



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:54 AM GMT

PDB ID : 3N7A  
Title : Crystal structure of 3-dehydroquinate dehydratase from Mycobacterium tuberculosis in complex with inhibitor 2  
Authors : Dias, M.V.B.; Snee, W.C.; Bromfield, K.M.; Payne, R.; Palaninathan, S.K.; Ciulli, A.; Howard, N.I.; Abell, C.; Sacchettini, J.C.; Blundell, T.L.  
Deposited on : 2010-05-26  
Resolution : 2.00 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

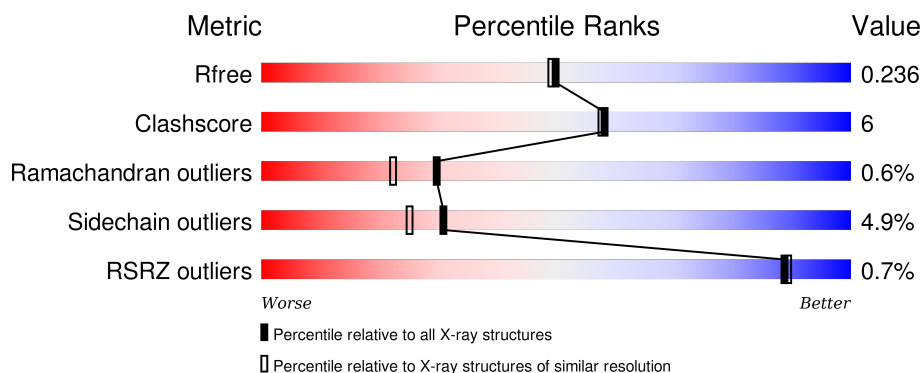
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
















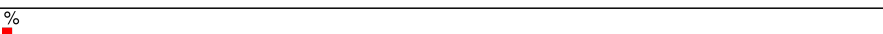





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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	147	 81% 13% . .
1	B	147	 84% 11% . .
1	C	147	 81% 12% .. 5%
1	D	147	 88% 6% . .
1	E	147	 78% 17% . .

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Mol	Chain	Length	Quality of chain
1	F	147	
1	G	147	
1	H	147	
1	I	147	
1	J	147	
1	K	147	
1	L	147	
1	M	147	
1	N	147	
1	O	147	
1	P	147	
1	Q	147	
1	R	147	
1	S	147	
1	T	147	
1	U	147	
1	V	147	
1	W	147	
1	X	147	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FA1	N	147	X	-	-	-
2	FA1	O	148	-	-	-	X
3	GOL	E	147	-	-	-	X
3	GOL	L	147	-	-	-	X
3	GOL	P	147	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	V	147	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28420 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 3-dehydroquinate dehydratase.

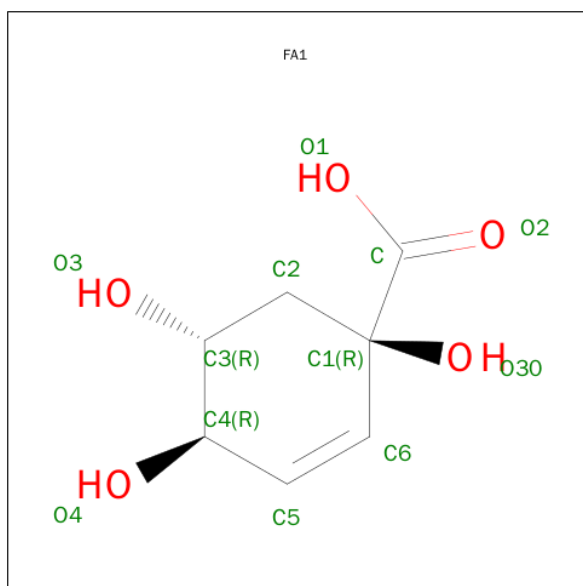
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1067	672	196	198	1			
1	B	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	C	139	Total	C	N	O	S	0	0	0
			1055	664	194	196	1			
1	D	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	E	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	F	137	Total	C	N	O	S	0	1	0
			1042	654	194	193	1			
1	G	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	H	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	I	141	Total	C	N	O	S	0	1	0
			1073	676	198	198	1			
1	J	141	Total	C	N	O	S	0	1	0
			1073	676	198	198	1			
1	K	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	L	141	Total	C	N	O	S	0	2	0
			1083	681	201	200	1			
1	M	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	N	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	O	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	P	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	141	Total	C	N	O	S	0	0	0
			1065	671	193	200	1			
1	R	141	Total	C	N	O	S	0	1	0
			1067	673	195	198	1			
1	S	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	T	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	U	141	Total	C	N	O	S	0	1	0
			1073	676	198	198	1			
1	V	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	W	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	X	137	Total	C	N	O	S	0	1	0
			1043	657	191	194	1			

- Molecule 2 is 2,3 -ANHYDRO-QUINIC ACID (three-letter code: FA1) (formula: C<sub>7</sub>H<sub>10</sub>O<sub>5</sub>).



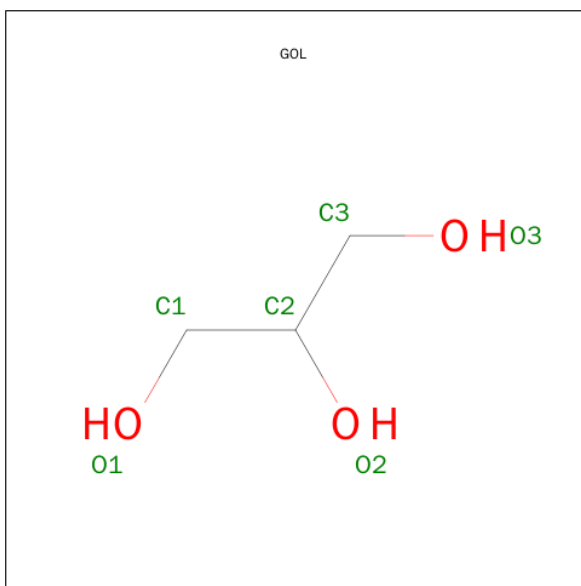
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	7	5		
2	B	1	Total	C	O	0	0
			12	7	5		
2	C	1	Total	C	O	0	0
			12	7	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			12	7	5		
2	E	1	Total	C	O	0	0
			12	7	5		
2	F	1	Total	C	O	0	0
			12	7	5		
2	G	1	Total	C	O	0	0
			12	7	5		
2	H	1	Total	C	O	0	0
			12	7	5		
2	I	1	Total	C	O	0	0
			12	7	5		
2	J	1	Total	C	O	0	0
			12	7	5		
2	K	1	Total	C	O	0	0
			12	7	5		
2	L	1	Total	C	O	0	0
			12	7	5		
2	M	1	Total	C	O	0	0
			12	7	5		
2	N	1	Total	C	O	0	0
			12	7	5		
2	O	1	Total	C	O	0	0
			12	7	5		
2	P	1	Total	C	O	0	0
			12	7	5		
2	Q	1	Total	C	O	0	0
			12	7	5		
2	R	1	Total	C	O	0	0
			12	7	5		
2	S	1	Total	C	O	0	0
			12	7	5		
2	T	1	Total	C	O	0	0
			12	7	5		
2	U	1	Total	C	O	0	0
			12	7	5		
2	V	1	Total	C	O	0	0
			12	7	5		
2	W	1	Total	C	O	0	0
			12	7	5		
2	X	1	Total	C	O	0	0
			12	7	5		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	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	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	O	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		
3	Q	1	Total	C	O	0	0
			6	3	3		
3	T	1	Total	C	O	0	0
			6	3	3		
3	U	1	Total	C	O	0	0
			6	3	3		
3	V	1	Total	C	O	0	0
			6	3	3		
3	X	1	Total	C	O	0	0
			6	3	3		



- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	82	Total O 82 82	0	0
4	B	95	Total O 95 95	0	0
4	C	96	Total O 96 96	0	0
4	D	84	Total O 84 84	0	0
4	E	84	Total O 84 84	0	0
4	F	85	Total O 85 85	0	0
4	G	101	Total O 101 101	0	0
4	H	106	Total O 106 106	0	0
4	I	99	Total O 99 99	0	0
4	J	125	Total O 125 125	0	0
4	K	92	Total O 92 92	0	0
4	L	127	Total O 127 127	0	0
4	M	112	Total O 112 112	0	0
4	N	85	Total O 85 85	0	0
4	O	85	Total O 85 85	0	0
4	P	102	Total O 102 102	0	0
4	Q	108	Total O 108 108	0	0
4	R	83	Total O 83 83	0	0
4	S	103	Total O 103 103	0	0
4	T	112	Total O 112 112	0	0
4	U	94	Total O 94 94	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	V	81	Total 81	O 81	0	0
4	W	109	Total 109	O 109	0	0
4	X	97	Total 97	O 97	0	0

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


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

- Molecule 1: 3-dehydroquinase dehydratase

Chain A: 




- Molecule 1: 3-dehydroquinase dehydratase

Chain B: 




- Molecule 1: 3-dehydroquinase dehydratase

Chain C: 




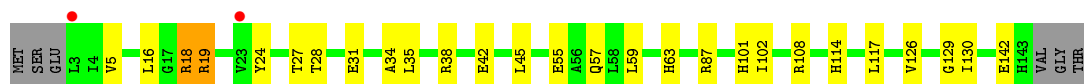
- Molecule 1: 3-dehydroquinase dehydratase

Chain D: 




- Molecule 1: 3-dehydroquinase dehydratase

Chain E: 



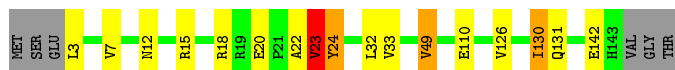
- Molecule 1: 3-dehydroquinase dehydratase

Chain F: 



- Molecule 1: 3-dehydroquinase dehydratase

Chain G: 84% 9% . . .



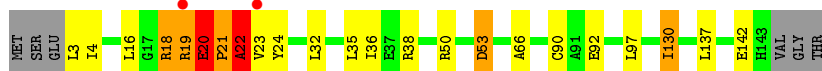
- Molecule 1: 3-dehydroquinase dehydratase

Chain H: 80% 13% . . .



- Molecule 1: 3-dehydroquinase dehydratase

Chain I: 80% 11% . . .



- Molecule 1: 3-dehydroquinase dehydratase

Chain J: 80% 10% . . .



- Molecule 1: 3-dehydroquinase dehydratase

Chain K: 82% 12% . . .



- Molecule 1: 3-dehydroquinase dehydratase

Chain L: 78% 15% . . .

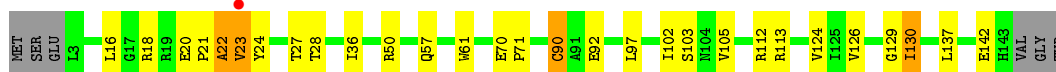
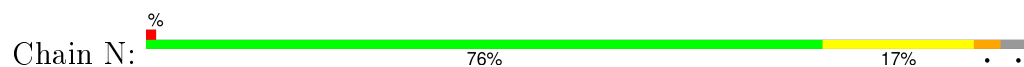


- Molecule 1: 3-dehydroquinase dehydratase

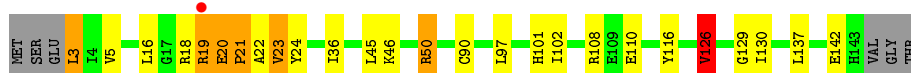
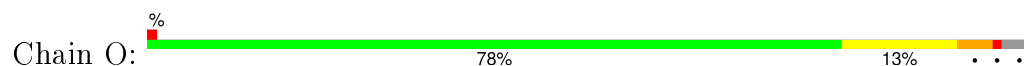
Chain M: 84% 8% . . .



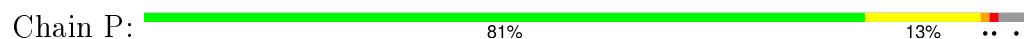
- Molecule 1: 3-dehydroquinase dehydratase



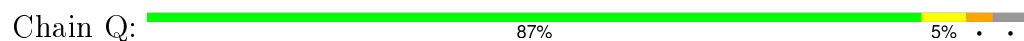
- Molecule 1: 3-dehydroquinase dehydratase



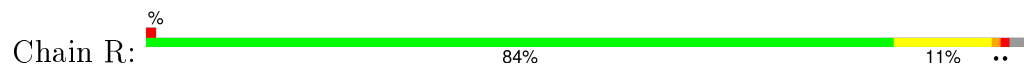
- Molecule 1: 3-dehydroquinase dehydratase



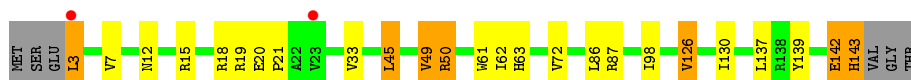
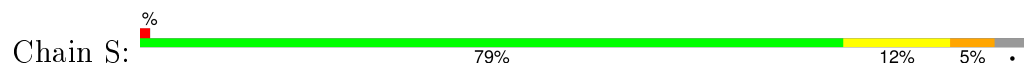
- Molecule 1: 3-dehydroquinase dehydratase



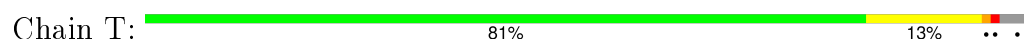
- Molecule 1: 3-dehydroquinase dehydratase



- Molecule 1: 3-dehydroquinase dehydratase

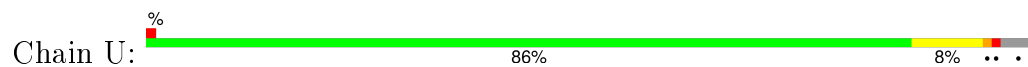


- Molecule 1: 3-dehydroquinase dehydratase

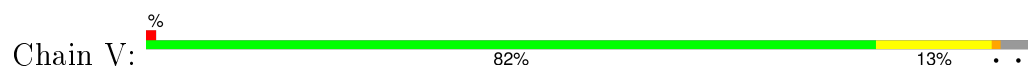




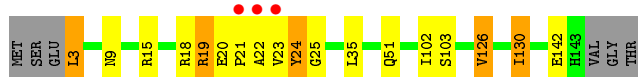
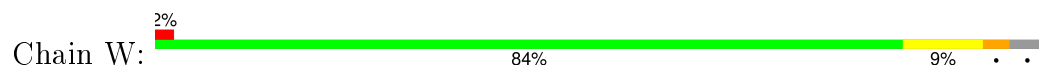
- Molecule 1: 3-dehydroquinase dehydratase



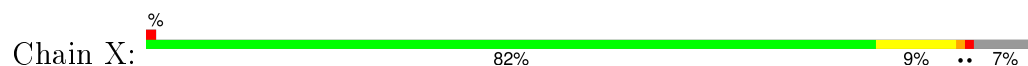
- Molecule 1: 3-dehydroquinase dehydratase



- Molecule 1: 3-dehydroquinase dehydratase



- Molecule 1: 3-dehydroquinase dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.91Å 95.56Å 124.47Å 79.93° 80.30° 77.60°	Depositor
Resolution (Å)	79.21 – 2.00 79.21 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (79.21-2.00) 90.3 (79.21-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.178 , 0.238 0.178 , 0.236	Depositor DCC
$R_{free}$ test set	12908 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.0	EDS
Estimated twinning fraction	0.011 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 256373 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	28420	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FA1

