



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:18 pm BST

PDB ID : 5DS0  
Title : Crystal structure of TET aminopeptidase from marine sediment archaeon Thaumarchaeota archaeon SCGC AB-539-E09  
Authors : Michalska, K.; Chhor, G.; Mootz, J.; Endres, M.; Jedrzejczak, R.; Babnigg, G.; Steen, A.; Lloyd, K.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2015-09-16  
Resolution : 2.80 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

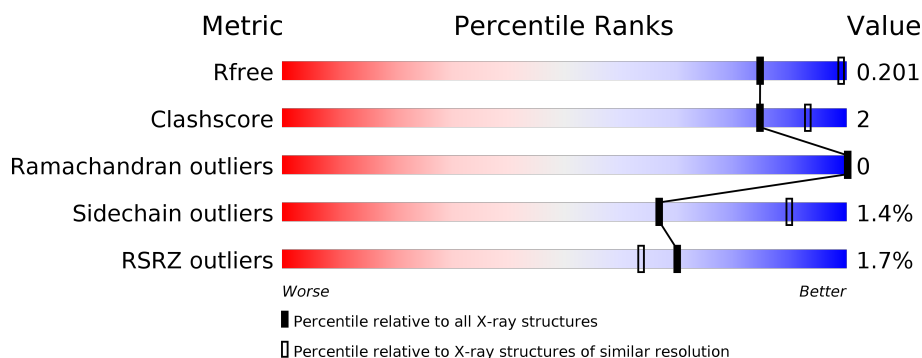
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	359	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	B	359	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	C	359	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	D	359	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	E	359	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	F	359	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	359	<div><div></div><div>3%</div><div>94%</div><div>7%</div><div>•</div><div>••</div></div>
1	H	359	<div><div></div><div>%</div><div>92%</div><div>7%</div><div>•</div></div>
1	I	359	<div><div></div><div>%</div><div>91%</div><div>7%</div><div>••</div></div>
1	J	359	<div><div></div><div>2%</div><div>92%</div><div>7%</div><div>•</div></div>
1	K	359	<div><div></div><div>2%</div><div>93%</div><div>6%</div><div>••</div></div>
1	L	359	<div><div></div><div>%</div><div>92%</div><div>6%</div><div>••</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32797 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 Peptidase M42.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	Se	0	0	0
			2728	1720	474	517	3	14			
1	B	356	Total	C	N	O	S	Se	0	0	0
			2718	1715	472	514	3	14			
1	C	359	Total	C	N	O	S	Se	0	0	0
			2744	1731	477	519	3	14			
1	D	358	Total	C	N	O	S	Se	0	0	0
			2732	1722	475	518	3	14			
1	E	357	Total	C	N	O	S	Se	0	0	0
			2728	1720	474	517	3	14			
1	F	356	Total	C	N	O	S	Se	0	0	0
			2723	1717	473	516	3	14			
1	G	356	Total	C	N	O	S	Se	0	0	0
			2723	1717	473	516	3	14			
1	H	356	Total	C	N	O	S	Se	0	0	0
			2723	1717	473	516	3	14			
1	I	354	Total	C	N	O	S	Se	0	0	0
			2709	1710	470	512	3	14			
1	J	356	Total	C	N	O	S	Se	0	0	0
			2723	1717	473	516	3	14			
1	K	356	Total	C	N	O	S	Se	0	0	0
			2723	1717	473	516	3	14			
1	L	355	Total	C	N	O	S	Se	0	0	0
			2709	1710	471	511	3	14			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP M7T295
A	2	ASN	-	expression tag	UNP M7T295
A	3	ALA	-	expression tag	UNP M7T295
B	1	SER	-	expression tag	UNP M7T295
B	2	ASN	-	expression tag	UNP M7T295

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	ALA	-	expression tag	UNP M7T295
C	1	SER	-	expression tag	UNP M7T295
C	2	ASN	-	expression tag	UNP M7T295
C	3	ALA	-	expression tag	UNP M7T295
D	1	SER	-	expression tag	UNP M7T295
D	2	ASN	-	expression tag	UNP M7T295
D	3	ALA	-	expression tag	UNP M7T295
E	1	SER	-	expression tag	UNP M7T295
E	2	ASN	-	expression tag	UNP M7T295
E	3	ALA	-	expression tag	UNP M7T295
F	1	SER	-	expression tag	UNP M7T295
F	2	ASN	-	expression tag	UNP M7T295
F	3	ALA	-	expression tag	UNP M7T295
G	1	SER	-	expression tag	UNP M7T295
G	2	ASN	-	expression tag	UNP M7T295
G	3	ALA	-	expression tag	UNP M7T295
H	1	SER	-	expression tag	UNP M7T295
H	2	ASN	-	expression tag	UNP M7T295
H	3	ALA	-	expression tag	UNP M7T295
I	1	SER	-	expression tag	UNP M7T295
I	2	ASN	-	expression tag	UNP M7T295
I	3	ALA	-	expression tag	UNP M7T295
J	1	SER	-	expression tag	UNP M7T295
J	2	ASN	-	expression tag	UNP M7T295
J	3	ALA	-	expression tag	UNP M7T295
K	1	SER	-	expression tag	UNP M7T295
K	2	ASN	-	expression tag	UNP M7T295
K	3	ALA	-	expression tag	UNP M7T295
L	1	SER	-	expression tag	UNP M7T295
L	2	ASN	-	expression tag	UNP M7T295
L	3	ALA	-	expression tag	UNP M7T295

