



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 03:01 am BST

PDB ID : 4R8K  
Title : Crystal structure of the guinea pig L-asparaginase 1 catalytic domain  
Authors : Schalk, A.M.; Lavie, A.  
Deposited on : 2014-09-02  
Resolution : 2.20 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

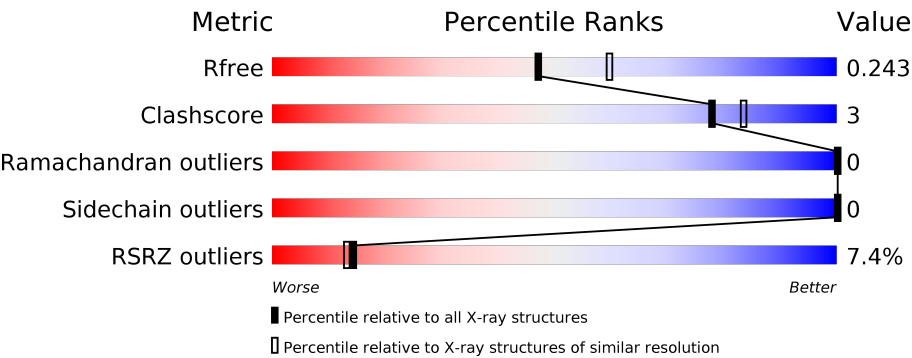
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	385	<div><div>5%</div><div><div></div><div>87%</div><div>5%</div><div>8%</div></div></div>
1	B	385	<div><div>6%</div><div><div></div><div>85%</div><div>5%</div><div>10%</div></div></div>
1	C	385	<div><div>4%</div><div><div></div><div>85%</div><div>7%</div><div>8%</div></div></div>
1	D	385	<div><div>5%</div><div><div></div><div>88%</div><div>5%</div><div>8%</div></div></div>
1	E	385	<div><div>9%</div><div><div></div><div>85%</div><div>7%</div><div>8%</div></div></div>
1	F	385	<div><div>10%</div><div><div></div><div>86%</div><div>6%</div><div>8%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	385	<div><div></div><div>7%</div><div>86%</div><div>5%</div><div>8%</div></div>
1	H	385	<div><div></div><div>7%</div><div>87%</div><div>5%</div><div>8%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22683 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2716	1737	469	494	16			
1	B	347	Total	C	N	O	S	0	0	0
			2667	1705	460	486	16			
1	C	355	Total	C	N	O	S	0	1	0
			2724	1743	471	494	16			
1	D	355	Total	C	N	O	S	0	0	0
			2717	1738	469	494	16			
1	E	353	Total	C	N	O	S	0	0	0
			2703	1729	466	492	16			
1	F	354	Total	C	N	O	S	0	1	0
			2717	1739	470	492	16			
1	G	354	Total	C	N	O	S	0	1	0
			2717	1739	470	492	16			
1	H	354	Total	C	N	O	S	0	0	0
			2710	1734	468	492	16			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP H0W0T5
A	-21	GLY	-	EXPRESSION TAG	UNP H0W0T5
A	-20	SER	-	EXPRESSION TAG	UNP H0W0T5
A	-19	SER	-	EXPRESSION TAG	UNP H0W0T5
A	-18	HIS	-	EXPRESSION TAG	UNP H0W0T5
A	-17	HIS	-	EXPRESSION TAG	UNP H0W0T5
A	-16	HIS	-	EXPRESSION TAG	UNP H0W0T5
A	-15	HIS	-	EXPRESSION TAG	UNP H0W0T5
A	-14	HIS	-	EXPRESSION TAG	UNP H0W0T5
A	-13	HIS	-	EXPRESSION TAG	UNP H0W0T5
A	-12	SER	-	EXPRESSION TAG	UNP H0W0T5
A	-11	SER	-	EXPRESSION TAG	UNP H0W0T5
A	-10	GLY	-	EXPRESSION TAG	UNP H0W0T5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	EXPRESSION TAG	UNP H0W0T5
A	-8	ASN	-	EXPRESSION TAG	UNP H0W0T5
A	-7	GLU	-	EXPRESSION TAG	UNP H0W0T5
A	-6	ASN	-	EXPRESSION TAG	UNP H0W0T5
A	-5	LEU	-	EXPRESSION TAG	UNP H0W0T5
A	-4	TYR	-	EXPRESSION TAG	UNP H0W0T5
A	-3	PHE	-	EXPRESSION TAG	UNP H0W0T5
A	-2	GLN	-	EXPRESSION TAG	UNP H0W0T5
A	-1	GLY	-	EXPRESSION TAG	UNP H0W0T5
A	0	HIS	-	EXPRESSION TAG	UNP H0W0T5
B	-22	MET	-	EXPRESSION TAG	UNP H0W0T5
B	-21	GLY	-	EXPRESSION TAG	UNP H0W0T5
B	-20	SER	-	EXPRESSION TAG	UNP H0W0T5
B	-19	SER	-	EXPRESSION TAG	UNP H0W0T5
B	-18	HIS	-	EXPRESSION TAG	UNP H0W0T5
B	-17	HIS	-	EXPRESSION TAG	UNP H0W0T5
B	-16	HIS	-	EXPRESSION TAG	UNP H0W0T5
B	-15	HIS	-	EXPRESSION TAG	UNP H0W0T5
B	-14	HIS	-	EXPRESSION TAG	UNP H0W0T5
B	-13	HIS	-	EXPRESSION TAG	UNP H0W0T5
B	-12	SER	-	EXPRESSION TAG	UNP H0W0T5
B	-11	SER	-	EXPRESSION TAG	UNP H0W0T5
B	-10	GLY	-	EXPRESSION TAG	UNP H0W0T5
B	-9	GLY	-	EXPRESSION TAG	UNP H0W0T5
B	-8	ASN	-	EXPRESSION TAG	UNP H0W0T5
B	-7	GLU	-	EXPRESSION TAG	UNP H0W0T5
B	-6	ASN	-	EXPRESSION TAG	UNP H0W0T5
B	-5	LEU	-	EXPRESSION TAG	UNP H0W0T5
B	-4	TYR	-	EXPRESSION TAG	UNP H0W0T5
B	-3	PHE	-	EXPRESSION TAG	UNP H0W0T5
B	-2	GLN	-	EXPRESSION TAG	UNP H0W0T5
B	-1	GLY	-	EXPRESSION TAG	UNP H0W0T5
B	0	HIS	-	EXPRESSION TAG	UNP H0W0T5
C	-22	MET	-	EXPRESSION TAG	UNP H0W0T5
C	-21	GLY	-	EXPRESSION TAG	UNP H0W0T5
C	-20	SER	-	EXPRESSION TAG	UNP H0W0T5
C	-19	SER	-	EXPRESSION TAG	UNP H0W0T5
C	-18	HIS	-	EXPRESSION TAG	UNP H0W0T5
C	-17	HIS	-	EXPRESSION TAG	UNP H0W0T5
C	-16	HIS	-	EXPRESSION TAG	UNP H0W0T5
C	-15	HIS	-	EXPRESSION TAG	UNP H0W0T5
C	-14	HIS	-	EXPRESSION TAG	UNP H0W0T5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	EXPRESSION TAG	UNP H0W0T5
C	-12	SER	-	EXPRESSION TAG	UNP H0W0T5
C	-11	SER	-	EXPRESSION TAG	UNP H0W0T5
C	-10	GLY	-	EXPRESSION TAG	UNP H0W0T5
C	-9	GLY	-	EXPRESSION TAG	UNP H0W0T5
C	-8	ASN	-	EXPRESSION TAG	UNP H0W0T5
C	-7	GLU	-	EXPRESSION TAG	UNP H0W0T5
C	-6	ASN	-	EXPRESSION TAG	UNP H0W0T5
C	-5	LEU	-	EXPRESSION TAG	UNP H0W0T5
C	-4	TYR	-	EXPRESSION TAG	UNP H0W0T5
C	-3	PHE	-	EXPRESSION TAG	UNP H0W0T5
C	-2	GLN	-	EXPRESSION TAG	UNP H0W0T5
C	-1	GLY	-	EXPRESSION TAG	UNP H0W0T5