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	1.05	0/1085	0.99	2/1478 (0.1%)
1	B	1.00	0/1100	0.97	1/1498 (0.1%)
1	C	1.04	1/1071 (0.1%)	0.99	6/1456 (0.4%)
1	D	0.99	1/1100 (0.1%)	0.94	0/1498
1	E	0.99	0/1100	0.96	4/1498 (0.3%)
1	F	1.05	2/1062 (0.2%)	0.92	3/1443 (0.2%)
1	G	1.10	0/1100	1.02	2/1498 (0.1%)
1	H	1.10	0/1089	1.02	2/1483 (0.1%)
1	I	1.10	0/1096	1.04	5/1493 (0.3%)
1	J	1.31	5/1096 (0.5%)	1.10	5/1493 (0.3%)
1	K	1.02	1/1100 (0.1%)	0.96	4/1498 (0.3%)
1	L	1.28	6/1111 (0.5%)	1.05	2/1512 (0.1%)
1	M	1.18	2/1100 (0.2%)	1.04	4/1498 (0.3%)
1	N	1.09	1/1100 (0.1%)	0.95	1/1498 (0.1%)
1	O	1.06	1/1100 (0.1%)	0.94	3/1498 (0.2%)
1	P	1.13	1/1089 (0.1%)	0.94	2/1483 (0.1%)
1	Q	1.17	2/1083 (0.2%)	0.98	1/1476 (0.1%)
1	R	1.02	0/1090	0.93	3/1486 (0.2%)
1	S	1.19	1/1100 (0.1%)	1.08	6/1498 (0.4%)
1	T	1.14	4/1100 (0.4%)	1.01	4/1498 (0.3%)
1	U	0.99	1/1096 (0.1%)	0.94	1/1493 (0.1%)
1	V	0.99	1/1100 (0.1%)	0.95	3/1498 (0.2%)
1	W	1.16	1/1100 (0.1%)	1.01	3/1498 (0.2%)
1	X	1.00	0/1064	0.95	3/1447 (0.2%)
All	All	1.09	31/26232 (0.1%)	0.99	70/35719 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.



Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	G	0	1
1	I	0	2
1	J	0	1
1	K	0	1
1	L	0	2
1	M	0	1
1	Q	0	1
1	U	0	2
1	X	0	1
All	All	0	13

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	126	VAL	CB-CG1	-9.90	1.32	1.52
1	U	90	CYS	CB-SG	-7.45	1.69	1.82
1	V	84	VAL	CB-CG2	7.14	1.67	1.52
1	T	84	VAL	CB-CG2	7.04	1.67	1.52
1	F	126	VAL	CB-CG1	-5.88	1.40	1.52
1	O	116	TYR	CE2-CZ	5.86	1.46	1.38
1	W	126	VAL	CB-CG1	-5.85	1.40	1.52
1	L	126	VAL	CB-CG1	-5.67	1.41	1.52
1	T	70	GLU	CD-OE1	5.65	1.31	1.25
1	J	124	VAL	CB-CG2	5.62	1.64	1.52
1	L	124	VAL	CB-CG1	5.61	1.64	1.52
1	L	85	ALA	CA-CB	5.55	1.64	1.52
1	K	90	CYS	CB-SG	-5.45	1.73	1.81
1	J	91	ALA	CA-CB	5.37	1.63	1.52
1	Q	111	PHE	CE1-CZ	5.35	1.47	1.37
1	C	85	ALA	CA-CB	5.34	1.63	1.52
1	S	72	VAL	CB-CG1	5.34	1.64	1.52
1	J	136	ALA	CA-CB	5.26	1.63	1.52
1	D	23	VAL	CA-CB	5.25	1.65	1.54
1	J	56	ALA	CA-CB	5.25	1.63	1.52
1	Q	99	GLU	CG-CD	5.22	1.59	1.51
1	N	90	CYS	CB-SG	-5.17	1.73	1.81
1	P	90	CYS	CB-SG	-5.16	1.73	1.81
1	T	31	GLU	CG-CD	5.15	1.59	1.51
1	F	48	VAL	CB-CG2	5.14	1.63	1.52
1	T	23	VAL	CB-CG2	5.12	1.63	1.52
1	L	76	ALA	CA-CB	5.11	1.63	1.52
1	M	99	GLU	CB-CG	5.11	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	92	GLU	CG-CD	5.03	1.59	1.51
1	L	70	GLU	CB-CG	5.01	1.61	1.52
1	J	133	TYR	CD1-CE1	5.00	1.46	1.39

