Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:15 PM GMT

PDB ID	:	4HNK
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

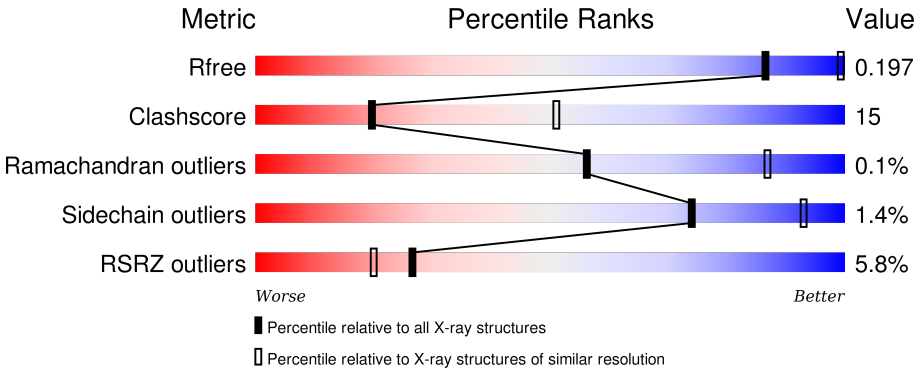
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 55% 24% 18%
1	B	219	2% 53% 20% 26%
1	C	219	% 58% 16% 24%
1	D	219	12% 58% 16% 26%
1	E	219	2% 60% 19% 18%

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Mol	Chain	Length	Quality of chain
1	F	219	3% 58% 17% 24%
1	G	219	4% 60% 17% 22%
1	H	219	4% 59% 21% 18%
1	I	219	% 54% 20% 25%
1	J	219	4% 58% 17% 24%
1	K	219	11% 54% 19% 26%
1	L	219	2% 58% 21% 20%
1	M	219	6% 54% 16% 29%
1	N	219	7% 58% 16% 25%

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	X
2	GOL	I	301	-	-	X	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
G	36	SER	-	EXPRESSION TAG	UNP Q8IL98
G	37	SER	-	EXPRESSION TAG	UNP Q8IL98
G	38	GLY	-	EXPRESSION TAG	UNP Q8IL98
G	39	ARG	-	EXPRESSION TAG	UNP Q8IL98
G	40	GLU	-	EXPRESSION TAG	UNP Q8IL98
G	41	ASN	-	EXPRESSION TAG	UNP Q8IL98
G	42	LEU	-	EXPRESSION TAG	UNP Q8IL98
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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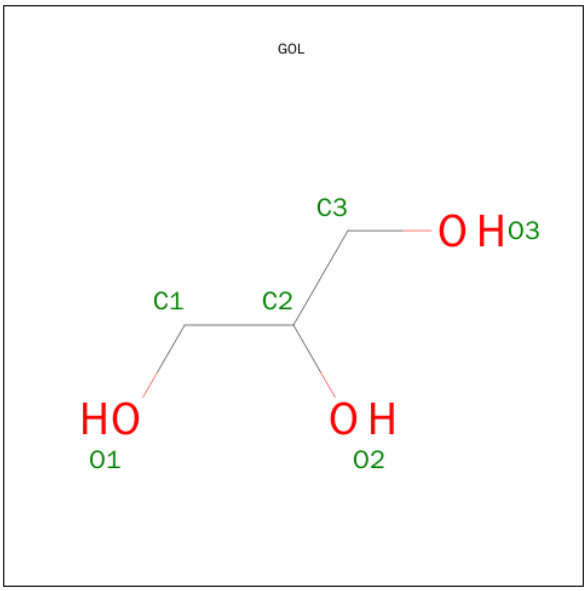
Chain	Residue	Modelled	Actual	Comment	Reference
M	45	GLN	-	EXPRESSION TAG	UNP Q8IL98
M	46	GLY	-	EXPRESSION TAG	UNP Q8IL98
M	47	HIS	-	EXPRESSION TAG	UNP Q8IL98
M	48	MET	-	EXPRESSION TAG	UNP Q8IL98
N	26	MET	-	EXPRESSION TAG	UNP Q8IL98
N	27	GLY	-	EXPRESSION TAG	UNP Q8IL98
N	28	SER	-	EXPRESSION TAG	UNP Q8IL98
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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

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

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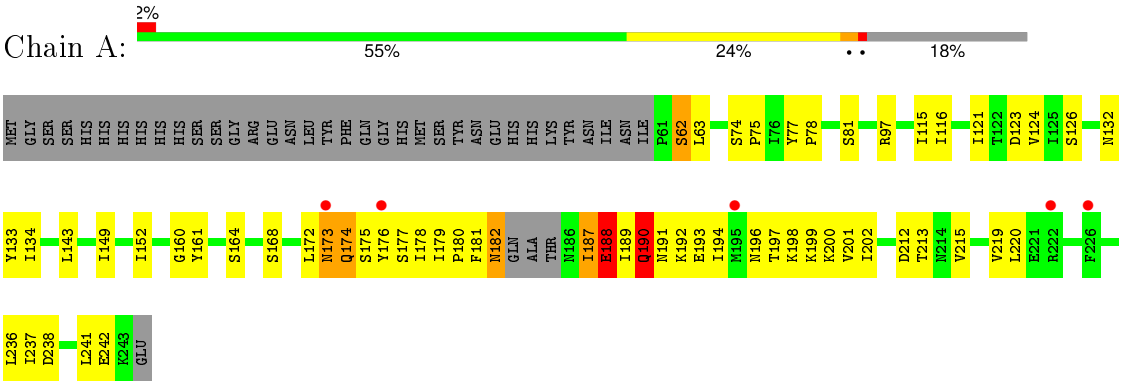
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	1	Total O 1 1	0	0
3	L	4	Total O 4 4	0	0
3	M	6	Total O 6 6	0	0
3	N	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

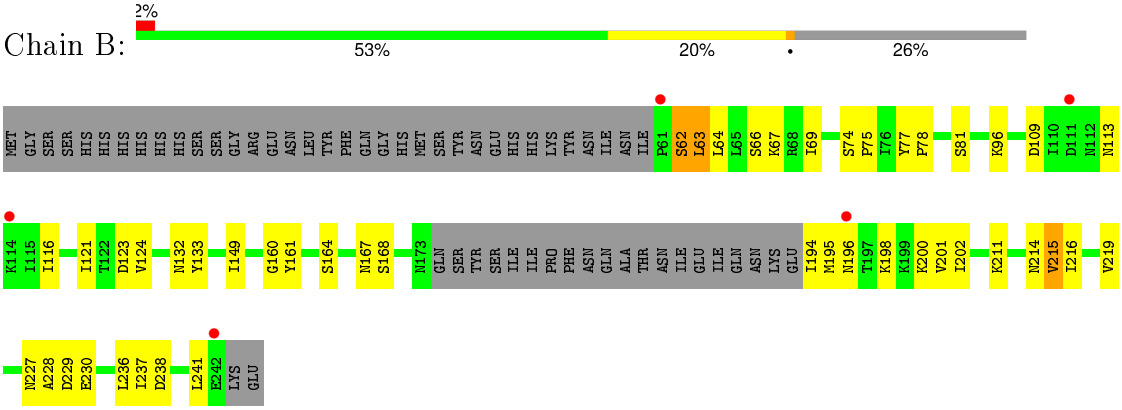
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



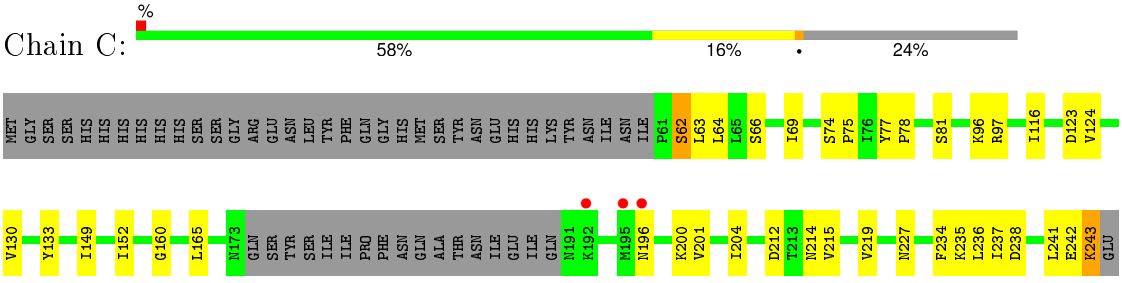
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:

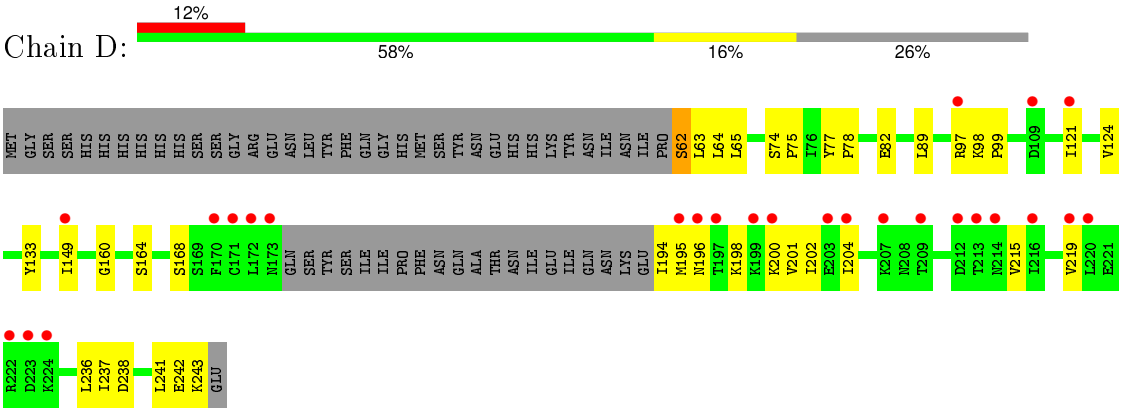


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

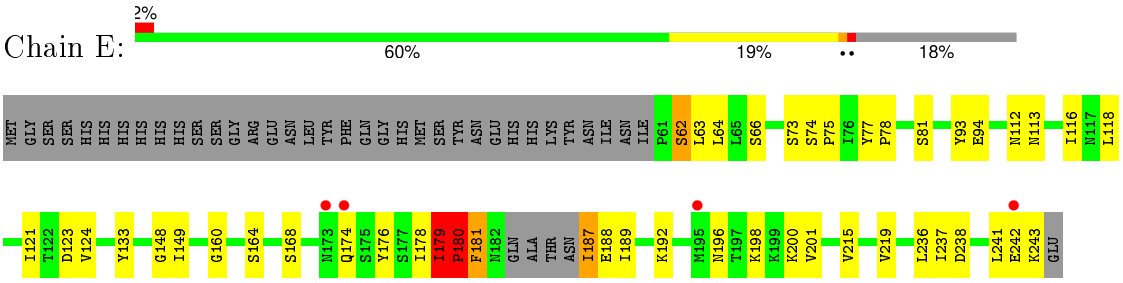
Chain C:



