
C	27	GLY	-	expression tag	UNP Q8IL98
C	28	SER	-	expression tag	UNP Q8IL98
C	29	SER	-	expression tag	UNP Q8IL98
C	30	HIS	-	expression tag	UNP Q8IL98
C	31	HIS	-	expression tag	UNP Q8IL98
C	32	HIS	-	expression tag	UNP Q8IL98
C	33	HIS	-	expression tag	UNP Q8IL98
C	34	HIS	-	expression tag	UNP Q8IL98
C	35	HIS	-	expression tag	UNP Q8IL98
C	36	SER	-	expression tag	UNP Q8IL98
C	37	SER	-	expression tag	UNP Q8IL98
C	38	GLY	-	expression tag	UNP Q8IL98
C	39	ARG	-	expression tag	UNP Q8IL98
C	40	GLU	-	expression tag	UNP Q8IL98
C	41	ASN	-	expression tag	UNP Q8IL98
C	42	LEU	-	expression tag	UNP Q8IL98
C	43	TYR	-	expression tag	UNP Q8IL98
C	44	PHE	-	expression tag	UNP Q8IL98
C	45	GLN	-	expression tag	UNP Q8IL98
C	46	GLY	-	expression tag	UNP Q8IL98
C	47	HIS	-	expression tag	UNP Q8IL98
C	48	MET	-	expression tag	UNP Q8IL98
D	26	MET	-	expression tag	UNP Q8IL98
D	27	GLY	-	expression tag	UNP Q8IL98
D	28	SER	-	expression tag	UNP Q8IL98
D	29	SER	-	expression tag	UNP Q8IL98
D	30	HIS	-	expression tag	UNP Q8IL98
D	31	HIS	-	expression tag	UNP Q8IL98
D	32	HIS	-	expression tag	UNP Q8IL98
D	33	HIS	-	expression tag	UNP Q8IL98
D	34	HIS	-	expression tag	UNP Q8IL98
D	35	HIS	-	expression tag	UNP Q8IL98
D	36	SER	-	expression tag	UNP Q8IL98
D	37	SER	-	expression tag	UNP Q8IL98
D	38	GLY	-	expression tag	UNP Q8IL98
D	39	ARG	-	expression tag	UNP Q8IL98
D	40	GLU	-	expression tag	UNP Q8IL98
D	41	ASN	-	expression tag	UNP Q8IL98

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Chain	Residue	Modelled	Actual	Comment	Reference
D	42	LEU	-	expression tag	UNP Q8IL98
D	43	TYR	-	expression tag	UNP Q8IL98
D	44	PHE	-	expression tag	UNP Q8IL98
D	45	GLN	-	expression tag	UNP Q8IL98
D	46	GLY	-	expression tag	UNP Q8IL98
D	47	HIS	-	expression tag	UNP Q8IL98
D	48	MET	-	expression tag	UNP Q8IL98
E	26	MET	-	expression tag	UNP Q8IL98
E	27	GLY	-	expression tag	UNP Q8IL98
E	28	SER	-	expression tag	UNP Q8IL98
E	29	SER	-	expression tag	UNP Q8IL98
E	30	HIS	-	expression tag	UNP Q8IL98
E	31	HIS	-	expression tag	UNP Q8IL98
E	32	HIS	-	expression tag	UNP Q8IL98
E	33	HIS	-	expression tag	UNP Q8IL98
E	34	HIS	-	expression tag	UNP Q8IL98
E	35	HIS	-	expression tag	UNP Q8IL98
E	36	SER	-	expression tag	UNP Q8IL98
E	37	SER	-	expression tag	UNP Q8IL98
E	38	GLY	-	expression tag	UNP Q8IL98
E	39	ARG	-	expression tag	UNP Q8IL98
E	40	GLU	-	expression tag	UNP Q8IL98
E	41	ASN	-	expression tag	UNP Q8IL98
E	42	LEU	-	expression tag	UNP Q8IL98
E	43	TYR	-	expression tag	UNP Q8IL98
E	44	PHE	-	expression tag	UNP Q8IL98
E	45	GLN	-	expression tag	UNP Q8IL98
E	46	GLY	-	expression tag	UNP Q8IL98
E	47	HIS	-	expression tag	UNP Q8IL98
E	48	MET	-	expression tag	UNP Q8IL98
F	26	MET	-	expression tag	UNP Q8IL98
F	27	GLY	-	expression tag	UNP Q8IL98
F	28	SER	-	expression tag	UNP Q8IL98
F	29	SER	-	expression tag	UNP Q8IL98
F	30	HIS	-	expression tag	UNP Q8IL98
F	31	HIS	-	expression tag	UNP Q8IL98
F	32	HIS	-	expression tag	UNP Q8IL98
F	33	HIS	-	expression tag	UNP Q8IL98
F	34	HIS	-	expression tag	UNP Q8IL98
F	35	HIS	-	expression tag	UNP Q8IL98
F	36	SER	-	expression tag	UNP Q8IL98
F	37	SER	-	expression tag	UNP Q8IL98

