



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2020 – 04:10 PM EDT

PDB ID : 6WA9  
Title : Structure of the Chlamydia pneumoniae CdsV and CdsO protein complex  
Authors : Jensen, J.L.; Spiller, B.W.  
Deposited on : 2020-03-24  
Resolution : 4.62 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

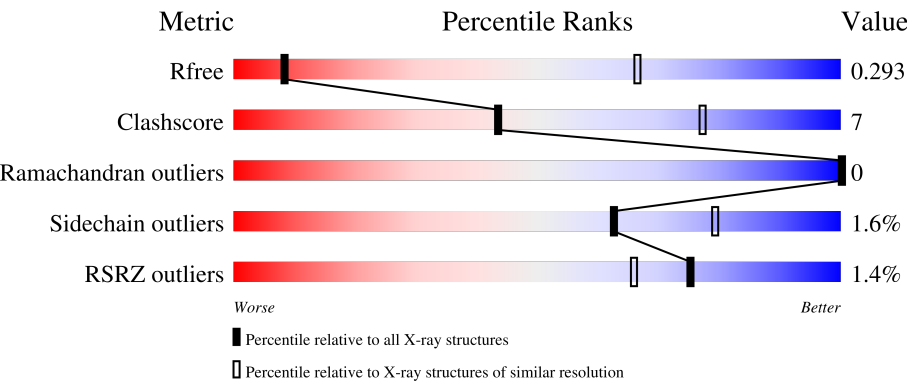
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.62 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.








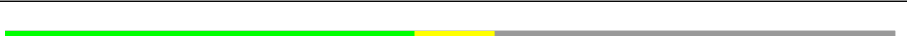
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1114 (5.54-3.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	387	
1	B	387	
1	C	387	
1	D	387	
1	E	387	

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Mol	Chain	Length	Quality of chain
1	F	387	
1	G	387	
1	H	387	
1	I	387	
2	L	107	
2	M	107	
2	N	107	
2	O	107	
2	P	107	
2	Q	107	
2	R	107	
2	S	107	
2	T	107	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29937 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 Low calcium response locus protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2643	1710	433	493	7			
1	B	348	Total	C	N	O	S	0	0	0
			2808	1815	463	523	7			
1	C	347	Total	C	N	O	S	0	0	0
			2800	1809	462	522	7			
1	D	331	Total	C	N	O	S	0	0	0
			2670	1722	440	501	7			
1	E	347	Total	C	N	O	S	0	0	0
			2800	1809	462	522	7			
1	F	346	Total	C	N	O	S	0	0	0
			2793	1806	460	520	7			
1	G	349	Total	C	N	O	S	0	0	0
			2819	1824	464	524	7			
1	H	344	Total	C	N	O	S	0	0	0
			2772	1792	455	518	7			
1	I	340	Total	C	N	O	S	0	0	0
			2754	1780	453	514	7			

There are 189 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	MET	-	initiating methionine	UNP Q9Z8L5
A	325	GLY	-	expression tag	UNP Q9Z8L5
A	326	SER	-	expression tag	UNP Q9Z8L5
A	327	SER	-	expression tag	UNP Q9Z8L5
A	328	HIS	-	expression tag	UNP Q9Z8L5
A	329	HIS	-	expression tag	UNP Q9Z8L5
A	330	HIS	-	expression tag	UNP Q9Z8L5
A	331	HIS	-	expression tag	UNP Q9Z8L5
A	332	HIS	-	expression tag	UNP Q9Z8L5
A	333	HIS	-	expression tag	UNP Q9Z8L5
A	334	SER	-	expression tag	UNP Q9Z8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	335	SER	-	expression tag	UNP Q9Z8L5
A	336	GLY	-	expression tag	UNP Q9Z8L5
A	337	LEU	-	expression tag	UNP Q9Z8L5
A	338	VAL	-	expression tag	UNP Q9Z8L5
A	339	PRO	-	expression tag	UNP Q9Z8L5
A	340	ARG	-	expression tag	UNP Q9Z8L5
A	341	GLY	-	expression tag	UNP Q9Z8L5
A	342	SER	-	expression tag	UNP Q9Z8L5
A	343	HIS	-	expression tag	UNP Q9Z8L5
A	344	MET	-	expression tag	UNP Q9Z8L5
B	324	MET	-	initiating methionine	UNP Q9Z8L5
B	325	GLY	-	expression tag	UNP Q9Z8L5
B	326	SER	-	expression tag	UNP Q9Z8L5
B	327	SER	-	expression tag	UNP Q9Z8L5
B	328	HIS	-	expression tag	UNP Q9Z8L5
B	329	HIS	-	expression tag	UNP Q9Z8L5
B	330	HIS	-	expression tag	UNP Q9Z8L5
B	331	HIS	-	expression tag	UNP Q9Z8L5
B	332	HIS	-	expression tag	UNP Q9Z8L5
B	333	HIS	-	expression tag	UNP Q9Z8L5
B	334	SER	-	expression tag	UNP Q9Z8L5
B	335	SER	-	expression tag	UNP Q9Z8L5
B	336	GLY	-	expression tag	UNP Q9Z8L5
B	337	LEU	-	expression tag	UNP Q9Z8L5
B	338	VAL	-	expression tag	UNP Q9Z8L5
B	339	PRO	-	expression tag	UNP Q9Z8L5
B	340	ARG	-	expression tag	UNP Q9Z8L5
B	341	GLY	-	expression tag	UNP Q9Z8L5
B	342	SER	-	expression tag	UNP Q9Z8L5
B	343	HIS	-	expression tag	UNP Q9Z8L5
B	344	MET	-	expression tag	UNP Q9Z8L5
C	324	MET	-	initiating methionine	UNP Q9Z8L5
C	325	GLY	-	expression tag	UNP Q9Z8L5
C	326	SER	-	expression tag	UNP Q9Z8L5
C	327	SER	-	expression tag	UNP Q9Z8L5
C	328	HIS	-	expression tag	UNP Q9Z8L5
C	329	HIS	-	expression tag	UNP Q9Z8L5
C	330	HIS	-	expression tag	UNP Q9Z8L5
C	331	HIS	-	expression tag	UNP Q9Z8L5
C	332	HIS	-	expression tag	UNP Q9Z8L5
C	333	HIS	-	expression tag	UNP Q9Z8L5
C	334	SER	-	expression tag	UNP Q9Z8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	335	SER	-	expression tag	UNP Q9Z8L5
C	336	GLY	-	expression tag	UNP Q9Z8L5
C	337	LEU	-	expression tag	UNP Q9Z8L5
C	338	VAL	-	expression tag	UNP Q9Z8L5
C	339	PRO	-	expression tag	UNP Q9Z8L5
C	340	ARG	-	expression tag	UNP Q9Z8L5
C	341	GLY	-	expression tag	UNP Q9Z8L5
C	342	SER	-	expression tag	UNP Q9Z8L5
C	343	HIS	-	expression tag	UNP Q9Z8L5
C	344	MET	-	expression tag	UNP Q9Z8L5
D	324	MET	-	initiating methionine	UNP Q9Z8L5
D	325	GLY	-	expression tag	UNP Q9Z8L5
D	326	SER	-	expression tag	UNP Q9Z8L5
D	327	SER	-	expression tag	UNP Q9Z8L5
D	328	HIS	-	expression tag	UNP Q9Z8L5
D	329	HIS	-	expression tag	UNP Q9Z8L5
D	330	HIS	-	expression tag	UNP Q9Z8L5
D	331	HIS	-	expression tag	UNP Q9Z8L5
D	332	HIS	-	expression tag	UNP Q9Z8L5
D	333	HIS	-	expression tag	UNP Q9Z8L5
D	334	SER	-	expression tag	UNP Q9Z8L5
D	335	SER	-	expression tag	UNP Q9Z8L5
D	336	GLY	-	expression tag	UNP Q9Z8L5
D	337	LEU	-	expression tag	UNP Q9Z8L5
D	338	VAL	-	expression tag	UNP Q9Z8L5
D	339	PRO	-	expression tag	UNP Q9Z8L5
D	340	ARG	-	expression tag	UNP Q9Z8L5
D	341	GLY	-	expression tag	UNP Q9Z8L5
D	342	SER	-	expression tag	UNP Q9Z8L5
D	343	HIS	-	expression tag	UNP Q9Z8L5
D	344	MET	-	expression tag	UNP Q9Z8L5
E	324	MET	-	initiating methionine	UNP Q9Z8L5
E	325	GLY	-	expression tag	UNP Q9Z8L5
E	326	SER	-	expression tag	UNP Q9Z8L5
E	327	SER	-	expression tag	UNP Q9Z8L5
E	328	HIS	-	expression tag	UNP Q9Z8L5
E	329	HIS	-	expression tag	UNP Q9Z8L5
E	330	HIS	-	expression tag	UNP Q9Z8L5
E	331	HIS	-	expression tag	UNP Q9Z8L5
E	332	HIS	-	expression tag	UNP Q9Z8L5
E	333	HIS	-	expression tag	UNP Q9Z8L5
E	334	SER	-	expression tag	UNP Q9Z8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	335	SER	-	expression tag	UNP Q9Z8L5
E	336	GLY	-	expression tag	UNP Q9Z8L5
E	337	LEU	-	expression tag	UNP Q9Z8L5
E	338	VAL	-	expression tag	UNP Q9Z8L5
E	339	PRO	-	expression tag	UNP Q9Z8L5
E	340	ARG	-	expression tag	UNP Q9Z8L5
E	341	GLY	-	expression tag	UNP Q9Z8L5
E	342	SER	-	expression tag	UNP Q9Z8L5
E	343	HIS	-	expression tag	UNP Q9Z8L5
E	344	MET	-	expression tag	UNP Q9Z8L5
F	324	MET	-	initiating methionine	UNP Q9Z8L5
F	325	GLY	-	expression tag	UNP Q9Z8L5
F	326	SER	-	expression tag	UNP Q9Z8L5
F	327	SER	-	expression tag	UNP Q9Z8L5
F	328	HIS	-	expression tag	UNP Q9Z8L5
F	329	HIS	-	expression tag	UNP Q9Z8L5
F	330	HIS	-	expression tag	UNP Q9Z8L5
F	331	HIS	-	expression tag	UNP Q9Z8L5
F	332	HIS	-	expression tag	UNP Q9Z8L5
F	333	HIS	-	expression tag	UNP Q9Z8L5
F	334	SER	-	expression tag	UNP Q9Z8L5
F	335	SER	-	expression tag	UNP Q9Z8L5
F	336	GLY	-	expression tag	UNP Q9Z8L5
F	337	LEU	-	expression tag	UNP Q9Z8L5
F	338	VAL	-	expression tag	UNP Q9Z8L5
F	339	PRO	-	expression tag	UNP Q9Z8L5
F	340	ARG	-	expression tag	UNP Q9Z8L5
F	341	GLY	-	expression tag	UNP Q9Z8L5
F	342	SER	-	expression tag	UNP Q9Z8L5
F	343	HIS	-	expression tag	UNP Q9Z8L5
F	344	MET	-	expression tag	UNP Q9Z8L5
G	324	MET	-	initiating methionine	UNP Q9Z8L5
G	325	GLY	-	expression tag	UNP Q9Z8L5
G	326	SER	-	expression tag	UNP Q9Z8L5
G	327	SER	-	expression tag	UNP Q9Z8L5
G	328	HIS	-	expression tag	UNP Q9Z8L5
G	329	HIS	-	expression tag	UNP Q9Z8L5
G	330	HIS	-	expression tag	UNP Q9Z8L5
G	331	HIS	-	expression tag	UNP Q9Z8L5
G	332	HIS	-	expression tag	UNP Q9Z8L5
G	333	HIS	-	expression tag	UNP Q9Z8L5
G	334	SER	-	expression tag	UNP Q9Z8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	335	SER	-	expression tag	UNP Q9Z8L5
G	336	GLY	-	expression tag	UNP Q9Z8L5
G	337	LEU	-	expression tag	UNP Q9Z8L5
G	338	VAL	-	expression tag	UNP Q9Z8L5
G	339	PRO	-	expression tag	UNP Q9Z8L5
G	340	ARG	-	expression tag	UNP Q9Z8L5
G	341	GLY	-	expression tag	UNP Q9Z8L5
G	342	SER	-	expression tag	UNP Q9Z8L5
G	343	HIS	-	expression tag	UNP Q9Z8L5
G	344	MET	-	expression tag	UNP Q9Z8L5
H	324	MET	-	initiating methionine	UNP Q9Z8L5
H	325	GLY	-	expression tag	UNP Q9Z8L5
H	326	SER	-	expression tag	UNP Q9Z8L5
H	327	SER	-	expression tag	UNP Q9Z8L5
H	328	HIS	-	expression tag	UNP Q9Z8L5
H	329	HIS	-	expression tag	UNP Q9Z8L5
H	330	HIS	-	expression tag	UNP Q9Z8L5
H	331	HIS	-	expression tag	UNP Q9Z8L5
H	332	HIS	-	expression tag	UNP Q9Z8L5
H	333	HIS	-	expression tag	UNP Q9Z8L5
H	334	SER	-	expression tag	UNP Q9Z8L5
H	335	SER	-	expression tag	UNP Q9Z8L5
H	336	GLY	-	expression tag	UNP Q9Z8L5
H	337	LEU	-	expression tag	UNP Q9Z8L5
H	338	VAL	-	expression tag	UNP Q9Z8L5
H	339	PRO	-	expression tag	UNP Q9Z8L5
H	340	ARG	-	expression tag	UNP Q9Z8L5
H	341	GLY	-	expression tag	UNP Q9Z8L5
H	342	SER	-	expression tag	UNP Q9Z8L5
H	343	HIS	-	expression tag	UNP Q9Z8L5
H	344	MET	-	expression tag	UNP Q9Z8L5
I	324	MET	-	initiating methionine	UNP Q9Z8L5
I	325	GLY	-	expression tag	UNP Q9Z8L5
I	326	SER	-	expression tag	UNP Q9Z8L5
I	327	SER	-	expression tag	UNP Q9Z8L5
I	328	HIS	-	expression tag	UNP Q9Z8L5
I	329	HIS	-	expression tag	UNP Q9Z8L5
I	330	HIS	-	expression tag	UNP Q9Z8L5
I	331	HIS	-	expression tag	UNP Q9Z8L5
I	332	HIS	-	expression tag	UNP Q9Z8L5
I	333	HIS	-	expression tag	UNP Q9Z8L5
I	334	SER	-	expression tag	UNP Q9Z8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	335	SER	-	expression tag	UNP Q9Z8L5
I	336	GLY	-	expression tag	UNP Q9Z8L5
I	337	LEU	-	expression tag	UNP Q9Z8L5
I	338	VAL	-	expression tag	UNP Q9Z8L5
I	339	PRO	-	expression tag	UNP Q9Z8L5
I	340	ARG	-	expression tag	UNP Q9Z8L5
I	341	GLY	-	expression tag	UNP Q9Z8L5
I	342	SER	-	expression tag	UNP Q9Z8L5
I	343	HIS	-	expression tag	UNP Q9Z8L5
I	344	MET	-	expression tag	UNP Q9Z8L5