C	0	HIS	-	EXPRESSION TAG	UNP H0W0T5
D	-22	MET	-	EXPRESSION TAG	UNP H0W0T5
D	-21	GLY	-	EXPRESSION TAG	UNP H0W0T5
D	-20	SER	-	EXPRESSION TAG	UNP H0W0T5
D	-19	SER	-	EXPRESSION TAG	UNP H0W0T5
D	-18	HIS	-	EXPRESSION TAG	UNP H0W0T5
D	-17	HIS	-	EXPRESSION TAG	UNP H0W0T5
D	-16	HIS	-	EXPRESSION TAG	UNP H0W0T5
D	-15	HIS	-	EXPRESSION TAG	UNP H0W0T5
D	-14	HIS	-	EXPRESSION TAG	UNP H0W0T5
D	-13	HIS	-	EXPRESSION TAG	UNP H0W0T5
D	-12	SER	-	EXPRESSION TAG	UNP H0W0T5
D	-11	SER	-	EXPRESSION TAG	UNP H0W0T5
D	-10	GLY	-	EXPRESSION TAG	UNP H0W0T5
D	-9	GLY	-	EXPRESSION TAG	UNP H0W0T5
D	-8	ASN	-	EXPRESSION TAG	UNP H0W0T5
D	-7	GLU	-	EXPRESSION TAG	UNP H0W0T5
D	-6	ASN	-	EXPRESSION TAG	UNP H0W0T5
D	-5	LEU	-	EXPRESSION TAG	UNP H0W0T5
D	-4	TYR	-	EXPRESSION TAG	UNP H0W0T5
D	-3	PHE	-	EXPRESSION TAG	UNP H0W0T5
D	-2	GLN	-	EXPRESSION TAG	UNP H0W0T5
D	-1	GLY	-	EXPRESSION TAG	UNP H0W0T5
D	0	HIS	-	EXPRESSION TAG	UNP H0W0T5
E	-22	MET	-	EXPRESSION TAG	UNP H0W0T5
E	-21	GLY	-	EXPRESSION TAG	UNP H0W0T5
E	-20	SER	-	EXPRESSION TAG	UNP H0W0T5
E	-19	SER	-	EXPRESSION TAG	UNP H0W0T5
E	-18	HIS	-	EXPRESSION TAG	UNP H0W0T5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-17	HIS	-	EXPRESSION TAG	UNP H0W0T5
E	-16	HIS	-	EXPRESSION TAG	UNP H0W0T5
E	-15	HIS	-	EXPRESSION TAG	UNP H0W0T5
E	-14	HIS	-	EXPRESSION TAG	UNP H0W0T5
E	-13	HIS	-	EXPRESSION TAG	UNP H0W0T5
E	-12	SER	-	EXPRESSION TAG	UNP H0W0T5
E	-11	SER	-	EXPRESSION TAG	UNP H0W0T5
E	-10	GLY	-	EXPRESSION TAG	UNP H0W0T5
E	-9	GLY	-	EXPRESSION TAG	UNP H0W0T5
E	-8	ASN	-	EXPRESSION TAG	UNP H0W0T5
E	-7	GLU	-	EXPRESSION TAG	UNP H0W0T5
E	-6	ASN	-	EXPRESSION TAG	UNP H0W0T5
E	-5	LEU	-	EXPRESSION TAG	UNP H0W0T5
E	-4	TYR	-	EXPRESSION TAG	UNP H0W0T5
E	-3	PHE	-	EXPRESSION TAG	UNP H0W0T5
E	-2	GLN	-	EXPRESSION TAG	UNP H0W0T5
E	-1	GLY	-	EXPRESSION TAG	UNP H0W0T5
E	0	HIS	-	EXPRESSION TAG	UNP H0W0T5
F	-22	MET	-	EXPRESSION TAG	UNP H0W0T5
F	-21	GLY	-	EXPRESSION TAG	UNP H0W0T5
F	-20	SER	-	EXPRESSION TAG	UNP H0W0T5
F	-19	SER	-	EXPRESSION TAG	UNP H0W0T5
F	-18	HIS	-	EXPRESSION TAG	UNP H0W0T5
F	-17	HIS	-	EXPRESSION TAG	UNP H0W0T5
F	-16	HIS	-	EXPRESSION TAG	UNP H0W0T5
F	-15	HIS	-	EXPRESSION TAG	UNP H0W0T5
F	-14	HIS	-	EXPRESSION TAG	UNP H0W0T5
F	-13	HIS	-	EXPRESSION TAG	UNP H0W0T5
F	-12	SER	-	EXPRESSION TAG	UNP H0W0T5
F	-11	SER	-	EXPRESSION TAG	UNP H0W0T5
F	-10	GLY	-	EXPRESSION TAG	UNP H0W0T5
F	-9	GLY	-	EXPRESSION TAG	UNP H0W0T5
F	-8	ASN	-	EXPRESSION TAG	UNP H0W0T5
F	-7	GLU	-	EXPRESSION TAG	UNP H0W0T5
F	-6	ASN	-	EXPRESSION TAG	UNP H0W0T5
F	-5	LEU	-	EXPRESSION TAG	UNP H0W0T5
F	-4	TYR	-	EXPRESSION TAG	UNP H0W0T5
F	-3	PHE	-	EXPRESSION TAG	UNP H0W0T5
F	-2	GLN	-	EXPRESSION TAG	UNP H0W0T5
F	-1	GLY	-	EXPRESSION TAG	UNP H0W0T5
F	0	HIS	-	EXPRESSION TAG	UNP H0W0T5
G	-22	MET	-	EXPRESSION TAG	UNP H0W0T5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-21	GLY	-	EXPRESSION TAG	UNP H0W0T5
G	-20	SER	-	EXPRESSION TAG	UNP H0W0T5
G	-19	SER	-	EXPRESSION TAG	UNP H0W0T5
G	-18	HIS	-	EXPRESSION TAG	UNP H0W0T5
G	-17	HIS	-	EXPRESSION TAG	UNP H0W0T5
G	-16	HIS	-	EXPRESSION TAG	UNP H0W0T5
G	-15	HIS	-	EXPRESSION TAG	UNP H0W0T5
G	-14	HIS	-	EXPRESSION TAG	UNP H0W0T5
G	-13	HIS	-	EXPRESSION TAG	UNP H0W0T5
G	-12	SER	-	EXPRESSION TAG	UNP H0W0T5
G	-11	SER	-	EXPRESSION TAG	UNP H0W0T5
G	-10	GLY	-	EXPRESSION TAG	UNP H0W0T5
G	-9	GLY	-	EXPRESSION TAG	UNP H0W0T5
G	-8	ASN	-	EXPRESSION TAG	UNP H0W0T5
G	-7	GLU	-	EXPRESSION TAG	UNP H0W0T5
G	-6	ASN	-	EXPRESSION TAG	UNP H0W0T5
G	-5	LEU	-	EXPRESSION TAG	UNP H0W0T5
G	-4	TYR	-	EXPRESSION TAG	UNP H0W0T5
G	-3	PHE	-	EXPRESSION TAG	UNP H0W0T5
G	-2	GLN	-	EXPRESSION TAG	UNP H0W0T5
G	-1	GLY	-	EXPRESSION TAG	UNP H0W0T5
G	0	HIS	-	EXPRESSION TAG	UNP H0W0T5
H	-22	MET	-	EXPRESSION TAG	UNP H0W0T5
H	-21	GLY	-	EXPRESSION TAG	UNP H0W0T5
H	-20	SER	-	EXPRESSION TAG	UNP H0W0T5
H	-19	SER	-	EXPRESSION TAG	UNP H0W0T5
H	-18	HIS	-	EXPRESSION TAG	UNP H0W0T5
H	-17	HIS	-	EXPRESSION TAG	UNP H0W0T5
H	-16	HIS	-	EXPRESSION TAG	UNP H0W0T5
H	-15	HIS	-	EXPRESSION TAG	UNP H0W0T5
H	-14	HIS	-	EXPRESSION TAG	UNP H0W0T5
H	-13	HIS	-	EXPRESSION TAG	UNP H0W0T5
H	-12	SER	-	EXPRESSION TAG	UNP H0W0T5
H	-11	SER	-	EXPRESSION TAG	UNP H0W0T5
H	-10	GLY	-	EXPRESSION TAG	UNP H0W0T5
H	-9	GLY	-	EXPRESSION TAG	UNP H0W0T5
H	-8	ASN	-	EXPRESSION TAG	UNP H0W0T5
H	-7	GLU	-	EXPRESSION TAG	UNP H0W0T5
H	-6	ASN	-	EXPRESSION TAG	UNP H0W0T5
H	-5	LEU	-	EXPRESSION TAG	UNP H0W0T5
H	-4	TYR	-	EXPRESSION TAG	UNP H0W0T5
H	-3	PHE	-	EXPRESSION TAG	UNP H0W0T5