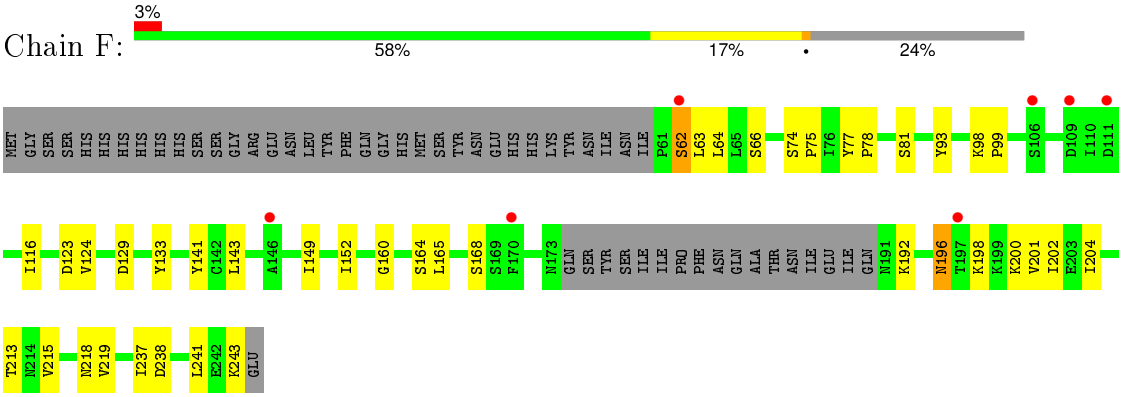
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



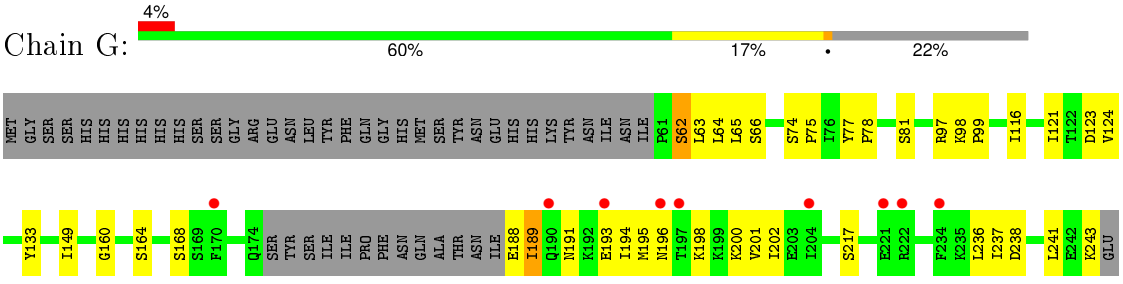
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



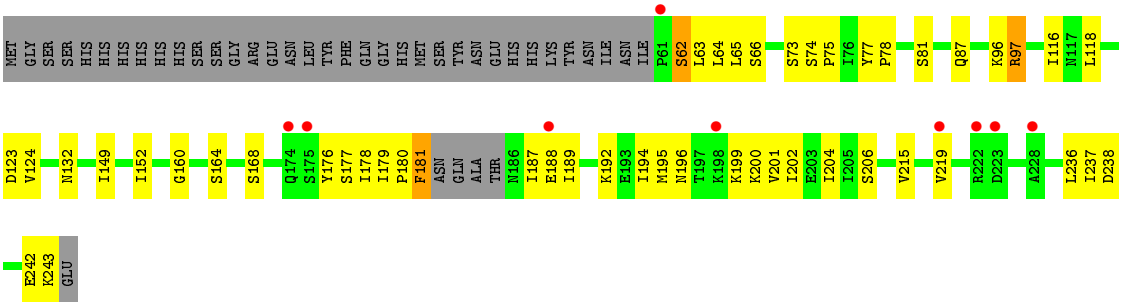
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

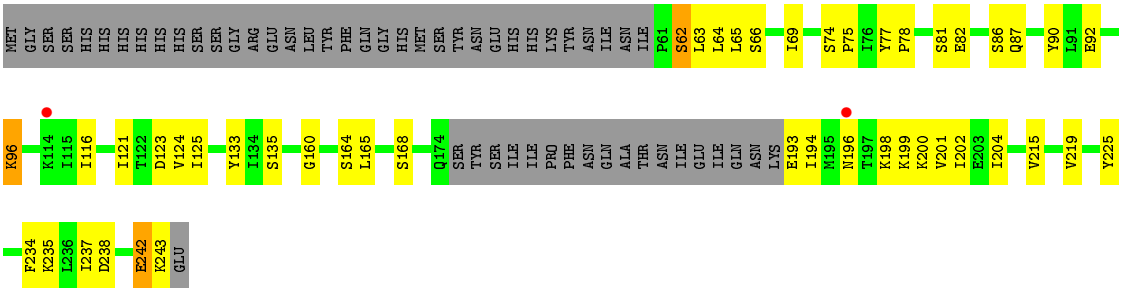


• Molecule 1: ATP-dependent Clp protease proteolytic subunit



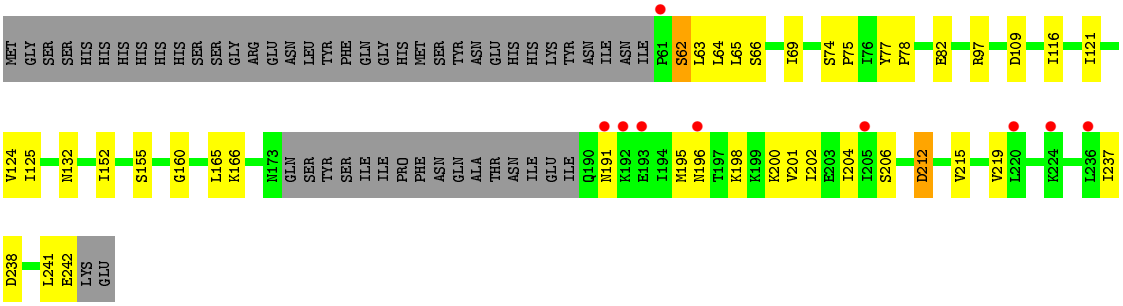
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:



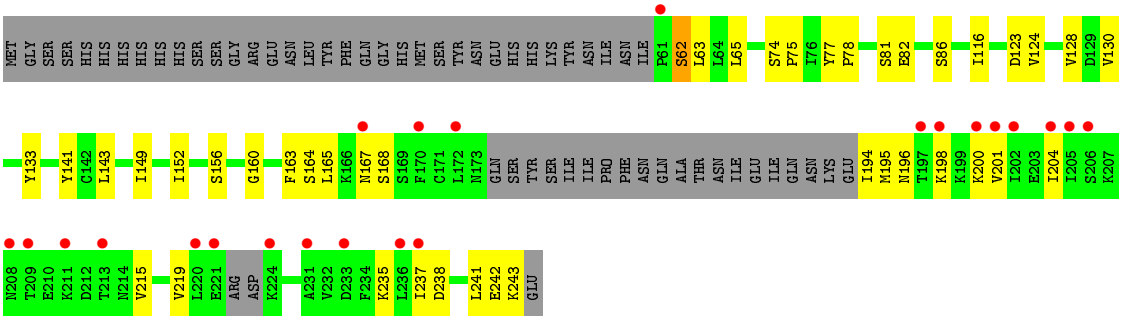
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



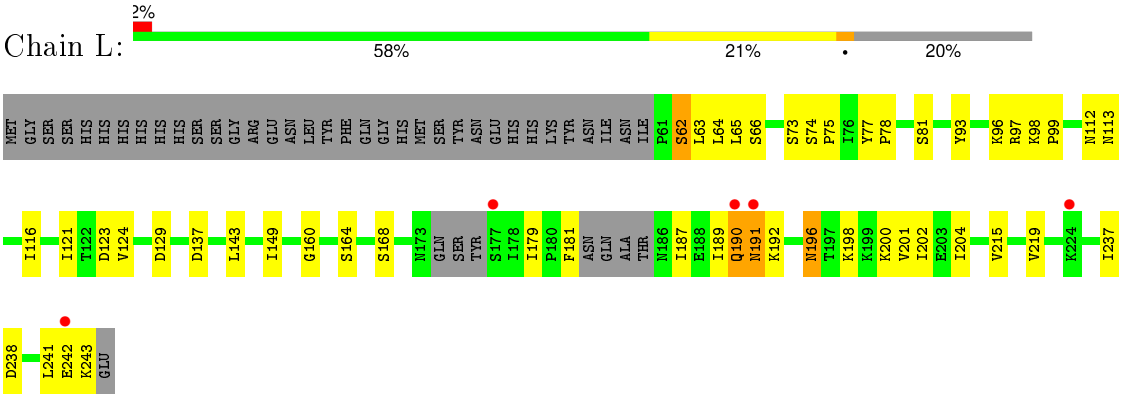
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