- Molecule 2 is a protein called CdsO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	83	Total	C	N	O	S	0	0	0
			687	427	124	134	2			
2	M	65	Total	C	N	O	S	0	0	0
			536	333	94	108	1			
2	N	86	Total	C	N	O	S	0	0	0
			709	441	126	141	1			
2	O	74	Total	C	N	O	S	0	0	0
			604	375	105	123	1			
2	P	65	Total	C	N	O	S	0	0	0
			536	333	94	108	1			
2	Q	71	Total	C	N	O	S	0	0	0
			578	358	101	118	1			
2	R	59	Total	C	N	O	S	0	0	0
			481	299	83	98	1			
2	S	40	Total	C	N	O	S	0	0	0
			325	205	58	61	1			
2	T	75	Total	C	N	O	S	0	0	0
			622	387	111	123	1			

There are 189 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	4	MET	-	initiating methionine	UNP Q9Z7J9
L	5	GLY	-	expression tag	UNP Q9Z7J9
L	6	SER	-	expression tag	UNP Q9Z7J9
L	7	SER	-	expression tag	UNP Q9Z7J9
L	8	HIS	-	expression tag	UNP Q9Z7J9
L	9	HIS	-	expression tag	UNP Q9Z7J9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	10	HIS	-	expression tag	UNP Q9Z7J9
L	11	HIS	-	expression tag	UNP Q9Z7J9
L	12	HIS	-	expression tag	UNP Q9Z7J9
L	13	HIS	-	expression tag	UNP Q9Z7J9
L	14	SER	-	expression tag	UNP Q9Z7J9
L	15	SER	-	expression tag	UNP Q9Z7J9
L	16	GLY	-	expression tag	UNP Q9Z7J9
L	17	LEU	-	expression tag	UNP Q9Z7J9
L	18	VAL	-	expression tag	UNP Q9Z7J9
L	19	PRO	-	expression tag	UNP Q9Z7J9
L	20	ARG	-	expression tag	UNP Q9Z7J9
L	21	GLY	-	expression tag	UNP Q9Z7J9
L	22	SER	-	expression tag	UNP Q9Z7J9
L	23	HIS	-	expression tag	UNP Q9Z7J9
L	24	MET	-	expression tag	UNP Q9Z7J9
M	4	MET	-	initiating methionine	UNP Q9Z7J9
M	5	GLY	-	expression tag	UNP Q9Z7J9
M	6	SER	-	expression tag	UNP Q9Z7J9
M	7	SER	-	expression tag	UNP Q9Z7J9
M	8	HIS	-	expression tag	UNP Q9Z7J9
M	9	HIS	-	expression tag	UNP Q9Z7J9
M	10	HIS	-	expression tag	UNP Q9Z7J9
M	11	HIS	-	expression tag	UNP Q9Z7J9
M	12	HIS	-	expression tag	UNP Q9Z7J9
M	13	HIS	-	expression tag	UNP Q9Z7J9
M	14	SER	-	expression tag	UNP Q9Z7J9
M	15	SER	-	expression tag	UNP Q9Z7J9
M	16	GLY	-	expression tag	UNP Q9Z7J9
M	17	LEU	-	expression tag	UNP Q9Z7J9
M	18	VAL	-	expression tag	UNP Q9Z7J9
M	19	PRO	-	expression tag	UNP Q9Z7J9
M	20	ARG	-	expression tag	UNP Q9Z7J9
M	21	GLY	-	expression tag	UNP Q9Z7J9
M	22	SER	-	expression tag	UNP Q9Z7J9
M	23	HIS	-	expression tag	UNP Q9Z7J9
M	24	MET	-	expression tag	UNP Q9Z7J9
N	4	MET	-	initiating methionine	UNP Q9Z7J9
N	5	GLY	-	expression tag	UNP Q9Z7J9
N	6	SER	-	expression tag	UNP Q9Z7J9
N	7	SER	-	expression tag	UNP Q9Z7J9
N	8	HIS	-	expression tag	UNP Q9Z7J9
N	9	HIS	-	expression tag	UNP Q9Z7J9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	10	HIS	-	expression tag	UNP Q9Z7J9
N	11	HIS	-	expression tag	UNP Q9Z7J9
N	12	HIS	-	expression tag	UNP Q9Z7J9
N	13	HIS	-	expression tag	UNP Q9Z7J9
N	14	SER	-	expression tag	UNP Q9Z7J9
N	15	SER	-	expression tag	UNP Q9Z7J9
N	16	GLY	-	expression tag	UNP Q9Z7J9
N	17	LEU	-	expression tag	UNP Q9Z7J9
N	18	VAL	-	expression tag	UNP Q9Z7J9
N	19	PRO	-	expression tag	UNP Q9Z7J9
N	20	ARG	-	expression tag	UNP Q9Z7J9
N	21	GLY	-	expression tag	UNP Q9Z7J9
N	22	SER	-	expression tag	UNP Q9Z7J9
N	23	HIS	-	expression tag	UNP Q9Z7J9
N	24	MET	-	expression tag	UNP Q9Z7J9
O	4	MET	-	initiating methionine	UNP Q9Z7J9
O	5	GLY	-	expression tag	UNP Q9Z7J9
O	6	SER	-	expression tag	UNP Q9Z7J9
O	7	SER	-	expression tag	UNP Q9Z7J9
O	8	HIS	-	expression tag	UNP Q9Z7J9
O	9	HIS	-	expression tag	UNP Q9Z7J9
O	10	HIS	-	expression tag	UNP Q9Z7J9
O	11	HIS	-	expression tag	UNP Q9Z7J9
O	12	HIS	-	expression tag	UNP Q9Z7J9
O	13	HIS	-	expression tag	UNP Q9Z7J9
O	14	SER	-	expression tag	UNP Q9Z7J9
O	15	SER	-	expression tag	UNP Q9Z7J9
O	16	GLY	-	expression tag	UNP Q9Z7J9
O	17	LEU	-	expression tag	UNP Q9Z7J9
O	18	VAL	-	expression tag	UNP Q9Z7J9
O	19	PRO	-	expression tag	UNP Q9Z7J9
O	20	ARG	-	expression tag	UNP Q9Z7J9
O	21	GLY	-	expression tag	UNP Q9Z7J9
O	22	SER	-	expression tag	UNP Q9Z7J9
O	23	HIS	-	expression tag	UNP Q9Z7J9
O	24	MET	-	expression tag	UNP Q9Z7J9
P	4	MET	-	initiating methionine	UNP Q9Z7J9
P	5	GLY	-	expression tag	UNP Q9Z7J9
P	6	SER	-	expression tag	UNP Q9Z7J9
P	7	SER	-	expression tag	UNP Q9Z7J9
P	8	HIS	-	expression tag	UNP Q9Z7J9
P	9	HIS	-	expression tag	UNP Q9Z7J9