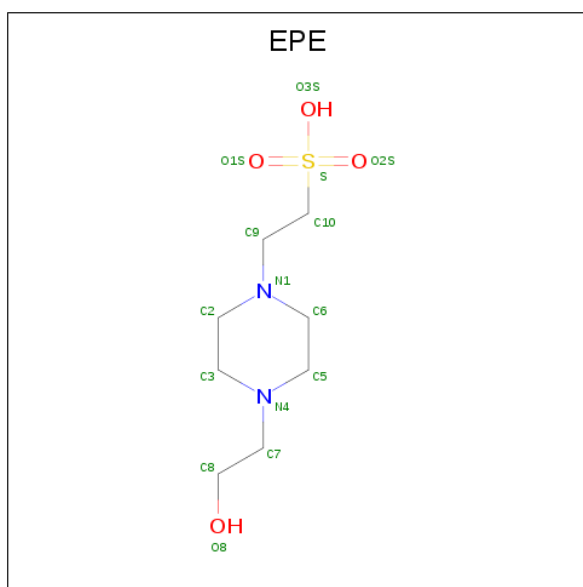
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	GLN	-	EXPRESSION TAG	UNP H0W0T5
H	-1	GLY	-	EXPRESSION TAG	UNP H0W0T5
H	0	HIS	-	EXPRESSION TAG	UNP H0W0T5

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

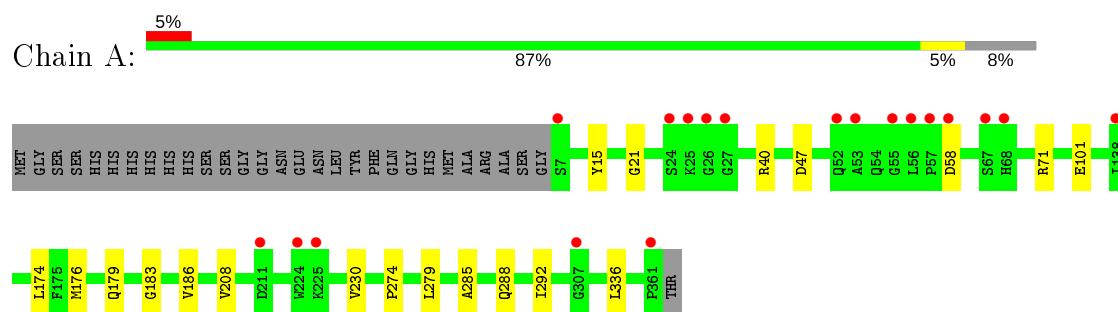
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total 119	O 119	0	0
3	B	76	Total 76	O 76	0	0
3	C	138	Total 138	O 138	0	0
3	D	140	Total 140	O 140	0	0
3	E	91	Total 91	O 91	0	0
3	F	94	Total 94	O 94	0	0
3	G	120	Total 120	O 120	0	0
3	H	114	Total 114	O 114	0	0

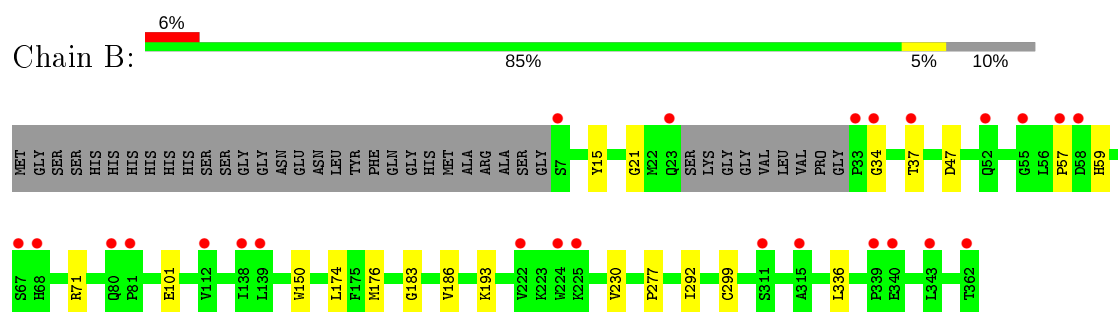
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