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

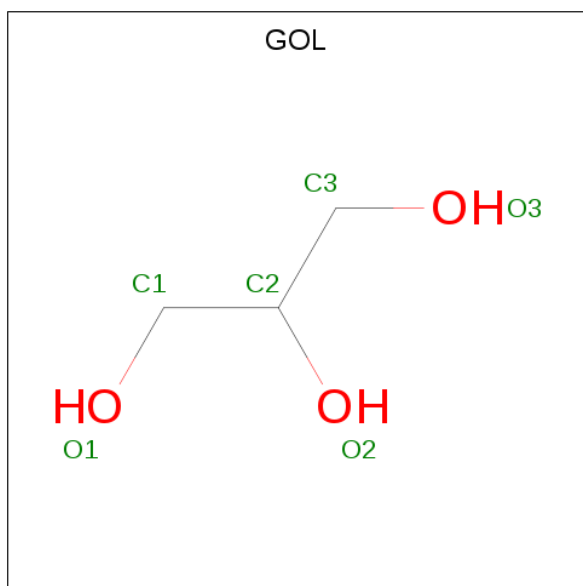
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Co 2 2	0	0
2	J	2	Total Co 2 2	0	0
2	D	2	Total Co 2 2	0	0
2	K	2	Total Co 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total 2	Co 2	0	0
2	H	2	Total 2	Co 2	0	0
2	B	2	Total 2	Co 2	0	0
2	I	2	Total 2	Co 2	0	0
2	C	2	Total 2	Co 2	0	0
2	A	2	Total 2	Co 2	0	0
2	L	2	Total 2	Co 2	0	0
2	F	2	Total 2	Co 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0

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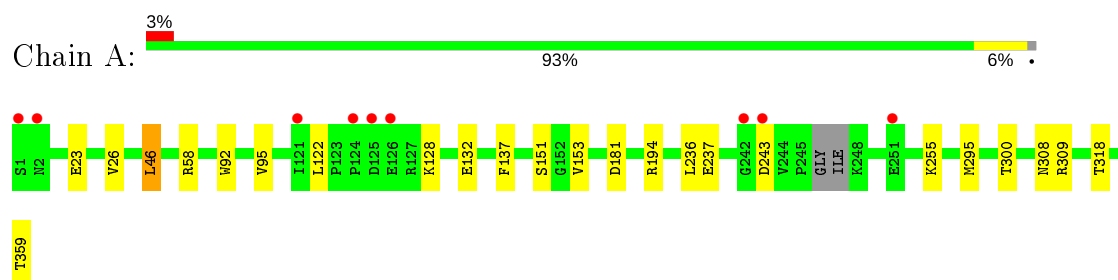
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		

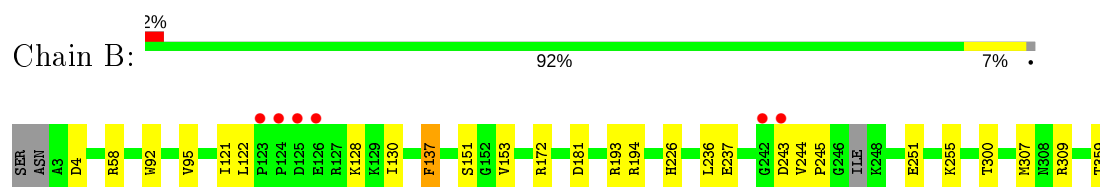
### 3 Residue-property plots [i](#)

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.