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Chain	Residue	Modelled	Actual	Comment	Reference
P	10	HIS	-	expression tag	UNP Q9Z7J9
P	11	HIS	-	expression tag	UNP Q9Z7J9
P	12	HIS	-	expression tag	UNP Q9Z7J9
P	13	HIS	-	expression tag	UNP Q9Z7J9
P	14	SER	-	expression tag	UNP Q9Z7J9
P	15	SER	-	expression tag	UNP Q9Z7J9
P	16	GLY	-	expression tag	UNP Q9Z7J9
P	17	LEU	-	expression tag	UNP Q9Z7J9
P	18	VAL	-	expression tag	UNP Q9Z7J9
P	19	PRO	-	expression tag	UNP Q9Z7J9
P	20	ARG	-	expression tag	UNP Q9Z7J9
P	21	GLY	-	expression tag	UNP Q9Z7J9
P	22	SER	-	expression tag	UNP Q9Z7J9
P	23	HIS	-	expression tag	UNP Q9Z7J9
P	24	MET	-	expression tag	UNP Q9Z7J9
Q	4	MET	-	initiating methionine	UNP Q9Z7J9
Q	5	GLY	-	expression tag	UNP Q9Z7J9
Q	6	SER	-	expression tag	UNP Q9Z7J9
Q	7	SER	-	expression tag	UNP Q9Z7J9
Q	8	HIS	-	expression tag	UNP Q9Z7J9
Q	9	HIS	-	expression tag	UNP Q9Z7J9
Q	10	HIS	-	expression tag	UNP Q9Z7J9
Q	11	HIS	-	expression tag	UNP Q9Z7J9
Q	12	HIS	-	expression tag	UNP Q9Z7J9
Q	13	HIS	-	expression tag	UNP Q9Z7J9
Q	14	SER	-	expression tag	UNP Q9Z7J9
Q	15	SER	-	expression tag	UNP Q9Z7J9
Q	16	GLY	-	expression tag	UNP Q9Z7J9
Q	17	LEU	-	expression tag	UNP Q9Z7J9
Q	18	VAL	-	expression tag	UNP Q9Z7J9
Q	19	PRO	-	expression tag	UNP Q9Z7J9
Q	20	ARG	-	expression tag	UNP Q9Z7J9
Q	21	GLY	-	expression tag	UNP Q9Z7J9
Q	22	SER	-	expression tag	UNP Q9Z7J9
Q	23	HIS	-	expression tag	UNP Q9Z7J9
Q	24	MET	-	expression tag	UNP Q9Z7J9
R	4	MET	-	initiating methionine	UNP Q9Z7J9
R	5	GLY	-	expression tag	UNP Q9Z7J9
R	6	SER	-	expression tag	UNP Q9Z7J9
R	7	SER	-	expression tag	UNP Q9Z7J9
R	8	HIS	-	expression tag	UNP Q9Z7J9
R	9	HIS	-	expression tag	UNP Q9Z7J9

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Chain	Residue	Modelled	Actual	Comment	Reference
R	10	HIS	-	expression tag	UNP Q9Z7J9
R	11	HIS	-	expression tag	UNP Q9Z7J9
R	12	HIS	-	expression tag	UNP Q9Z7J9
R	13	HIS	-	expression tag	UNP Q9Z7J9
R	14	SER	-	expression tag	UNP Q9Z7J9
R	15	SER	-	expression tag	UNP Q9Z7J9
R	16	GLY	-	expression tag	UNP Q9Z7J9
R	17	LEU	-	expression tag	UNP Q9Z7J9
R	18	VAL	-	expression tag	UNP Q9Z7J9
R	19	PRO	-	expression tag	UNP Q9Z7J9
R	20	ARG	-	expression tag	UNP Q9Z7J9
R	21	GLY	-	expression tag	UNP Q9Z7J9
R	22	SER	-	expression tag	UNP Q9Z7J9
R	23	HIS	-	expression tag	UNP Q9Z7J9
R	24	MET	-	expression tag	UNP Q9Z7J9
S	4	MET	-	initiating methionine	UNP Q9Z7J9
S	5	GLY	-	expression tag	UNP Q9Z7J9
S	6	SER	-	expression tag	UNP Q9Z7J9
S	7	SER	-	expression tag	UNP Q9Z7J9
S	8	HIS	-	expression tag	UNP Q9Z7J9
S	9	HIS	-	expression tag	UNP Q9Z7J9
S	10	HIS	-	expression tag	UNP Q9Z7J9
S	11	HIS	-	expression tag	UNP Q9Z7J9
S	12	HIS	-	expression tag	UNP Q9Z7J9
S	13	HIS	-	expression tag	UNP Q9Z7J9
S	14	SER	-	expression tag	UNP Q9Z7J9
S	15	SER	-	expression tag	UNP Q9Z7J9
S	16	GLY	-	expression tag	UNP Q9Z7J9
S	17	LEU	-	expression tag	UNP Q9Z7J9
S	18	VAL	-	expression tag	UNP Q9Z7J9
S	19	PRO	-	expression tag	UNP Q9Z7J9
S	20	ARG	-	expression tag	UNP Q9Z7J9
S	21	GLY	-	expression tag	UNP Q9Z7J9
S	22	SER	-	expression tag	UNP Q9Z7J9
S	23	HIS	-	expression tag	UNP Q9Z7J9
S	24	MET	-	expression tag	UNP Q9Z7J9
T	4	MET	-	initiating methionine	UNP Q9Z7J9
T	5	GLY	-	expression tag	UNP Q9Z7J9
T	6	SER	-	expression tag	UNP Q9Z7J9
T	7	SER	-	expression tag	UNP Q9Z7J9
T	8	HIS	-	expression tag	UNP Q9Z7J9
T	9	HIS	-	expression tag	UNP Q9Z7J9

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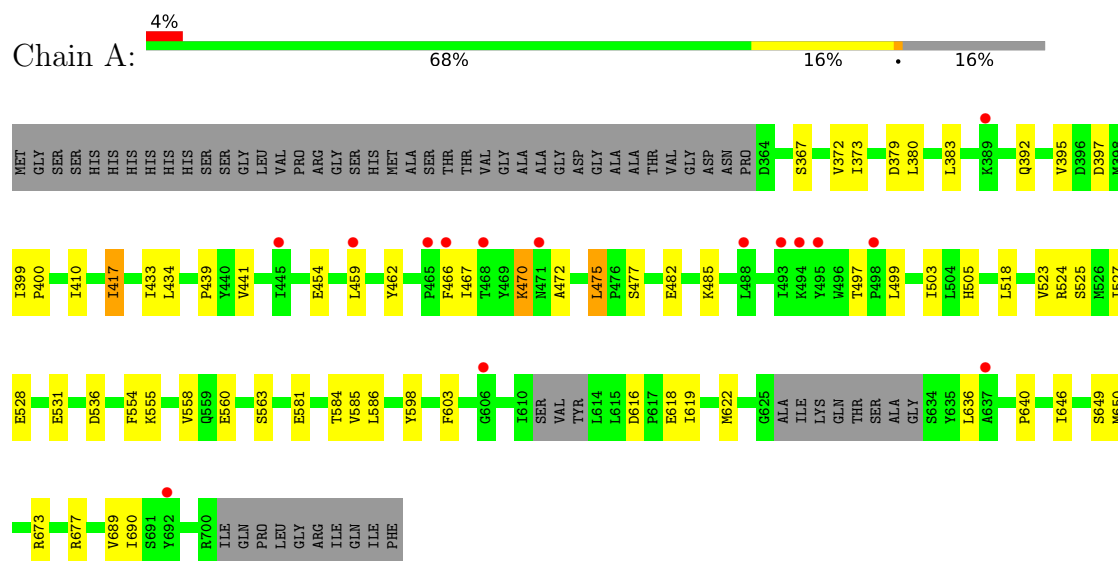
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Chain	Residue	Modelled	Actual	Comment	Reference
T	10	HIS	-	expression tag	UNP Q9Z7J9
T	11	HIS	-	expression tag	UNP Q9Z7J9
T	12	HIS	-	expression tag	UNP Q9Z7J9
T	13	HIS	-	expression tag	UNP Q9Z7J9
T	14	SER	-	expression tag	UNP Q9Z7J9
T	15	SER	-	expression tag	UNP Q9Z7J9
T	16	GLY	-	expression tag	UNP Q9Z7J9
T	17	LEU	-	expression tag	UNP Q9Z7J9
T	18	VAL	-	expression tag	UNP Q9Z7J9
T	19	PRO	-	expression tag	UNP Q9Z7J9
T	20	ARG	-	expression tag	UNP Q9Z7J9
T	21	GLY	-	expression tag	UNP Q9Z7J9
T	22	SER	-	expression tag	UNP Q9Z7J9
T	23	HIS	-	expression tag	UNP Q9Z7J9
T	24	MET	-	expression tag	UNP Q9Z7J9

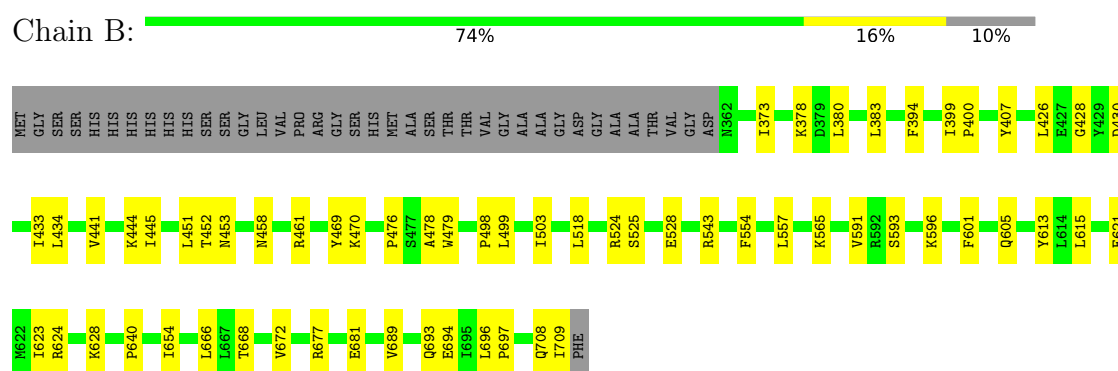
### 3 Residue-property plots [i](#)

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

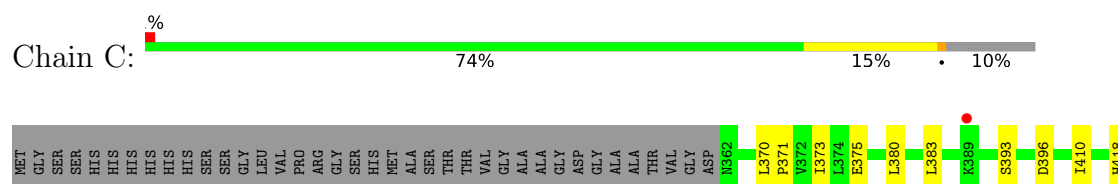
#### • Molecule 1: Low calcium response locus protein D