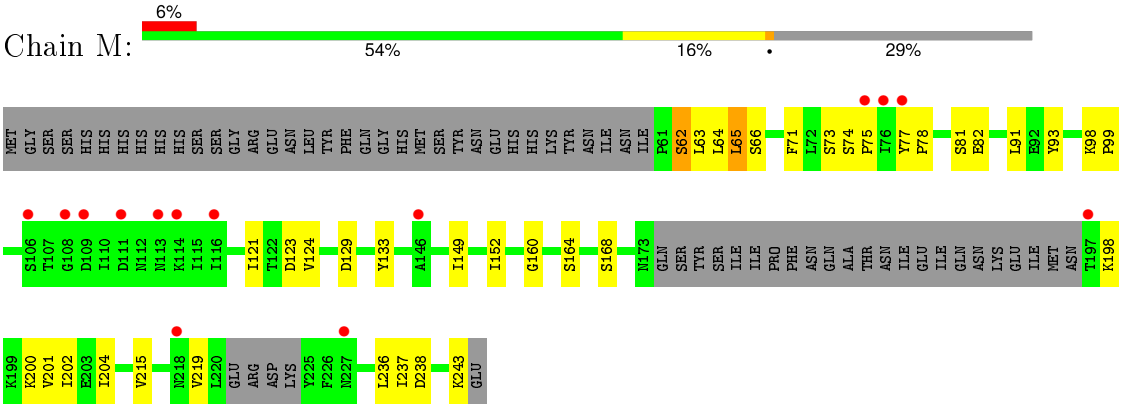
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



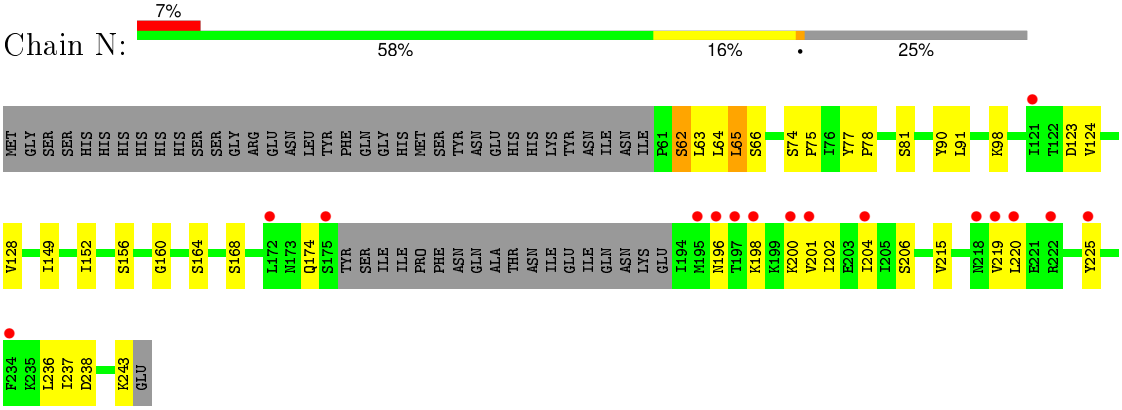
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:



4 Data and refinement statistics (i)

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 47.08 – 2.88	Depositor EDS
% Data completeness (in resolution range)	88.6 (45.54-2.90) 95.3 (47.08-2.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.202 , 0.243 0.203 , 0.197	Depositor DCC
R_{free} test set	3328 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 80.9	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	3 of 66495 reflections (0.005%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.39	0/1467	0.65	1/1979 (0.1%)
1	B	0.36	0/1315	0.57	0/1774
1	C	0.37	0/1350	0.93	3/1819 (0.2%)
1	D	0.34	0/1316	0.57	0/1774
1	E	0.40	0/1462	0.62	1/1972 (0.1%)
1	F	0.35	0/1358	0.60	0/1830
1	G	0.36	0/1385	0.57	0/1866
1	H	0.35	0/1462	0.56	0/1972
1	I	0.33	0/1342	0.56	0/1809
1	J	0.35	0/1350	0.92	3/1820 (0.2%)
1	K	0.34	0/1304	0.55	0/1757
1	L	0.35	0/1433	0.54	0/1931
1	M	0.34	0/1262	0.54	0/1702
1	N	0.34	0/1339	0.57	0/1805
All	All	0.36	0/19145	0.64	8/25810 (0.0%)

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.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	97	ARG	NE-CZ-NH1	-22.61	108.99	120.30
1	J	97	ARG	NE-CZ-NH1	-21.46	109.57	120.30
1	J	97	ARG	NE-CZ-NH2	21.31	130.96	120.30
1	C	97	ARG	NE-CZ-NH2	20.33	130.47	120.30
1	J	97	ARG	CD-NE-CZ	10.62	138.47	123.60
1	C	97	ARG	CD-NE-CZ	10.18	137.84	123.60
1	E	179	ILE	C-N-CD	-6.75	105.75	120.60
1	A	190	GLN	CB-CA-C	-6.70	96.99	110.40

There are no chirality outliers.

All (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
1	B	62	SER	Peptide
1	C	62	SER	Peptide
1	D	62	SER	Peptide
1	E	179	ILE	Peptide
1	E	180	PRO	Peptide
1	E	181	PHE	Peptide
1	E	62	SER	Peptide
1	F	62	SER	Peptide
1	G	62	SER	Peptide
1	H	62	SER	Peptide
1	I	242	GLU	Peptide
1	I	62	SER	Peptide

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Mol	Chain	Res	Type	Group
1	J	62	SER	Peptide
1	K	62	SER	Peptide
1	L	62	SER	Peptide
1	M	62	SER	Peptide
1	N	62	SER	Peptide

5.2 Too-close contacts (i)

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	65	0
1	B	1295	0	1334	44	0
1	C	1330	0	1372	36	0
1	D	1297	0	1339	30	0
1	E	1439	0	1479	58	0
1	F	1338	0	1377	35	0
1	G	1365	0	1405	48	0
1	H	1439	0	1479	55	0
1	I	1322	0	1361	60	0
1	J	1330	0	1367	41	0
1	K	1285	0	1329	39	0
1	L	1412	0	1456	42	0
1	M	1243	0	1284	45	0
1	N	1319	0	1360	42	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	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	6	0	0	2	0
3	N	1	0	0	0	0
All	All	18940	0	19439	572	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 15.