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ASP	CB-CG-OD1	8.19	125.67	118.30
1	I	20	GLU	C-N-CD	-8.01	102.98	120.60
1	S	87	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	M	53	ASP	CB-CG-OD1	7.54	125.09	118.30
1	G	23	VAL	C-N-CA	7.50	140.45	121.70
1	K	3	LEU	CA-CB-CG	-7.41	98.25	115.30
1	C	112	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	S	3	LEU	CA-CB-CG	7.22	131.91	115.30
1	M	3	LEU	CA-CB-CG	7.19	131.84	115.30
1	A	67	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	M	108	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	K	87	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	Q	126	VAL	CG1-CB-CG2	6.77	121.73	110.90
1	E	87	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	T	112	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	C	87	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	J	20	GLU	C-N-CD	-6.44	106.43	120.60
1	M	50	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	S	137	LEU	CB-CG-CD1	-6.37	100.18	111.00
1	E	108	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	R	87	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	S	15	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	F	126	VAL	CG1-CB-CG2	6.23	120.86	110.90
1	V	79	LEU	CB-CG-CD1	-6.22	100.43	111.00
1	I	20	GLU	C-N-CA	6.13	147.75	122.00
1	S	45	LEU	CA-CB-CG	6.12	129.38	115.30
1	C	87	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	H	3	LEU	CB-CG-CD1	6.08	121.34	111.00
1	U	20	GLU	N-CA-C	6.08	127.42	111.00
1	O	3	LEU	CA-CB-CG	6.03	129.16	115.30
1	W	18	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	P	3	LEU	CA-CB-CG	6.00	129.09	115.30
1	K	87	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	R	87	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	F	3	LEU	CA-CB-CG	5.89	128.85	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	130	ILE	CG1-CB-CG2	5.84	124.25	111.40
1	I	53	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	V	87	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	P	19	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	W	18	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	J	22	ALA	N-CA-C	5.67	126.31	111.00
1	T	16	LEU	CB-CG-CD2	5.67	120.63	111.00
1	N	112	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	W	130	ILE	CG1-CB-CG2	5.63	123.78	111.40
1	O	108	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	L	126	VAL	CA-CB-CG2	5.57	119.25	110.90
1	O	126	VAL	CG1-CB-CG2	5.53	119.75	110.90
1	I	53	ASP	CB-CG-OD1	5.51	123.26	118.30
1	R	3	LEU	CA-CB-CG	5.43	127.80	115.30
1	J	3	LEU	CA-CB-CG	5.42	127.77	115.30
1	X	126	VAL	CG1-CB-CG2	5.41	119.56	110.90
1	C	112	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	G	24	TYR	N-CA-CB	5.39	120.31	110.60
1	T	3	LEU	CA-CB-CG	5.39	127.70	115.30
1	C	18	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	T	16	LEU	CA-CB-CG	5.36	127.63	115.30
1	K	16	LEU	CA-CB-CG	5.34	127.58	115.30
1	H	60	ASP	CB-CG-OD1	5.33	123.09	118.30
1	I	22	ALA	N-CA-C	5.32	125.36	111.00
1	B	112	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	X	35	LEU	CA-CB-CG	5.30	127.49	115.30
1	S	126	VAL	CA-CB-CG1	5.30	118.85	110.90
1	L	21	PRO	N-CA-C	5.18	125.56	112.10
1	F	15	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	J	21	PRO	N-CA-C	5.15	125.48	112.10
1	J	126	VAL	CG1-CB-CG2	5.12	119.09	110.90
1	E	117	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	C	53	ASP	CB-CG-OD1	5.05	122.85	118.30
1	V	87	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	E	87	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	19	ARG	Peptide
1	G	23	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	I	20	GLU	Peptide
1	I	22	ALA	Peptide
1	J	22	ALA	Peptide
1	K	142	GLU	Peptide
1	L	142	GLU	Peptide
1	L	21	PRO	Peptide
1	M	142	GLU	Peptide
1	Q	142	GLU	Peptide
1	U	19	ARG	Peptide
1	U	20	GLU	Peptide
1	X	142	GLU	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1067	0	1075	11	0
1	B	1077	0	1082	11	0
1	C	1055	0	1062	13	0
1	D	1077	0	1082	10	0
1	E	1077	0	1082	14	0
1	F	1042	0	1047	10	0
1	G	1077	0	1082	8	0
1	H	1071	0	1079	15	0
1	I	1073	0	1078	34	0
1	J	1073	0	1078	20	0
1	K	1077	0	1082	7	0
1	L	1083	0	1091	16	1
1	M	1077	0	1082	9	0
1	N	1077	0	1082	19	0
1	O	1077	0	1082	18	0
1	P	1071	0	1079	11	0
1	Q	1065	0	1068	4	0
1	R	1067	0	1067	11	0
1	S	1077	0	1082	18	0
1	T	1077	0	1082	13	0
1	U	1073	0	1078	6	0
1	V	1077	0	1082	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1077	0	1082	19	0
1	X	1043	0	1043	8	0
2	A	12	0	10	0	0
2	B	12	0	10	1	0
2	C	12	0	10	0	0
2	D	12	0	10	0	0
2	E	12	0	10	0	0
2	F	12	0	10	0	0
2	G	12	0	10	0	0
2	H	12	0	10	0	0
2	I	12	0	10	0	0
2	J	12	0	9	0	0
2	K	12	0	10	0	0
2	L	12	0	10	0	0
2	M	12	0	10	0	0
2	N	12	0	10	2	0
2	O	12	0	10	0	0
2	P	12	0	10	0	0
2	Q	12	0	10	0	0
2	R	12	0	8	0	0
2	S	12	0	10	0	0
2	T	12	0	10	0	0
2	U	12	0	10	0	0
2	V	12	0	10	0	0
2	W	12	0	10	0	0
2	X	12	0	10	0	0
3	B	6	0	8	0	0
3	E	6	0	8	1	0
3	G	6	0	8	1	0
3	H	6	0	8	0	0
3	I	6	0	8	0	0
3	L	6	0	8	0	0
3	O	6	0	8	2	0
3	P	6	0	8	0	0
3	Q	6	0	8	0	0
3	T	6	0	8	0	0
3	U	6	0	8	0	0
3	V	6	0	8	0	0
3	X	6	0	8	0	0
4	A	82	0	0	3	0
4	B	95	0	0	5	0
4	C	96	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	84	0	0	2	0
4	E	84	0	0	2	0
4	F	85	0	0	4	0
4	G	101	0	0	2	0
4	H	106	0	0	2	0
4	I	99	0	0	1	0
4	J	125	0	0	3	0
4	K	92	0	0	3	0
4	L	127	0	0	7	0
4	M	112	0	0	1	0
4	N	85	0	0	4	0
4	O	85	0	0	3	0
4	P	102	0	0	1	0
4	Q	108	0	0	0	0
4	R	83	0	0	3	0
4	S	103	0	0	3	0
4	T	112	0	0	5	0
4	U	94	0	0	4	0
4	V	81	0	0	3	0
4	W	109	0	0	5	1
4	X	97	0	0	2	0
All	All	28420	0	26170	309	1

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 6.