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Chain	Residue	Modelled	Actual	Comment	Reference
F	38	GLY	-	expression tag	UNP Q8IL98
F	39	ARG	-	expression tag	UNP Q8IL98
F	40	GLU	-	expression tag	UNP Q8IL98
F	41	ASN	-	expression tag	UNP Q8IL98
F	42	LEU	-	expression tag	UNP Q8IL98
F	43	TYR	-	expression tag	UNP Q8IL98
F	44	PHE	-	expression tag	UNP Q8IL98
F	45	GLN	-	expression tag	UNP Q8IL98
F	46	GLY	-	expression tag	UNP Q8IL98
F	47	HIS	-	expression tag	UNP Q8IL98
F	48	MET	-	expression tag	UNP Q8IL98
G	26	MET	-	expression tag	UNP Q8IL98
G	27	GLY	-	expression tag	UNP Q8IL98
G	28	SER	-	expression tag	UNP Q8IL98
G	29	SER	-	expression tag	UNP Q8IL98
G	30	HIS	-	expression tag	UNP Q8IL98
G	31	HIS	-	expression tag	UNP Q8IL98
G	32	HIS	-	expression tag	UNP Q8IL98
G	33	HIS	-	expression tag	UNP Q8IL98
G	34	HIS	-	expression tag	UNP Q8IL98
G	35	HIS	-	expression tag	UNP Q8IL98
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G	43	TYR	-	expression tag	UNP Q8IL98
G	44	PHE	-	expression tag	UNP Q8IL98
G	45	GLN	-	expression tag	UNP Q8IL98
G	46	GLY	-	expression tag	UNP Q8IL98
G	47	HIS	-	expression tag	UNP Q8IL98
G	48	MET	-	expression tag	UNP Q8IL98
H	26	MET	-	expression tag	UNP Q8IL98
H	27	GLY	-	expression tag	UNP Q8IL98
H	28	SER	-	expression tag	UNP Q8IL98
H	29	SER	-	expression tag	UNP Q8IL98
H	30	HIS	-	expression tag	UNP Q8IL98
H	31	HIS	-	expression tag	UNP Q8IL98
H	32	HIS	-	expression tag	UNP Q8IL98
H	33	HIS	-	expression tag	UNP Q8IL98

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Chain	Residue	Modelled	Actual	Comment	Reference
H	34	HIS	-	expression tag	UNP Q8IL98
H	35	HIS	-	expression tag	UNP Q8IL98
H	36	SER	-	expression tag	UNP Q8IL98
H	37	SER	-	expression tag	UNP Q8IL98
H	38	GLY	-	expression tag	UNP Q8IL98
H	39	ARG	-	expression tag	UNP Q8IL98
H	40	GLU	-	expression tag	UNP Q8IL98
H	41	ASN	-	expression tag	UNP Q8IL98
H	42	LEU	-	expression tag	UNP Q8IL98
H	43	TYR	-	expression tag	UNP Q8IL98
H	44	PHE	-	expression tag	UNP Q8IL98
H	45	GLN	-	expression tag	UNP Q8IL98
H	46	GLY	-	expression tag	UNP Q8IL98
H	47	HIS	-	expression tag	UNP Q8IL98
H	48	MET	-	expression tag	UNP Q8IL98
I	26	MET	-	expression tag	UNP Q8IL98
I	27	GLY	-	expression tag	UNP Q8IL98
I	28	SER	-	expression tag	UNP Q8IL98
I	29	SER	-	expression tag	UNP Q8IL98
I	30	HIS	-	expression tag	UNP Q8IL98
I	31	HIS	-	expression tag	UNP Q8IL98
I	32	HIS	-	expression tag	UNP Q8IL98
I	33	HIS	-	expression tag	UNP Q8IL98
I	34	HIS	-	expression tag	UNP Q8IL98
I	35	HIS	-	expression tag	UNP Q8IL98
I	36	SER	-	expression tag	UNP Q8IL98
I	37	SER	-	expression tag	UNP Q8IL98
I	38	GLY	-	expression tag	UNP Q8IL98
I	39	ARG	-	expression tag	UNP Q8IL98
I	40	GLU	-	expression tag	UNP Q8IL98
I	41	ASN	-	expression tag	UNP Q8IL98
I	42	LEU	-	expression tag	UNP Q8IL98
I	43	TYR	-	expression tag	UNP Q8IL98
I	44	PHE	-	expression tag	UNP Q8IL98
I	45	GLN	-	expression tag	UNP Q8IL98
I	46	GLY	-	expression tag	UNP Q8IL98
I	47	HIS	-	expression tag	UNP Q8IL98
I	48	MET	-	expression tag	UNP Q8IL98
J	26	MET	-	expression tag	UNP Q8IL98
J	27	GLY	-	expression tag	UNP Q8IL98
J	28	SER	-	expression tag	UNP Q8IL98
J	29	SER	-	expression tag	UNP Q8IL98