All (572) 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:H:187:ILE:HG23	1:H:189:ILE:H	1.10	1.16
1:G:124:VAL:HG21	1:G:149:ILE:HB	1.17	1.16
1:N:124:VAL:HG21	1:N:149:ILE:HB	1.25	1.15
1:K:124:VAL:HG21	1:K:149:ILE:HB	1.13	1.12
1:M:124:VAL:HG21	1:M:149:ILE:HB	1.16	1.12
1:A:124:VAL:HG21	1:A:149:ILE:HB	1.25	1.11
1:F:124:VAL:HG21	1:F:149:ILE:HB	1.22	1.10
1:H:124:VAL:HG21	1:H:149:ILE:HB	1.17	1.09
1:C:124:VAL:HG21	1:C:149:ILE:HB	1.14	1.09
1:D:124:VAL:HG21	1:D:149:ILE:HB	1.19	1.09
1:M:82:GLU:HG3	3:M:306:HOH:O	1.50	1.08
1:B:124:VAL:HG21	1:B:149:ILE:HB	1.23	1.08
1:A:187:ILE:HG22	1:A:190:GLN:H	1.23	1.04
1:A:173:ASN:OD1	1:A:174:GLN:HG2	1.61	0.99
1:J:241:LEU:HD23	1:M:133:TYR:CE1	1.99	0.96
1:H:187:ILE:HG13	1:H:188:GLU:N	1.73	0.96
1:A:174:GLN:HB3	1:A:175:SER:HB3	1.46	0.96
1:A:189:ILE:O	1:A:192:LYS:HB3	1.70	0.92
1:H:118:LEU:HD22	1:H:178:ILE:HG21	1.49	0.92
1:K:235:LYS:HA	3:K:301:HOH:O	1.68	0.91
1:I:90:TYR:CE1	1:M:63:LEU:HG	2.05	0.91
1:L:112:ASN:O	1:L:113:ASN:HB2	1.72	0.90
1:J:166:LYS:HD3	1:J:242:GLU:OE1	1.73	0.89
1:E:179:ILE:O	1:E:179:ILE:HG22	1.71	0.88
1:I:165:LEU:HD13	1:L:129:ASP:HB3	1.53	0.88
1:H:187:ILE:HG23	1:H:189:ILE:N	1.88	0.88
1:H:187:ILE:CG1	1:H:188:GLU:H	1.87	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLN:HG3	1:A:191:ASN:N	1.91	0.85
1:E:188:GLU:HG3	1:E:189:ILE:H	1.40	0.84
1:E:188:GLU:HG3	1:E:189:ILE:N	1.93	0.84
1:M:124:VAL:HG21	1:M:149:ILE:CB	2.06	0.84
1:C:124:VAL:HG21	1:C:149:ILE:CB	2.06	0.83
1:H:73:SER:HB2	1:J:82:GLU:HG2	1.59	0.83
1:G:191:ASN:O	1:G:194:ILE:HG22	1.78	0.83
1:G:98:LYS:HE3	1:N:98:LYS:NZ	1.92	0.82
1:K:124:VAL:HG21	1:K:149:ILE:CB	2.04	0.81
1:H:124:VAL:HG21	1:H:149:ILE:CB	2.08	0.80
1:G:188:GLU:HG2	1:G:189:ILE:H	1.46	0.78
1:E:180:PRO:O	1:E:181:PHE:HD2	1.66	0.78
1:K:242:GLU:O	1:K:243:LYS:CB	2.32	0.78
1:F:192:LYS:O	1:F:196:ASN:HB2	1.84	0.78
1:I:92:GLU:HG2	2:I:301:GOL:H11	1.66	0.77
1:J:121:ILE:O	1:J:124:VAL:HG12	1.84	0.77
1:H:189:ILE:HG12	1:N:225:TYR:CD1	2.19	0.77
1:A:187:ILE:HG22	1:A:188:GLU:N	1.99	0.76
1:A:173:ASN:OD1	1:A:174:GLN:CG	2.34	0.76
1:E:188:GLU:CG	1:E:189:ILE:H	1.98	0.76
1:I:242:GLU:HG3	1:I:243:LYS:HG2	1.67	0.75
1:I:193:GLU:HG2	1:I:194:ILE:H	1.51	0.75
1:J:166:LYS:CD	1:J:242:GLU:OE1	2.34	0.74
1:K:242:GLU:O	1:K:243:LYS:HB2	1.87	0.74
1:I:96:LYS:HE2	2:I:301:GOL:O1	1.88	0.74
1:J:241:LEU:HD23	1:M:133:TYR:CD1	2.23	0.74
1:I:242:GLU:CD	1:I:243:LYS:HE2	2.07	0.74
1:C:242:GLU:O	1:C:243:LYS:HG3	1.87	0.73
1:E:112:ASN:O	1:E:113:ASN:HB2	1.86	0.73
1:J:191:ASN:O	1:J:195:MET:HG2	1.88	0.73
1:A:187:ILE:CG2	1:A:190:GLN:H	2.01	0.73
1:G:124:VAL:HG21	1:G:149:ILE:CB	2.10	0.72
1:N:174:GLN:HB2	1:N:220:LEU:O	1.90	0.72
1:A:133:TYR:CE1	1:G:241:LEU:HD13	2.25	0.71
1:I:193:GLU:HG2	1:I:194:ILE:N	2.06	0.71
1:I:96:LYS:CE	2:I:301:GOL:O1	2.38	0.71
1:H:189:ILE:HG12	1:N:225:TYR:CE1	2.25	0.71
1:G:194:ILE:HG23	1:G:195:MET:N	2.06	0.70
1:I:121:ILE:O	1:I:124:VAL:HG12	1.91	0.70
1:E:174:GLN:O	1:E:174:GLN:HG3	1.91	0.69
1:G:124:VAL:CG2	1:G:149:ILE:HB	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:SER:O	1:L:63:LEU:C	2.31	0.69
1:E:192:LYS:O	1:E:196:ASN:HB2	1.93	0.68
1:A:182:ASN:CG	1:A:182:ASN:O	2.32	0.68
1:B:133:TYR:CE1	1:F:241:LEU:HD13	2.28	0.68
1:I:225:TYR:CE1	1:L:189:ILE:HD13	2.29	0.67
1:A:188:GLU:HA	1:A:190:GLN:HB3	1.77	0.67
1:L:63:LEU:O	1:L:66:SER:N	2.25	0.67
1:L:124:VAL:HG21	1:L:149:ILE:CB	2.16	0.67
1:D:124:VAL:HG21	1:D:149:ILE:CB	2.11	0.67
1:A:191:ASN:HA	1:A:194:ILE:HG13	1.77	0.66
1:B:67:LYS:NZ	1:E:94:GLU:HA	2.10	0.66
1:G:194:ILE:CG2	1:G:195:MET:H	2.08	0.66
1:B:230:GLU:HG3	3:B:307:HOH:O	1.95	0.66
1:B:124:VAL:HG21	1:B:149:ILE:CB	2.14	0.66
1:G:191:ASN:HA	1:G:194:ILE:HG22	1.77	0.66
1:M:62:SER:O	1:M:63:LEU:C	2.35	0.65
1:B:132:ASN:O	1:F:243:LYS:HB2	1.96	0.65
1:L:242:GLU:O	1:L:243:LYS:C	2.35	0.65
1:K:167:ASN:ND2	1:N:200:LYS:HD3	2.11	0.65
1:M:63:LEU:O	1:M:66:SER:N	2.29	0.64
1:A:152:ILE:HD13	1:A:201:VAL:HG23	1.80	0.64
1:H:152:ILE:HD13	1:H:201:VAL:HG23	1.79	0.64
1:L:179:ILE:HG13	1:L:179:ILE:O	1.98	0.64
1:K:152:ILE:HD13	1:K:201:VAL:HG23	1.80	0.64
1:E:118:LEU:HD22	1:E:178:ILE:HG21	1.80	0.63
1:D:242:GLU:O	1:D:243:LYS:CB	2.46	0.63
1:J:241:LEU:HD23	1:M:133:TYR:HE1	1.60	0.63
1:C:242:GLU:C	1:C:243:LYS:HG3	2.18	0.63
1:D:124:VAL:CG2	1:D:149:ILE:HB	2.13	0.63
1:H:189:ILE:HG21	1:N:225:TYR:CZ	2.32	0.62
1:F:124:VAL:HG21	1:F:149:ILE:CB	2.14	0.62
1:E:196:ASN:OD1	1:E:200:LYS:HE3	2.01	0.61
1:E:189:ILE:HG22	1:E:189:ILE:O	2.00	0.61
1:G:194:ILE:CG2	1:G:195:MET:N	2.63	0.61
3:H:306:HOH:O	1:N:243:LYS:NZ	2.28	0.61
1:I:62:SER:O	1:I:63:LEU:C	2.39	0.61
1:D:194:ILE:HG22	1:D:195:MET:N	2.14	0.61
1:H:179:ILE:O	1:H:179:ILE:HG22	1.99	0.61
1:I:63:LEU:O	1:I:66:SER:N	2.31	0.61
1:C:152:ILE:HD13	1:C:201:VAL:HG23	1.81	0.60
1:E:124:VAL:HG21	1:E:149:ILE:CB	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LYS:HZ2	1:E:94:GLU:HA	1.65	0.60
1:A:194:ILE:CG2	1:A:198:LYS:HE3	2.31	0.60
1:I:133:TYR:OH	2:I:301:GOL:C3	2.48	0.60
1:I:242:GLU:C	1:I:243:LYS:HG2	2.22	0.60
1:C:63:LEU:O	1:C:66:SER:N	2.31	0.60
1:D:82:GLU:HG2	1:E:73:SER:HB2	1.84	0.60
1:A:121:ILE:HD11	1:A:174:GLN:CD	2.22	0.59
1:N:62:SER:O	1:N:63:LEU:C	2.40	0.59
1:D:242:GLU:O	1:D:243:LYS:HB2	2.01	0.59
1:I:135:SER:HA	1:M:243:LYS:HE3	1.83	0.59
1:A:194:ILE:HG22	1:A:198:LYS:HE3	1.84	0.59
1:C:62:SER:O	1:C:63:LEU:C	2.41	0.59
1:J:165:LEU:HD13	1:M:129:ASP:HB3	1.84	0.59
1:J:63:LEU:O	1:J:66:SER:N	2.32	0.59
1:I:165:LEU:CD1	1:L:129:ASP:HB3	2.28	0.59
1:G:194:ILE:HG23	1:G:195:MET:H	1.65	0.59
1:I:133:TYR:OH	2:I:301:GOL:H32	2.02	0.59
1:G:63:LEU:O	1:G:66:SER:N	2.29	0.59
1:A:174:GLN:HB3	1:A:175:SER:CB	2.28	0.59
1:D:242:GLU:O	1:D:243:LYS:HG3	2.02	0.59
1:H:81:SER:OG	1:H:123:ASP:HB3	2.03	0.59
1:A:241:LEU:HD13	1:C:133:TYR:CE1	2.37	0.58
1:E:179:ILE:O	1:E:179:ILE:CG2	2.45	0.58
1:D:97:ARG:HG2	3:D:302:HOH:O	2.02	0.58
1:G:81:SER:OG	1:G:123:ASP:HB3	2.03	0.58
1:I:82:GLU:HG2	1:M:73:SER:HB2	1.85	0.58
1:I:65:LEU:HD13	1:I:87:GLN:OE1	2.04	0.58
1:J:241:LEU:CD2	1:M:133:TYR:CE1	2.81	0.58
1:G:62:SER:O	1:G:63:LEU:C	2.41	0.58
1:N:81:SER:OG	1:N:123:ASP:HB3	2.03	0.58
1:E:178:ILE:O	1:E:180:PRO:HD2	2.04	0.58
1:L:112:ASN:O	1:L:113:ASN:CB	2.49	0.57
1:N:63:LEU:O	1:N:66:SER:N	2.27	0.57
1:I:81:SER:OG	1:I:123:ASP:HB3	2.04	0.57
1:M:81:SER:OG	1:M:123:ASP:HB3	2.04	0.57
1:N:124:VAL:HG21	1:N:149:ILE:CB	2.17	0.57
1:F:81:SER:OG	1:F:123:ASP:HB3	2.04	0.57
1:F:124:VAL:CG2	1:F:149:ILE:HB	2.15	0.57
1:J:62:SER:O	1:J:63:LEU:C	2.43	0.57
1:C:81:SER:OG	1:C:123:ASP:HB3	2.05	0.57
1:H:243:LYS:NZ	1:J:132:ASN:O	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:242:GLU:CG	1:I:243:LYS:HG2	2.35	0.56
1:H:62:SER:O	1:H:63:LEU:C	2.43	0.56
1:A:121:ILE:HD11	1:A:174:GLN:OE1	2.05	0.56
1:H:63:LEU:O	1:H:66:SER:N	2.30	0.56
1:B:81:SER:OG	1:B:123:ASP:HB3	2.05	0.56
1:C:212:ASP:OD2	1:C:214:ASN:ND2	2.24	0.56
1:J:241:LEU:O	1:J:242:GLU:HB3	2.05	0.56
1:K:81:SER:OG	1:K:123:ASP:HB3	2.06	0.56
1:N:128:VAL:HG11	1:N:204:ILE:HD13	1.88	0.56
1:C:165:LEU:HD13	1:F:129:ASP:HB3	1.86	0.56
1:I:82:GLU:OE1	1:M:73:SER:O	2.25	0.55
1:B:74:SER:HB2	1:B:75:PRO:HD2	1.88	0.55
1:I:74:SER:HB2	1:I:75:PRO:HD2	1.88	0.55
1:H:187:ILE:HG13	1:H:188:GLU:HG2	1.87	0.55
1:B:167:ASN:HB3	1:E:200:LYS:NZ	2.21	0.55
1:B:67:LYS:CE	1:E:94:GLU:HG2	2.36	0.55
1:I:82:GLU:CG	1:M:73:SER:HB2	2.36	0.55
1:A:81:SER:OG	1:A:123:ASP:HB3	2.06	0.55
1:F:63:LEU:O	1:F:66:SER:N	2.34	0.55
1:G:191:ASN:HA	1:G:194:ILE:CG2	2.37	0.55
1:G:98:LYS:HE3	1:N:98:LYS:HZ3	1.70	0.55
1:A:187:ILE:HG22	1:A:190:GLN:N	2.08	0.55
1:E:192:LYS:O	1:E:196:ASN:CB	2.55	0.55
1:A:115:ILE:HD11	1:A:176:TYR:CD2	2.42	0.54
1:I:86:SER:HG	1:M:71:PHE:HE2	1.52	0.54
1:N:196:ASN:O	1:N:200:LYS:HG3	2.08	0.54
1:G:74:SER:HB2	1:G:75:PRO:HD2	1.90	0.54
1:C:160:GLY:N	1:C:238:ASP:OD2	2.35	0.54
1:A:212:ASP:OD1	1:A:213:THR:N	2.40	0.54
1:I:92:GLU:CG	2:I:301:GOL:H11	2.36	0.54
1:L:196:ASN:O	1:L:200:LYS:HG3	2.08	0.54
1:E:62:SER:O	1:E:62:SER:OG	2.26	0.54
1:F:74:SER:HB2	1:F:75:PRO:HD2	1.90	0.54
1:G:98:LYS:HE3	1:N:98:LYS:HZ1	1.71	0.54
1:I:86:SER:OG	1:M:71:PHE:CD2	2.59	0.53
1:L:81:SER:OG	1:L:123:ASP:HB3	2.09	0.53
1:F:160:GLY:N	1:F:238:ASP:OD2	2.37	0.53
1:E:62:SER:O	1:E:63:LEU:C	2.47	0.53
1:F:196:ASN:O	1:F:200:LYS:HG3	2.09	0.53
1:K:128:VAL:HG11	1:K:204:ILE:HD13	1.90	0.53