All (309) 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:W:23:VAL:HG21	1:W:103:SER:CB	1.80	1.12
1:J:21:PRO:HB3	1:J:23:VAL:H	0.96	1.10
1:J:21:PRO:HB3	1:J:23:VAL:N	1.65	1.10
1:O:50:ARG:HG3	1:O:50:ARG:HH11	0.98	1.09
1:L:3:LEU:HD12	4:L:1155:HOH:O	1.57	1.05
1:W:23:VAL:HG21	1:W:103:SER:HB2	1.35	1.03
1:J:20:GLU:CB	1:J:21:PRO:HD2	1.86	1.03
1:I:21:PRO:HB3	1:I:23:VAL:N	1.75	1.01
1:O:50:ARG:NH1	1:O:50:ARG:HG3	1.75	0.97
1:V:3:LEU:HA	4:V:1643:HOH:O	1.65	0.95
1:U:110:GLU:HG2	4:U:1509:HOH:O	1.67	0.94
1:J:21:PRO:CB	1:J:23:VAL:H	1.81	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:3:LEU:HA	4:R:1482:HOH:O	1.69	0.92
1:V:18:ARG:HG3	1:V:18:ARG:HH11	1.33	0.91
1:M:3:LEU:HA	4:M:1213:HOH:O	1.72	0.88
1:T:38:ARG:HG3	4:T:1568:HOH:O	1.75	0.86
1:I:21:PRO:CB	1:I:22:ALA:HA	2.06	0.85
1:W:23:VAL:CG2	1:W:103:SER:CB	2.55	0.85
1:N:24:TYR:HA	1:N:102:ILE:HG21	1.57	0.84
1:E:34:ALA:HB1	1:E:38:ARG:NH2	1.93	0.84
1:E:114[A]:HIS:CD2	4:K:937:HOH:O	2.32	0.82
1:I:92:GLU:OE1	1:J:19:ARG:HB2	1.80	0.81
1:O:3:LEU:HD12	4:O:597:HOH:O	1.78	0.81
1:I:21:PRO:CB	1:I:24:TYR:H	1.94	0.80
1:I:21:PRO:HB3	1:I:22:ALA:HA	1.64	0.79
1:C:18:ARG:HG3	1:C:18:ARG:HH11	1.45	0.79
1:K:57:GLN:HG2	4:K:757:HOH:O	1.80	0.79
1:D:18:ARG:CG	1:D:18:ARG:HH11	1.95	0.79
1:V:101:HIS:HB2	1:V:126:VAL:HG22	1.66	0.78
1:O:20:GLU:HG3	1:O:23:VAL:HG13	1.66	0.78
1:N:20:GLU:O	1:N:23:VAL:O	2.03	0.76
1:R:101:HIS:HB2	1:R:126:VAL:HG22	1.67	0.75
1:J:21:PRO:HG3	1:J:23:VAL:HB	1.70	0.74
1:I:21:PRO:CG	1:I:24:TYR:H	2.01	0.73
1:W:23:VAL:CG2	1:W:103:SER:HB2	2.14	0.71
1:C:18:ARG:O	1:C:19:ARG:HB2	1.90	0.71
1:I:21:PRO:HB3	1:I:23:VAL:H	1.54	0.71
1:Q:32:LEU:HD13	1:Q:130:ILE:HG13	1.73	0.71
1:W:23:VAL:CG2	1:W:103:SER:HB3	2.20	0.71
1:H:32:LEU:HD13	1:H:130:ILE:HG12	1.71	0.71
1:I:21:PRO:HB3	1:I:24:TYR:H	1.55	0.70
1:V:18:ARG:CG	1:V:18:ARG:HH11	2.03	0.70
1:L:20:GLU:C	1:L:22:ALA:HB3	2.11	0.70
1:D:18:ARG:HG3	1:D:18:ARG:HH11	1.56	0.69
1:L:21:PRO:N	1:L:22:ALA:HB3	2.07	0.69
1:R:36:ILE:HG23	1:R:137:LEU:HD11	1.74	0.69
1:H:32:LEU:HD13	1:H:130:ILE:CG1	2.23	0.69
1:E:101:HIS:HB2	1:E:126:VAL:HG22	1.76	0.68
1:S:63:HIS:HD2	4:S:374:HOH:O	1.76	0.68
1:X:32:LEU:HD13	1:X:130:ILE:HG12	1.76	0.67
1:T:16:LEU:HD11	1:T:130:ILE:HD11	1.77	0.67
1:K:50:ARG:HB3	1:K:61:TRP:CZ3	2.29	0.66
1:P:29:HIS:O	1:P:33:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:LEU:HD12	1:I:53:ASP:HB3	1.77	0.66
1:T:50:ARG:NH1	4:T:1550:HOH:O	2.29	0.65
1:N:24:TYR:HA	1:N:102:ILE:CG2	2.27	0.64
1:U:19:ARG:O	1:U:21:PRO:HD3	1.98	0.64
1:H:50:ARG:HD2	4:H:1001:HOH:O	1.97	0.64
1:C:18:ARG:HH11	1:C:18:ARG:CG	2.10	0.64
1:T:32:LEU:HD13	1:T:130:ILE:HG12	1.80	0.64
1:N:92:GLU:HB3	1:O:19:ARG:HD2	1.80	0.64
1:D:18:ARG:HG3	1:D:18:ARG:NH1	2.12	0.63
1:J:32:LEU:HD13	1:J:130:ILE:HG12	1.81	0.63
1:W:24:TYR:HA	1:W:102:ILE:HG21	1.79	0.63
1:S:142:GLU:O	1:S:143:HIS:ND1	2.31	0.62
1:C:36:ILE:HG23	1:C:137:LEU:HD11	1.81	0.62
1:N:113:ARG:NH2	4:N:2293:HOH:O	2.26	0.62
1:H:101:HIS:HB2	1:H:126:VAL:HG22	1.81	0.61
1:A:32:LEU:HD13	1:A:130:ILE:HD12	1.83	0.60
1:L:21:PRO:O	1:L:25:GLY:HA2	2.00	0.60
1:O:19:ARG:HB2	1:O:19:ARG:HH11	1.65	0.60
1:G:3:LEU:N	4:G:852:HOH:O	2.34	0.60
1:J:21:PRO:HB3	1:J:24:TYR:H	1.66	0.60
1:B:50:ARG:HD2	4:B:783:HOH:O	2.02	0.59
1:O:3:LEU:N	4:O:1340:HOH:O	2.35	0.59
1:B:101:HIS:HB2	1:B:126:VAL:HG22	1.84	0.59
1:I:21:PRO:CB	1:I:23:VAL:H	2.15	0.59
1:X:139:TYR:O	1:X:143:HIS:N	2.35	0.59
1:I:3:LEU:HG	1:I:4:ILE:N	2.16	0.59
1:R:63:HIS:HD2	4:R:1492:HOH:O	1.85	0.59
1:I:21:PRO:CB	1:I:23:VAL:N	2.60	0.59
1:B:32:LEU:HD13	1:B:130:ILE:HG13	1.83	0.59
1:S:49:VAL:C	1:S:50:ARG:HD3	2.22	0.59
1:V:113:ARG:HD2	4:V:1674:HOH:O	2.03	0.59
1:K:101:HIS:HB2	1:K:126:VAL:HG22	1.85	0.58
1:I:21:PRO:HG3	1:I:24:TYR:H	1.68	0.58
1:I:66:ALA:HB1	1:J:19:ARG:HD3	1.85	0.58
1:L:38[A]:ARG:CD	4:L:1201:HOH:O	2.52	0.58
1:N:105:VAL:HG12	2:N:147:FA1:H5	1.85	0.58
1:I:21:PRO:HB3	1:I:24:TYR:N	2.18	0.58
1:G:32:LEU:HD13	1:G:130:ILE:HG12	1.86	0.58
1:J:20:GLU:CB	1:J:21:PRO:CD	2.75	0.58
1:M:143:HIS:ND1	1:M:143:HIS:N	2.51	0.58
1:K:48:VAL:HG12	1:K:50:ARG:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:LEU:N	4:H:1000:HOH:O	2.36	0.57
1:W:21:PRO:HB3	1:W:25:GLY:H	1.69	0.57
1:J:32:LEU:HD13	1:J:130:ILE:CG1	2.35	0.57
1:F:46:LYS:HD3	4:F:945:HOH:O	2.04	0.56
1:V:18:ARG:NH1	1:V:18:ARG:HG3	2.08	0.56
1:T:32:LEU:HD13	1:T:130:ILE:CG1	2.36	0.56
1:E:18:ARG:O	1:E:19:ARG:HB2	2.06	0.56
1:X:48:VAL:HG12	1:X:50:ARG:HD2	1.87	0.56
1:F:48:VAL:HG12	1:F:50:ARG:HD2	1.88	0.56
1:I:18:ARG:O	1:I:20:GLU:CB	2.54	0.55
1:A:41:ALA:HA	4:A:1780:HOH:O	2.06	0.55
1:L:113:ARG:NH2	4:L:1126:HOH:O	2.39	0.55
1:O:21:PRO:O	1:O:23:VAL:N	2.36	0.55
4:U:537:HOH:O	1:V:15:ARG:HB2	2.05	0.55
1:J:21:PRO:HB3	1:J:22:ALA:HA	1.89	0.55
1:L:21:PRO:O	1:L:25:GLY:CA	2.55	0.55
1:S:50:ARG:NH2	4:S:1530:HOH:O	2.39	0.55
1:P:48:VAL:HG12	1:P:50:ARG:HD2	1.88	0.55
1:S:3:LEU:HG	1:S:45:LEU:HD23	1.89	0.54
1:I:32:LEU:HD13	1:I:130:ILE:HG12	1.89	0.54
1:N:50:ARG:HD3	1:N:61:TRP:CE2	2.41	0.54
1:I:3:LEU:HG	1:I:4:ILE:H	1.72	0.54
1:D:27:THR:HB	4:D:860:HOH:O	2.06	0.54
1:P:35:LEU:HD23	1:P:38:ARG:HH21	1.71	0.54
1:W:23:VAL:HG23	1:W:103:SER:HB3	1.89	0.53
1:V:18:ARG:HD2	1:V:19:ARG:HH12	1.73	0.53
1:K:143:HIS:CE1	4:K:1179:HOH:O	2.61	0.53
1:V:113:ARG:NH2	4:V:1754:HOH:O	2.42	0.53
1:I:18:ARG:O	1:I:19:ARG:C	2.46	0.53
1:M:5:VAL:HG22	1:M:71:PRO:HG2	1.91	0.53
1:F:25:GLY:N	4:F:946:HOH:O	2.41	0.53
1:V:48:VAL:HG12	1:V:50:ARG:HD2	1.90	0.53
1:G:33:VAL:HG22	1:G:49:VAL:HG22	1.91	0.52
1:W:23:VAL:HG21	1:W:103:SER:CA	2.39	0.52
1:Q:19:ARG:O	1:Q:20:GLU:HB2	2.09	0.52
1:M:48:VAL:HG12	1:M:50:ARG:HD2	1.91	0.52
1:W:19:ARG:HG2	4:W:1262:HOH:O	2.09	0.52
1:I:21:PRO:HB3	1:I:22:ALA:CA	2.37	0.52
1:L:50:ARG:HD3	1:L:61:TRP:CE2	2.43	0.52
1:L:38[A]:ARG:NE	4:L:1201:HOH:O	2.42	0.52
1:S:142:GLU:C	1:S:143:HIS:ND1	2.64	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:HIS:HE1	1:G:12:ASN:OD1	1.93	0.52
1:R:63:HIS:HE1	1:S:12:ASN:OD1	1.93	0.52
1:E:38:ARG:O	1:E:42:GLU:HG2	2.09	0.52
1:F:63:HIS:HD2	4:F:949:HOH:O	1.92	0.51
1:G:22:ALA:HB3	4:G:2009:HOH:O	2.10	0.51
1:B:97:LEU:HD23	1:B:121:ALA:HA	1.93	0.51
1:L:142:GLU:HG3	4:L:2030:HOH:O	2.10	0.51
1:I:50:ARG:HD2	4:I:1064:HOH:O	2.10	0.51
1:D:113:ARG:HD2	4:D:893:HOH:O	2.09	0.51
1:J:21:PRO:CB	1:J:24:TYR:H	2.24	0.51
1:I:21:PRO:HB2	1:I:22:ALA:HA	1.92	0.51
1:J:3:LEU:HA	4:J:1089:HOH:O	2.10	0.50
1:X:7:VAL:HG11	1:X:36:ILE:HD13	1.92	0.50
1:N:57:GLN:HG2	4:N:1299:HOH:O	2.11	0.50
1:O:101:HIS:HB2	1:O:126:VAL:HG22	1.93	0.50
1:I:36:ILE:HG23	1:I:137:LEU:HD11	1.94	0.50
1:W:3:LEU:N	4:W:2119:HOH:O	2.44	0.50
1:H:60:ASP:OD2	1:H:64:GLN:NE2	2.44	0.49
1:P:19:ARG:HG3	1:P:19:ARG:NH1	2.27	0.49
1:O:50:ARG:NH2	4:O:1351:HOH:O	2.45	0.49