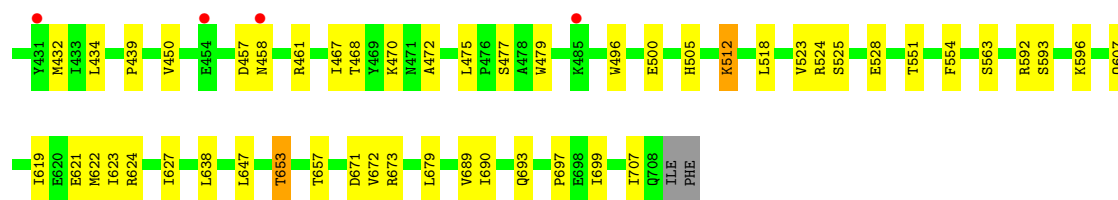


#### • Molecule 1: Low calcium response locus protein D

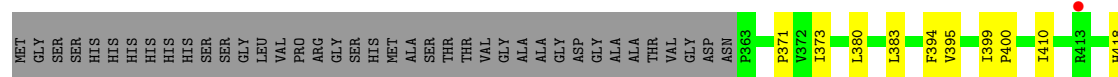


#### • Molecule 1: Low calcium response locus protein D

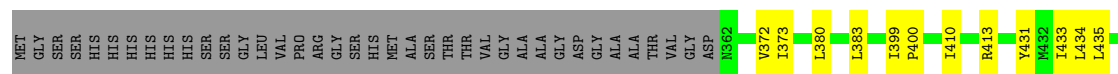
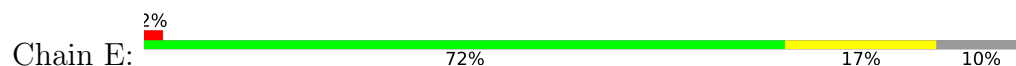




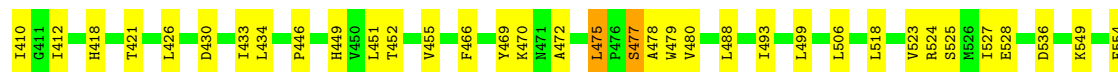
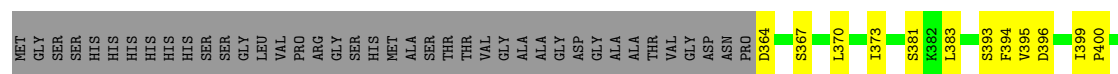
• Molecule 1: Low calcium response locus protein D



• Molecule 1: Low calcium response locus protein D

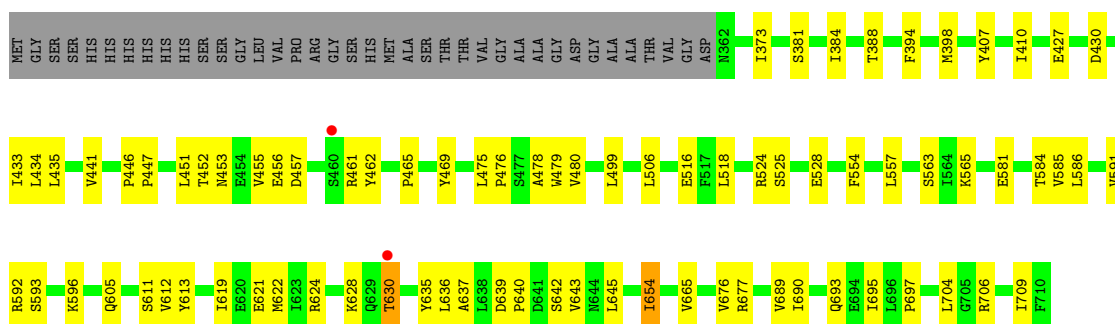


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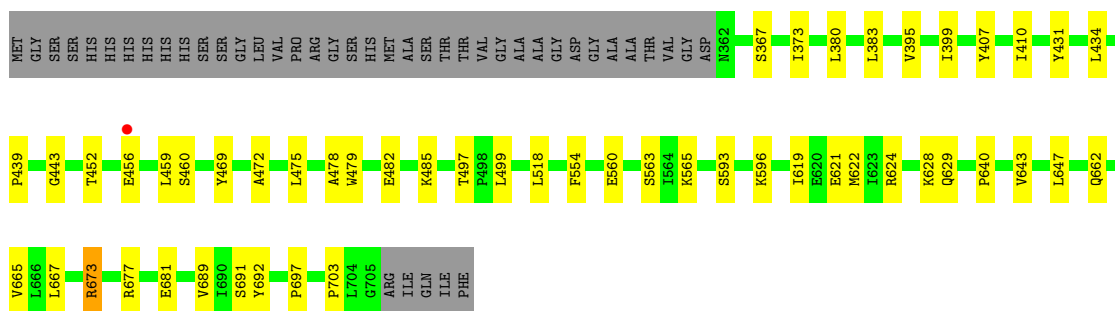


• Molecule 1: Low calcium response locus protein D

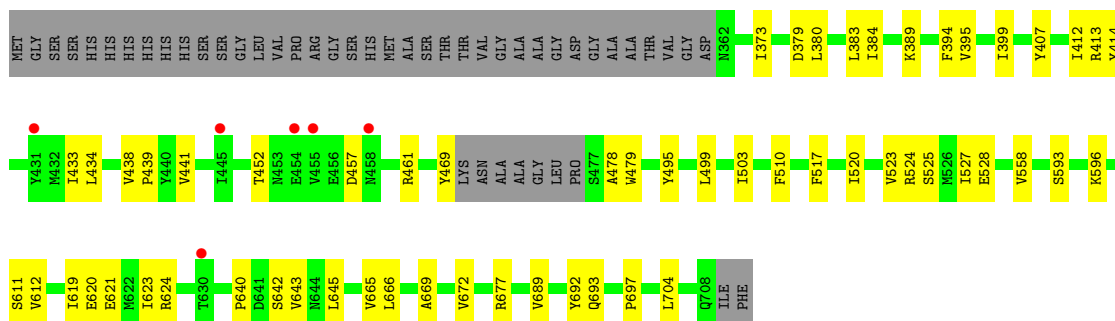




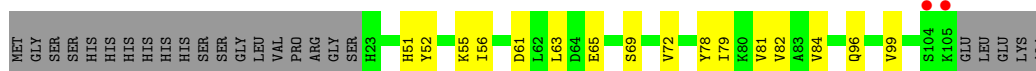
• Molecule 1: Low calcium response locus protein D



• Molecule 1: Low calcium response locus protein D

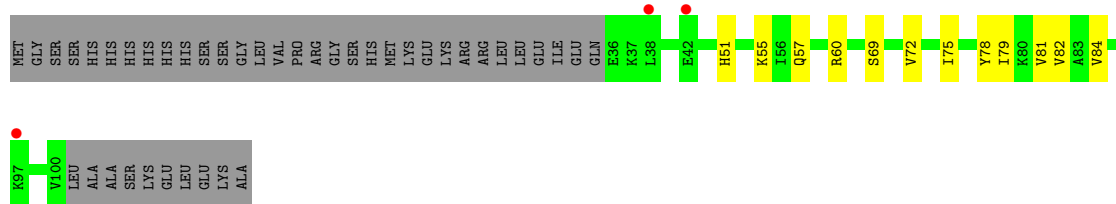


• Molecule 2: CdsO



• Molecule 2: CdsO

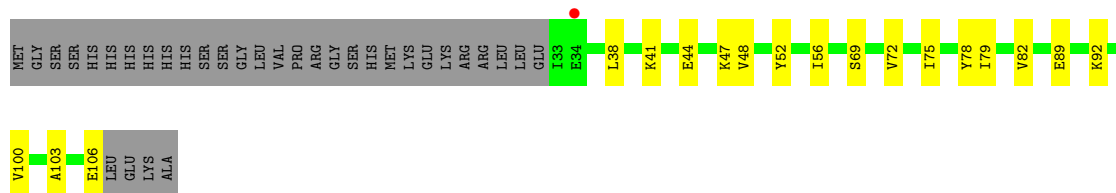




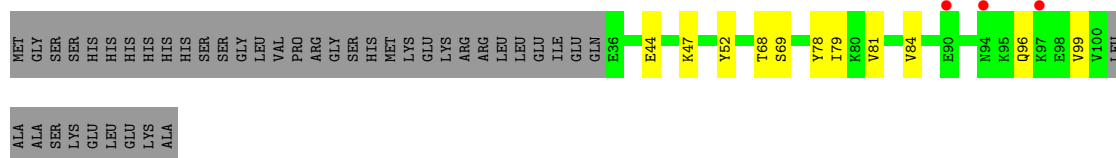
• Molecule 2: CdsO



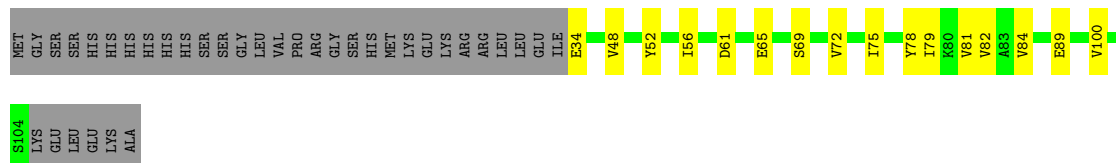
• Molecule 2: CdsO



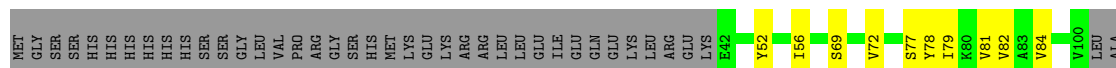
• Molecule 2: CdsO



• Molecule 2: CdsO



• Molecule 2: CdsO



ALA  
SER  
LYS  
GLU  
LEU  
GLU  
LYS  
ALA

● Molecule 2: CdsO



MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET LYS GLU LYS ARG ARG LEU LEU TLE GLN GLN LYS LEU ARG GLU LYS ALA ALA R45 Y52 Y56 L59 R60 D61 L62 L63 D64 E65 A71 I75 K76 S77

Y78 I79 R80 V81 V82 A83 V84 GLN LEU SER SER SER SER GLY GLU GLU VAL LYS VAL ASN LYS GLN LYS MET LYS VAL VAL VAL LEU ALA ALA SER LYS GLU LEU GLN LYS

● Molecule 2: CdsO



MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET LYS GLU LYS R28 E44 K47 Y52 K55 I56 S69 V72 Y78 I79 K80 V81 V82 A83 V84 Q96 V99 A102 ALA SER LYS GLU LEU GLU LYS ALA

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.41Å 206.61Å 280.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.22 – 4.62 52.22 – 4.62	Depositor EDS
% Data completeness (in resolution range)	99.4 (52.22-4.62) 99.4 (52.22-4.62)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 4.64Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874-000	Depositor
R, $R_{free}$	0.241 , 0.285 0.246 , 0.293	Depositor DCC
$R_{free}$ test set	2498 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	228.0	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 243.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	29937	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	307.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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	0.32	0/2698	0.47	0/3658
1	B	0.30	0/2868	0.47	0/3893
1	C	0.33	0/2860	0.46	0/3882
1	D	0.29	0/2723	0.44	0/3688
1	E	0.28	0/2860	0.45	0/3882
1	F	0.31	0/2852	0.47	0/3870
1	G	0.35	0/2880	0.49	0/3909
1	H	0.29	0/2832	0.45	0/3845
1	I	0.28	0/2812	0.43	0/3815
2	L	0.23	0/690	0.36	0/917
2	M	0.23	0/538	0.38	0/717
2	N	0.25	0/711	0.40	0/945
2	O	0.23	0/606	0.37	0/808
2	P	0.23	0/538	0.40	0/717
2	Q	0.23	0/580	0.37	0/774
2	R	0.23	0/483	0.37	0/646
2	S	0.33	0/327	0.43	0/438
2	T	0.23	0/624	0.38	0/832
All	All	0.30	0/30482	0.45	0/41236

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2643	0	2707	34	0
1	B	2808	0	2885	40	0
1	C	2800	0	2874	38	0
1	D	2670	0	2735	34	0
1	E	2800	0	2874	42	0
1	F	2793	0	2872	49	0
1	G	2819	0	2894	47	0
1	H	2772	0	2842	32	0
1	I	2754	0	2823	38	0
2	L	687	0	722	15	0
2	M	536	0	556	11	0
2	N	709	0	747	11	0
2	O	604	0	626	11	0
2	P	536	0	556	8	0
2	Q	578	0	596	12	0
2	R	481	0	494	7	0
2	S	325	0	343	6	0
2	T	622	0	651	9	0
All	All	29937	0	30797	408	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 7.