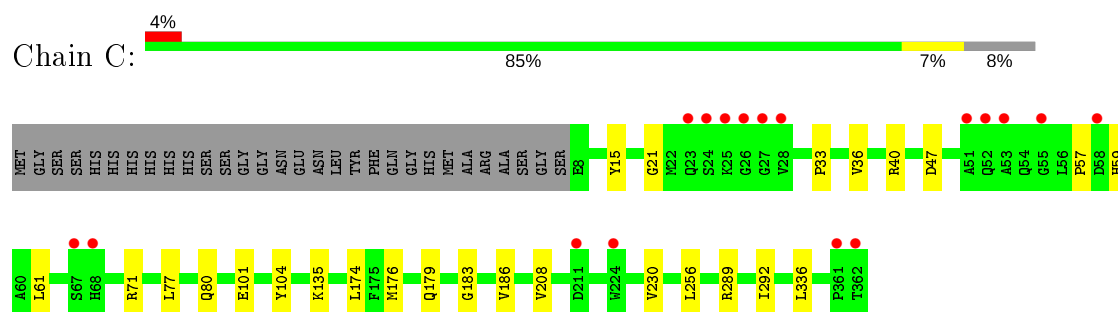
- Molecule 1: Uncharacterized protein



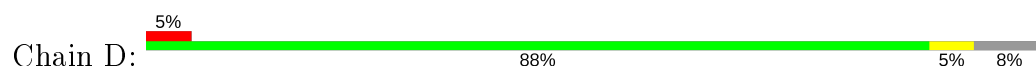
- Molecule 1: Uncharacterized protein

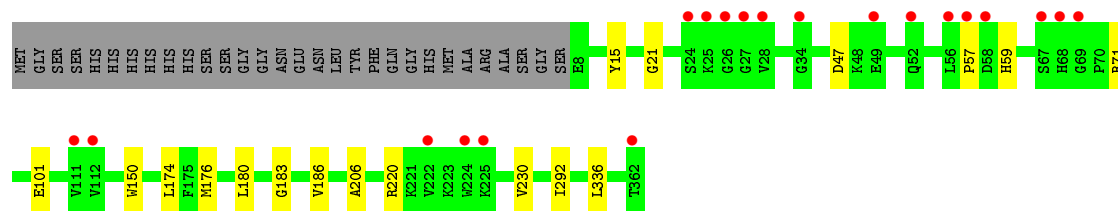


- Molecule 1: Uncharacterized protein

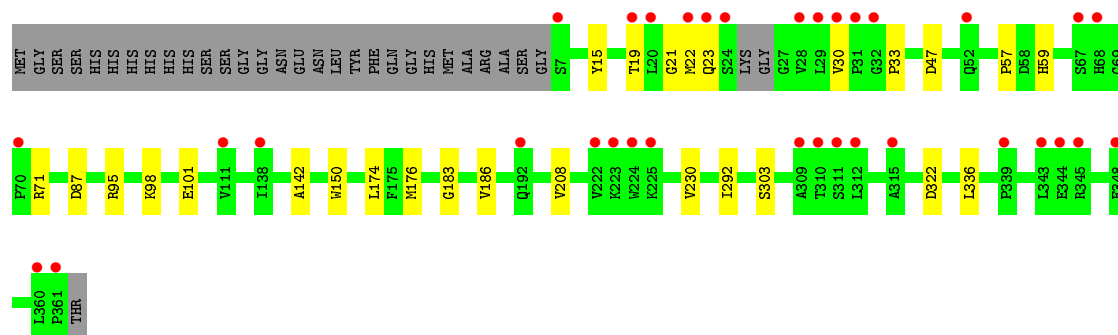
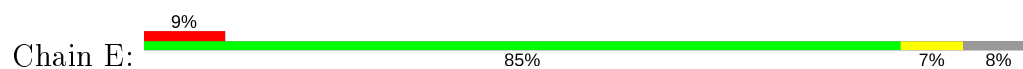


- Molecule 1: Uncharacterized protein

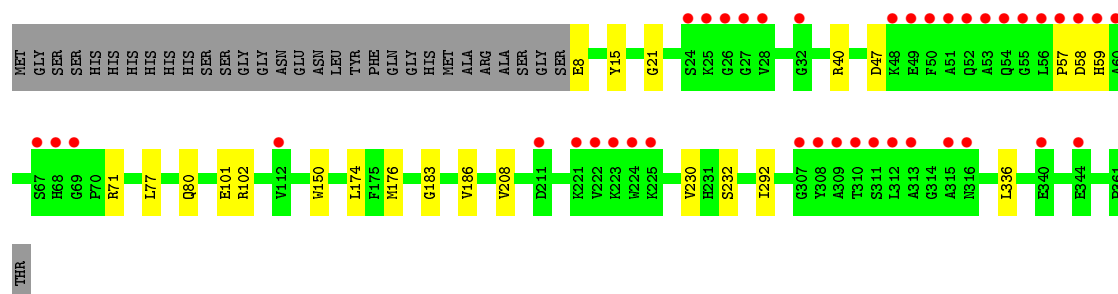
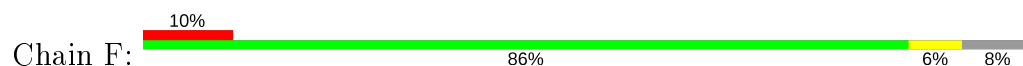




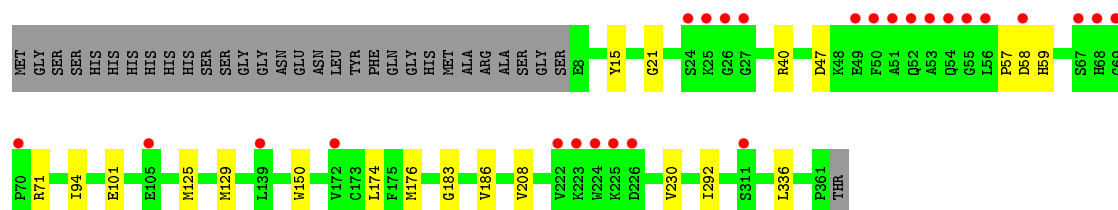
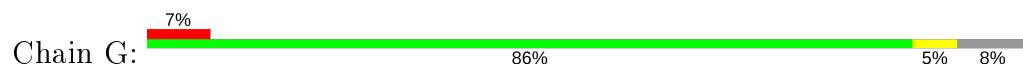
• Molecule 1: Uncharacterized protein