1:S:50:ARG:HB3	1:S:61:TRP:CZ3	2.47	0.49
1:O:19:ARG:HB2	1:O:19:ARG:NH1	2.26	0.49
1:P:3:LEU:HA	4:P:1381:HOH:O	2.12	0.49
1:P:36:ILE:HG23	1:P:137:LEU:HD11	1.94	0.49
1:G:32:LEU:HD13	1:G:130:ILE:CG1	2.41	0.49
1:P:19:ARG:HG3	1:P:19:ARG:HH11	1.78	0.49
1:T:16:LEU:O	1:T:28:THR:HA	2.12	0.49
1:Q:43:LEU:HD21	1:Q:138:ARG:CZ	2.43	0.48
1:I:21:PRO:HG3	1:I:24:TYR:CD1	2.48	0.48
1:B:18:ARG:HD2	4:B:786:HOH:O	2.12	0.48
1:W:21:PRO:HB2	1:W:22:ALA:HA	1.95	0.48
1:C:102:ILE:HG23	1:C:129:GLY:HA2	1.94	0.48
1:X:45:LEU:HD11	1:X:141:ALA:HB2	1.95	0.48
1:M:62:ILE:CD1	1:M:86:LEU:HD11	2.44	0.48
1:E:102:ILE:HG23	1:E:129:GLY:HA2	1.95	0.48
1:H:19:ARG:NH2	1:J:67:ASP:OD1	2.47	0.48
1:J:38:ARG:NH1	4:J:148:HOH:O	2.47	0.48
1:D:50:ARG:HB3	1:D:61:TRP:CZ3	2.49	0.48
1:U:18:ARG:HG3	4:U:1606:HOH:O	2.13	0.47
1:O:5:VAL:HG21	1:O:45:LEU:HD13	1.96	0.47
1:V:31:GLU:O	1:V:35:LEU:HD12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:113:ARG:NH2	4:T:1974:HOH:O	2.46	0.47
1:S:7:VAL:HB	1:S:49:VAL:HB	1.96	0.47
1:J:21:PRO:CB	1:J:22:ALA:HA	2.44	0.47
1:O:24:TYR:CD1	3:O:147:GOL:H12	2.48	0.47
1:A:101:HIS:HB2	1:A:126:VAL:HG22	1.96	0.47
1:P:73:ILE:HD13	1:P:136:ALA:HB3	1.96	0.47
1:T:97:LEU:HD23	1:T:121:ALA:HA	1.97	0.47
1:W:9:ASN:O	1:W:51:GLN:HA	2.14	0.47
1:H:94:SER:HB3	1:I:19:ARG:HH22	1.79	0.47
1:N:23:VAL:HG12	1:N:103:SER:HB3	1.97	0.47
1:H:32:LEU:HD13	1:H:130:ILE:HG13	1.96	0.47
1:K:58:LEU:O	1:K:62:ILE:HG12	2.14	0.47
1:U:3:LEU:HA	4:U:2201:HOH:O	2.14	0.47
1:D:18:ARG:NH1	1:D:18:ARG:CG	2.62	0.46
1:T:57:GLN:NE2	1:T:61:TRP:NE1	2.63	0.46
1:E:57:GLN:HG2	4:E:911:HOH:O	2.15	0.46
1:C:18:ARG:O	1:C:19:ARG:CB	2.60	0.46
1:H:94:SER:CB	1:I:19:ARG:HH22	2.29	0.46
1:E:27:THR:HG22	1:E:31:GLU:HB2	1.96	0.46
1:M:62:ILE:CD1	1:M:86:LEU:CD1	2.94	0.46
1:W:19:ARG:NH1	4:W:1248:HOH:O	2.43	0.46
1:Q:143:HIS:N	1:Q:143:HIS:ND1	2.64	0.46
1:A:18:ARG:O	1:A:19:ARG:O	2.33	0.46
1:E:28:THR:OG1	1:E:31:GLU:HG3	2.16	0.46
1:O:36:ILE:HG23	1:O:137:LEU:HD11	1.98	0.46
1:E:63:HIS:HD2	4:E:162:HOH:O	1.99	0.45
1:W:23:VAL:CG1	4:W:2006:HOH:O	2.65	0.45
1:D:18:ARG:HH11	1:D:18:ARG:HG2	1.77	0.45
1:I:20:GLU:HA	1:I:21:PRO:HD2	1.55	0.45
1:A:36:ILE:HG23	1:A:137:LEU:HD11	1.97	0.45
1:R:118:SER:HB2	1:R:119:PRO:HD3	1.99	0.45
1:T:3:LEU:HD12	4:T:1545:HOH:O	2.16	0.45
1:I:21:PRO:CB	1:I:22:ALA:CA	2.84	0.45
1:C:18:ARG:HG3	1:C:18:ARG:NH1	2.23	0.45
1:N:21:PRO:O	1:N:22:ALA:CB	2.65	0.45
1:S:20:GLU:N	1:S:21:PRO:HD3	2.31	0.45
1:N:50:ARG:HG2	4:N:1286:HOH:O	2.17	0.45
1:V:28:THR:OG1	1:V:31:GLU:HG3	2.17	0.45
1:L:15:ARG:HD2	4:L:168:HOH:O	2.16	0.45
1:A:11:PRO:HA	1:A:53:ASP:OD1	2.17	0.45
1:I:21:PRO:HB3	1:I:22:ALA:C	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:104:ASN:HA	1:R:126:VAL:HG13	1.99	0.45
1:S:50:ARG:HB3	1:S:61:TRP:CH2	2.52	0.45
1:U:29:HIS:O	1:U:33:VAL:HG23	2.17	0.45
1:J:15:ARG:NH2	1:J:19:ARG:HG3	2.32	0.44
1:L:36:ILE:HG23	1:L:137:LEU:HD11	1.98	0.44
1:U:50:ARG:HB3	1:U:61:TRP:CZ3	2.53	0.44
1:D:22:ALA:HA	1:D:23:VAL:HA	1.73	0.44
1:S:18:ARG:O	1:S:19:ARG:HB3	2.16	0.44
1:I:21:PRO:CG	1:I:24:TYR:HD1	2.31	0.44
1:S:3:LEU:N	4:S:2026:HOH:O	2.49	0.44
1:C:4:ILE:HA	1:C:46:LYS:O	2.17	0.44
1:O:50:ARG:CG	1:O:50:ARG:NH1	2.60	0.44
1:A:106:HIS:HA	1:A:113:ARG:HG2	1.98	0.44
1:V:98:ILE:N	1:V:98:ILE:HD12	2.32	0.44
1:G:7:VAL:HB	1:G:49:VAL:HB	2.00	0.44
1:A:48:VAL:HG21	4:A:1777:HOH:O	2.18	0.44
1:F:29:HIS:O	1:F:33:VAL:HG23	2.17	0.44
1:W:35:LEU:HD21	4:W:1698:HOH:O	2.17	0.44
1:E:18:ARG:O	1:E:19:ARG:CB	2.65	0.43
1:T:11:PRO:HD3	1:T:58:LEU:HD11	1.99	0.43
1:R:39:GLU:CB	1:R:134:LEU:HD22	2.48	0.43
1:L:143:HIS:ND1	1:L:143:HIS:N	2.66	0.43
1:B:110:GLU:HG2	4:B:809:HOH:O	2.18	0.43
1:N:90:CYS:HB3	1:N:97:LEU:HD22	1.99	0.43
1:S:33:VAL:HG22	1:S:49:VAL:HG22	2.01	0.43
1:N:105:VAL:CG1	2:N:147:FA1:H5	2.46	0.43
1:O:24:TYR:CE1	3:O:147:GOL:H12	2.53	0.43
1:M:124:VAL:HG12	1:M:126:VAL:HG23	1.99	0.43
1:B:3:LEU:N	4:B:1829:HOH:O	2.52	0.43
1:N:124:VAL:HG12	1:N:126:VAL:HG23	2.01	0.43
1:H:5:VAL:HG21	1:H:45:LEU:HD13	2.00	0.43
1:T:118:SER:N	1:T:119:PRO:CD	2.82	0.43
1:J:50:ARG:HD3	1:J:61:TRP:CE2	2.53	0.43
1:S:98:ILE:HD11	1:S:139:TYR:CD2	2.54	0.43
1:N:130:ILE:HD13	4:N:1294:HOH:O	2.17	0.43
1:A:143:HIS:HB3	4:A:779:HOH:O	2.19	0.43
1:N:102:ILE:HG23	1:N:129:GLY:HA2	2.01	0.43
1:L:106:HIS:HA	1:L:113:ARG:HG2	2.01	0.42
1:D:48:VAL:HG12	1:D:50:ARG:HD2	2.01	0.42
1:S:50:ARG:N	1:S:50:ARG:HD3	2.34	0.42
1:W:21:PRO:HB3	1:W:25:GLY:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:31:GLU:O	1:L:35:LEU:HG	2.19	0.42
1:F:3:LEU:HD23	4:F:964:HOH:O	2.19	0.42
1:C:28:THR:HB	4:C:822:HOH:O	2.19	0.42
1:F:32:LEU:HD13	1:F:130:ILE:HG12	2.01	0.42
1:T:18:ARG:HD3	4:T:1556:HOH:O	2.19	0.42
1:S:62:ILE:CD1	1:S:86:LEU:HD11	2.50	0.42
1:L:90:CYS:HB3	1:L:97:LEU:HD22	2.00	0.42
1:C:13:LEU:HD23	1:C:13:LEU:HA	1.78	0.42
1:V:4:ILE:HG12	1:V:46:LYS:HD3	2.01	0.42
1:I:3:LEU:CG	1:I:4:ILE:N	2.81	0.42
1:A:41:ALA:O	1:A:43:LEU:N	2.52	0.42
1:A:82:THR:HG22	4:L:1163:HOH:O	2.20	0.42
1:N:70:GLU:HA	1:N:71:PRO:HD3	1.86	0.42
1:M:63:HIS:CG	1:W:15:ARG:HD3	2.55	0.42
1:P:102:ILE:HG23	1:P:129:GLY:HA2	2.02	0.41
1:B:114[A]:HIS:CD2	4:B:677:HOH:O	2.72	0.41
1:B:103:SER:H	2:B:148:FA1:H1	1.67	0.41
1:E:5:VAL:HG21	1:E:45:LEU:HD13	2.02	0.41
1:W:23:VAL:O	1:W:24:TYR:CB	2.68	0.41
1:I:90:CYS:HB3	1:I:97:LEU:HD22	2.02	0.41
1:X:3:LEU:N	4:X:1732:HOH:O	2.53	0.41
1:O:102:ILE:HG23	1:O:129:GLY:HA2	2.02	0.41
1:H:73:ILE:HD13	1:H:136:ALA:HB3	2.02	0.41
1:B:32:LEU:HD13	1:B:130:ILE:CG1	2.48	0.41
1:F:13:LEU:HD23	1:F:13:LEU:HA	1.89	0.41
1:X:143:HIS:HE1	4:X:2041:HOH:O	2.04	0.41
1:M:62:ILE:HD11	1:M:86:LEU:HD11	2.02	0.41
1:S:50:ARG:NH2	1:S:50:ARG:HG2	2.35	0.41
1:I:21:PRO:CA	1:I:23:VAL:H	2.33	0.41
1:E:24:TYR:CE1	3:E:147:GOL:H12	2.56	0.41
1:G:24:TYR:CE2	3:G:147:GOL:H12	2.56	0.41
1:H:98:ILE:HD11	1:H:139:TYR:CD2	2.55	0.41
1:O:90:CYS:HB3	1:O:97:LEU:HD22	2.02	0.41
1:R:102:ILE:HD13	1:R:130:ILE:CD1	2.51	0.41
1:R:102:ILE:HD13	1:R:130:ILE:HD12	2.02	0.41
1:C:35:LEU:HA	1:C:35:LEU:HD23	1.88	0.41
1:B:102:ILE:HG23	1:B:129:GLY:HA2	2.02	0.41
1:E:55:GLU:O	1:E:59:LEU:HG	2.21	0.41
1:K:70:GLU:HA	1:K:71:PRO:HD3	1.93	0.41
1:R:26:GLY:HA3	4:R:636:HOH:O	2.20	0.41
1:F:9:ASN:OD1	1:F:75:ASN:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:32:LEU:HD13	1:P:130:ILE:CG1	2.52	0.40
1:J:3:LEU:CA	4:J:1089:HOH:O	2.69	0.40
1:N:27:THR:HG22	1:N:28:THR:O	2.21	0.40
1:H:11:PRO:HA	1:H:53:ASP:HA	2.03	0.40
1:I:32:LEU:HD13	1:I:130:ILE:CG1	2.50	0.40
1:C:3:LEU:HG	1:C:4:ILE:N	2.36	0.40
1:N:36:ILE:HG23	1:N:137:LEU:HD11	2.04	0.40
1:X:36:ILE:HG23	1:X:137:LEU:HD11	2.04	0.40
1:C:50:ARG:NH2	4:C:2295:HOH:O	2.54	0.40
1:P:80:THR:HG21	1:P:101:HIS:CE1	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:46:LYS:NZ	4:W:1243:HOH:O[1_655]	2.15	0.05