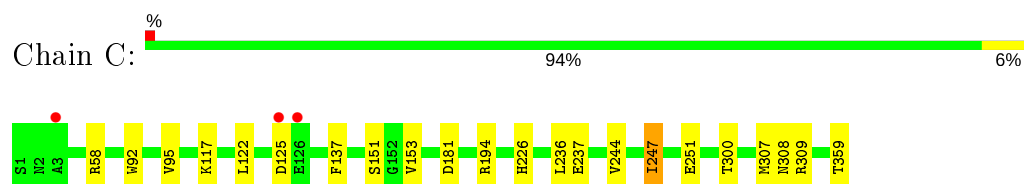
#### • Molecule 1: Peptidase M42



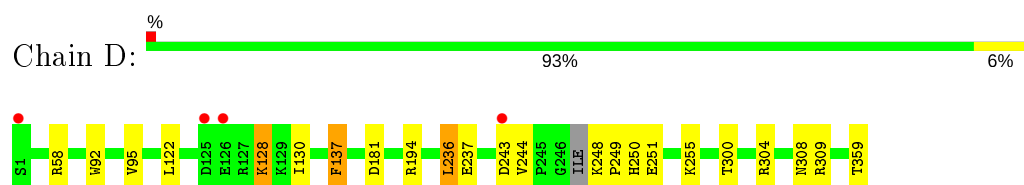
#### • Molecule 1: Peptidase M42



#### • Molecule 1: Peptidase M42



#### • Molecule 1: Peptidase M42



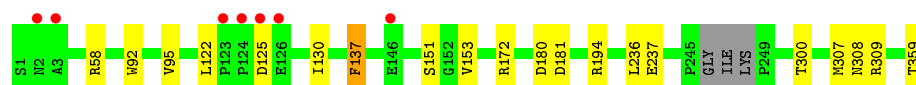
#### • Molecule 1: Peptidase M42







- Molecule 1: Peptidase M42



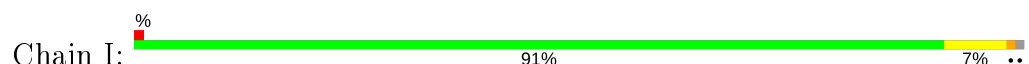
- Molecule 1: Peptidase M42



- Molecule 1: Peptidase M42



- Molecule 1: Peptidase M42



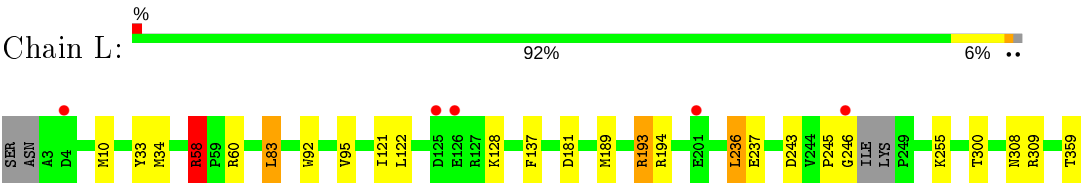
- Molecule 1: Peptidase M42



- Molecule 1: Peptidase M42



● Molecule 1: Peptidase M42



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.64Å 165.37Å 125.79Å 90.00° 90.87° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 45.67 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.80) 98.9 (45.67-2.78)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.193 , 0.206 0.194 , 0.201	Depositor DCC
$R_{free}$ test set	1850 reflections (1.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 18.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32797	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.52	1/2764 (0.0%)	0.73	4/3717 (0.1%)
1	B	0.53	0/2754	0.85	7/3703 (0.2%)
1	C	0.50	0/2781	0.72	3/3740 (0.1%)
1	D	0.49	0/2768	0.78	5/3722 (0.1%)
1	E	0.51	0/2764	0.78	4/3717 (0.1%)
1	F	0.49	0/2759	0.73	4/3709 (0.1%)
1	G	0.52	0/2759	0.74	5/3709 (0.1%)
1	H	0.51	0/2759	0.76	5/3709 (0.1%)
1	I	0.51	0/2745	0.75	3/3691 (0.1%)
1	J	0.50	1/2759 (0.0%)	0.73	4/3709 (0.1%)
1	K	0.48	0/2759	0.71	5/3709 (0.1%)
1	L	0.49	0/2745	0.80	8/3690 (0.2%)
All	All	0.50	2/33116 (0.0%)	0.76	57/44525 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	GLU	CD-OE1	6.44	1.32	1.25
1	J	251	GLU	CG-CD	5.46	1.60	1.51

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	ARG	NE-CZ-NH1	18.70	129.65	120.30
1	B	194	ARG	NE-CZ-NH2	-17.25	111.67	120.30
1	E	194	ARG	NE-CZ-NH2	-16.37	112.11	120.30
1	L	194	ARG	NE-CZ-NH2	-16.22	112.19	120.30
1	D	194	ARG	NE-CZ-NH2	-16.11	112.25	120.30
1	I	194	ARG	NE-CZ-NH2	-15.63	112.48	120.30
1	D	194	ARG	NE-CZ-NH1	12.58	126.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	194	ARG	NE-CZ-NH1	12.53	126.56	120.30
1	E	194	ARG	NE-CZ-NH1	12.46	126.53	120.30
1	L	194	ARG	NE-CZ-NH1	12.31	126.46	120.30
1	H	341	ARG	NE-CZ-NH2	-11.60	114.50	120.30
1	H	194	ARG	NE-CZ-NH2	11.53	126.07	120.30
1	A	194	ARG	NE-CZ-NH2	11.49	126.05	120.30
1	J	194	ARG	NE-CZ-NH2	11.39	126.00	120.30
1	G	194	ARG	NE-CZ-NH2	11.26	125.93	120.30
1	H	341	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	C	194	ARG	NE-CZ-NH2	10.97	125.79	120.30
1	F	194	ARG	NE-CZ-NH2	10.87	125.73	120.30
1	A	194	ARG	NE-CZ-NH1	-10.08	115.26	120.30
1	G	194	ARG	NE-CZ-NH1	-9.93	115.34	120.30
1	J	194	ARG	NE-CZ-NH1	-9.88	115.36	120.30
1	H	194	ARG	NE-CZ-NH1	-9.72	115.44	120.30
1	C	194	ARG	NE-CZ-NH1	-9.45	115.58	120.30
1	F	194	ARG	NE-CZ-NH1	-9.28	115.66	120.30
1	E	58	ARG	NE-CZ-NH2	9.24	124.92	120.30
1	K	194	ARG	NE-CZ-NH1	-8.81	115.89	120.30
1	G	58	ARG	NE-CZ-NH2	8.21	124.41	120.30
1	L	122	LEU	CB-CG-CD1	7.23	123.29	111.00
1	B	193	ARG	CG-CD-NE	-7.18	96.72	111.80
1	K	122	LEU	CB-CG-CD1	7.02	122.94	111.00
1	F	122	LEU	CB-CG-CD1	6.88	122.70	111.00
1	D	122	LEU	CB-CG-CD1	6.85	122.64	111.00
1	H	122	LEU	CB-CG-CD1	6.81	122.57	111.00
1	B	122	LEU	CB-CG-CD1	6.78	122.53	111.00
1	G	309	ARG	CG-CD-NE	-6.68	97.76	111.80
1	A	132	GLU	CG-CD-OE1	6.50	131.30	118.30
1	D	304	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	C	122	LEU	CB-CG-CD2	6.31	121.73	111.00
1	E	122	LEU	CB-CG-CD2	6.27	121.65	111.00
1	I	122	LEU	CB-CG-CD2	6.26	121.65	111.00
1	J	122	LEU	CB-CG-CD2	6.24	121.61	111.00
1	G	122	LEU	CB-CG-CD2	6.20	121.55	111.00
1	A	46	LEU	CB-CG-CD1	6.19	121.52	111.00
1	L	236	LEU	CB-CG-CD2	6.05	121.28	111.00
1	K	194	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	B	251	GLU	CG-CD-OE1	-5.82	106.67	118.30
1	D	236	LEU	CB-CG-CD2	5.81	120.87	111.00
1	F	172	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	L	83	LEU	CB-CG-CD2	5.52	120.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	58	ARG	CB-CG-CD	5.47	125.83	111.60
1	B	251	GLU	CG-CD-OE2	5.42	129.14	118.30
1	J	193	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	172	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	K	34	MSE	CG-SE-CE	5.21	110.35	98.90
1	L	83	LEU	CA-CB-CG	5.08	126.99	115.30
1	K	172	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	L	58	ARG	CA-CB-CG	5.04	124.50	113.40