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Chain	Residue	Modelled	Actual	Comment	Reference
J	30	HIS	-	expression tag	UNP Q8IL98
J	31	HIS	-	expression tag	UNP Q8IL98
J	32	HIS	-	expression tag	UNP Q8IL98
J	33	HIS	-	expression tag	UNP Q8IL98
J	34	HIS	-	expression tag	UNP Q8IL98
J	35	HIS	-	expression tag	UNP Q8IL98
J	36	SER	-	expression tag	UNP Q8IL98
J	37	SER	-	expression tag	UNP Q8IL98
J	38	GLY	-	expression tag	UNP Q8IL98
J	39	ARG	-	expression tag	UNP Q8IL98
J	40	GLU	-	expression tag	UNP Q8IL98
J	41	ASN	-	expression tag	UNP Q8IL98
J	42	LEU	-	expression tag	UNP Q8IL98
J	43	TYR	-	expression tag	UNP Q8IL98
J	44	PHE	-	expression tag	UNP Q8IL98
J	45	GLN	-	expression tag	UNP Q8IL98
J	46	GLY	-	expression tag	UNP Q8IL98
J	47	HIS	-	expression tag	UNP Q8IL98
J	48	MET	-	expression tag	UNP Q8IL98
K	26	MET	-	expression tag	UNP Q8IL98
K	27	GLY	-	expression tag	UNP Q8IL98
K	28	SER	-	expression tag	UNP Q8IL98
K	29	SER	-	expression tag	UNP Q8IL98
K	30	HIS	-	expression tag	UNP Q8IL98
K	31	HIS	-	expression tag	UNP Q8IL98
K	32	HIS	-	expression tag	UNP Q8IL98
K	33	HIS	-	expression tag	UNP Q8IL98
K	34	HIS	-	expression tag	UNP Q8IL98
K	35	HIS	-	expression tag	UNP Q8IL98
K	36	SER	-	expression tag	UNP Q8IL98
K	37	SER	-	expression tag	UNP Q8IL98
K	38	GLY	-	expression tag	UNP Q8IL98
K	39	ARG	-	expression tag	UNP Q8IL98
K	40	GLU	-	expression tag	UNP Q8IL98
K	41	ASN	-	expression tag	UNP Q8IL98
K	42	LEU	-	expression tag	UNP Q8IL98
K	43	TYR	-	expression tag	UNP Q8IL98
K	44	PHE	-	expression tag	UNP Q8IL98
K	45	GLN	-	expression tag	UNP Q8IL98
K	46	GLY	-	expression tag	UNP Q8IL98
K	47	HIS	-	expression tag	UNP Q8IL98
K	48	MET	-	expression tag	UNP Q8IL98

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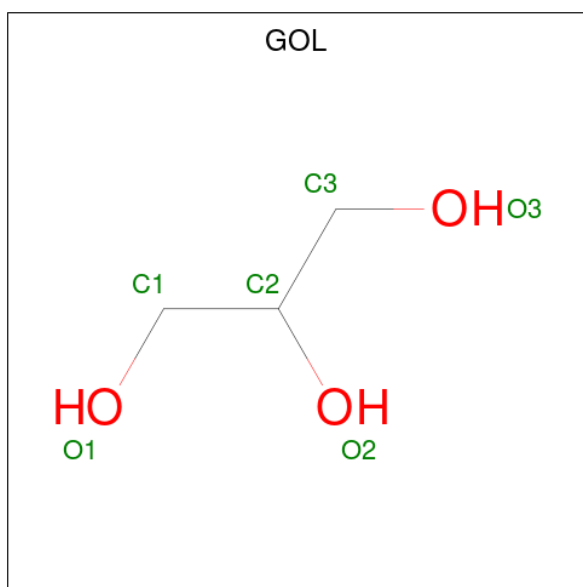
Chain	Residue	Modelled	Actual	Comment	Reference
L	26	MET	-	expression tag	UNP Q8IL98
L	27	GLY	-	expression tag	UNP Q8IL98
L	28	SER	-	expression tag	UNP Q8IL98
L	29	SER	-	expression tag	UNP Q8IL98
L	30	HIS	-	expression tag	UNP Q8IL98
L	31	HIS	-	expression tag	UNP Q8IL98
L	32	HIS	-	expression tag	UNP Q8IL98
L	33	HIS	-	expression tag	UNP Q8IL98
L	34	HIS	-	expression tag	UNP Q8IL98
L	35	HIS	-	expression tag	UNP Q8IL98
L	36	SER	-	expression tag	UNP Q8IL98
L	37	SER	-	expression tag	UNP Q8IL98
L	38	GLY	-	expression tag	UNP Q8IL98
L	39	ARG	-	expression tag	UNP Q8IL98
L	40	GLU	-	expression tag	UNP Q8IL98
L	41	ASN	-	expression tag	UNP Q8IL98
L	42	LEU	-	expression tag	UNP Q8IL98
L	43	TYR	-	expression tag	UNP Q8IL98
L	44	PHE	-	expression tag	UNP Q8IL98
L	45	GLN	-	expression tag	UNP Q8IL98
L	46	GLY	-	expression tag	UNP Q8IL98
L	47	HIS	-	expression tag	UNP Q8IL98
L	48	MET	-	expression tag	UNP Q8IL98
M	26	MET	-	expression tag	UNP Q8IL98
M	27	GLY	-	expression tag	UNP Q8IL98
M	28	SER	-	expression tag	UNP Q8IL98
M	29	SER	-	expression tag	UNP Q8IL98
M	30	HIS	-	expression tag	UNP Q8IL98
M	31	HIS	-	expression tag	UNP Q8IL98
M	32	HIS	-	expression tag	UNP Q8IL98
M	33	HIS	-	expression tag	UNP Q8IL98
M	34	HIS	-	expression tag	UNP Q8IL98
M	35	HIS	-	expression tag	UNP Q8IL98
M	36	SER	-	expression tag	UNP Q8IL98
M	37	SER	-	expression tag	UNP Q8IL98
M	38	GLY	-	expression tag	UNP Q8IL98
M	39	ARG	-	expression tag	UNP Q8IL98
M	40	GLU	-	expression tag	UNP Q8IL98
M	41	ASN	-	expression tag	UNP Q8IL98
M	42	LEU	-	expression tag	UNP Q8IL98
M	43	TYR	-	expression tag	UNP Q8IL98
M	44	PHE	-	expression tag	UNP Q8IL98