## 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	139/147 (95%)	131 (94%)	6 (4%)	2 (1%)	14	6
1	B	140/147 (95%)	138 (99%)	2 (1%)	0	100	100
1	C	135/147 (92%)	128 (95%)	6 (4%)	1 (1%)	26	19
1	D	140/147 (95%)	136 (97%)	4 (3%)	0	100	100
1	E	140/147 (95%)	132 (94%)	7 (5%)	1 (1%)	26	19
1	F	134/147 (91%)	131 (98%)	2 (2%)	1 (1%)	26	19
1	G	140/147 (95%)	135 (96%)	4 (3%)	1 (1%)	26	19
1	H	139/147 (95%)	137 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	140/147 (95%)	132 (94%)	5 (4%)	3 (2%)	9	3
1	J	140/147 (95%)	134 (96%)	4 (3%)	2 (1%)	14	6
1	K	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	L	141/147 (96%)	137 (97%)	3 (2%)	1 (1%)	26	19
1	M	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	N	140/147 (95%)	134 (96%)	5 (4%)	1 (1%)	26	19
1	O	140/147 (95%)	135 (96%)	3 (2%)	2 (1%)	14	6
1	P	139/147 (95%)	135 (97%)	4 (3%)	0	100	100
1	Q	139/147 (95%)	135 (97%)	3 (2%)	1 (1%)	26	19
1	R	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	S	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	T	140/147 (95%)	138 (99%)	2 (1%)	0	100	100
1	U	140/147 (95%)	134 (96%)	5 (4%)	1 (1%)	26	19
1	V	140/147 (95%)	135 (96%)	5 (4%)	0	100	100
1	W	140/147 (95%)	133 (95%)	5 (4%)	2 (1%)	14	6
1	X	134/147 (91%)	132 (98%)	2 (2%)	0	100	100
All	All	3340/3528 (95%)	3230 (97%)	91 (3%)	19 (1%)	30	22