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	2728	0	2752	10	0
1	B	2718	0	2741	20	0
1	C	2744	0	2778	11	0
1	D	2732	0	2755	23	0
1	E	2728	0	2752	15	0
1	F	2723	0	2751	14	0
1	G	2723	0	2751	8	0
1	H	2723	0	2751	15	0
1	I	2709	0	2733	24	0
1	J	2723	0	2751	13	0
1	K	2723	0	2751	14	0
1	L	2709	0	2736	18	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	6	0	8	0	0
3	B	12	0	16	0	0
3	C	12	0	16	0	0
3	E	6	0	8	0	0
3	G	12	0	16	0	0
3	H	12	0	16	0	0
3	I	12	0	16	1	0
3	J	6	0	8	0	0
3	K	6	0	8	1	0
3	L	6	0	8	0	0
All	All	32797	0	33122	150	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 2.

All (150) 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:I:34:MSE:HG2	1:I:189:MSE:HE3	1.31	1.10
1:D:248:LYS:CB	1:D:249:PRO:HD2	1.81	1.10
1:B:130:ILE:HG13	1:D:130:ILE:HG22	1.54	0.87
1:I:34:MSE:CG	1:I:189:MSE:HE3	2.05	0.86
1:D:248:LYS:CB	1:D:249:PRO:CD	2.56	0.82
1:E:130:ILE:HG22	1:F:130:ILE:HG13	1.68	0.75
1:L:33:TYR:CD2	1:L:189:MSE:CE	2.79	0.66
1:I:33:TYR:CD2	1:I:189:MSE:HE2	2.32	0.65
1:C:117:LYS:HD3	1:L:246:GLY:HA3	1.80	0.64
1:I:33:TYR:HB3	1:I:189:MSE:HE1	1.82	0.62
1:C:251:GLU:HG3	1:L:121:ILE:HG23	1.81	0.62
1:J:121:ILE:HG23	1:K:251:GLU:HG3	1.84	0.60
1:L:193:ARG:HB3	1:L:193:ARG:HH11	1.66	0.60
1:G:226:HIS:O	1:G:309:ARG:NH2	2.36	0.58
1:J:151:SER:OG	1:J:153:VAL:HG23	2.04	0.58
1:C:151:SER:OG	1:C:153:VAL:HG23	2.04	0.57
1:B:244:VAL:HG13	1:D:137:PHE:CE1	2.39	0.57
1:B:151:SER:OG	1:B:153:VAL:HG23	2.05	0.57
1:I:151:SER:OG	1:I:153:VAL:HG23	2.05	0.57
1:A:151:SER:OG	1:A:153:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:151:SER:OG	1:H:153:VAL:HG23	2.05	0.57
1:K:151:SER:OG	1:K:153:VAL:HG23	2.05	0.57
1:H:323:HIS:HA	3:I:404:GOL:H11	1.87	0.57
1:F:151:SER:OG	1:F:153:VAL:HG23	2.04	0.56
1:E:151:SER:OG	1:E:153:VAL:HG23	2.05	0.56
1:H:244:VAL:HG13	1:I:137:PHE:CE1	2.41	0.55
1:B:244:VAL:CG1	1:D:137:PHE:CZ	2.89	0.54
1:L:308:ASN:OD1	1:L:309:ARG:NH2	2.41	0.54
1:B:137:PHE:CE1	1:D:244:VAL:HG13	2.43	0.54
1:I:308:ASN:OD1	1:I:309:ARG:NH2	2.41	0.53
1:E:244:VAL:HG13	1:F:137:PHE:CE1	2.43	0.53
1:F:308:ASN:OD1	1:F:309:ARG:NH2	2.41	0.53
1:A:128:LYS:O	1:G:130:ILE:HD12	2.09	0.52
1:K:308:ASN:OD1	1:K:309:ARG:NH2	2.42	0.52
1:H:244:VAL:CG1	1:I:137:PHE:CZ	2.92	0.52
1:B:137:PHE:CZ	1:D:244:VAL:CG1	2.93	0.52
1:H:308:ASN:OD1	1:H:309:ARG:NH1	2.43	0.52
1:L:34:MSE:HG2	1:L:189:MSE:HE3	1.90	0.52
1:A:308:ASN:OD1	1:A:309:ARG:NH1	2.43	0.51
1:L:359:THR:HG22	1:L:359:THR:OXT	2.10	0.51
1:E:244:VAL:CG1	1:F:137:PHE:CZ	2.93	0.51
1:B:121:ILE:HG13	1:D:251:GLU:HB2	1.92	0.51
1:D:308:ASN:OD1	1:D:309:ARG:NH1	2.44	0.51
1:J:308:ASN:OD1	1:J:309:ARG:NH1	2.44	0.51
1:C:308:ASN:OD1	1:C:309:ARG:NH1	2.44	0.51
1:E:308:ASN:OD1	1:E:309:ARG:NH1	2.44	0.50
1:J:121:ILE:HG23	1:K:251:GLU:HB2	1.94	0.50
1:I:359:THR:OXT	1:I:359:THR:HG22	2.11	0.50
1:A:359:THR:OXT	1:A:359:THR:HG22	2.12	0.49
1:B:244:VAL:CG1	1:D:137:PHE:HZ	2.24	0.49
1:D:359:THR:OXT	1:D:359:THR:HG22	2.12	0.49
1:B:359:THR:OXT	1:B:359:THR:HG22	2.12	0.49
1:K:359:THR:HG22	1:K:359:THR:OXT	2.13	0.49
1:F:359:THR:HG22	1:F:359:THR:OXT	2.12	0.49
1:H:244:VAL:CG1	1:I:137:PHE:HZ	2.26	0.49
1:C:359:THR:OXT	1:C:359:THR:HG22	2.12	0.49
1:J:359:THR:OXT	1:J:359:THR:HG22	2.13	0.49
1:B:137:PHE:HZ	1:D:244:VAL:CG1	2.27	0.48
1:A:295:MSE:CE	1:A:318:THR:HG21	2.43	0.48
1:H:359:THR:HG22	1:H:359:THR:OXT	2.13	0.48
1:J:295:MSE:CE	1:J:318:THR:HG21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:THR:OXT	1:E:359:THR:HG22	2.13	0.47
1:H:244:VAL:HG13	1:I:137:PHE:CZ	2.50	0.47
1:H:130:ILE:HD12	1:I:128:LYS:O	2.14	0.47
1:E:244:VAL:CG1	1:F:137:PHE:HZ	2.28	0.47
1:L:33:TYR:HD2	1:L:189:MSE:HE3	1.79	0.47
1:L:245:PRO:O	1:L:246:GLY:C	2.53	0.46
1:L:58:ARG:NH2	1:L:60:ARG:NE	2.63	0.46
1:A:237:GLU:HG3	1:A:300:THR:HG22	1.98	0.46
1:B:244:VAL:HG13	1:D:137:PHE:CZ	2.50	0.46
1:C:237:GLU:HG3	1:C:300:THR:HG22	1.98	0.46
1:B:137:PHE:CZ	1:D:244:VAL:HG13	2.50	0.46
1:D:250:HIS:NE2	1:D:251:GLU:OE1	2.48	0.46
1:I:33:TYR:HD2	1:I:189:MSE:HE2	1.75	0.46
1:D:237:GLU:HG3	1:D:300:THR:HG22	1.97	0.45
1:G:237:GLU:HG3	1:G:300:THR:HG22	1.98	0.45
1:K:237:GLU:HG3	1:K:300:THR:HG22	1.98	0.45
1:J:237:GLU:HG3	1:J:300:THR:HG22	1.99	0.45
1:G:2:ASN:N	1:G:2:ASN:OD1	2.36	0.45
1:H:237:GLU:HG3	1:H:300:THR:HG22	1.98	0.45
1:J:244:VAL:HG21	1:K:118:PRO:HD3	1.98	0.45