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Chain	Residue	Modelled	Actual	Comment	Reference
M	45	GLN	-	expression tag	UNP Q8IL98
M	46	GLY	-	expression tag	UNP Q8IL98
M	47	HIS	-	expression tag	UNP Q8IL98
M	48	MET	-	expression tag	UNP Q8IL98
N	26	MET	-	expression tag	UNP Q8IL98
N	27	GLY	-	expression tag	UNP Q8IL98
N	28	SER	-	expression tag	UNP Q8IL98
N	29	SER	-	expression tag	UNP Q8IL98
N	30	HIS	-	expression tag	UNP Q8IL98
N	31	HIS	-	expression tag	UNP Q8IL98
N	32	HIS	-	expression tag	UNP Q8IL98
N	33	HIS	-	expression tag	UNP Q8IL98
N	34	HIS	-	expression tag	UNP Q8IL98
N	35	HIS	-	expression tag	UNP Q8IL98
N	36	SER	-	expression tag	UNP Q8IL98
N	37	SER	-	expression tag	UNP Q8IL98
N	38	GLY	-	expression tag	UNP Q8IL98
N	39	ARG	-	expression tag	UNP Q8IL98
N	40	GLU	-	expression tag	UNP Q8IL98
N	41	ASN	-	expression tag	UNP Q8IL98
N	42	LEU	-	expression tag	UNP Q8IL98
N	43	TYR	-	expression tag	UNP Q8IL98
N	44	PHE	-	expression tag	UNP Q8IL98
N	45	GLN	-	expression tag	UNP Q8IL98
N	46	GLY	-	expression tag	UNP Q8IL98
N	47	HIS	-	expression tag	UNP Q8IL98
N	48	MET	-	expression tag	UNP Q8IL98

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		

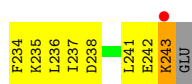
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	8	Total	O	0	0
			8	8		
3	C	11	Total	O	0	0
			11	11		
3	D	2	Total	O	0	0
			2	2		
3	E	6	Total	O	0	0
			6	6		
3	F	7	Total	O	0	0
			7	7		
3	G	3	Total	O	0	0
			3	3		
3	H	6	Total	O	0	0
			6	6		
3	I	3	Total	O	0	0
			3	3		
3	J	2	Total	O	0	0
			2	2		

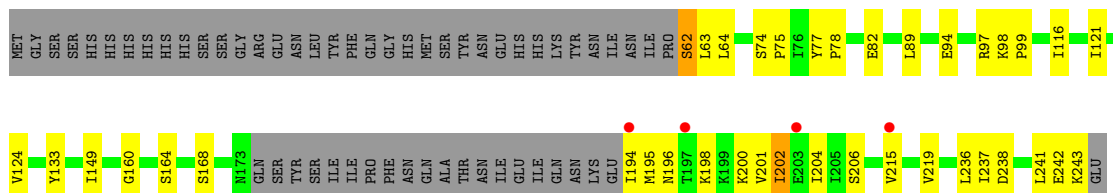
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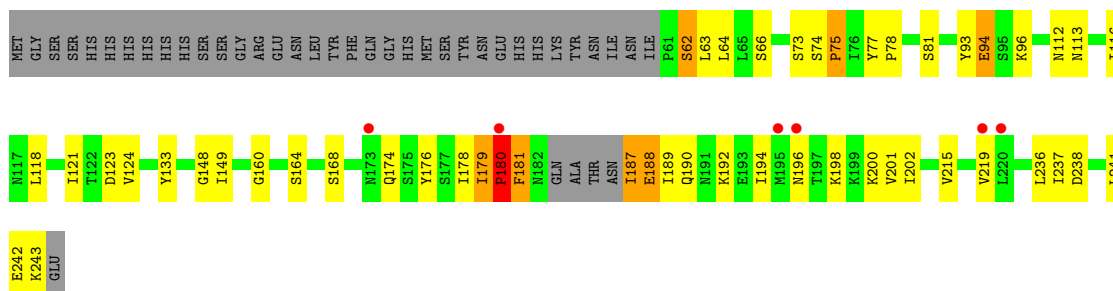
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	1	Total 1	O 1	0	0
3	L	4	Total 4	O 4	0	0
3	M	6	Total 6	O 6	0	0
3	N	1	Total 1	O 1	0	0