1:B:62:SER:O	1:B:63:LEU:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:HB3	1:A:194:ILE:HD13	1.90	0.53
1:F:62:SER:O	1:F:63:LEU:C	2.46	0.53
1:K:165:LEU:HD23	1:K:241:LEU:HB2	1.90	0.53
1:G:193:GLU:HA	1:G:196:ASN:HB2	1.90	0.53
1:B:74:SER:HB2	1:B:75:PRO:CD	2.38	0.53
1:J:160:GLY:N	1:J:238:ASP:OD2	2.39	0.52
1:E:81:SER:OG	1:E:123:ASP:HB3	2.09	0.52
1:M:121:ILE:HG23	1:M:201:VAL:HG21	1.91	0.52
1:D:241:LEU:HD13	1:G:133:TYR:CE1	2.44	0.52
1:J:196:ASN:O	1:J:200:LYS:HG3	2.10	0.52
1:G:160:GLY:N	1:G:238:ASP:OD2	2.41	0.52
1:C:74:SER:HB2	1:C:75:PRO:HD2	1.91	0.52
1:N:74:SER:HB2	1:N:75:PRO:HD2	1.92	0.52
1:I:196:ASN:O	1:I:200:LYS:HG3	2.08	0.52
1:B:62:SER:OG	1:B:62:SER:O	2.27	0.52
1:K:128:VAL:HG23	1:K:156:SER:HB3	1.92	0.52
1:A:74:SER:HB2	1:A:75:PRO:HD2	1.92	0.52
1:G:193:GLU:O	1:G:196:ASN:HB3	2.10	0.52
1:M:152:ILE:HD13	1:M:201:VAL:HG13	1.90	0.52
1:H:118:LEU:CD2	1:H:178:ILE:HG21	2.31	0.52
1:H:73:SER:HB2	1:J:82:GLU:CG	2.37	0.52
1:J:74:SER:HB2	1:J:75:PRO:HD2	1.91	0.52
1:E:74:SER:HB2	1:E:75:PRO:HD2	1.91	0.52
1:D:196:ASN:O	1:D:200:LYS:HG3	2.10	0.51
1:B:77:TYR:HB3	1:B:78:PRO:HD2	1.91	0.51
1:M:74:SER:HB2	1:M:75:PRO:HD2	1.91	0.51
1:N:77:TYR:HB3	1:N:78:PRO:HD2	1.93	0.51
1:A:182:ASN:OD1	1:A:182:ASN:O	2.29	0.51
1:N:160:GLY:N	1:N:238:ASP:OD2	2.40	0.51
1:G:98:LYS:HE3	1:N:98:LYS:CE	2.40	0.51
1:H:196:ASN:O	1:H:200:LYS:HG3	2.10	0.51
1:D:215:VAL:O	1:D:219:VAL:HG23	2.11	0.51
1:K:194:ILE:O	1:K:198:LYS:HD3	2.10	0.51
1:K:74:SER:HB2	1:K:75:PRO:HD2	1.93	0.51
1:D:62:SER:O	1:D:62:SER:OG	2.29	0.51
1:M:160:GLY:N	1:M:238:ASP:OD2	2.39	0.51
1:B:63:LEU:O	1:B:66:SER:N	2.40	0.51
1:K:77:TYR:HB3	1:K:78:PRO:HD2	1.91	0.51
1:K:196:ASN:O	1:K:200:LYS:HG3	2.11	0.50
1:A:175:SER:O	1:A:176:TYR:HD1	1.95	0.50
1:B:194:ILE:HG23	1:B:195:MET:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LYS:HZ1	1:E:94:GLU:HG2	1.77	0.50
1:L:242:GLU:O	1:L:243:LYS:O	2.30	0.50
1:L:74:SER:HB2	1:L:75:PRO:HD2	1.92	0.50
1:C:196:ASN:O	1:C:200:LYS:HG3	2.11	0.50
1:L:63:LEU:O	1:L:65:LEU:N	2.45	0.50
1:G:191:ASN:CA	1:G:194:ILE:HG22	2.41	0.50
1:K:86:SER:HB3	1:L:64:LEU:HD11	1.94	0.50
1:D:77:TYR:HB3	1:D:78:PRO:HD2	1.94	0.50
1:D:74:SER:HB2	1:D:75:PRO:HD2	1.94	0.50
1:D:160:GLY:N	1:D:238:ASP:OD2	2.40	0.50
1:G:196:ASN:O	1:G:200:LYS:HG3	2.12	0.50
1:F:213:THR:HG23	3:F:304:HOH:O	2.11	0.50
1:H:77:TYR:HB3	1:H:78:PRO:HD2	1.94	0.49
1:N:62:SER:O	1:N:62:SER:OG	2.30	0.49
1:G:77:TYR:HB3	1:G:78:PRO:HD2	1.94	0.49
1:A:196:ASN:O	1:A:200:LYS:HG3	2.11	0.49
1:F:77:TYR:HB3	1:F:78:PRO:HD2	1.94	0.49
1:M:78:PRO:O	3:M:306:HOH:O	2.20	0.49
1:D:242:GLU:O	1:D:243:LYS:CG	2.60	0.49
1:N:215:VAL:O	1:N:219:VAL:HG23	2.12	0.49
1:A:215:VAL:O	1:A:219:VAL:HG23	2.12	0.49
1:H:237:ILE:HG22	1:H:238:ASP:N	2.27	0.49
1:H:160:GLY:N	1:H:238:ASP:OD2	2.42	0.49
1:A:124:VAL:HG21	1:A:149:ILE:CB	2.16	0.49
1:I:96:LYS:NZ	2:I:301:GOL:O1	2.46	0.49
1:F:215:VAL:O	1:F:219:VAL:HG23	2.12	0.49
1:K:63:LEU:HG	1:N:90:TYR:CE1	2.47	0.49
1:I:193:GLU:CG	1:I:194:ILE:H	2.17	0.49
1:N:152:ILE:HD13	1:N:201:VAL:HG23	1.95	0.49
1:C:77:TYR:HB3	1:C:78:PRO:HD2	1.94	0.49
1:A:179:ILE:HG13	1:A:179:ILE:O	2.11	0.49
1:M:62:SER:O	1:M:64:LEU:N	2.45	0.49
1:M:65:LEU:CD2	1:M:91:LEU:HD21	2.42	0.49
1:E:63:LEU:O	1:E:66:SER:N	2.40	0.49
1:H:176:TYR:N	1:H:176:TYR:CD2	2.80	0.49
1:B:69:ILE:HD11	1:E:93:TYR:CD2	2.48	0.48
1:H:74:SER:HB2	1:H:75:PRO:HD2	1.95	0.48
1:C:215:VAL:O	1:C:219:VAL:HG23	2.13	0.48
1:A:190:GLN:C	1:A:192:LYS:H	2.16	0.48
1:E:77:TYR:HB3	1:E:78:PRO:HD2	1.95	0.48
1:B:211:LYS:HB2	1:B:216:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:237:ILE:HG22	1:L:238:ASP:N	2.29	0.48
1:B:160:GLY:N	1:B:238:ASP:OD2	2.39	0.48
1:A:97:ARG:HH21	1:H:97:ARG:H	1.62	0.48
1:I:74:SER:HB2	1:I:75:PRO:CD	2.44	0.48
1:J:77:TYR:HB3	1:J:78:PRO:HD2	1.95	0.48
1:L:77:TYR:HB3	1:L:78:PRO:HD2	1.94	0.48
1:A:77:TYR:HB3	1:A:78:PRO:HD2	1.95	0.48
1:H:187:ILE:HG22	1:H:189:ILE:HG22	1.96	0.48
1:M:77:TYR:HB3	1:M:78:PRO:HD2	1.95	0.48
1:H:180:PRO:O	1:H:181:PHE:CD2	2.67	0.48
1:H:242:GLU:O	1:H:243:LYS:C	2.52	0.48
1:I:86:SER:HG	1:M:71:PHE:HD2	1.50	0.48
1:I:69:ILE:HD11	1:L:93:TYR:CD2	2.48	0.48
1:K:62:SER:OG	1:K:62:SER:O	2.31	0.48
1:B:215:VAL:O	1:B:219:VAL:HG23	2.13	0.48
1:I:215:VAL:O	1:I:219:VAL:HG23	2.13	0.48
1:E:188:GLU:HG3	1:E:189:ILE:HG13	1.96	0.48
1:C:62:SER:OG	1:C:62:SER:O	2.28	0.48
1:A:97:ARG:HB2	1:H:97:ARG:HB2	1.95	0.48
1:L:215:VAL:O	1:L:219:VAL:HG23	2.13	0.48
1:K:215:VAL:O	1:K:219:VAL:HG23	2.14	0.47
1:A:116:ILE:HD12	1:A:116:ILE:C	2.34	0.47
1:N:128:VAL:HG23	1:N:156:SER:HB3	1.95	0.47
1:A:237:ILE:HG22	1:A:238:ASP:N	2.29	0.47
1:H:62:SER:OG	1:H:62:SER:O	2.29	0.47
1:B:196:ASN:O	1:B:200:LYS:HG3	2.14	0.47
1:E:242:GLU:O	1:E:243:LYS:C	2.52	0.47
1:M:215:VAL:O	1:M:219:VAL:HG23	2.13	0.47
1:I:62:SER:O	1:I:64:LEU:N	2.47	0.47
1:I:77:TYR:HB3	1:I:78:PRO:HD2	1.95	0.47
1:G:62:SER:OG	1:G:62:SER:O	2.28	0.47
1:D:63:LEU:HB3	1:D:64:LEU:H	1.55	0.47
1:F:116:ILE:HD12	1:F:116:ILE:C	2.35	0.47
1:L:62:SER:O	1:L:64:LEU:N	2.47	0.47
1:C:63:LEU:HD12	1:C:63:LEU:HA	1.77	0.47
1:B:198:LYS:HE2	1:B:202:ILE:HD11	1.97	0.47
1:B:113:ASN:HD21	1:E:187:ILE:HG12	1.80	0.47
1:B:124:VAL:CG2	1:B:149:ILE:HB	2.17	0.47
1:E:62:SER:O	1:E:64:LEU:N	2.48	0.47
1:L:187:ILE:HG23	1:L:191:ASN:HB2	1.96	0.47
1:J:215:VAL:O	1:J:219:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLU:O	1:A:197:THR:N	2.45	0.47
1:M:63:LEU:HA	1:M:63:LEU:HD12	1.78	0.47
1:E:237:ILE:HG22	1:E:238:ASP:N	2.30	0.47
1:J:69:ILE:HD11	1:M:93:TYR:CD2	2.50	0.47
1:I:133:TYR:CZ	2:I:301:GOL:H32	2.50	0.46
1:B:237:ILE:HG22	1:B:238:ASP:N	2.30	0.46
1:K:160:GLY:N	1:K:238:ASP:OD2	2.43	0.46
1:D:133:TYR:CE1	1:E:241:LEU:HD13	2.50	0.46
1:J:69:ILE:HD11	1:M:93:TYR:CG	2.51	0.46
1:L:121:ILE:HG23	1:L:201:VAL:HG21	1.96	0.46
1:J:121:ILE:HG23	1:J:201:VAL:HG21	1.97	0.46
1:B:241:LEU:HD13	1:E:133:TYR:CE1	2.49	0.46
1:I:160:GLY:N	1:I:238:ASP:OD2	2.42	0.46
1:F:152:ILE:HD13	1:F:201:VAL:HG23	1.97	0.46
1:I:242:GLU:CB	1:I:243:LYS:HG2	2.46	0.46
1:L:200:LYS:O	1:L:204:ILE:HG13	2.16	0.46
1:C:96:LYS:HE2	2:C:301:GOL:H31	1.98	0.46
1:G:116:ILE:C	1:G:116:ILE:HD12	2.35	0.46
1:L:164:SER:OG	1:L:168:SER:HB2	2.16	0.46
1:A:181:PHE:O	1:A:182:ASN:C	2.53	0.46
1:N:237:ILE:HG22	1:N:238:ASP:N	2.31	0.46
1:G:236:LEU:O	1:G:237:ILE:HD13	2.16	0.46
1:I:62:SER:OG	1:I:62:SER:O	2.30	0.45
1:N:65:LEU:HD22	1:N:91:LEU:HD21	1.98	0.45
1:J:74:SER:HB2	1:J:75:PRO:CD	2.46	0.45
1:E:148:GLY:HA3	3:E:303:HOH:O	2.15	0.45
1:G:188:GLU:HG2	1:G:189:ILE:N	2.23	0.45
1:A:187:ILE:CG2	1:A:188:GLU:N	2.65	0.45
1:J:63:LEU:HA	1:J:63:LEU:HD12	1.71	0.45
1:G:74:SER:HB2	1:G:75:PRO:CD	2.45	0.45
1:J:237:ILE:HG22	1:J:238:ASP:N	2.31	0.45
1:H:187:ILE:CG2	1:H:189:ILE:HG22	2.46	0.45
1:E:174:GLN:O	1:E:176:TYR:HD2	2.00	0.45
1:H:63:LEU:HA	1:H:63:LEU:HD12	1.77	0.45
1:K:194:ILE:HG13	1:K:195:MET:N	2.32	0.45
1:B:69:ILE:HD11	1:E:93:TYR:CG	2.52	0.45
1:H:116:ILE:C	1:H:116:ILE:HD12	2.37	0.45
1:K:65:LEU:HA	1:K:65:LEU:HD12	1.80	0.45
1:A:115:ILE:HD11	1:A:176:TYR:CG	2.52	0.45
1:I:121:ILE:HG23	1:I:201:VAL:HG21	1.99	0.45
1:C:74:SER:HB2	1:C:75:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ASP:N	1:B:109:ASP:OD1	2.48	0.45
1:C:62:SER:O	1:C:64:LEU:N	2.50	0.45
1:H:65:LEU:HD13	1:H:87:GLN:OE1	2.17	0.45
1:E:116:ILE:HD12	1:E:116:ILE:C	2.36	0.45
1:I:121:ILE:CG2	1:I:201:VAL:HG21	2.47	0.45
1:K:200:LYS:O	1:K:204:ILE:HG13	2.17	0.45
1:A:134:ILE:O	1:G:243:LYS:NZ	2.27	0.45
1:G:62:SER:O	1:G:64:LEU:N	2.50	0.44
1:A:132:ASN:O	1:G:243:LYS:HG3	2.16	0.44
1:E:121:ILE:CG2	1:E:201:VAL:HG21	2.47	0.44
1:H:195:MET:O	1:H:199:LYS:HG3	2.16	0.44
1:H:180:PRO:O	1:H:181:PHE:HD2	1.99	0.44
1:C:237:ILE:HG22	1:C:238:ASP:N	2.32	0.44
1:B:62:SER:O	1:B:64:LEU:N	2.50	0.44
1:G:237:ILE:HG22	1:G:238:ASP:N	2.32	0.44
1:L:121:ILE:CG2	1:L:201:VAL:HG21	2.47	0.44
1:G:121:ILE:CG2	1:G:201:VAL:HG21	2.47	0.44
1:E:215:VAL:O	1:E:219:VAL:HG23	2.17	0.44
1:M:237:ILE:HG22	1:M:238:ASP:N	2.33	0.44
1:J:109:ASP:OD1	1:J:109:ASP:N	2.50	0.44
1:I:90:TYR:CD1	1:M:63:LEU:HG	2.48	0.44
1:E:179:ILE:HA	1:E:180:PRO:HD2	1.36	0.44
1:I:63:LEU:HD12	1:I:63:LEU:HA	1.68	0.44
1:H:180:PRO:HG2	1:H:181:PHE:H	1.81	0.44
1:A:97:ARG:HB2	1:H:97:ARG:CB	2.48	0.44
1:M:164:SER:OG	1:M:168:SER:HB2	2.17	0.44
1:E:112:ASN:O	1:E:113:ASN:CB	2.58	0.44
1:I:237:ILE:HG22	1:I:238:ASP:N	2.32	0.44