1:J:79:LYS:O	1:J:79:LYS:HG3	2.17	0.45
1:I:237:GLU:HG3	1:I:300:THR:HG22	1.98	0.45
1:B:237:GLU:HG3	1:B:300:THR:HG22	1.98	0.45
1:E:79:LYS:HG3	1:E:79:LYS:O	2.17	0.45
1:K:34:MSE:HE3	1:K:189:MSE:HB3	1.99	0.45
1:F:237:GLU:HG3	1:F:300:THR:HG22	1.99	0.45
1:L:33:TYR:CD2	1:L:189:MSE:HE2	2.52	0.45
1:B:130:ILE:HD12	1:D:128:LYS:O	2.17	0.44
1:E:237:GLU:HG3	1:E:300:THR:HG22	1.98	0.44
1:D:243:ASP:OD1	1:D:255:LYS:HA	2.18	0.44
1:L:237:GLU:HG3	1:L:300:THR:HG22	1.99	0.44
1:C:247:ILE:HD12	1:L:121:ILE:CD1	2.47	0.43
1:E:128:LYS:O	1:F:130:ILE:HD12	2.18	0.43
1:L:33:TYR:HB3	1:L:189:MSE:HE1	2.01	0.43
1:I:243:ASP:OD1	1:I:255:LYS:HA	2.19	0.43
1:B:243:ASP:OD1	1:B:255:LYS:HA	2.18	0.43
1:G:5:LYS:HE2	1:G:5:LYS:HB3	1.86	0.43
1:K:33:TYR:CD2	1:K:34:MSE:CE	3.02	0.43
1:J:243:ASP:OD1	1:J:255:LYS:HA	2.18	0.43
1:L:181:ASP:OD2	1:L:236:LEU:O	2.37	0.43
1:K:33:TYR:CD2	1:K:34:MSE:HE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:245:PRO:HD2	1:F:137:PHE:CZ	2.54	0.42
1:H:243:ASP:OD1	1:H:255:LYS:HA	2.19	0.42
1:L:243:ASP:OD1	1:L:255:LYS:HA	2.19	0.42
1:C:181:ASP:OD2	1:C:236:LEU:O	2.38	0.42
1:K:323:HIS:HA	3:K:403:GOL:O1	2.18	0.42
1:A:243:ASP:OD1	1:A:255:LYS:HA	2.19	0.42
1:B:181:ASP:OD2	1:B:236:LEU:O	2.38	0.42
1:E:181:ASP:OD2	1:E:236:LEU:O	2.38	0.42
1:F:181:ASP:OD2	1:F:236:LEU:O	2.38	0.42
1:H:245:PRO:HD2	1:I:137:PHE:CZ	2.55	0.42
1:A:181:ASP:OD2	1:A:236:LEU:O	2.37	0.42
1:E:244:VAL:HG13	1:F:137:PHE:CZ	2.54	0.42
1:H:181:ASP:OD2	1:H:236:LEU:O	2.38	0.42
1:J:121:ILE:HG23	1:K:251:GLU:CB	2.50	0.42
1:L:33:TYR:CD2	1:L:189:MSE:HE3	2.52	0.42
1:C:226:HIS:CE1	1:D:309:ARG:HG2	2.55	0.42
1:B:121:ILE:HD11	1:D:248:LYS:O	2.20	0.41
1:D:181:ASP:OD2	1:D:236:LEU:O	2.38	0.41
1:E:92:TRP:O	1:E:95:VAL:HG22	2.20	0.41
1:K:181:ASP:OD2	1:K:236:LEU:O	2.37	0.41
1:B:226:HIS:O	1:B:309:ARG:NH1	2.43	0.41
1:D:92:TRP:O	1:D:95:VAL:HG22	2.20	0.41
1:I:181:ASP:OD2	1:I:236:LEU:O	2.38	0.41
1:J:181:ASP:OD2	1:J:236:LEU:O	2.38	0.41
1:H:92:TRP:O	1:H:95:VAL:HG22	2.20	0.41
1:G:243:ASP:OD1	1:G:255:LYS:HA	2.21	0.41
1:I:180:ASP:HA	1:I:181:ASP:HA	1.86	0.41
1:I:92:TRP:O	1:I:95:VAL:HG22	2.20	0.41
1:G:181:ASP:OD2	1:G:236:LEU:O	2.38	0.41
1:I:33:TYR:CD2	1:I:189:MSE:CE	3.02	0.41
1:A:23:GLU:O	1:A:26:VAL:HG12	2.21	0.41
1:E:128:LYS:HG2	1:E:128:LYS:O	2.19	0.41
1:G:92:TRP:O	1:G:95:VAL:HG22	2.20	0.41
1:A:92:TRP:O	1:A:95:VAL:HG22	2.20	0.41
1:C:92:TRP:O	1:C:95:VAL:HG22	2.21	0.41
1:J:92:TRP:O	1:J:95:VAL:HG22	2.21	0.41
1:F:180:ASP:HA	1:F:181:ASP:HA	1.86	0.41
1:F:92:TRP:O	1:F:95:VAL:HG22	2.21	0.41
1:I:130:ILE:H	1:I:130:ILE:HG22	1.56	0.41
1:I:33:TYR:HB3	1:I:189:MSE:CE	2.49	0.41
1:K:92:TRP:O	1:K:95:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:VAL:O	1:C:247:ILE:HB	2.20	0.40
1:I:23:GLU:O	1:I:26:VAL:HG12	2.21	0.40
1:B:92:TRP:O	1:B:95:VAL:HG22	2.21	0.40
1:I:161:PRO:HB3	1:I:327:HIS:CD2	2.56	0.40
1:L:92:TRP:O	1:L:95:VAL:HG22	2.20	0.40
1:B:245:PRO:HD2	1:D:137:PHE:CZ	2.57	0.40
1:H:23:GLU:O	1:H:26:VAL:HG12	2.21	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	353/359 (98%)	341 (97%)	12 (3%)	0	100	100
1	B	352/359 (98%)	341 (97%)	11 (3%)	0	100	100
1	C	357/359 (99%)	344 (96%)	13 (4%)	0	100	100
1	D	354/359 (99%)	343 (97%)	11 (3%)	0	100	100
1	E	353/359 (98%)	341 (97%)	12 (3%)	0	100	100
1	F	352/359 (98%)	339 (96%)	13 (4%)	0	100	100
1	G	352/359 (98%)	340 (97%)	12 (3%)	0	100	100
1	H	352/359 (98%)	340 (97%)	12 (3%)	0	100	100
1	I	350/359 (98%)	338 (97%)	12 (3%)	0	100	100
1	J	352/359 (98%)	339 (96%)	13 (4%)	0	100	100
1	K	352/359 (98%)	341 (97%)	11 (3%)	0	100	100
1	L	351/359 (98%)	339 (97%)	12 (3%)	0	100	100
All	All	4230/4308 (98%)	4086 (97%)	144 (3%)	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	298/286 (104%)	294 (99%)	4 (1%)	69	91
1	B	296/286 (104%)	291 (98%)	5 (2%)	60	87
1	C	300/286 (105%)	295 (98%)	5 (2%)	60	87
1	D	298/286 (104%)	295 (99%)	3 (1%)	76	93
1	E	298/286 (104%)	295 (99%)	3 (1%)	76	93
1	F	298/286 (104%)	294 (99%)	4 (1%)	69	91
1	G	298/286 (104%)	294 (99%)	4 (1%)	69	91
1	H	298/286 (104%)	294 (99%)	4 (1%)	69	91
1	I	296/286 (104%)	292 (99%)	4 (1%)	67	90
1	J	298/286 (104%)	294 (99%)	4 (1%)	69	91
1	K	298/286 (104%)	294 (99%)	4 (1%)	69	91
1	L	295/286 (103%)	289 (98%)	6 (2%)	55	84
All	All	3571/3432 (104%)	3521 (99%)	50 (1%)	67	90