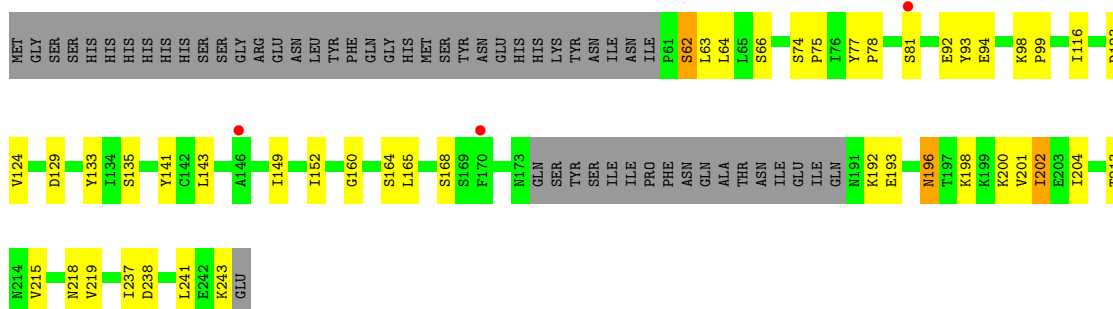
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



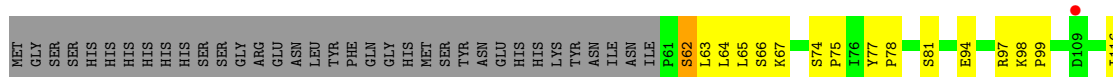
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

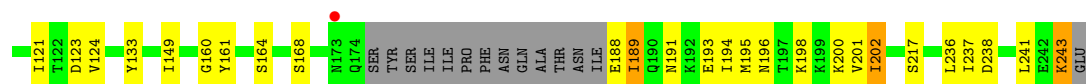


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

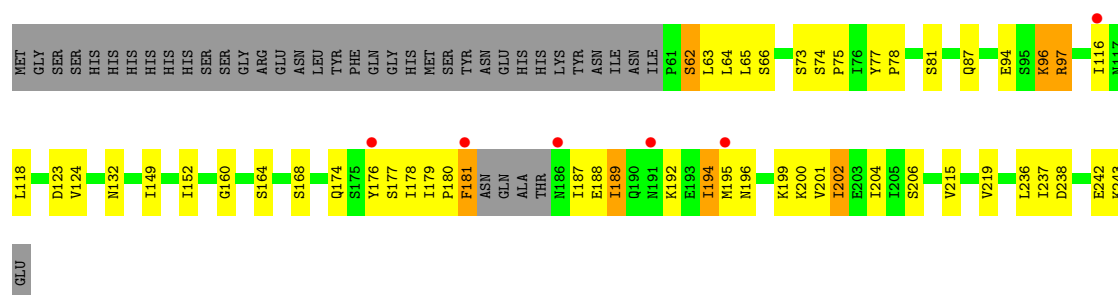


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

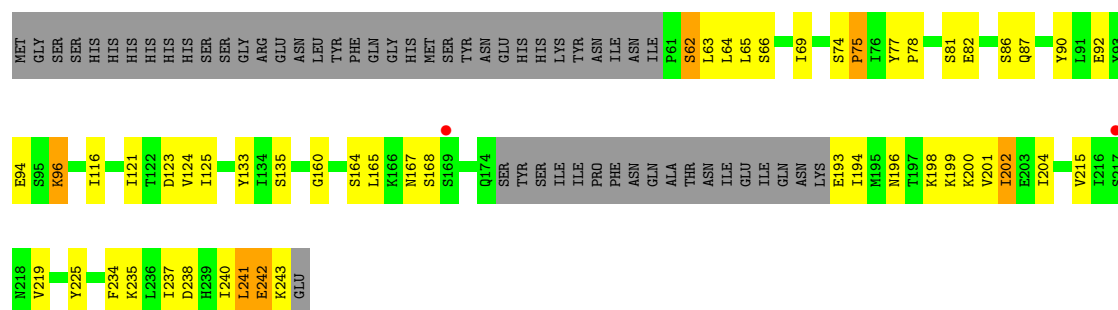




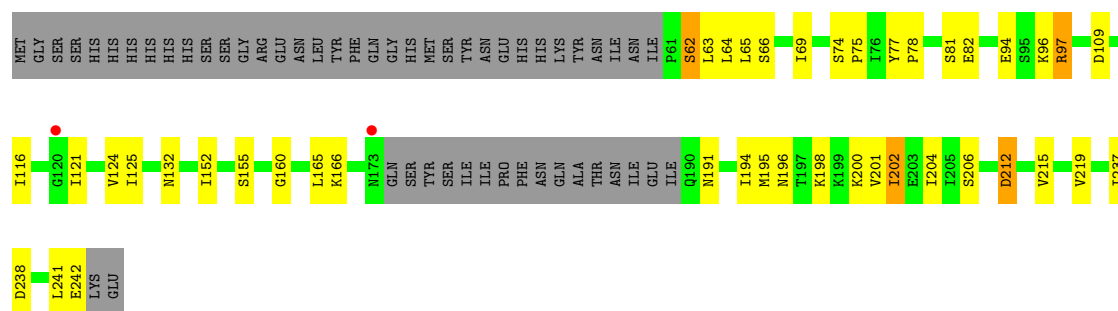
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