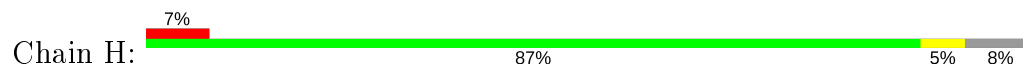
• Molecule 1: Uncharacterized protein

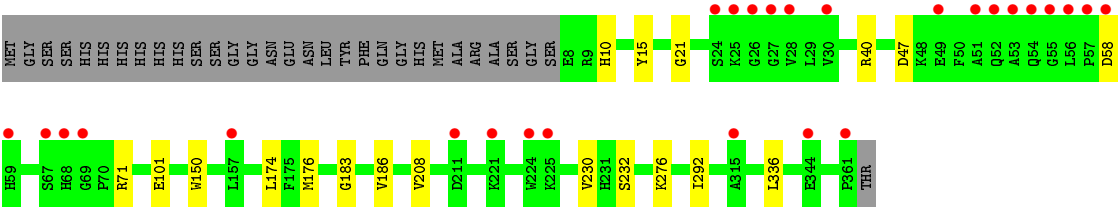


• Molecule 1: Uncharacterized protein



• Molecule 1: Uncharacterized protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.55Å 123.31Å 120.56Å 90.00° 92.35° 90.00°	Depositor
Resolution (Å)	29.62 – 2.20 29.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.62-2.20) 99.2 (29.62-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.207 , 0.238 0.212 , 0.243	Depositor DCC
$R_{free}$ test set	7281 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.000 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22683	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	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 38.88 % 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 3.4498e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.55	0/2773	0.68	0/3771
1	B	0.53	0/2722	0.68	0/3700
1	C	0.56	0/2785	0.68	0/3788
1	D	0.55	0/2774	0.67	0/3773
1	E	0.56	0/2759	0.70	0/3752
1	F	0.54	0/2778	0.68	0/3778
1	G	0.53	0/2778	0.68	0/3778
1	H	0.54	0/2767	0.68	0/3763
All	All	0.54	0/22136	0.68	0/30103

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 [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	2716	0	2786	16	0
1	B	2667	0	2730	18	0
1	C	2724	0	2795	23	0
1	D	2717	0	2788	15	0
1	E	2703	0	2769	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2717	0	2788	28	0
1	G	2717	0	2788	17	0
1	H	2710	0	2781	12	0
2	A	15	0	18	0	0
2	B	15	0	18	0	0
2	C	15	0	18	1	0
2	D	15	0	17	0	0
2	E	15	0	17	0	0
2	F	15	0	18	0	0
2	G	15	0	17	0	0
2	H	15	0	17	0	0
3	A	119	0	0	1	0
3	B	76	0	0	3	0
3	C	138	0	0	1	0
3	D	140	0	0	1	0
3	E	91	0	0	4	0
3	F	94	0	0	1	0
3	G	120	0	0	0	0
3	H	114	0	0	2	0
All	All	22683	0	22365	126	0