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	58	ARG
1	A	122	LEU
1	A	137	PHE
1	B	4	ASP
1	B	58	ARG
1	B	128	LYS
1	B	137	PHE
1	B	307	MSE
1	C	58	ARG
1	C	125	ASP
1	C	137	PHE
1	C	247	ILE
1	C	307	MSE

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Mol	Chain	Res	Type
1	D	58	ARG
1	D	128	LYS
1	D	137	PHE
1	E	58	ARG
1	E	128	LYS
1	E	137	PHE
1	F	58	ARG
1	F	125	ASP
1	F	137	PHE
1	F	307	MSE
1	G	2	ASN
1	G	58	ARG
1	G	137	PHE
1	G	307	MSE
1	H	58	ARG
1	H	125	ASP
1	H	137	PHE
1	H	307	MSE
1	I	58	ARG
1	I	128	LYS
1	I	137	PHE
1	I	307	MSE
1	J	58	ARG
1	J	128	LYS
1	J	137	PHE
1	J	307	MSE
1	K	58	ARG
1	K	122	LEU
1	K	137	PHE
1	K	307	MSE
1	L	10	MSE
1	L	58	ARG
1	L	83	LEU
1	L	128	LYS
1	L	137	PHE
1	L	193	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	226	HIS
1	C	226	HIS