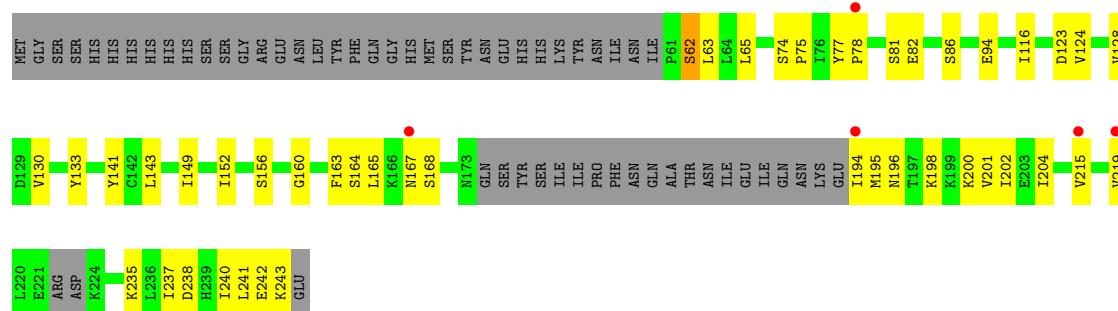


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

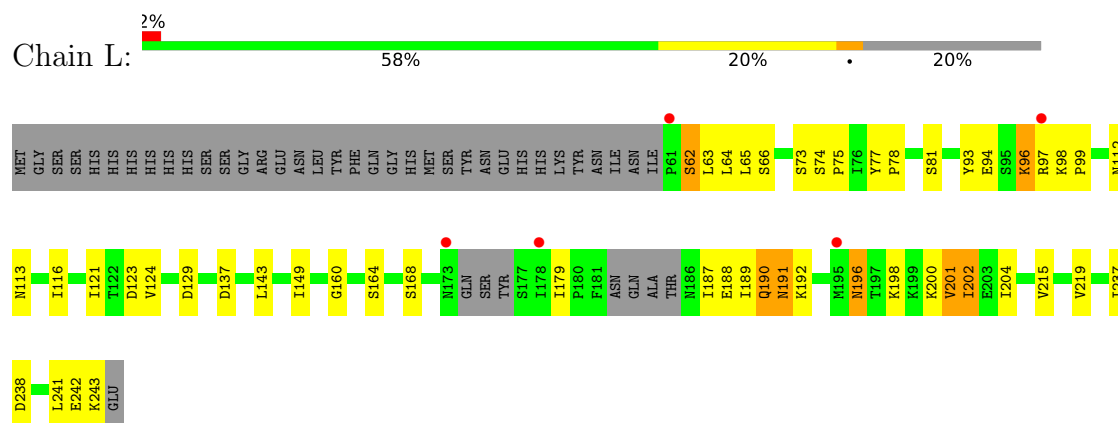


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

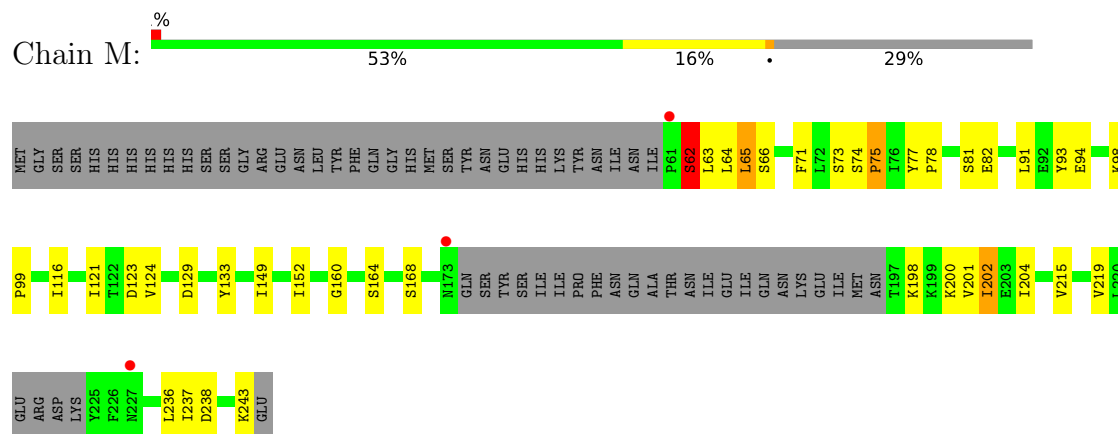




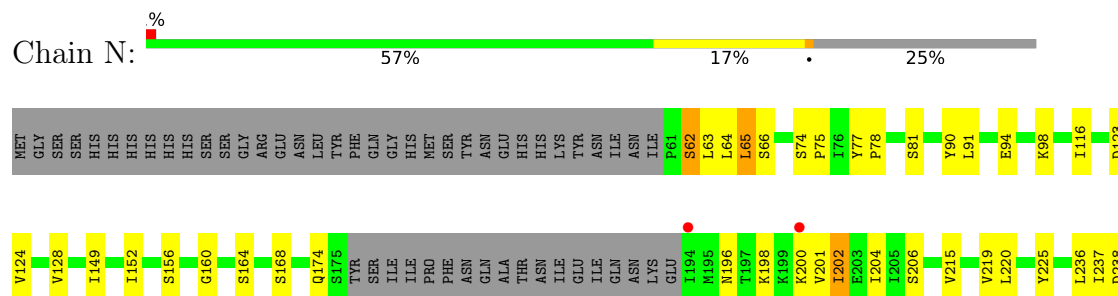
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



• Molecule 1: ATP-dependent Clp protease proteolytic subunit



• Molecule 1: ATP-dependent Clp protease proteolytic subunit





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.78Å 105.85Å 186.40Å 90.00° 118.10° 90.00°	Depositor
Resolution (Å)	45.54 – 2.90 45.54 – 2.90	Depositor EDS
% Data completeness (in resolution range)	88.6 (45.54-2.90) 96.7 (45.54-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.202 , 0.243 0.198 , 0.190	Depositor DCC
R_{free} test set	3354 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 99.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18940	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0580e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.52	0/1467	0.96	9/1979 (0.5%)
1	B	0.44	0/1315	0.82	2/1774 (0.1%)
1	C	0.48	0/1350	0.97	7/1819 (0.4%)
1	D	0.42	0/1316	0.82	0/1774
1	E	0.51	0/1462	0.90	6/1972 (0.3%)
1	F	0.43	0/1358	0.84	0/1830
1	G	0.46	0/1385	0.87	1/1866 (0.1%)
1	H	0.44	0/1462	0.84	3/1972 (0.2%)
1	I	0.41	0/1342	0.82	2/1809 (0.1%)
1	J	0.41	0/1350	0.94	4/1820 (0.2%)
1	K	0.41	0/1304	0.81	0/1757