All (408) 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:E:457:ASP:O	1:E:461:ARG:HG3	1.53	1.08
1:C:457:ASP:O	1:C:461:ARG:HG3	1.63	0.97
1:I:697:PRO:HA	2:T:69:SER:HB3	1.54	0.89
1:G:581:GLU:HG2	1:G:586:LEU:HD22	1.57	0.85
1:H:697:PRO:HA	2:L:69:SER:HB3	1.58	0.84
1:A:373:ILE:HB	1:A:434:LEU:HB2	1.59	0.83
1:G:457:ASP:O	1:G:461:ARG:HG3	1.80	0.82
1:C:653:THR:HG21	1:C:707:ILE:HG12	1.62	0.81
1:A:581:GLU:HG2	1:A:586:LEU:HD22	1.61	0.81
1:C:697:PRO:HA	2:Q:69:SER:HB3	1.62	0.80
1:G:697:PRO:HA	2:M:69:SER:HB3	1.62	0.80
1:D:697:PRO:HA	2:P:69:SER:HB3	1.63	0.80
1:E:673:ARG:HG2	1:E:689:VAL:HG12	1.65	0.78
1:B:697:PRO:HA	2:R:69:SER:HB3	1.64	0.78
1:F:697:PRO:HA	2:N:69:SER:HB3	1.65	0.77
1:F:373:ILE:HB	1:F:434:LEU:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:457:ASP:HB3	1:E:461:ARG:HE	1.53	0.74
1:F:670:ILE:HA	1:F:691:SER:OG	1.87	0.74
1:B:518:LEU:HD21	1:B:554:PHE:HB3	1.71	0.72
1:H:640:PRO:HG3	2:T:78:TYR:HB3	1.71	0.72
1:F:410:ILE:HG13	1:F:563:SER:HA	1.72	0.71
1:E:410:ILE:HD12	1:E:563:SER:HA	1.71	0.71
1:B:623:ILE:HG21	1:B:672:VAL:HG23	1.73	0.70
1:F:524:ARG:HH12	1:F:528:GLU:HB3	1.56	0.70
1:A:673:ARG:HG2	1:A:689:VAL:HG12	1.72	0.69
1:G:373:ILE:HB	1:G:434:LEU:HB2	1.73	0.69
1:F:640:PRO:HG3	2:M:78:TYR:HB3	1.75	0.68
1:H:518:LEU:HD21	1:H:554:PHE:HB3	1.74	0.68
1:B:640:PRO:HG3	2:Q:78:TYR:HB3	1.76	0.68
1:E:640:PRO:HG3	2:N:78:TYR:HB3	1.74	0.67
1:B:708:GLN:HG3	1:B:709:ILE:H	1.58	0.67
1:H:373:ILE:HB	1:H:434:LEU:HB2	1.74	0.67
1:D:700:ARG:HA	2:P:68:THR:HG22	1.76	0.66
1:C:467:ILE:HB	1:C:479:TRP:HB2	1.77	0.66
1:G:518:LEU:HD21	1:G:554:PHE:HB3	1.77	0.66
1:F:394:PHE:HB2	1:F:499:LEU:HD23	1.78	0.66
1:A:472:ALA:HB3	1:A:475:LEU:HB2	1.78	0.65
1:H:410:ILE:HG13	1:H:563:SER:HA	1.78	0.65
1:B:373:ILE:HB	1:B:434:LEU:HB2	1.77	0.65
1:E:697:PRO:HA	2:O:69:SER:HB3	1.78	0.65
1:C:373:ILE:HB	1:C:434:LEU:HB2	1.79	0.65
1:C:673:ARG:HG2	1:C:689:VAL:HG12	1.78	0.65
1:G:640:PRO:HG3	2:L:78:TYR:HB3	1.79	0.65
1:G:613:TYR:HE2	1:G:654:ILE:HA	1.61	0.65
1:A:518:LEU:HD21	1:A:554:PHE:HB3	1.79	0.64
1:D:628:LYS:HB2	1:D:635:TYR:HB3	1.80	0.64
1:D:518:LEU:HD21	1:D:554:PHE:HB3	1.79	0.64
2:M:57:GLN:HE22	2:M:60:ARG:HH21	1.46	0.64
1:C:475:LEU:HD11	1:C:505:HIS:HB2	1.80	0.63
1:E:413:ARG:HH21	1:E:522:GLU:HG3	1.64	0.63
1:H:380:LEU:HD23	1:H:383:LEU:HD12	1.81	0.63
1:G:435:LEU:HD21	1:G:516:GLU:HG3	1.81	0.62
1:E:518:LEU:HD21	1:E:554:PHE:HB3	1.82	0.62
1:B:613:TYR:HE2	1:B:654:ILE:HA	1.64	0.62
1:E:642:SER:HA	1:E:645:LEU:HB2	1.81	0.61
1:F:524:ARG:NH1	1:F:528:GLU:HB3	2.15	0.61
1:F:549:LYS:HD2	1:F:584:THR:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:472:ALA:H	1:F:475:LEU:HB2	1.66	0.60
1:B:380:LEU:HD23	1:B:383:LEU:HD12	1.84	0.60
1:C:524:ARG:HH12	1:C:528:GLU:HB3	1.67	0.60
1:D:497:THR:HG22	1:D:499:LEU:H	1.65	0.60
1:H:621:GLU:HA	1:H:624:ARG:HD3	1.83	0.59
1:D:410:ILE:HG13	1:D:563:SER:HA	1.84	0.59
1:H:640:PRO:HB2	2:T:55:LYS:HE2	1.83	0.59
1:C:621:GLU:HA	1:C:624:ARG:HD3	1.84	0.59
1:H:431:TYR:CZ	1:H:443:GLY:HA3	2.38	0.59
1:I:510:PHE:HE1	1:I:517:PHE:HE2	1.50	0.59
1:H:472:ALA:N	1:H:475:LEU:HD12	2.19	0.58
1:H:472:ALA:H	1:H:475:LEU:HD12	1.68	0.58
1:E:380:LEU:HD23	1:E:383:LEU:HD12	1.83	0.58
1:G:524:ARG:NH1	1:G:528:GLU:HB3	2.19	0.58
1:E:621:GLU:HA	1:E:624:ARG:HD3	1.85	0.57
1:B:621:GLU:HA	1:B:624:ARG:HD3	1.85	0.57
1:A:410:ILE:HG13	1:A:563:SER:HA	1.86	0.57
1:H:452:THR:O	1:H:478:ALA:HB3	2.05	0.57
2:M:81:VAL:O	2:M:84:VAL:HG12	2.05	0.57
2:Q:81:VAL:O	2:Q:84:VAL:HG12	2.05	0.57
1:E:455:VAL:HG12	1:E:457:ASP:H	1.70	0.56
1:D:619:ILE:O	1:D:623:ILE:HG12	2.05	0.56
1:I:373:ILE:HB	1:I:434:LEU:HB2	1.88	0.56
1:C:619:ILE:O	1:C:623:ILE:HG12	2.06	0.56
2:N:44:GLU:HA	2:N:47:LYS:HE3	1.88	0.55
1:E:435:LEU:HD23	1:F:597:LEU:HD22	1.87	0.55
1:F:469:TYR:HB3	1:F:479:TRP:CD1	2.41	0.55
1:B:452:THR:O	1:B:478:ALA:HB3	2.06	0.55
1:D:431:TYR:CZ	1:D:443:GLY:HA3	2.41	0.55
1:D:619:ILE:HA	1:D:622:MET:HG2	1.88	0.55
1:G:524:ARG:HH12	1:G:528:GLU:HB3	1.71	0.55
1:C:470:LYS:HG3	1:C:477:SER:HB3	1.89	0.55
1:F:383:LEU:HD22	1:F:499:LEU:HD11	1.90	0.54
2:L:51:HIS:O	2:L:55:LYS:HG2	2.07	0.54
1:G:621:GLU:HA	1:G:624:ARG:HD3	1.89	0.54
1:E:611:SER:HB3	1:E:704:LEU:HD21	1.88	0.54
1:B:524:ARG:NH1	1:B:528:GLU:HB3	2.22	0.54
2:R:81:VAL:O	2:R:84:VAL:HG22	2.07	0.54
1:D:452:THR:HG22	1:D:495:TYR:HA	1.87	0.54
1:I:642:SER:HA	1:I:645:LEU:HB2	1.90	0.53
1:E:431:TYR:CZ	1:E:443:GLY:HA3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:81:VAL:O	2:P:84:VAL:HG12	2.08	0.53
1:D:472:ALA:H	1:D:475:LEU:HD12	1.73	0.53
1:G:452:THR:O	1:G:478:ALA:HB3	2.09	0.53
1:C:410:ILE:HG13	1:C:563:SER:HA	1.91	0.53
1:I:524:ARG:NH1	1:I:528:GLU:HB3	2.23	0.53
1:C:434:LEU:HA	1:C:439:PRO:HA	1.91	0.53
1:G:410:ILE:HG13	1:G:563:SER:HA	1.91	0.53
1:G:619:ILE:HD11	1:G:709:ILE:HB	1.90	0.53
2:N:81:VAL:O	2:N:84:VAL:HG12	2.08	0.52
2:T:96:GLN:HA	2:T:99:VAL:HG12	1.90	0.52
1:F:470:LYS:HB2	1:F:477:SER:HB3	1.91	0.52
1:B:453:ASN:HB2	1:B:476:PRO:HB3	1.90	0.52
1:C:593:SER:HB2	1:C:693:GLN:HG2	1.90	0.52
1:B:433:ILE:HG22	1:B:441:VAL:O	2.09	0.52
1:I:412:ILE:HD11	1:I:558:VAL:HG11	1.91	0.52
2:P:78:TYR:HA	2:P:81:VAL:HG12	1.91	0.52
1:F:488:LEU:HD22	1:F:493:ILE:HB	1.92	0.52
1:G:642:SER:HA	1:G:645:LEU:HB2	1.90	0.52
1:I:593:SER:HB2	1:I:693:GLN:HG2	1.92	0.52
1:F:412:ILE:HD11	1:F:558:VAL:HG11	1.92	0.52
2:N:105:LYS:HA	2:N:108:GLU:HG2	1.91	0.52
1:G:593:SER:HB2	1:G:693:GLN:HG2	1.92	0.52
1:H:395:VAL:HA	1:H:399:ILE:HD12	1.92	0.52
1:E:524:ARG:HG2	1:F:536:ASP:OD2	2.10	0.51
1:I:620:GLU:O	1:I:624:ARG:HD2	2.10	0.51
2:L:81:VAL:O	2:L:84:VAL:HG12	2.10	0.51
1:F:518:LEU:HD21	1:F:554:PHE:HB3	1.92	0.51
1:D:593:SER:HB2	1:D:693:GLN:HG2	1.93	0.51
1:E:647:LEU:O	1:E:650:MET:HB2	2.10	0.51
2:S:59:LEU:HB2	2:S:75:ILE:HG21	1.93	0.51
1:C:524:ARG:NH1	1:C:528:GLU:HB3	2.25	0.51
1:E:497:THR:HG22	1:E:499:LEU:H	1.75	0.51
1:C:592:ARG:HE	1:C:673:ARG:NH2	2.09	0.51
1:E:453:ASN:HB2	1:E:476:PRO:HB3	1.93	0.51
1:A:470:LYS:HG3	1:A:477:SER:HB3	1.94	0.50
2:T:81:VAL:O	2:T:84:VAL:HG12	2.11	0.50
1:A:525:SER:O	1:A:528:GLU:HG3	2.12	0.50
1:B:593:SER:O	1:B:596:LYS:HG3	2.12	0.50
1:H:367:SER:HB3	1:I:407:TYR:HE2	1.74	0.50
1:G:525:SER:O	1:G:528:GLU:HG3	2.12	0.50
1:B:557:LEU:HD11	1:B:591:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:LEU:HD21	1:C:554:PHE:HB3	1.94	0.49
1:E:373:ILE:HB	1:E:434:LEU:HB2	1.94	0.49
2:P:96:GLN:HA	2:P:99:VAL:HG12	1.92	0.49
1:B:605:GLN:HG2	1:B:605:GLN:O	2.12	0.49
1:F:646:ILE:HG13	1:F:709:ILE:HD13	1.93	0.49
1:I:469:TYR:HB3	1:I:479:TRP:CD1	2.47	0.49
2:M:57:GLN:NE2	2:M:60:ARG:HH21	2.11	0.49
1:A:395:VAL:HA	1:A:399:ILE:HD12	1.94	0.49
1:A:392:GLN:HG2	1:A:397:ASP:OD2	2.11	0.49