1:C:116:ILE:C	1:C:116:ILE:HD12	2.38	0.44
1:D:121:ILE:HG23	1:D:201:VAL:HG21	1.99	0.44
1:H:177:SER:OG	1:H:194:ILE:HD13	2.17	0.44
1:I:116:ILE:HD12	1:I:116:ILE:C	2.38	0.44
1:K:116:ILE:C	1:K:116:ILE:HD12	2.38	0.44
1:C:236:LEU:O	1:C:237:ILE:HD13	2.17	0.44
1:M:74:SER:HB2	1:M:75:PRO:CD	2.47	0.44
1:N:236:LEU:O	1:N:237:ILE:HD13	2.18	0.44
1:H:237:ILE:CG2	1:H:238:ASP:N	2.81	0.44
1:A:236:LEU:O	1:A:237:ILE:HD13	2.17	0.44
1:C:234:PHE:O	1:C:235:LYS:HB2	2.18	0.44
1:H:202:ILE:O	1:H:206:SER:OG	2.34	0.44
1:C:200:LYS:O	1:C:204:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:LEU:O	1:E:237:ILE:HD13	2.17	0.44
1:B:116:ILE:C	1:B:116:ILE:HD12	2.38	0.44
1:A:143:LEU:HD22	1:C:130:VAL:HG22	1.99	0.44
1:A:74:SER:HB2	1:A:75:PRO:CD	2.48	0.44
1:K:63:LEU:HD12	1:K:63:LEU:HA	1.81	0.44
1:A:164:SER:OG	1:A:168:SER:HB2	2.18	0.44
1:G:191:ASN:C	1:G:194:ILE:HG22	2.37	0.43
1:G:98:LYS:NZ	1:N:98:LYS:CE	2.81	0.43
1:H:132:ASN:O	1:N:243:LYS:HG3	2.17	0.43
1:J:62:SER:O	1:J:64:LEU:N	2.51	0.43
1:F:62:SER:O	1:F:64:LEU:N	2.51	0.43
1:H:200:LYS:O	1:H:204:ILE:HG13	2.17	0.43
1:G:121:ILE:HG23	1:G:201:VAL:HG21	2.00	0.43
1:D:98:LYS:HA	1:D:99:PRO:HD3	1.89	0.43
1:M:63:LEU:O	1:M:65:LEU:N	2.51	0.43
1:K:243:LYS:O	1:K:243:LYS:HG2	2.17	0.43
1:F:237:ILE:HG22	1:F:238:ASP:N	2.33	0.43
1:M:121:ILE:CG2	1:M:201:VAL:HG21	2.48	0.43
1:E:74:SER:HB2	1:E:75:PRO:CD	2.48	0.43
1:K:237:ILE:HG22	1:K:238:ASP:N	2.32	0.43
1:H:215:VAL:O	1:H:219:VAL:HG23	2.18	0.43
1:F:74:SER:HB2	1:F:75:PRO:CD	2.47	0.43
1:D:236:LEU:O	1:D:237:ILE:HD13	2.18	0.43
1:J:124:VAL:HG13	1:J:125:ILE:N	2.33	0.43
1:L:74:SER:HB2	1:L:75:PRO:CD	2.49	0.43
1:I:234:PHE:O	1:I:235:LYS:HB2	2.18	0.43
1:G:198:LYS:O	1:G:202:ILE:HD13	2.18	0.43
1:J:65:LEU:HA	1:J:65:LEU:HD12	1.84	0.43
1:J:62:SER:OG	1:J:62:SER:O	2.31	0.43
1:K:130:VAL:HG22	1:L:143:LEU:HD22	2.00	0.43
1:L:116:ILE:HD12	1:L:116:ILE:C	2.39	0.43
1:J:121:ILE:CG2	1:J:201:VAL:HG21	2.48	0.43
1:D:121:ILE:CG2	1:D:201:VAL:HG21	2.49	0.43
1:A:62:SER:OG	1:A:62:SER:O	2.34	0.43
1:C:152:ILE:CD1	1:C:201:VAL:CG2	2.97	0.43
1:N:198:LYS:O	1:N:201:VAL:HG12	2.19	0.43
1:A:237:ILE:CG2	1:A:238:ASP:N	2.82	0.43
1:J:202:ILE:O	1:J:206:SER:OG	2.31	0.43
1:I:65:LEU:HD11	1:I:87:GLN:HG2	2.01	0.43
1:K:77:TYR:HB3	1:K:78:PRO:CD	2.49	0.43
1:L:237:ILE:CG2	1:L:238:ASP:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:179:ILE:O	1:H:180:PRO:C	2.57	0.42
1:K:141:TYR:HD2	1:K:241:LEU:HD11	1.83	0.42
1:H:118:LEU:HD22	1:H:178:ILE:CG2	2.36	0.42
1:A:152:ILE:CD1	1:A:201:VAL:HG23	2.48	0.42
1:I:82:GLU:CD	1:M:73:SER:O	2.58	0.42
1:B:227:ASN:O	1:B:228:ALA:C	2.57	0.42
1:A:115:ILE:CD1	1:A:176:TYR:CD2	3.02	0.42
1:E:160:GLY:N	1:E:238:ASP:OD2	2.45	0.42
1:A:198:LYS:O	1:A:202:ILE:HD13	2.19	0.42
1:C:152:ILE:CD1	1:C:201:VAL:HG23	2.47	0.42
1:B:77:TYR:HB3	1:B:78:PRO:CD	2.49	0.42
1:D:63:LEU:HA	1:D:63:LEU:HD12	1.83	0.42
1:D:164:SER:OG	1:D:168:SER:HB2	2.19	0.42
1:E:164:SER:OG	1:E:168:SER:HB2	2.20	0.42
1:G:191:ASN:O	1:G:194:ILE:N	2.52	0.42
1:I:242:GLU:C	1:I:243:LYS:CG	2.88	0.42
1:C:69:ILE:HD11	1:F:93:TYR:CG	2.55	0.42
1:E:192:LYS:HA	1:E:192:LYS:HD3	1.88	0.42
1:K:164:SER:OG	1:K:168:SER:HB2	2.19	0.42
1:E:118:LEU:HD22	1:E:178:ILE:CG2	2.49	0.42
1:I:82:GLU:HB3	1:M:73:SER:HB2	2.01	0.42
1:J:212:ASP:O	1:J:215:VAL:HG12	2.20	0.42
1:L:98:LYS:HA	1:L:99:PRO:HD3	1.89	0.42
1:A:173:ASN:ND2	1:A:220:LEU:HB3	2.35	0.42
1:M:63:LEU:O	1:M:64:LEU:C	2.58	0.42
1:D:198:LYS:O	1:D:202:ILE:HD13	2.19	0.42
1:I:63:LEU:HB3	1:I:64:LEU:H	1.76	0.42
1:N:62:SER:O	1:N:64:LEU:N	2.52	0.42
1:H:62:SER:O	1:H:64:LEU:N	2.53	0.42
1:F:62:SER:O	1:F:62:SER:OG	2.31	0.42
1:N:74:SER:HB2	1:N:75:PRO:CD	2.49	0.42
1:L:137:ASP:OD1	3:L:301:HOH:O	2.22	0.42
1:J:152:ILE:HD13	1:J:201:VAL:HG13	2.02	0.42
1:N:63:LEU:HD12	1:N:63:LEU:HA	1.82	0.42
1:K:141:TYR:CD1	1:K:141:TYR:N	2.88	0.42
1:F:198:LYS:O	1:F:202:ILE:HD13	2.19	0.42
1:H:164:SER:OG	1:H:168:SER:HB2	2.20	0.42
1:D:74:SER:HB2	1:D:75:PRO:CD	2.50	0.41
1:F:201:VAL:HG13	1:F:202:ILE:N	2.35	0.41
1:L:198:LYS:O	1:L:202:ILE:HD13	2.20	0.41
1:K:82:GLU:HG2	1:L:73:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ILE:HG22	1:A:188:GLU:H	1.79	0.41
1:D:237:ILE:HG22	1:D:238:ASP:N	2.34	0.41
1:E:77:TYR:HB3	1:E:78:PRO:CD	2.50	0.41
1:B:236:LEU:O	1:B:237:ILE:HD13	2.20	0.41
1:A:242:GLU:OE1	1:A:242:GLU:N	2.52	0.41
1:N:124:VAL:CG2	1:N:149:ILE:HB	2.19	0.41
1:F:200:LYS:O	1:F:204:ILE:HG13	2.20	0.41
1:E:174:GLN:CG	1:E:174:GLN:O	2.60	0.41
1:A:152:ILE:CD1	1:A:201:VAL:CG2	2.97	0.41
1:K:152:ILE:CD1	1:K:201:VAL:HG23	2.49	0.41
1:K:143:LEU:HD22	1:K:165:LEU:HD11	2.03	0.41
1:K:74:SER:HB2	1:K:75:PRO:CD	2.49	0.41
1:B:198:LYS:O	1:B:202:ILE:HD13	2.20	0.41
1:K:133:TYR:CE1	1:L:241:LEU:HD13	2.56	0.41
1:M:198:LYS:O	1:M:202:ILE:HD13	2.20	0.41
1:I:124:VAL:HG13	1:I:125:ILE:N	2.34	0.41
1:N:237:ILE:CG2	1:N:238:ASP:N	2.84	0.41
1:H:236:LEU:O	1:H:237:ILE:HD13	2.20	0.41
1:C:96:LYS:CE	2:C:301:GOL:C3	2.97	0.41
1:F:143:LEU:HD22	1:F:165:LEU:HD11	2.02	0.41
1:B:229:ASP:OD2	3:B:306:HOH:O	2.21	0.41
1:N:200:LYS:O	1:N:204:ILE:HG13	2.20	0.41
1:F:215:VAL:O	1:F:218[B]:ASN:HB3	2.20	0.41
1:A:173:ASN:CG	1:A:174:GLN:N	2.74	0.41
1:H:152:ILE:CD1	1:H:201:VAL:CG2	2.99	0.41
1:F:198:LYS:O	1:F:201:VAL:HG12	2.19	0.41
1:C:96:LYS:CE	2:C:301:GOL:H32	2.51	0.41
1:N:164:SER:OG	1:N:168:SER:HB2	2.20	0.41
1:J:116:ILE:C	1:J:116:ILE:HD12	2.40	0.41
1:G:98:LYS:HA	1:G:99:PRO:HD3	1.91	0.41
1:L:65:LEU:HA	1:L:65:LEU:HD12	1.94	0.41
1:N:201:VAL:HG13	1:N:202:ILE:N	2.36	0.41
1:N:202:ILE:O	1:N:206:SER:OG	2.33	0.41
1:B:237:ILE:CG2	1:B:238:ASP:N	2.83	0.41
1:A:77:TYR:HB3	1:A:78:PRO:CD	2.51	0.41
1:J:155:SER:O	3:J:301:HOH:O	2.22	0.41
1:D:89:LEU:HD23	1:D:89:LEU:HA	1.88	0.41
1:E:237:ILE:CG2	1:E:238:ASP:N	2.84	0.41
1:J:166:LYS:CG	1:J:242:GLU:OE1	2.68	0.41
1:I:65:LEU:CD1	1:I:87:GLN:OE1	2.67	0.41
1:N:63:LEU:O	1:N:64:LEU:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:LEU:HA	1:G:63:LEU:HD12	1.78	0.41
1:G:63:LEU:O	1:G:65:LEU:N	2.54	0.41
1:H:63:LEU:O	1:H:65:LEU:N	2.54	0.41
1:I:200:LYS:O	1:I:204:ILE:HG13	2.21	0.41
1:N:198:LYS:O	1:N:202:ILE:HD13	2.19	0.41
1:L:160:GLY:N	1:L:238:ASP:OD2	2.45	0.41
1:A:160:GLY:N	1:A:238:ASP:OD2	2.46	0.41
1:A:62:SER:O	1:A:63:LEU:C	2.59	0.41
1:B:161:TYR:N	1:B:161:TYR:CD2	2.89	0.41
1:B:121:ILE:HG23	1:B:201:VAL:HG21	2.02	0.41
1:I:164:SER:OG	1:I:168:SER:HB2	2.21	0.41
1:B:67:LYS:NZ	1:E:94:GLU:HG2	2.35	0.41
1:I:63:LEU:O	1:I:65:LEU:N	2.54	0.41
1:G:193:GLU:O	1:G:193:GLU:CD	2.59	0.41
1:G:237:ILE:CG2	1:G:238:ASP:N	2.84	0.41
1:D:200:LYS:O	1:D:204:ILE:HG13	2.21	0.41
1:M:236:LEU:O	1:M:237:ILE:HD13	2.21	0.41
1:A:199:LYS:HE2	1:A:199:LYS:HB3	1.98	0.41
1:B:167:ASN:HB3	1:E:200:LYS:HZ1	1.87	0.40
1:J:237:ILE:CG2	1:J:238:ASP:N	2.84	0.40
1:A:179:ILE:HA	1:A:180:PRO:HD2	1.93	0.40
1:C:96:LYS:HE2	2:C:301:GOL:C3	2.51	0.40
1:C:227:ASN:HB2	3:C:408:HOH:O	2.21	0.40
1:M:200:LYS:O	1:M:204:ILE:HG13	2.20	0.40
1:I:199:LYS:HB3	1:I:199:LYS:HE2	1.97	0.40
1:E:124:VAL:CG2	1:E:149:ILE:HB	2.19	0.40
1:E:178:ILE:O	1:E:179:ILE:HD13	2.21	0.40
1:K:152:ILE:CD1	1:K:201:VAL:CG2	2.99	0.40
1:E:63:LEU:HA	1:E:63:LEU:HD12	1.75	0.40
1:K:163:PHE:HB3	1:K:241:LEU:HG	2.02	0.40
1:J:198:LYS:O	1:J:202:ILE:HD13	2.22	0.40
1:F:143:LEU:CD2	1:F:165:LEU:HD11	2.51	0.40
1:F:164:SER:OG	1:F:168:SER:HB2	2.21	0.40
1:M:152:ILE:CD1	1:M:201:VAL:HG13	2.52	0.40
1:J:200:LYS:O	1:J:204:ILE:HG13	2.20	0.40
1:H:192:LYS:O	1:H:196:ASN:CG	2.60	0.40
1:L:77:TYR:HB3	1:L:78:PRO:CD	2.51	0.40
1:C:69:ILE:HD11	1:F:93:TYR:CD2	2.56	0.40
1:C:241:LEU:HD13	1:F:133:TYR:CE1	2.56	0.40
1:F:141:TYR:CD1	1:F:141:TYR:N	2.90	0.40
1:I:198:LYS:O	1:I:202:ILE:HD13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:VAL:CG2	1:L:149:ILE:HB	2.19	0.40
1:L:187:ILE:HA	1:L:190:GLN:HB2	2.03	0.40
1:F:98:LYS:HA	1:F:99:PRO:HD3	1.92	0.40
1:A:161:TYR:CD2	1:A:161:TYR:N	2.89	0.40
1:L:189:ILE:O	1:L:192:LYS:N	2.54	0.40
1:G:164:SER:OG	1:G:168:SER:HB2	2.21	0.40
1:B:164:SER:OG	1:B:168:SER:HB2	2.22	0.40
1:M:98:LYS:HA	1:M:99:PRO:HD3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	176/219 (80%)	163 (93%)	12 (7%)	1 (1%)	30	67
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%)	30	67
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	161/219 (74%)	157 (98%)	4 (2%)	0	100 100
All	All	2292/3066 (75%)	2200 (96%)	90 (4%)	2 (0%)	56 87