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

All (126) 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:C:80:GLN:HG3	1:F:77:LEU:HD11	1.44	0.99
1:E:208:VAL:CG1	1:F:150:TRP:HE1	1.86	0.88
1:E:208:VAL:CG1	1:F:150:TRP:NE1	2.36	0.87
1:E:208:VAL:HG11	1:F:150:TRP:NE1	1.97	0.79
1:C:208:VAL:CG1	1:D:150:TRP:HE1	1.98	0.76
1:B:193:LYS:HE2	3:B:846:HOH:O	1.85	0.75
1:C:208:VAL:CG1	1:D:150:TRP:NE1	2.48	0.75
1:G:125:MET:HE3	1:G:129:MET:CE	2.17	0.75
1:E:208:VAL:HG11	1:F:150:TRP:CE2	2.22	0.75
1:A:208:VAL:CG1	1:B:150:TRP:HE1	2.02	0.73
1:H:40:ARG:NH2	1:H:58:ASP:O	2.22	0.73
1:A:40:ARG:NH2	1:A:58:ASP:O	2.22	0.72
1:F:40:ARG:NH2	1:F:58:ASP:O	2.23	0.72
1:E:208:VAL:HG12	1:F:150:TRP:HE1	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:ARG:NH2	1:G:58:ASP:O	2.24	0.70
1:C:80:GLN:HG3	1:F:77:LEU:CD1	2.20	0.69
1:A:208:VAL:CG1	1:B:150:TRP:NE1	2.56	0.68
1:B:34:GLY:O	1:B:37:THR:HG22	1.94	0.67
1:G:125:MET:HE3	1:G:129:MET:HE2	1.77	0.66
1:C:256:LEU:O	1:C:289:ARG:NH2	2.28	0.65
1:B:277:PRO:HG2	1:F:232:SER:HB2	1.80	0.64
1:C:77:LEU:HD11	1:F:80:GLN:HG3	1.80	0.64
1:C:208:VAL:HG11	1:D:150:TRP:NE1	2.12	0.64
1:C:208:VAL:HG11	1:D:150:TRP:CE2	2.33	0.63
1:C:208:VAL:HG12	1:D:150:TRP:HE1	1.65	0.61
1:G:125:MET:CE	1:G:129:MET:CE	2.78	0.61
1:G:125:MET:HE3	1:G:129:MET:HE3	1.82	0.60
1:E:150:TRP:NE1	1:F:208:VAL:CG1	2.65	0.60
1:C:36:VAL:O	1:C:40:ARG:HG3	2.02	0.60
1:G:125:MET:CE	1:G:129:MET:HE3	2.33	0.58
1:A:208:VAL:HG11	1:B:150:TRP:CE2	2.38	0.58
1:E:150:TRP:HE1	1:F:208:VAL:CG1	2.16	0.58
1:A:208:VAL:HG11	1:B:150:TRP:NE1	2.18	0.57
1:E:23:GLN:OE1	1:E:33:PRO:HD3	2.06	0.55
1:G:47:ASP:OD2	1:G:71:ARG:NH2	2.40	0.55
1:A:179:GLN:HG3	3:A:829:HOH:O	2.06	0.54
1:E:150:TRP:CE2	1:F:208:VAL:HG11	2.42	0.54
1:F:8:GLU:N	3:F:864:HOH:O	2.40	0.53
1:G:94:ILE:HG13	1:G:129:MET:HE1	1.90	0.53
1:A:47:ASP:OD2	1:A:71:ARG:NH2	2.41	0.53
1:H:10:HIS:HB2	3:H:910:HOH:O	2.09	0.52
1:B:47:ASP:OD2	1:B:71:ARG:NH2	2.41	0.52
1:G:292:ILE:HD12	1:G:336:LEU:HD21	1.92	0.52
1:C:80:GLN:CG	1:F:77:LEU:HD11	2.28	0.51
1:A:292:ILE:HD12	1:A:336:LEU:HD21	1.92	0.51
1:D:292:ILE:HD12	1:D:336:LEU:HD21	1.92	0.51
1:C:292:ILE:HD12	1:C:336:LEU:HD21	1.92	0.51
1:E:98:LYS:HE2	3:E:873:HOH:O	2.11	0.51
1:E:208:VAL:HG11	1:F:150:TRP:CZ2	2.46	0.51
1:A:208:VAL:HG12	1:B:150:TRP:HE1	1.74	0.51
1:H:47:ASP:OD2	1:H:71:ARG:NH2	2.42	0.51
1:C:179:GLN:HG3	3:C:898:HOH:O	2.11	0.51
1:D:47:ASP:OD2	1:D:71:ARG:NH2	2.41	0.51
1:E:22:MET:SD	1:E:30:VAL:O	2.68	0.50
1:E:19:THR:OG1	1:E:142:ALA:O	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:ILE:HD12	1:E:336:LEU:HD21	1.92	0.50
1:F:292:ILE:HD12	1:F:336:LEU:HD21	1.93	0.50
1:C:57:PRO:HB2	1:C:59:HIS:CE1	2.47	0.50
1:E:15:TYR:OH	1:E:21:GLY:HA3	2.11	0.50
1:B:292:ILE:HD12	1:B:336:LEU:HD21	1.93	0.49
1:A:15:TYR:OH	1:A:21:GLY:HA3	2.12	0.49
1:F:47:ASP:OD2	1:F:71:ARG:NH2	2.41	0.49
1:F:57:PRO:HB2	1:F:59:HIS:CE1	2.47	0.49
1:A:274:PRO:HB2	1:A:279:LEU:HD23	1.94	0.49
1:H:15:TYR:OH	1:H:21:GLY:HA3	2.13	0.49
1:B:299:CYS:O	3:B:876:HOH:O	2.20	0.49
1:F:15:TYR:OH	1:F:21:GLY:HA3	2.13	0.49
1:C:47:ASP:OD2	1:C:71:ARG:NH2	2.42	0.49
1:E:47:ASP:OD2	1:E:71:ARG:NH2	2.42	0.49
3:B:802:HOH:O	2:C:700:EPE:H21	2.12	0.48
1:D:57:PRO:HB2	1:D:59:HIS:CE1	2.48	0.48
1:G:57:PRO:HB2	1:G:59:HIS:CE1	2.48	0.48
1:E:150:TRP:NE1	1:F:208:VAL:HG11	2.28	0.48
1:B:15:TYR:OH	1:B:21:GLY:HA3	2.13	0.48
1:C:15:TYR:OH	1:C:21:GLY:HA3	2.13	0.48
1:D:101:GLU:HB2	1:D:230:VAL:HG21	1.96	0.48
1:A:208:VAL:HG11	1:B:150:TRP:CZ2	2.50	0.47
1:B:57:PRO:HB2	1:B:59:HIS:CE1	2.50	0.47
1:E:303:SER:HB3	1:E:322:ASP:HB3	1.96	0.47
1:E:23:GLN:OE1	1:E:33:PRO:CD	2.63	0.47
1:G:150:TRP:CZ2	1:H:208:VAL:HG21	2.49	0.47
1:B:101:GLU:HB2	1:B:230:VAL:HG21	1.97	0.47
1:F:101:GLU:HB2	1:F:230:VAL:HG21	1.96	0.47
1:G:15:TYR:OH	1:G:21:GLY:HA3	2.15	0.47
1:H:292:ILE:HD12	1:H:336:LEU:HD21	1.95	0.47
1:E:98:LYS:CE	3:E:873:HOH:O	2.63	0.46
1:G:101:GLU:HB2	1:G:230:VAL:HG21	1.96	0.46
1:E:57:PRO:HB2	1:E:59:HIS:CE1	2.50	0.46
1:E:101:GLU:HB2	1:E:230:VAL:HG21	1.97	0.46
1:C:208:VAL:HG11	1:D:150:TRP:CZ2	2.51	0.46
1:B:277:PRO:CG	1:F:232:SER:HB2	2.45	0.46
1:A:101:GLU:HB2	1:A:230:VAL:HG21	1.98	0.45
1:H:101:GLU:HB2	1:H:230:VAL:HG21	1.98	0.45
1:D:15:TYR:OH	1:D:21:GLY:HA3	2.16	0.45
1:C:101:GLU:HB2	1:C:230:VAL:HG21	1.99	0.45
1:E:87:ASP:O	1:H:276:LYS:NZ	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:LEU:HD21	1:E:176:MET:HG3	1.98	0.44
1:B:174:LEU:HD21	1:B:176:MET:HG3	1.98	0.44
1:G:174:LEU:HD21	1:G:176:MET:HG3	2.00	0.44
1:F:174:LEU:HD21	1:F:176:MET:HG3	2.00	0.44
1:E:150:TRP:CZ2	1:F:208:VAL:HG11	2.52	0.44
1:A:285:ALA:HA	1:A:288:GLN:HE21	1.83	0.44
1:A:183:GLY:O	1:A:186:VAL:HG22	2.18	0.43
1:H:174:LEU:HD21	1:H:176:MET:HG3	2.00	0.43
1:A:174:LEU:HD21	1:A:176:MET:HG3	2.00	0.43
1:F:183:GLY:O	1:F:186:VAL:HG22	2.19	0.43
1:D:183:GLY:O	1:D:186:VAL:HG22	2.19	0.42
1:G:208:VAL:HG21	1:H:150:TRP:CZ2	2.55	0.42
1:C:174:LEU:HD21	1:C:176:MET:HG3	2.01	0.42
1:H:183:GLY:O	1:H:186:VAL:HG22	2.19	0.42
1:D:220:ARG:NH1	3:D:938:HOH:O	2.36	0.42
1:C:183:GLY:O	1:C:186:VAL:HG22	2.19	0.42
1:D:174:LEU:HD21	1:D:176:MET:HG3	2.02	0.42
1:G:125:MET:CE	1:G:129:MET:HE2	2.45	0.42
1:E:183:GLY:O	1:E:186:VAL:HG22	2.19	0.42
1:E:150:TRP:HE1	1:F:208:VAL:HG12	1.84	0.42
1:B:183:GLY:O	1:B:186:VAL:HG22	2.20	0.42
1:G:183:GLY:O	1:G:186:VAL:HG22	2.20	0.42
1:H:232:SER:HB3	3:H:906:HOH:O	2.18	0.41
1:D:180:LEU:HB3	1:D:206:ALA:HB3	2.03	0.41
1:C:33:PRO:HG3	1:F:102:ARG:HH21	1.85	0.41
1:C:40:ARG:HG2	1:C:61:LEU:HD21	2.02	0.41
1:E:98:LYS:HE3	3:E:853:HOH:O	2.19	0.41
1:C:104:TYR:O	1:C:135:LYS:NZ	2.53	0.40
1:E:22:MET:SD	1:E:30:VAL:C	3.00	0.40
1:E:95:ARG:HD2	3:E:890:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	353/385 (92%)	343 (97%)	10 (3%)	0	100	100
1	B	343/385 (89%)	336 (98%)	7 (2%)	0	100	100
1	C	354/385 (92%)	346 (98%)	8 (2%)	0	100	100
1	D	353/385 (92%)	344 (98%)	9 (2%)	0	100	100
1	E	349/385 (91%)	341 (98%)	8 (2%)	0	100	100
1	F	353/385 (92%)	343 (97%)	10 (3%)	0	100	100
1	G	353/385 (92%)	344 (98%)	9 (2%)	0	100	100
1	H	352/385 (91%)	343 (97%)	9 (3%)	0	100	100
All	All	2810/3080 (91%)	2740 (98%)	70 (2%)	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	297/320 (93%)	297 (100%)	0	100	100
1	B	292/320 (91%)	292 (100%)	0	100	100
1	C	298/320 (93%)	298 (100%)	0	100	100
1	D	297/320 (93%)	297 (100%)	0	100	100
1	E	296/320 (92%)	296 (100%)	0	100	100
1	F	297/320 (93%)	297 (100%)	0	100	100
1	G	297/320 (93%)	297 (100%)	0	100	100
1	H	296/320 (92%)	296 (100%)	0	100	100
All	All	2370/2560 (93%)	2370 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

such sidechains identified.