1:I:666:LEU:HD23	1:I:689:VAL:HG22	1.95	0.49
1:I:669:ALA:HB3	1:I:672:VAL:HG22	1.95	0.49
1:G:605:GLN:HG2	1:G:605:GLN:O	2.12	0.48
1:G:640:PRO:HG2	2:L:55:LYS:HD2	1.94	0.48
1:I:612:VAL:HG12	1:I:665:VAL:HB	1.95	0.48
1:F:433:ILE:HD12	1:F:506:LEU:HD23	1.95	0.48
1:F:452:THR:O	1:F:478:ALA:HB3	2.12	0.48
2:Q:69:SER:HA	2:Q:72:VAL:HG12	1.94	0.48
1:A:524:ARG:NH1	1:A:528:GLU:HB3	2.28	0.48
2:S:76:LYS:HE3	2:S:80:LYS:HE3	1.95	0.48
2:L:96:GLN:HA	2:L:99:VAL:HG12	1.96	0.48
1:D:371:PRO:HD2	1:D:418:HIS:CE1	2.49	0.48
1:D:433:ILE:HG23	1:D:440:TYR:HB3	1.95	0.48
1:F:593:SER:HB2	1:F:693:GLN:HG2	1.94	0.48
1:H:677:ARG:HD3	1:H:689:VAL:H	1.79	0.48
1:H:662:GLN:O	1:H:662:GLN:HG2	2.12	0.48
1:F:640:PRO:HG2	2:M:55:LYS:HD2	1.96	0.48
1:G:676:VAL:HB	1:G:689:VAL:HG11	1.96	0.48
1:A:616:ASP:HB3	1:A:619:ILE:HG12	1.96	0.47
1:C:472:ALA:H	1:C:475:LEU:HB2	1.78	0.47
1:C:525:SER:O	1:C:528:GLU:HG3	2.14	0.47
1:D:395:VAL:HA	1:D:399:ILE:HD12	1.96	0.47
1:I:434:LEU:HA	1:I:439:PRO:HA	1.96	0.47
1:D:556:ARG:CZ	1:D:585:VAL:HG22	2.44	0.47
1:I:524:ARG:HH12	1:I:528:GLU:HB3	1.78	0.47
2:M:72:VAL:HA	2:M:75:ILE:HG22	1.96	0.47
2:L:69:SER:HA	2:L:72:VAL:HG12	1.96	0.47
2:O:44:GLU:HA	2:O:47:LYS:HE3	1.97	0.47
1:C:470:LYS:CG	1:C:477:SER:HB3	2.44	0.47
1:F:640:PRO:O	1:F:643:VAL:HG12	2.14	0.47
1:H:407:TYR:CE2	1:H:565:LYS:HE2	2.50	0.47
1:I:452:THR:O	1:I:478:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:69:SER:HA	2:T:72:VAL:HG12	1.97	0.47
1:A:380:LEU:HD23	1:A:383:LEU:HD12	1.96	0.47
1:F:393:SER:HB3	1:F:396:ASP:HB3	1.96	0.47
1:I:394:PHE:HB2	1:I:499:LEU:HD23	1.97	0.47
1:I:510:PHE:CE1	1:I:517:PHE:HE2	2.32	0.47
1:D:380:LEU:HD23	1:D:383:LEU:HD12	1.97	0.47
1:E:593:SER:HB2	1:E:693:GLN:HG2	1.97	0.47
1:G:584:THR:HG23	1:G:585:VAL:HG23	1.97	0.47
1:F:399:ILE:HB	1:F:400:PRO:HD3	1.97	0.46
1:G:677:ARG:HB2	1:G:689:VAL:HB	1.96	0.46
1:E:524:ARG:NH1	1:E:528:GLU:HB2	2.30	0.46
1:I:457:ASP:O	1:I:461:ARG:HG3	2.15	0.46
1:I:499:LEU:O	1:I:503:ILE:HG12	2.16	0.46
1:A:367:SER:HB3	1:B:407:TYR:HE2	1.81	0.46
1:C:380:LEU:HD23	1:C:383:LEU:HD12	1.97	0.46
1:G:433:ILE:HG22	1:G:441:VAL:O	2.16	0.46
1:H:673:ARG:HB3	1:H:691:SER:HB3	1.97	0.46
1:B:525:SER:O	1:B:528:GLU:HG3	2.15	0.46
1:C:370:LEU:HD22	1:C:418:HIS:NE2	2.31	0.46
1:F:466:PHE:HD1	1:F:480:VAL:HG22	1.80	0.46
2:O:79:ILE:HA	2:O:82:VAL:HG22	1.98	0.46
1:E:512:LYS:HA	1:E:512:LYS:HD3	1.78	0.46
1:I:621:GLU:HA	1:I:624:ARG:HD3	1.96	0.46
2:N:27:LYS:HD2	2:N:106:GLU:HG3	1.98	0.46
1:B:445:ILE:HD13	1:B:498:PRO:HB3	1.98	0.46
1:I:669:ALA:HA	1:I:692:TYR:CE2	2.51	0.46
1:F:451:LEU:HD13	1:F:479:TRP:CE2	2.51	0.46
1:F:593:SER:O	1:F:596:LYS:HG3	2.15	0.46
2:M:51:HIS:O	2:M:55:LYS:HG2	2.16	0.46
1:H:593:SER:O	1:H:596:LYS:HG3	2.16	0.45
2:O:38:LEU:HB2	2:O:100:VAL:HG21	1.98	0.45
1:E:457:ASP:HB3	1:E:461:ARG:NE	2.26	0.45
2:N:55:LYS:HA	2:N:55:LYS:HD2	1.66	0.45
1:F:676:VAL:HB	1:F:689:VAL:HG11	1.97	0.45
1:H:677:ARG:NH1	1:H:681:GLU:HB3	2.31	0.45
1:A:439:PRO:HD2	1:B:601:PHE:CZ	2.52	0.45
1:E:619:ILE:HA	1:E:622:MET:HG2	1.99	0.45
1:A:482:GLU:O	1:A:485:LYS:HG3	2.17	0.45
1:E:482:GLU:O	1:E:485:LYS:HG3	2.17	0.45
1:F:370:LEU:HD22	1:F:418:HIS:CE1	2.52	0.45
1:F:367:SER:HB3	1:G:407:TYR:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:71:ALA:O	2:S:75:ILE:HG12	2.17	0.45
1:A:499:LEU:O	1:A:503:ILE:HG12	2.17	0.45
1:B:394:PHE:HB2	1:B:499:LEU:HD23	1.99	0.45
1:B:615:LEU:HD11	1:B:668:THR:HG22	1.99	0.45
2:Q:52:TYR:CE2	2:Q:56:ILE:HD11	2.52	0.45
2:T:44:GLU:HA	2:T:47:LYS:HE3	1.99	0.45
1:C:371:PRO:HD2	1:C:418:HIS:HE1	1.81	0.45
1:F:426:LEU:HB3	1:F:430:ASP:HB2	1.99	0.45
1:G:640:PRO:HA	2:L:78:TYR:CD2	2.52	0.45
1:G:465:PRO:O	1:G:480:VAL:HA	2.18	0.44
1:C:496:TRP:HD1	1:C:500:GLU:HB3	1.82	0.44
1:D:394:PHE:HB2	1:D:499:LEU:HD23	1.99	0.44
1:G:619:ILE:HA	1:G:622:MET:HG2	1.98	0.44
2:O:41:LYS:NZ	2:O:92:LYS:HD3	2.32	0.44
1:C:523:VAL:HG21	1:C:551:THR:HG23	1.99	0.44
1:D:593:SER:O	1:D:596:LYS:HG3	2.17	0.44
1:I:407:TYR:CD1	1:I:413:ARG:HB2	2.52	0.44
2:O:52:TYR:CE2	2:O:56:ILE:HD11	2.52	0.44
2:P:44:GLU:HA	2:P:47:LYS:HE3	2.00	0.44
2:S:52:TYR:CE2	2:S:56:ILE:HD11	2.53	0.44
1:B:426:LEU:HB3	1:B:430:ASP:HB2	1.99	0.44
2:L:52:TYR:CE2	2:L:56:ILE:HD11	2.52	0.44
1:D:525:SER:O	1:D:528:GLU:HG3	2.16	0.44
1:G:557:LEU:HD11	1:G:591:VAL:HG11	1.99	0.44
1:G:611:SER:HB3	1:G:704:LEU:HD11	2.00	0.44
1:I:525:SER:O	1:I:528:GLU:HG3	2.17	0.44
2:S:77:SER:O	2:S:81:VAL:HG23	2.17	0.44
1:B:666:LEU:HD23	1:B:689:VAL:HG22	1.99	0.44
1:C:375:GLU:HG3	1:C:432:MET:HE2	1.99	0.44
1:E:433:ILE:HD12	1:E:506:LEU:HD23	2.00	0.44
1:E:451:LEU:HD13	1:E:479:TRP:CE2	2.53	0.44
1:G:451:LEU:HD13	1:G:479:TRP:CE2	2.53	0.44
1:I:593:SER:O	1:I:596:LYS:HG3	2.17	0.44
2:R:52:TYR:CE2	2:R:56:ILE:HD11	2.53	0.44
1:A:527:ILE:O	1:A:531:GLU:HG3	2.18	0.44
1:D:653:THR:HG21	1:D:707:ILE:HG12	2.00	0.44
1:E:628:LYS:HD2	1:E:628:LYS:HA	1.70	0.44
1:G:451:LEU:HB2	1:G:479:TRP:CZ3	2.53	0.44
1:C:647:LEU:HD11	1:C:679:LEU:HD21	2.00	0.44
1:G:695:ILE:HD11	2:M:69:SER:HB2	1.99	0.44
1:I:640:PRO:O	1:I:643:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:611:SER:HB3	1:I:704:LEU:HD22	2.00	0.44
1:C:512:LYS:HA	1:C:512:LYS:HD2	1.73	0.43
1:E:676:VAL:O	1:E:680:ILE:HG12	2.17	0.43
1:F:475:LEU:HD22	1:F:475:LEU:HA	1.77	0.43
2:Q:34:GLU:HB3	2:Q:100:VAL:HG22	2.00	0.43
2:Q:79:ILE:HA	2:Q:82:VAL:HG22	2.00	0.43
2:R:69:SER:HA	2:R:72:VAL:HG12	2.00	0.43
2:T:79:ILE:HA	2:T:82:VAL:HG22	2.00	0.43
1:A:497:THR:HG22	1:A:499:LEU:H	1.82	0.43
1:D:371:PRO:HD2	1:D:418:HIS:HE1	1.82	0.43
1:D:373:ILE:HB	1:D:434:LEU:HB2	2.00	0.43
1:I:414:TYR:HD1	1:I:517:PHE:HD2	1.65	0.43
2:O:72:VAL:HA	2:O:75:ILE:HG22	1.99	0.43
1:A:454:GLU:O	1:A:454:GLU:HG2	2.17	0.43
1:F:523:VAL:O	1:F:527:ILE:HG12	2.19	0.43
1:G:427:GLU:HB2	1:G:430:ASP:OD2	2.17	0.43
1:B:640:PRO:HG3	2:Q:78:TYR:CB	2.47	0.43
1:H:640:PRO:O	1:H:643:VAL:HG12	2.18	0.43
1:A:433:ILE:HG22	1:A:441:VAL:O	2.19	0.43
1:D:399:ILE:HB	1:D:400:PRO:HD3	2.00	0.43
1:I:395:VAL:HA	1:I:399:ILE:HD12	2.00	0.43
2:Q:48:VAL:HG21	2:Q:89:GLU:HG3	2.01	0.43
1:C:524:ARG:HG2	1:D:536:ASP:OD2	2.18	0.43
1:E:584:THR:HG23	1:E:585:VAL:HG23	2.00	0.43
1:C:450:VAL:HB	1:C:496:TRP:O	2.19	0.43
1:E:452:THR:O	1:E:478:ALA:HB3	2.18	0.43
1:F:410:ILE:HA	1:F:563:SER:OG	2.18	0.43
1:F:381:SER:HB3	1:F:421:THR:HB	2.01	0.43
2:T:52:TYR:CE2	2:T:56:ILE:HD11	2.54	0.43
1:B:399:ILE:HB	1:B:400:PRO:HD3	2.01	0.43
1:B:451:LEU:HD12	1:B:478:ALA:O	2.19	0.43
1:H:482:GLU:O	1:H:485:LYS:HG3	2.19	0.43
1:H:667:LEU:HD12	1:H:667:LEU:HA	1.86	0.43
2:O:69:SER:HA	2:O:72:VAL:HG12	2.00	0.43
1:B:499:LEU:O	1:B:503:ILE:HG12	2.19	0.43
1:F:642:SER:HA	1:F:645:LEU:HB2	2.00	0.43
1:G:453:ASN:HB2	1:G:476:PRO:HB3	2.01	0.43