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Mol	Chain	Res	Type
1	D	226	HIS
1	F	2	ASN
1	H	226	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 24 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	C	404	-	5,5,5	0.50	0	5,5,5	0.69	0
3	GOL	B	404	-	5,5,5	0.49	0	5,5,5	0.45	0
3	GOL	H	404	-	5,5,5	0.47	0	5,5,5	0.38	0
3	GOL	B	403	-	5,5,5	0.51	0	5,5,5	0.61	0
3	GOL	E	403	-	5,5,5	0.66	0	5,5,5	0.90	0
3	GOL	C	403	-	5,5,5	0.37	0	5,5,5	0.66	0
3	GOL	A	403	-	5,5,5	0.29	0	5,5,5	0.59	0
3	GOL	L	403	-	5,5,5	0.26	0	5,5,5	0.23	0
3	GOL	J	403	-	5,5,5	0.55	0	5,5,5	0.59	0
3	GOL	G	404	-	5,5,5	0.35	0	5,5,5	0.51	0
3	GOL	K	403	-	5,5,5	0.27	0	5,5,5	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	I	404	-	5,5,5	0.24	0	5,5,5	0.55	0
3	GOL	I	403	-	5,5,5	0.54	0	5,5,5	0.85	0
3	GOL	G	403	-	5,5,5	0.20	0	5,5,5	0.64	0
3	GOL	H	403	-	5,5,5	0.50	0	5,5,5	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	404	-	-	4/4/4/4	-
3	GOL	B	404	-	-	1/4/4/4	-
3	GOL	H	404	-	-	2/4/4/4	-
3	GOL	B	403	-	-	3/4/4/4	-
3	GOL	E	403	-	-	4/4/4/4	-
3	GOL	C	403	-	-	2/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	L	403	-	-	2/4/4/4	-
3	GOL	J	403	-	-	2/4/4/4	-
3	GOL	G	404	-	-	2/4/4/4	-
3	GOL	K	403	-	-	4/4/4/4	-
3	GOL	I	404	-	-	0/4/4/4	-
3	GOL	I	403	-	-	2/4/4/4	-
3	GOL	G	403	-	-	4/4/4/4	-
3	GOL	H	403	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	404	GOL	O1-C1-C2-C3
3	J	403	GOL	O1-C1-C2-C3
3	A	403	GOL	O1-C1-C2-C3
3	K	403	GOL	O1-C1-C2-C3
3	K	403	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	I	403	GOL	C1-C2-C3-O3
3	C	404	GOL	C1-C2-C3-O3
3	B	403	GOL	O1-C1-C2-C3
3	C	403	GOL	O1-C1-C2-C3
3	G	404	GOL	O1-C1-C2-C3
3	G	403	GOL	O1-C1-C2-O2
3	G	403	GOL	O1-C1-C2-C3
3	G	403	GOL	C1-C2-C3-O3
3	G	403	GOL	O2-C2-C3-O3
3	H	403	GOL	O1-C1-C2-O2
3	H	403	GOL	O1-C1-C2-C3
3	H	403	GOL	C1-C2-C3-O3
3	L	403	GOL	O1-C1-C2-C3
3	J	403	GOL	O1-C1-C2-O2
3	C	404	GOL	O2-C2-C3-O3
3	H	403	GOL	O2-C2-C3-O3
3	E	403	GOL	O1-C1-C2-C3
3	E	403	GOL	C1-C2-C3-O3
3	K	403	GOL	C1-C2-C3-O3
3	C	404	GOL	O1-C1-C2-C3
3	B	403	GOL	C1-C2-C3-O3
3	E	403	GOL	O1-C1-C2-O2
3	E	403	GOL	O2-C2-C3-O3
3	H	404	GOL	O1-C1-C2-O2
3	A	403	GOL	O1-C1-C2-O2
3	I	403	GOL	O2-C2-C3-O3
3	C	403	GOL	O1-C1-C2-O2
3	L	403	GOL	O1-C1-C2-O2
3	C	404	GOL	O1-C1-C2-O2
3	G	404	GOL	O1-C1-C2-O2
3	K	403	GOL	O1-C1-C2-O2
3	B	404	GOL	O1-C1-C2-C3
3	B	403	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	403	GOL	1	0
3	I	404	GOL	1	0