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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%)	163 (97%)	5 (3%)	48 83
1	B	151/204 (74%)	147 (97%)	4 (3%)	54 85
1	C	155/204 (76%)	154 (99%)	1 (1%)	90 97
1	D	151/204 (74%)	150 (99%)	1 (1%)	88 97
1	E	168/204 (82%)	165 (98%)	3 (2%)	66 90
1	F	156/204 (76%)	155 (99%)	1 (1%)	90 97
1	G	159/204 (78%)	156 (98%)	3 (2%)	65 89
1	H	168/204 (82%)	165 (98%)	3 (2%)	66 90
1	I	154/204 (76%)	153 (99%)	1 (1%)	90 97
1	J	155/204 (76%)	154 (99%)	1 (1%)	90 97
1	K	150/204 (74%)	150 (100%)	0	100 100
1	L	165/204 (81%)	159 (96%)	6 (4%)	42 78
1	M	145/204 (71%)	144 (99%)	1 (1%)	88 97
1	N	154/204 (76%)	153 (99%)	1 (1%)	90 97
All	All	2199/2856 (77%)	2168 (99%)	31 (1%)	74 93

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	SER
1	A	178	ILE
1	A	182	ASN
1	A	188	GLU
1	A	190	GLN
1	B	63	LEU
1	B	96	LYS
1	B	214	ASN
1	B	215	VAL
1	C	243	LYS
1	D	65	LEU
1	E	180	PRO
1	E	187	ILE
1	E	198	LYS
1	F	196	ASN
1	G	97	ARG
1	G	189	ILE
1	G	217	SER
1	H	96	LYS
1	H	97	ARG
1	H	181	PHE
1	I	96	LYS
1	J	212	ASP
1	L	96	LYS
1	L	97	ARG
1	L	181	PHE
1	L	190	GLN
1	L	191	ASN
1	L	196	ASN
1	M	65	LEU
1	N	65	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	B	83	GLN
1	C	83	GLN
1	D	83	GLN
1	E	83	GLN
1	F	83	GLN
1	G	83	GLN
1	H	83	GLN