1:G:612:VAL:HG12	1:G:665:VAL:HB	2.00	0.43
1:H:497:THR:HG22	1:H:499:LEU:H	1.83	0.43
2:O:48:VAL:HG21	2:O:89:GLU:HG3	2.01	0.43
1:D:640:PRO:HB3	2:O:78:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ALA:HB2	1:A:505:HIS:CD2	2.54	0.43
1:C:607:GLN:O	1:C:699:ILE:HD11	2.18	0.43
1:F:525:SER:O	1:F:528:GLU:HG3	2.19	0.43
2:L:61:ASP:O	2:L:65:GLU:HG2	2.19	0.43
1:H:434:LEU:HA	1:H:439:PRO:HA	2.00	0.42
1:A:523:VAL:O	1:A:527:ILE:HG12	2.19	0.42
1:C:593:SER:O	1:C:596:LYS:HG3	2.19	0.42
1:C:619:ILE:HA	1:C:622:MET:HG2	2.01	0.42
1:D:627:ILE:O	1:D:627:ILE:HG13	2.20	0.42
2:L:51:HIS:CD2	2:L:55:LYS:HE3	2.54	0.42
2:S:52:TYR:HE1	2:S:79:ILE:HG23	1.85	0.42
1:E:438:VAL:HG11	1:F:597:LEU:HG	2.01	0.42
1:G:455:VAL:HG12	1:G:457:ASP:H	1.85	0.42
1:H:456:GLU:HA	1:H:459:LEU:HD12	2.01	0.42
1:G:640:PRO:O	1:G:643:VAL:HG12	2.19	0.42
1:I:379:ASP:O	1:I:383:LEU:HG	2.19	0.42
1:B:430:ASP:OD1	1:B:444:LYS:HG2	2.19	0.42
1:D:684:PHE:HB3	1:D:687:ILE:HD12	2.01	0.42
1:E:499:LEU:O	1:E:503:ILE:HG12	2.20	0.42
1:F:395:VAL:HA	1:F:399:ILE:HD12	2.01	0.42
2:M:79:ILE:HA	2:M:82:VAL:HG22	2.00	0.42
1:C:671:ASP:OD1	1:C:672:VAL:HG13	2.20	0.42
1:D:451:LEU:HD12	1:D:478:ALA:O	2.20	0.42
1:D:499:LEU:O	1:D:503:ILE:HG12	2.20	0.42
1:D:647:LEU:HD11	1:D:683:GLU:OE1	2.19	0.42
2:L:79:ILE:HA	2:L:82:VAL:HG22	2.02	0.42
1:A:603:PHE:HD2	1:A:690:ILE:HD13	1.84	0.42
1:B:596:LYS:HE2	1:B:693:GLN:O	2.20	0.42
1:C:592:ARG:HH21	1:C:690:ILE:HG22	1.85	0.42
2:N:52:TYR:CE2	2:N:56:ILE:HD11	2.54	0.42
1:A:372:VAL:HG12	1:A:417:ILE:HG23	2.01	0.42
1:A:584:THR:HG23	1:A:585:VAL:HG23	2.01	0.42
1:D:597:LEU:HD12	1:D:696:LEU:HD11	2.02	0.42
1:E:399:ILE:HB	1:E:400:PRO:HD3	2.02	0.42
1:F:466:PHE:CD1	1:F:480:VAL:HG22	2.55	0.42
1:G:433:ILE:HD12	1:G:506:LEU:HD23	2.02	0.42
1:H:643:VAL:O	1:H:647:LEU:HD13	2.19	0.42
1:B:378:LYS:N	1:B:428:GLY:HA2	2.35	0.42
1:B:677:ARG:NH1	1:B:681:GLU:HB3	2.35	0.42
1:F:621:GLU:HA	1:F:624:ARG:HD3	2.01	0.42
1:G:637:ALA:HA	2:L:81:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:77:SER:O	2:R:81:VAL:HG23	2.20	0.42
1:C:393:SER:HB3	1:C:396:ASP:HB2	2.01	0.41
1:G:388:THR:HG21	1:G:398:MET:HE1	2.01	0.41
1:H:703:PRO:HG2	2:L:63:LEU:O	2.20	0.41
1:I:433:ILE:HG22	1:I:441:VAL:O	2.20	0.41
2:R:79:ILE:HA	2:R:82:VAL:HG22	2.00	0.41
1:B:458:ASN:HA	1:B:461:ARG:HB3	2.01	0.41
1:H:619:ILE:HA	1:H:622:MET:HG2	2.01	0.41
2:N:34:GLU:HG3	2:N:103:ALA:HB2	2.02	0.41
1:G:446:PRO:HA	1:G:447:PRO:HD3	1.90	0.41
1:B:696:LEU:HA	1:B:697:PRO:HD3	1.87	0.41
1:I:389:LYS:HE2	1:I:495:TYR:OH	2.20	0.41
1:I:619:ILE:O	1:I:623:ILE:HG12	2.20	0.41
1:B:407:TYR:CE2	1:B:565:LYS:HE2	2.55	0.41
1:E:451:LEU:HG	1:E:476:PRO:HB2	2.02	0.41
1:F:641:ASP:O	1:F:645:LEU:HG	2.20	0.41
2:Q:61:ASP:O	2:Q:65:GLU:HG2	2.20	0.41
2:Q:72:VAL:HA	2:Q:75:ILE:HG22	2.02	0.41
1:E:372:VAL:HA	1:E:434:LEU:O	2.20	0.41
1:G:407:TYR:CE2	1:G:565:LYS:HE2	2.55	0.41
1:C:370:LEU:HA	1:C:371:PRO:HD3	1.94	0.41
1:E:614:LEU:HD21	1:E:667:LEU:HD23	2.03	0.41
1:F:651:ARG:HD3	1:F:683:GLU:OE2	2.21	0.41
1:G:593:SER:O	1:G:596:LYS:HG3	2.21	0.41
1:G:628:LYS:HG2	1:G:630:THR:HG23	2.03	0.41
2:N:34:GLU:HB3	2:N:100:VAL:HG22	2.02	0.41
1:A:536:ASP:OD2	1:I:524:ARG:HG2	2.20	0.41
1:I:523:VAL:O	1:I:527:ILE:HG12	2.21	0.41
2:N:72:VAL:HA	2:N:75:ILE:HG22	2.03	0.41
2:P:52:TYR:CE1	2:P:79:ILE:HG23	2.56	0.41
1:A:399:ILE:HB	1:A:400:PRO:HD3	2.03	0.41
1:A:618:GLU:O	1:A:622:MET:HB2	2.21	0.41
1:E:684:PHE:HB3	1:E:687:ILE:HG12	2.01	0.41
1:G:381:SER:HA	1:G:384:ILE:HG12	2.03	0.41
1:G:592:ARG:NH2	1:G:690:ILE:HG22	2.36	0.41
1:I:380:LEU:HD23	1:I:383:LEU:HD12	2.02	0.41
1:I:380:LEU:O	1:I:384:ILE:HG23	2.21	0.41
1:A:598:TYR:HD1	1:I:438:VAL:HG22	1.86	0.41
1:E:434:LEU:HA	1:E:439:PRO:HA	2.02	0.41
1:F:446:PRO:HB2	1:F:449:HIS:HB2	2.03	0.41
2:M:69:SER:HA	2:M:72:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:GLU:HG3	1:A:677:ARG:HG2	2.03	0.40
1:E:446:PRO:HD2	1:E:479:TRP:CZ3	2.56	0.40
1:F:616:ASP:HB2	1:F:707:ILE:O	2.22	0.40
1:H:469:TYR:HB3	1:H:479:TRP:CD1	2.55	0.40
2:P:78:TYR:O	2:P:81:VAL:HG12	2.22	0.40
1:B:469:TYR:HB3	1:B:479:TRP:CD1	2.57	0.40
1:B:596:LYS:HA	1:B:694:GLU:O	2.22	0.40
1:D:523:VAL:HG21	1:D:551:THR:HG23	2.03	0.40
1:D:544:LEU:HD13	1:D:578:ALA:C	2.42	0.40
1:H:560:GLU:HG3	1:H:677:ARG:HG2	2.02	0.40
1:H:692:TYR:CE1	2:L:72:VAL:HG21	2.56	0.40
1:A:379:ASP:O	1:A:383:LEU:HG	2.21	0.40
1:A:555:LYS:HA	1:A:558:VAL:HG22	2.02	0.40
1:F:619:ILE:HA	1:F:622:MET:HG2	2.03	0.40
1:G:394:PHE:HB2	1:G:499:LEU:HD23	2.02	0.40
1:B:672:VAL:O	1:B:672:VAL:HG22	2.21	0.40
1:C:627:ILE:HG13	1:C:627:ILE:O	2.22	0.40
1:E:640:PRO:O	1:E:643:VAL:HG12	2.22	0.40
1:F:643:VAL:O	1:F:647:LEU:HD13	2.21	0.40
2:O:103:ALA:O	2:O:106:GLU:HB2	2.21	0.40
1:B:628:LYS:NZ	2:Q:81:VAL:HG22	2.36	0.40
1:A:640:PRO:HA	2:R:78:TYR:CD2	2.56	0.40
1:B:623:ILE:HG21	1:B:672:VAL:CG2	2.49	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	320/387 (83%)	304 (95%)	16 (5%)	0	100	100
1	B	346/387 (89%)	330 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	345/387 (89%)	325 (94%)	20 (6%)	0	100	100
1	D	323/387 (84%)	308 (95%)	15 (5%)	0	100	100
1	E	345/387 (89%)	332 (96%)	13 (4%)	0	100	100
1	F	344/387 (89%)	333 (97%)	11 (3%)	0	100	100
1	G	347/387 (90%)	334 (96%)	13 (4%)	0	100	100
1	H	342/387 (88%)	327 (96%)	15 (4%)	0	100	100
1	I	336/387 (87%)	323 (96%)	13 (4%)	0	100	100
2	L	81/107 (76%)	81 (100%)	0	0	100	100
2	M	63/107 (59%)	63 (100%)	0	0	100	100
2	N	84/107 (78%)	83 (99%)	1 (1%)	0	100	100
2	O	72/107 (67%)	72 (100%)	0	0	100	100
2	P	63/107 (59%)	62 (98%)	1 (2%)	0	100	100
2	Q	69/107 (64%)	69 (100%)	0	0	100	100
2	R	57/107 (53%)	56 (98%)	1 (2%)	0	100	100
2	S	38/107 (36%)	38 (100%)	0	0	100	100
2	T	73/107 (68%)	72 (99%)	1 (1%)	0	100	100
All	All	3648/4446 (82%)	3512 (96%)	136 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	300/345 (87%)	289 (96%)	11 (4%)	34	59
1	B	318/345 (92%)	316 (99%)	2 (1%)	86	92
1	C	317/345 (92%)	311 (98%)	6 (2%)	57	75
1	D	302/345 (88%)	298 (99%)	4 (1%)	69	82
1	E	317/345 (92%)	313 (99%)	4 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	316/345 (92%)	309 (98%)	7 (2%)	52	71
1	G	319/345 (92%)	309 (97%)	10 (3%)	40	62
1	H	314/345 (91%)	309 (98%)	5 (2%)	62	79
1	I	313/345 (91%)	311 (99%)	2 (1%)	86	92
2	L	77/97 (79%)	77 (100%)	0	100	100
2	M	61/97 (63%)	61 (100%)	0	100	100
2	N	79/97 (81%)	78 (99%)	1 (1%)	69	82
2	O	68/97 (70%)	68 (100%)	0	100	100
2	P	61/97 (63%)	61 (100%)	0	100	100
2	Q	65/97 (67%)	65 (100%)	0	100	100
2	R	55/97 (57%)	55 (100%)	0	100	100
2	S	37/97 (38%)	34 (92%)	3 (8%)	11	37
2	T	70/97 (72%)	70 (100%)	0	100	100
All	All	3389/3978 (85%)	3334 (98%)	55 (2%)	62	79