### 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 ⓘ

8 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	EPE	F	700	-	15,15,15	1.91	1 (6%)	18,20,20	1.27	2 (11%)
2	EPE	C	700	-	15,15,15	1.94	1 (6%)	18,20,20	1.79	5 (27%)
2	EPE	A	700	-	15,15,15	2.13	1 (6%)	18,20,20	1.50	2 (11%)
2	EPE	G	700	-	15,15,15	1.97	1 (6%)	18,20,20	1.61	4 (22%)
2	EPE	D	700	-	15,15,15	2.18	1 (6%)	18,20,20	1.05	1 (5%)
2	EPE	E	700	-	15,15,15	1.94	1 (6%)	18,20,20	2.09	3 (16%)
2	EPE	B	700	-	15,15,15	2.08	1 (6%)	18,20,20	1.70	2 (11%)
2	EPE	H	700	-	15,15,15	2.24	1 (6%)	18,20,20	1.66	4 (22%)

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	EPE	F	700	-	-	2/9/19/19	0/1/1/1
2	EPE	C	700	-	-	7/9/19/19	0/1/1/1
2	EPE	A	700	-	-	2/9/19/19	0/1/1/1
2	EPE	G	700	-	-	7/9/19/19	0/1/1/1
2	EPE	D	700	-	-	2/9/19/19	0/1/1/1
2	EPE	E	700	-	-	4/9/19/19	0/1/1/1
2	EPE	B	700	-	-	5/9/19/19	0/1/1/1
2	EPE	H	700	-	-	2/9/19/19	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	700	EPE	C10-S	-8.29	1.65	1.77
2	D	700	EPE	C10-S	-8.23	1.65	1.77
2	A	700	EPE	C10-S	-7.87	1.66	1.77
2	B	700	EPE	C10-S	-7.79	1.66	1.77
2	G	700	EPE	C10-S	-7.44	1.66	1.77
2	C	700	EPE	C10-S	-7.35	1.67	1.77
2	F	700	EPE	C10-S	-7.17	1.67	1.77
2	E	700	EPE	C10-S	-7.07	1.67	1.77

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	700	EPE	O1S-S-C10	6.18	114.36	106.92
2	H	700	EPE	O2S-S-C10	4.97	112.89	106.92
2	A	700	EPE	O1S-S-C10	4.62	112.47	106.92
2	C	700	EPE	O3S-S-C10	4.23	112.61	105.77
2	G	700	EPE	O1S-S-C10	4.01	111.74	106.92
2	E	700	EPE	O2S-S-O1S	-3.94	100.30	113.95
2	B	700	EPE	O2S-S-C10	3.80	111.49	106.92
2	E	700	EPE	C6-C5-N4	-3.39	103.69	110.64
2	F	700	EPE	O1S-S-C10	3.26	110.85	106.92
2	C	700	EPE	C9-N1-C2	3.08	119.11	111.23
2	D	700	EPE	O2S-S-C10	3.05	110.59	106.92
2	A	700	EPE	O3S-S-C10	2.98	110.59	105.77
2	B	700	EPE	C6-C5-N4	-2.98	104.52	110.64
2	F	700	EPE	O3S-S-C10	2.90	110.45	105.77
2	G	700	EPE	C6-C5-N4	-2.76	104.97	110.64
2	G	700	EPE	O3S-S-O2S	-2.47	105.23	111.27
2	G	700	EPE	O3S-S-C10	2.34	109.56	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	700	EPE	O3S-S-C10	2.32	109.52	105.77
2	C	700	EPE	C7-N4-C3	2.31	117.14	111.23
2	H	700	EPE	O3S-S-O2S	-2.16	106.00	111.27
2	C	700	EPE	C7-N4-C5	-2.14	105.77	111.23
2	C	700	EPE	C9-N1-C6	-2.12	105.82	111.23
2	H	700	EPE	C5-N4-C3	2.01	113.36	108.83

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	700	EPE	C10-C9-N1-C2
2	C	700	EPE	C9-C10-S-O1S
2	G	700	EPE	C8-C7-N4-C3
2	G	700	EPE	C9-C10-S-O2S
2	E	700	EPE	C9-C10-S-O2S
2	B	700	EPE	C10-C9-N1-C2
2	B	700	EPE	S-C10-C9-N1
2	B	700	EPE	C9-C10-S-O2S
2	C	700	EPE	C9-C10-S-O3S
2	G	700	EPE	C9-C10-S-O3S
2	B	700	EPE	C9-C10-S-O3S
2	C	700	EPE	C8-C7-N4-C3
2	E	700	EPE	C9-C10-S-O3S
2	C	700	EPE	N4-C7-C8-O8
2	E	700	EPE	S-C10-C9-N1
2	A	700	EPE	N4-C7-C8-O8
2	G	700	EPE	C10-C9-N1-C2
2	G	700	EPE	C10-C9-N1-C6
2	D	700	EPE	C8-C7-N4-C3
2	D	700	EPE	C8-C7-N4-C5
2	C	700	EPE	C9-C10-S-O2S
2	G	700	EPE	C9-C10-S-O1S
2	B	700	EPE	C9-C10-S-O1S
2	H	700	EPE	C8-C7-N4-C5
2	E	700	EPE	N4-C7-C8-O8
2	C	700	EPE	S-C10-C9-N1
2	F	700	EPE	C8-C7-N4-C3
2	F	700	EPE	C8-C7-N4-C5
2	H	700	EPE	C8-C7-N4-C3
2	A	700	EPE	C8-C7-N4-C5
2	G	700	EPE	C8-C7-N4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	700	EPE	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	355/385 (92%)	0.05	19 (5%)	25	24	17, 30, 71, 104	0
1	B	347/385 (90%)	0.20	25 (7%)	15	14	21, 34, 80, 110	0
1	C	355/385 (92%)	-0.03	17 (4%)	30	29	18, 27, 67, 102	0
1	D	355/385 (92%)	0.01	20 (5%)	24	23	18, 28, 67, 110	0
1	E	353/385 (91%)	0.30	34 (9%)	8	6	21, 36, 79, 113	0
1	F	354/385 (91%)	0.39	40 (11%)	5	4	19, 33, 92, 129	0
1	G	354/385 (91%)	0.11	26 (7%)	15	14	19, 32, 71, 106	0
1	H	354/385 (91%)	0.18	27 (7%)	13	12	18, 31, 81, 120	0
All	All	2827/3080 (91%)	0.15	208 (7%)	14	13	17, 31, 76, 129	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	53	ALA	13.4
1	E	30	VAL	8.1
1	F	27	GLY	7.2
1	H	224	TRP	7.1
1	H	53	ALA	7.1
1	H	26	GLY	6.7
1	F	56	LEU	6.7
1	C	27	GLY	6.6
1	E	31	PRO	6.5
1	F	26	GLY	6.5
1	H	68	HIS	6.3
1	F	68	HIS	6.1
1	H	67	SER	5.9
1	E	224	TRP	5.7
1	H	55	GLY	5.6
1	C	362	THR	5.6