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Mol	Chain	Res	Type
1	I	83	GLN
1	J	83	GLN
1	K	83	GLN
1	L	83	GLN
1	M	83	GLN
1	N	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 carbohydrates 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	C	301	-	5,5,5	0.35	0	5,5,5	0.24	0
2	GOL	I	301	-	5,5,5	0.36	0	5,5,5	0.24	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	C	301	-	-	0/4/4/4	0/0/0/0
2	GOL	I	301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	GOL	4	0
2	I	301	GOL	8	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	180/219 (82%)	0.09	5 (2%) 56 50	28, 67, 152, 166	0
1	B	162/219 (73%)	-0.10	5 (3%) 52 45	35, 78, 145, 166	0
1	C	166/219 (75%)	-0.04	3 (1%) 71 68	32, 69, 148, 176	0
1	D	162/219 (73%)	0.61	26 (16%) 3 1	41, 93, 153, 181	0
1	E	179/219 (81%)	0.04	4 (2%) 65 60	36, 68, 144, 215	0
1	F	166/219 (75%)	0.04	7 (4%) 40 33	39, 80, 151, 165	0
1	G	170/219 (77%)	0.14	9 (5%) 30 23	37, 78, 156, 187	0
1	H	179/219 (81%)	0.16	9 (5%) 32 26	35, 79, 160, 206	0
1	I	165/219 (75%)	-0.03	2 (1%) 81 78	42, 79, 151, 171	0
1	J	166/219 (75%)	0.12	9 (5%) 29 23	46, 87, 155, 182	0
1	K	161/219 (73%)	0.64	23 (14%) 4 2	53, 95, 154, 184	0
1	L	176/219 (80%)	0.02	5 (2%) 56 50	42, 80, 155, 191	0
1	M	156/219 (71%)	0.44	14 (8%) 12 7	51, 90, 142, 161	0
1	N	165/219 (75%)	0.39	16 (9%) 10 6	43, 83, 152, 168	0
All	All	2353/3066 (76%)	0.18	137 (5%) 26 20	28, 81, 153, 215	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	THR	6.4
1	N	197	THR	6.1
1	D	196	ASN	5.6
1	K	209	THR	5.6
1	N	200	LYS	5.2
1	N	175	SER	5.2
1	K	167	ASN	5.2
1	H	175	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	222	ARG	5.0
1	E	174	GLN	4.8
1	D	223	ASP	4.8
1	M	197	THR	4.8
1	D	204	ILE	4.7
1	D	220	LEU	4.6
1	D	172	LEU	4.6
1	D	203	GLU	4.5
1	G	222	ARG	4.3
1	G	197	THR	4.2
1	K	204	ILE	4.1
1	D	170	PHE	4.1
1	K	201	VAL	3.9
1	D	224	LYS	3.9
1	N	195	MET	3.8
1	K	220	LEU	3.8
1	K	233	ASP	3.7
1	M	77	TYR	3.7
1	D	171	CYS	3.7
1	D	213	THR	3.6
1	C	196	ASN	3.5
1	J	220	LEU	3.5
1	K	205	ILE	3.5
1	E	195	MET	3.5
1	N	198	LYS	3.5
1	D	173	ASN	3.5
1	N	204	ILE	3.5
1	N	220	LEU	3.4
1	H	219	VAL	3.4
1	J	192	LYS	3.4
1	J	193	GLU	3.3
1	C	192	LYS	3.2
1	I	196	ASN	3.2
1	K	224	LYS	3.2
1	K	236	LEU	3.2
1	B	111	ASP	3.2
1	D	200	LYS	3.1
1	L	242	GLU	3.1
1	G	196	ASN	3.1
1	F	170	PHE	3.1
1	A	173	ASN	3.1
1	H	228	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	219	VAL	3.0
1	D	216	ILE	3.0
1	K	206	SER	3.0
1	N	172	LEU	3.0
1	B	196	ASN	3.0
1	M	111	ASP	3.0
1	K	61	PRO	3.0
1	N	201	VAL	2.9
1	E	242	GLU	2.9
1	A	222	ARG	2.9
1	F	111	ASP	2.9
1	K	197	THR	2.9
1	K	208	ASN	2.9
1	N	222	ARG	2.9
1	D	219	VAL	2.9
1	K	172	LEU	2.9
1	H	174	GLN	2.9
1	N	196	ASN	2.9
1	K	221	GLU	2.9
1	M	146	ALA	2.8
1	M	106	SER	2.8
1	K	200	LYS	2.8
1	K	237	ILE	2.8
1	L	191	ASN	2.8
1	M	116	ILE	2.7
1	L	224	LYS	2.7
1	D	195	MET	2.7
1	B	114	LYS	2.7
1	M	75	PRO	2.7
1	D	212	ASP	2.6
1	L	190	GLN	2.6
1	K	202	ILE	2.6
1	D	149	ILE	2.6
1	F	62	SER	2.5
1	F	106	SER	2.5
1	J	191	ASN	2.5
1	M	76	ILE	2.5
1	A	226	PHE	2.5
1	N	225	TYR	2.5
1	H	222	ARG	2.5
1	D	209	THR	2.5
1	A	176	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	198	LYS	2.4
1	N	121	ILE	2.4
1	K	211	LYS	2.4
1	H	61	PRO	2.4
1	I	114	LYS	2.4
1	M	218	ASN	2.4
1	N	234	PHE	2.3
1	H	223	ASP	2.3
1	L	177	SER	2.3
1	G	204	ILE	2.3
1	M	227	ASN	2.3
1	F	109	ASP	2.3
1	H	188	GLU	2.3
1	G	190	GLN	2.3
1	J	196	ASN	2.2
1	A	195	MET	2.2
1	N	218	ASN	2.2
1	K	213	THR	2.2
1	K	231	ALA	2.2
1	B	242	GLU	2.2
1	G	170	PHE	2.2
1	D	207	LYS	2.2
1	J	224	LYS	2.2
1	G	193	GLU	2.1
1	D	97	ARG	2.1
1	K	170	PHE	2.1
1	G	221	GLU	2.1
1	F	146	ALA	2.1
1	B	61	PRO	2.1
1	M	114	LYS	2.1
1	C	195	MET	2.1
1	F	197	THR	2.1
1	D	214	ASN	2.1
1	H	198	LYS	2.1
1	J	205	ILE	2.1
1	D	121	ILE	2.0
1	J	61	PRO	2.0
1	G	234	PHE	2.0
1	E	173	ASN	2.0
1	M	109	ASP	2.0
1	D	199	LYS	2.0
1	J	236	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	109	ASP	2.0
1	M	108	GLY	2.0
1	M	113	ASN	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	I	301	6/6	0.65	0.34	7.90	89,128,153,155	0
2	GOL	C	301	6/6	0.91	0.28	2.28	74,88,102,112	0

6.5 Other polymers (i)

There are no such residues in this entry.