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	343/359 (95%)	-0.34	9 (2%)	56	46	29, 43, 84, 123	0
1	B	342/359 (95%)	-0.23	6 (1%)	68	61	28, 48, 79, 111	0
1	C	345/359 (96%)	-0.35	3 (0%)	84	80	28, 41, 81, 117	0
1	D	344/359 (95%)	-0.41	4 (1%)	79	73	27, 42, 80, 124	0
1	E	343/359 (95%)	-0.35	3 (0%)	84	80	31, 44, 78, 112	0
1	F	342/359 (95%)	-0.24	7 (2%)	65	56	31, 49, 88, 122	0
1	G	342/359 (95%)	-0.18	12 (3%)	44	34	26, 47, 84, 115	0
1	H	342/359 (95%)	-0.43	3 (0%)	84	80	23, 41, 71, 128	0
1	I	340/359 (94%)	-0.47	2 (0%)	89	86	24, 38, 70, 104	0
1	J	342/359 (95%)	-0.27	6 (1%)	68	61	27, 48, 85, 113	0
1	K	342/359 (95%)	-0.25	8 (2%)	60	51	28, 46, 77, 110	0
1	L	341/359 (94%)	-0.26	5 (1%)	73	68	26, 44, 81, 115	0
All	All	4108/4308 (95%)	-0.31	68 (1%)	70	63	23, 44, 82, 128	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	1	SER	5.4
1	A	1	SER	4.6
1	G	1	SER	3.9
1	K	126	GLU	3.8
1	G	2	ASN	3.6
1	H	126	GLU	3.6
1	G	123	PRO	3.5
1	F	3	ALA	3.5
1	J	251	GLU	3.4
1	F	2	ASN	3.4
1	C	3	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	126	GLU	3.1
1	J	126	GLU	3.1
1	J	2	ASN	3.1
1	B	125	ASP	3.0
1	G	3	ALA	3.0
1	G	242	GLY	2.9
1	D	1	SER	2.9
1	B	126	GLU	2.9
1	A	251	GLU	2.8
1	A	2	ASN	2.7
1	G	251	GLU	2.7
1	L	125	ASP	2.7
1	A	126	GLU	2.7
1	J	1	SER	2.6
1	J	3	ALA	2.6
1	C	125	ASP	2.6
1	G	126	GLU	2.6
1	E	38	ALA	2.6
1	C	126	GLU	2.6
1	F	125	ASP	2.6
1	L	201	GLU	2.5
1	K	125	ASP	2.5
1	A	121	ILE	2.5
1	B	124	PRO	2.5
1	L	4	ASP	2.5
1	G	125	ASP	2.4
1	G	199	GLY	2.4
1	B	242	GLY	2.4
1	A	125	ASP	2.4
1	L	246	GLY	2.4
1	D	243	ASP	2.4
1	G	57	ASP	2.3
1	B	123	PRO	2.3
1	E	243	ASP	2.3
1	F	123	PRO	2.3
1	E	1	SER	2.3
1	K	54	LYS	2.3
1	A	243	ASP	2.3
1	G	124	PRO	2.2
1	K	123	PRO	2.2
1	H	121	ILE	2.2
1	A	242	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	128	LYS	2.2
1	K	117	LYS	2.2
1	A	124	PRO	2.1
1	K	243	ASP	2.1
1	I	125	ASP	2.1
1	J	242	GLY	2.1
1	D	125	ASP	2.1
1	G	117	LYS	2.1
1	B	243	ASP	2.0
1	H	125	ASP	2.0
1	F	126	GLU	2.0
1	F	146	GLU	2.0
1	L	126	GLU	2.0
1	K	127	ARG	2.0
1	F	124	PRO	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
3	GOL	E	403	6/6	0.86	0.21	49,54,58,60	0
3	GOL	J	403	6/6	0.87	0.22	56,62,64,64	0
3	GOL	G	403	6/6	0.87	0.28	62,63,67,70	0
3	GOL	H	403	6/6	0.89	0.24	44,46,48,49	0
3	GOL	I	403	6/6	0.90	0.16	43,46,46,48	0
3	GOL	C	404	6/6	0.91	0.24	64,64,65,66	0
3	GOL	C	403	6/6	0.92	0.25	40,44,50,55	0
3	GOL	B	404	6/6	0.92	0.18	41,48,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	G	404	6/6	0.92	0.19	48,54,55,57	0
3	GOL	A	403	6/6	0.92	0.18	45,46,50,52	0
3	GOL	K	403	6/6	0.92	0.22	54,56,57,59	0
3	GOL	L	403	6/6	0.92	0.21	50,52,55,60	0
3	GOL	B	403	6/6	0.93	0.15	43,46,48,50	0
3	GOL	H	404	6/6	0.93	0.21	55,57,61,62	0
3	GOL	I	404	6/6	0.93	0.20	44,46,48,48	0
2	CO	L	401	1/1	0.98	0.13	28,28,28,28	0
2	CO	J	402	1/1	0.98	0.12	25,25,25,25	0
2	CO	B	401	1/1	0.98	0.16	35,35,35,35	0
2	CO	G	402	1/1	0.98	0.10	30,30,30,30	0
2	CO	I	401	1/1	0.98	0.11	26,26,26,26	0
2	CO	C	402	1/1	0.99	0.14	29,29,29,29	0
2	CO	E	401	1/1	0.99	0.12	27,27,27,27	0
2	CO	K	401	1/1	0.99	0.14	31,31,31,31	0
2	CO	E	402	1/1	0.99	0.14	30,30,30,30	0
2	CO	F	401	1/1	0.99	0.13	38,38,38,38	0
2	CO	D	402	1/1	0.99	0.12	30,30,30,30	0
2	CO	A	402	1/1	0.99	0.14	23,23,23,23	0
2	CO	K	402	1/1	0.99	0.11	26,26,26,26	0
2	CO	D	401	1/1	0.99	0.14	23,23,23,23	0
2	CO	H	401	1/1	0.99	0.11	27,27,27,27	0
2	CO	J	401	1/1	0.99	0.12	29,29,29,29	0
2	CO	A	401	1/1	0.99	0.14	28,28,28,28	0
2	CO	F	402	1/1	0.99	0.14	26,26,26,26	0
2	CO	G	401	1/1	0.99	0.13	24,24,24,24	0
2	CO	I	402	1/1	0.99	0.12	22,22,22,22	0
2	CO	B	402	1/1	0.99	0.12	27,27,27,27	0
2	CO	H	402	1/1	0.99	0.11	24,24,24,24	0
2	CO	C	401	1/1	0.99	0.12	22,22,22,22	0
2	CO	L	402	1/1	0.99	0.12	26,26,26,26	0

## 6.5 Other polymers

There are no such residues in this entry.