1	L	0.42	0/1433	0.83	3/1931 (0.2%)
1	M	0.41	0/1262	0.82	3/1702 (0.2%)
1	N	0.41	0/1339	0.82	0/1805
All	All	0.44	0/19145	0.86	40/25810 (0.2%)

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	5
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	4
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
All	All	0	22

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	97	ARG	NE-CZ-NH2	13.06	130.96	119.20
1	C	97	ARG	NE-CZ-NH2	12.52	130.47	119.20
1	C	97	ARG	NE-CZ-NH1	-12.51	108.99	121.50
1	J	97	ARG	NE-CZ-NH1	-11.93	109.57	121.50
1	A	189	ILE	N-CA-C	-10.78	99.62	110.62

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	LEU	Peptide
1	A	173	ASN	Peptide
1	A	174	GLN	Peptide
1	A	188	GLU	Peptide
1	A	62	SER	Peptide

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	1444	0	1481	67	0
1	B	1295	0	1334	45	0
1	C	1330	0	1372	38	0
1	D	1297	0	1339	33	0
1	E	1439	0	1479	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1338	0	1377	38	0
1	G	1365	0	1405	51	0
1	H	1439	0	1479	56	0
1	I	1322	0	1361	63	0
1	J	1330	0	1367	42	0
1	K	1285	0	1329	40	0
1	L	1412	0	1456	46	0
1	M	1243	0	1284	46	0
1	N	1319	0	1360	43	0
2	C	6	0	8	4	0
2	I	6	0	8	8	0
3	A	10	0	0	0	0
3	B	8	0	0	3	0
3	C	11	0	0	1	0
3	D	2	0	0	1	0
3	E	6	0	0	1	0
3	F	7	0	0	1	0
3	G	3	0	0	0	0
3	H	6	0	0	0	0
3	I	3	0	0	0	0
3	J	2	0	0	1	0
3	K	1	0	0	1	0
3	L	4	0	0	1	0
3	M	6	0	0	2	0
3	N	1	0	0	0	0
All	All	18940	0	19439	596	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 16.