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	417	ILE
1	A	459	LEU
1	A	462	TYR
1	A	466	PHE
1	A	467	ILE
1	A	470	LYS
1	A	475	LEU
1	A	636	LEU
1	A	646	ILE
1	A	649	SER
1	A	650	MET
1	B	470	LYS
1	B	543	ARG
1	C	458	ASN
1	C	468	THR
1	C	512	LYS
1	C	638	LEU
1	C	653	THR
1	C	657	THR

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Mol	Chain	Res	Type
1	D	455	VAL
1	D	608	SER
1	D	610	ILE
1	D	674	ARG
1	E	454	GLU
1	E	628	LYS
1	E	662	GLN
1	E	665	VAL
1	F	364	ASP
1	F	455	VAL
1	F	475	LEU
1	F	477	SER
1	F	655	THR
1	F	657	THR
1	F	662	GLN
1	G	456	GLU
1	G	462	TYR
1	G	469	TYR
1	G	475	LEU
1	G	630	THR
1	G	635	TYR
1	G	636	LEU
1	G	639	ASP
1	G	654	ILE
1	G	706	ARG
1	H	460	SER
1	H	628	LYS
1	H	629	GLN
1	H	665	VAL
1	H	673	ARG
1	I	520	ILE
1	I	677	ARG
2	N	55	LYS
2	S	59	LEU
2	S	61	ASP
2	S	63	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	326/387 (84%)	0.08	15 (4%) 32 28	245, 340, 416, 450	0
1	B	348/387 (89%)	-0.25	0 100 100	197, 256, 356, 433	0
1	C	347/387 (89%)	-0.11	5 (1%) 75 66	211, 293, 376, 409	0
1	D	331/387 (85%)	-0.11	5 (1%) 73 64	221, 312, 416, 447	0
1	E	347/387 (89%)	-0.19	6 (1%) 70 61	200, 257, 331, 401	0
1	F	346/387 (89%)	-0.21	0 100 100	174, 238, 342, 419	0
1	G	349/387 (90%)	-0.15	2 (0%) 89 84	194, 251, 326, 376	0
1	H	344/387 (88%)	-0.28	1 (0%) 94 90	191, 259, 341, 403	0
1	I	340/387 (87%)	-0.15	6 (1%) 68 60	198, 315, 395, 431	0
2	L	83/107 (77%)	0.13	2 (2%) 59 49	285, 399, 491, 496	0
2	M	65/107 (60%)	0.19	3 (4%) 32 28	263, 369, 437, 445	0
2	N	86/107 (80%)	-0.06	0 100 100	295, 369, 452, 465	0
2	O	74/107 (69%)	0.35	1 (1%) 75 66	386, 493, 544, 553	0
2	P	65/107 (60%)	0.64	3 (4%) 32 28	457, 498, 528, 536	0
2	Q	71/107 (66%)	-0.21	0 100 100	291, 406, 494, 507	0
2	R	59/107 (55%)	-0.06	0 100 100	330, 387, 431, 448	0
2	S	40/107 (37%)	0.69	4 (10%) 7 7	423, 483, 569, 579	0
2	T	75/107 (70%)	-0.08	0 100 100	310, 383, 437, 456	0
All	All	3696/4446 (83%)	-0.10	53 (1%) 75 66	174, 292, 462, 579	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	705	GLY	5.6
1	D	454	GLU	5.0
1	A	692	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	471	ASN	4.3
1	A	493	ILE	4.2
2	S	65	GLU	3.8
2	L	105	LYS	3.8
1	C	485	LYS	3.7
1	A	389	LYS	3.6
1	A	637	ALA	3.3
1	C	454	GLU	3.3
1	I	455	VAL	3.1
2	L	104	SER	3.1
1	G	630	THR	3.0
1	A	488	LEU	2.9
1	D	692	TYR	2.8
2	S	82	VAL	2.8
1	I	630	THR	2.7
2	P	90	GLU	2.7
1	C	458	ASN	2.7
1	D	468	THR	2.7
1	A	495	TYR	2.6
1	A	498	PRO	2.5
1	A	459	LEU	2.5
1	I	458	ASN	2.5
2	S	79	ILE	2.5
1	A	466	PHE	2.4
1	H	456	GLU	2.4
2	M	97	LYS	2.4
1	A	445	ILE	2.4
1	I	454	GLU	2.4
1	G	460	SER	2.4
1	E	614	LEU	2.3
1	A	494	LYS	2.3
1	C	431	TYR	2.2
1	E	465	PRO	2.2
1	D	413	ARG	2.2
2	P	97	LYS	2.2
2	O	34	GLU	2.2
1	C	389	LYS	2.2
1	A	606	GLY	2.1
1	A	465	PRO	2.1
1	I	431	TYR	2.1
2	M	42	GLU	2.1
1	A	468	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	612	VAL	2.1
1	E	464	LEU	2.1
1	D	498	PRO	2.1
2	P	94	ASN	2.1
2	S	76	LYS	2.1
1	E	445	ILE	2.1
2	M	38	LEU	2.0
1	I	445	ILE	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.