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Mol	Chain	Res	Type	RSRZ
1	F	52	GLN	5.5
1	C	26	GLY	5.5
1	D	26	GLY	5.4
1	G	68	HIS	5.4
1	B	68	HIS	5.2
1	H	56	LEU	5.2
1	E	68	HIS	5.2
1	A	26	GLY	5.0
1	B	362	THR	5.0
1	B	224	TRP	5.0
1	D	224	TRP	5.0
1	F	50	PHE	4.9
1	D	27	GLY	4.9
1	B	58	ASP	4.8
1	H	58	ASP	4.7
1	C	68	HIS	4.7
1	F	315	ALA	4.7
1	G	53	ALA	4.7
1	D	68	HIS	4.6
1	G	52	GLN	4.5
1	C	28	VAL	4.5
1	F	224	TRP	4.5
1	F	58	ASP	4.5
1	F	69	GLY	4.2
1	A	68	HIS	4.2
1	E	315	ALA	4.2
1	G	69	GLY	4.2
1	G	27	GLY	4.1
1	C	67	SER	4.1
1	F	312	LEU	4.1
1	G	224	TRP	4.0
1	F	59	HIS	4.0
1	F	340	GLU	4.0
1	F	32	GLY	4.0
1	A	52	GLN	4.0
1	H	225	LYS	4.0
1	A	225	LYS	4.0
1	B	23	GLN	3.9
1	H	52	GLN	3.9
1	H	27	GLY	3.9
1	F	225	LYS	3.9
1	F	316	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	67	SER	3.8
1	A	27	GLY	3.8
1	C	25	LYS	3.8
1	A	55	GLY	3.7
1	E	343	LEU	3.7
1	D	67	SER	3.6
1	E	24	SER	3.6
1	H	28	VAL	3.6
1	G	225	LYS	3.5
1	D	225	LYS	3.5
1	A	224	TRP	3.5
1	C	224	TRP	3.5
1	F	311	SER	3.5
1	A	138	ILE	3.5
1	A	307	GLY	3.5
1	B	315	ALA	3.5
1	C	58	ASP	3.5
1	A	67	SER	3.4
1	B	55	GLY	3.4
1	F	28	VAL	3.4
1	F	54	GLN	3.3
1	B	340	GLU	3.3
1	A	211	ASP	3.3
1	F	222	VAL	3.3
1	F	211	ASP	3.3
1	C	55	GLY	3.3
1	E	339	PRO	3.3
1	B	52	GLN	3.2
1	E	22	MET	3.2
1	E	225	LYS	3.2
1	C	53	ALA	3.2
1	B	7	SER	3.2
1	E	361	PRO	3.2
1	E	29	LEU	3.2
1	B	138	ILE	3.2
1	A	58	ASP	3.2
1	G	49	GLU	3.2
1	H	59	HIS	3.2
1	H	344	GLU	3.1
1	D	362	THR	3.1
1	H	69	GLY	3.1
1	C	211	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	315	ALA	3.1
1	G	311	SER	3.0
1	B	81	PRO	3.0
1	G	55	GLY	3.0
1	F	24	SER	3.0
1	F	55	GLY	3.0
1	E	28	VAL	3.0
1	C	52	GLN	3.0
1	E	192	GLN	3.0
1	E	32	GLY	3.0
1	G	56	LEU	2.9
1	F	221	LYS	2.9
1	F	25	LYS	2.9
1	B	222	VAL	2.9
1	H	211	ASP	2.9
1	D	222	VAL	2.9
1	H	25	LYS	2.9
1	F	308	TYR	2.8
1	D	69	GLY	2.8
1	H	24	SER	2.8
1	E	310	THR	2.8
1	H	361	PRO	2.8
1	H	30	VAL	2.8
1	C	51	ALA	2.8
1	B	80	GLN	2.8
1	A	24	SER	2.7
1	C	24	SER	2.7
1	E	19	THR	2.7
1	G	25	LYS	2.7
1	G	51	ALA	2.7
1	D	28	VAL	2.7
1	E	360	LEU	2.7
1	E	67	SER	2.7
1	B	311	SER	2.7
1	B	34	GLY	2.7
1	A	25	LYS	2.6
1	G	67	SER	2.6
1	D	58	ASP	2.6
1	E	222	VAL	2.6
1	E	311	SER	2.6
1	F	57	PRO	2.6
1	G	223	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	26	GLY	2.6
1	D	24	SER	2.6
1	B	139	LEU	2.6
1	G	222	VAL	2.6
1	F	49	GLU	2.6
1	B	225	LYS	2.5
1	D	25	LYS	2.5
1	E	23	GLN	2.5
1	E	20	LEU	2.5
1	H	51	ALA	2.5
1	E	344	GLU	2.5
1	E	312	LEU	2.5
1	E	52	GLN	2.5
1	A	57	PRO	2.5
1	B	33	PRO	2.4
1	B	57	PRO	2.4
1	G	54	GLN	2.4
1	A	56	LEU	2.4
1	D	34	GLY	2.4
1	A	7	SER	2.4
1	F	309	ALA	2.4
1	H	157	LEU	2.4
1	F	51	ALA	2.4
1	E	223	LYS	2.3
1	H	57	PRO	2.3
1	D	49	GLU	2.3
1	E	138	ILE	2.3
1	B	67	SER	2.3
1	G	139	LEU	2.2
1	F	344	GLU	2.2
1	F	48	LYS	2.2
1	F	223	LYS	2.2
1	E	348	GLU	2.2
1	E	345	ARG	2.2
1	B	37	THR	2.2
1	D	52	GLN	2.2
1	G	70	PRO	2.2
1	G	172	VAL	2.2
1	G	58	ASP	2.2
1	D	56	LEU	2.2
1	H	221	LYS	2.2
1	C	361	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	50	PHE	2.2
1	E	309	ALA	2.2
1	G	105	GLU	2.2
1	A	53	ALA	2.1
1	B	339	PRO	2.1
1	D	57	PRO	2.1
1	D	112	VAL	2.1
1	F	310	THR	2.1
1	F	313	ALA	2.1
1	H	54	GLN	2.1
1	E	111	VAL	2.1
1	E	70	PRO	2.1
1	G	24	SER	2.1
1	A	361	PRO	2.1
1	B	343	LEU	2.1
1	B	112	VAL	2.1
1	D	111	VAL	2.1
1	F	60	ALA	2.1
1	F	112	VAL	2.0
1	F	307	GLY	2.0
1	G	226	ASP	2.0
1	H	49	GLU	2.0
1	C	23	GLN	2.0
1	E	7	SER	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EPE	G	700	15/15	0.96	0.13	27,43,59,63	0
2	EPE	E	700	15/15	0.97	0.13	29,44,58,60	0
2	EPE	A	700	15/15	0.98	0.13	20,29,51,55	0
2	EPE	F	700	15/15	0.98	0.13	18,31,49,54	0
2	EPE	D	700	15/15	0.98	0.10	28,35,51,59	0
2	EPE	C	700	15/15	0.98	0.14	19,35,52,57	0
2	EPE	B	700	15/15	0.98	0.09	30,38,44,46	0
2	EPE	H	700	15/15	0.98	0.12	23,32,42,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.