The worst 5 of 596 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ASN:HB3	3:B:307:HOH:O	1.34	1.22
1:H:187:ILE:HG13	1:H:188:GLU:H	1.06	1.18
1:E:124:VAL:HG21	1:E:149:ILE:HB	1.25	1.17
1:L:124:VAL:HG21	1:L:149:ILE:HB	1.25	1.17
1:G:124:VAL:HG21	1:G:149:ILE:HB	1.17	1.16

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	176/219 (80%)	163 (93%)	12 (7%)	1 (1%)	21	51
1	B	158/219 (72%)	152 (96%)	6 (4%)	0	100	100
1	C	162/219 (74%)	156 (96%)	6 (4%)	0	100	100
1	D	158/219 (72%)	152 (96%)	6 (4%)	0	100	100
1	E	175/219 (80%)	166 (95%)	8 (5%)	1 (1%)	21	51
1	F	163/219 (74%)	157 (96%)	6 (4%)	0	100	100
1	G	166/219 (76%)	160 (96%)	6 (4%)	0	100	100
1	H	175/219 (80%)	167 (95%)	8 (5%)	0	100	100
1	I	161/219 (74%)	156 (97%)	5 (3%)	0	100	100
1	J	162/219 (74%)	156 (96%)	6 (4%)	0	100	100
1	K	155/219 (71%)	149 (96%)	6 (4%)	0	100	100
1	L	170/219 (78%)	163 (96%)	7 (4%)	0	100	100
1	M	150/219 (68%)	146 (97%)	4 (3%)	0	100	100
1	N	161/219 (74%)	157 (98%)	4 (2%)	0	100	100
All	All	2292/3066 (75%)	2200 (96%)	90 (4%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	180	PRO
1	A	187	ILE

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	168/204 (82%)	162 (96%)	6 (4%)	31	65
1	B	151/204 (74%)	147 (97%)	4 (3%)	40	73
1	C	155/204 (76%)	152 (98%)	3 (2%)	50	79
1	D	151/204 (74%)	149 (99%)	2 (1%)	61	86
1	E	168/204 (82%)	163 (97%)	5 (3%)	36	70
1	F	156/204 (76%)	152 (97%)	4 (3%)	40	73
1	G	159/204 (78%)	153 (96%)	6 (4%)	29	64
1	H	168/204 (82%)	162 (96%)	6 (4%)	31	65
1	I	154/204 (76%)	150 (97%)	4 (3%)	40	73
1	J	155/204 (76%)	149 (96%)	6 (4%)	28	63
1	K	150/204 (74%)	147 (98%)	3 (2%)	48	78
1	L	165/204 (81%)	158 (96%)	7 (4%)	26	60
1	M	145/204 (71%)	142 (98%)	3 (2%)	47	77
1	N	154/204 (76%)	151 (98%)	3 (2%)	50	79
All	All	2199/2856 (77%)	2137 (97%)	62 (3%)	38	72

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	217	SER
1	L	202	ILE
1	H	202	ILE
1	L	196	ASN
1	N	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	83	GLN
1	N	83	GLN
1	M	83	GLN
1	F	83	GLN
1	K	83	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 ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	I	301	-	5,5,5	0.38	0	5,5,5	0.32	0
2	GOL	C	301	-	5,5,5	0.37	0	5,5,5	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	I	301	-	-	4/4/4/4	-
2	GOL	C	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	GOL	C1-C2-C3-O3
2	I	301	GOL	O1-C1-C2-C3
2	I	301	GOL	C1-C2-C3-O3
2	C	301	GOL	O1-C1-C2-O2
2	I	301	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	301	GOL	8	0
2	C	301	GOL	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	180/219 (82%)	0.08	14 (7%)	19	16	28, 67, 152, 166	0
1	B	162/219 (73%)	-0.14	3 (1%)	66	58	35, 78, 145, 166	0
1	C	166/219 (75%)	-0.04	5 (3%)	52	43	32, 69, 148, 176	0
1	D	162/219 (73%)	0.17	4 (2%)	58	48	41, 93, 153, 181	0
1	E	179/219 (81%)	0.06	6 (3%)	48	39	36, 68, 144, 215	0
1	F	166/219 (75%)	-0.02	3 (1%)	67	59	39, 80, 151, 165	1 (0%)
1	G	170/219 (77%)	-0.15	2 (1%)	76	69	37, 78, 156, 187	0
1	H	179/219 (81%)	-0.02	6 (3%)	48	39	35, 78, 160, 206	0
1	I	165/219 (75%)	-0.07	2 (1%)	76	69	42, 79, 151, 171	0
1	J	166/219 (75%)	0.00	2 (1%)	76	69	46, 87, 155, 182	0
1	K	161/219 (73%)	0.18	5 (3%)	51	42	53, 95, 154, 184	0
1	L	176/219 (80%)	0.01	5 (2%)	55	46	42, 80, 155, 191	0
1	M	156/219 (71%)	0.24	3 (1%)	66	58	51, 90, 142, 161	0
1	N	165/219 (75%)	-0.12	2 (1%)	76	69	43, 83, 152, 168	0
All	All	2353/3066 (76%)	0.01	62 (2%)	57	48	28, 81, 153, 215	1 (0%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	167	ASN	4.1
1	A	173	ASN	3.8
1	C	173	ASN	3.8
1	C	148	GLY	3.6
1	A	182	ASN	3.5

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($\text{\AA}^2$)	Q<0.9
2	GOL	I	301	6/6	0.71	0.11	89,128,153,155	0
2	GOL	C	301	6/6	0.87	0.10	74,88,102,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.