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	C	19	ARG
1	E	19	ARG
1	I	21	PRO
1	J	21	PRO
1	N	22	ALA
1	U	20	GLU
1	W	20	GLU
1	A	42	GLU
1	F	19	ARG
1	G	23	VAL
1	O	21	PRO
1	W	24	TYR
1	J	18	ARG
1	O	22	ALA

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Mol	Chain	Res	Type
1	I	19	ARG
1	I	20	GLU
1	L	22	ALA
1	Q	20	GLU

### 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	109/115 (95%)	104 (95%)	5 (5%)	33	28
1	B	111/115 (96%)	108 (97%)	3 (3%)	52	52
1	C	108/115 (94%)	103 (95%)	5 (5%)	33	28
1	D	111/115 (96%)	106 (96%)	5 (4%)	34	29
1	E	111/115 (96%)	106 (96%)	5 (4%)	34	29
1	F	107/115 (93%)	104 (97%)	3 (3%)	51	50
1	G	111/115 (96%)	102 (92%)	9 (8%)	15	9
1	H	110/115 (96%)	104 (94%)	6 (6%)	27	21
1	I	110/115 (96%)	104 (94%)	6 (6%)	27	21
1	J	110/115 (96%)	103 (94%)	7 (6%)	22	15
1	K	111/115 (96%)	103 (93%)	8 (7%)	18	12
1	L	112/115 (97%)	108 (96%)	4 (4%)	42	39
1	M	111/115 (96%)	106 (96%)	5 (4%)	34	29
1	N	111/115 (96%)	106 (96%)	5 (4%)	34	29
1	O	111/115 (96%)	100 (90%)	11 (10%)	10	5
1	P	110/115 (96%)	105 (96%)	5 (4%)	34	29
1	Q	109/115 (95%)	103 (94%)	6 (6%)	27	21
1	R	109/115 (95%)	104 (95%)	5 (5%)	33	28
1	S	111/115 (96%)	105 (95%)	6 (5%)	27	21
1	T	111/115 (96%)	109 (98%)	2 (2%)	66	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	110/115 (96%)	105 (96%)	5 (4%)	34	29
1	V	111/115 (96%)	108 (97%)	3 (3%)	52	52
1	W	111/115 (96%)	106 (96%)	5 (4%)	34	29
1	X	107/115 (93%)	103 (96%)	4 (4%)	41	38
All	All	2643/2760 (96%)	2515 (95%)	128 (5%)	31	26

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	45	LEU
1	A	50	ARG
1	A	96	PRO
1	A	126	VAL
1	B	16	LEU
1	B	46	LYS
1	B	126	VAL
1	C	3	LEU
1	C	15	ARG
1	C	18	ARG
1	C	130	ILE
1	C	142	GLU
1	D	18	ARG
1	D	19	ARG
1	D	126	VAL
1	D	130	ILE
1	D	142	GLU
1	E	16	LEU
1	E	18	ARG
1	E	35	LEU
1	E	130	ILE
1	E	142	GLU
1	F	19	ARG
1	F	126	VAL
1	F	130	ILE
1	G	15	ARG
1	G	18	ARG
1	G	20	GLU
1	G	49	VAL
1	G	110	GLU
1	G	126	VAL

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Mol	Chain	Res	Type
1	G	130	ILE
1	G	131	GLN
1	G	142	GLU
1	H	23	VAL
1	H	38	ARG
1	H	46	LYS
1	H	126	VAL
1	H	130	ILE
1	H	142	GLU
1	I	16	LEU
1	I	18	ARG
1	I	35	LEU
1	I	38	ARG
1	I	130	ILE
1	I	142	GLU
1	J	18	ARG
1	J	21	PRO
1	J	38	ARG
1	J	42	GLU
1	J	126	VAL
1	J	130	ILE
1	J	142	GLU
1	K	3	LEU
1	K	15	ARG
1	K	18	ARG
1	K	20	GLU
1	K	35	LEU
1	K	50	ARG
1	K	126	VAL
1	K	130	ILE
1	L	126	VAL
1	L	130	ILE
1	L	142	GLU
1	L	143	HIS
1	M	3	LEU
1	M	4	ILE
1	M	130	ILE
1	M	142	GLU
1	M	143	HIS
1	N	16	LEU
1	N	18	ARG
1	N	23	VAL

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Mol	Chain	Res	Type
1	N	130	ILE
1	N	142	GLU
1	O	16	LEU
1	O	18	ARG
1	O	19	ARG
1	O	20	GLU
1	O	23	VAL
1	O	46	LYS
1	O	50	ARG
1	O	110	GLU
1	O	126	VAL
1	O	130	ILE
1	O	142	GLU
1	P	19	ARG
1	P	110	GLU
1	P	126	VAL
1	P	130	ILE
1	P	142	GLU
1	Q	110	GLU
1	Q	126	VAL
1	Q	130	ILE
1	Q	131	GLN
1	Q	142	GLU
1	Q	143	HIS
1	R	3	LEU
1	R	15	ARG
1	R	57	GLN
1	R	130	ILE
1	R	131	GLN
1	S	49	VAL
1	S	50	ARG
1	S	126	VAL
1	S	130	ILE
1	S	142	GLU
1	S	143	HIS
1	T	16	LEU
1	T	130	ILE
1	U	15	ARG
1	U	18	ARG
1	U	45	LEU
1	U	51	GLN
1	U	130	ILE

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Mol	Chain	Res	Type
1	V	18	ARG
1	V	45	LEU
1	V	130	ILE
1	W	3	LEU
1	W	19	ARG
1	W	126	VAL
1	W	130	ILE
1	W	142	GLU
1	X	42	GLU
1	X	50	ARG
1	X	126	VAL
1	X	130	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	E	57	GLN
1	E	131	GLN
1	F	63	HIS
1	G	131	GLN
1	I	51	GLN
1	I	131	GLN
1	J	64	GLN
1	J	143	HIS
1	R	57	GLN
1	R	63	HIS
1	S	57	GLN
1	T	57	GLN
1	T	131	GLN
1	U	131	GLN
1	V	131	GLN
1	V	143	HIS

### 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 ⓘ

37 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	FA1	A	147	-	7,12,12	4.38	3 (42%)	7,18,18	1.58	2 (28%)
3	GOL	B	147	-	5,5,5	0.32	0	5,5,5	0.76	0
2	FA1	B	148	-	7,12,12	4.44	4 (57%)	7,18,18	1.78	2 (28%)
2	FA1	C	147	-	7,12,12	4.31	3 (42%)	7,18,18	1.49	2 (28%)
2	FA1	D	147	-	7,12,12	5.16	5 (71%)	7,18,18	1.54	2 (28%)
3	GOL	E	147	-	5,5,5	0.34	0	5,5,5	0.48	0
2	FA1	E	148	-	7,12,12	4.15	2 (28%)	7,18,18	1.99	2 (28%)
2	FA1	F	147	-	7,12,12	4.22	2 (28%)	7,18,18	1.73	2 (28%)
3	GOL	G	147	-	5,5,5	0.41	0	5,5,5	0.34	0
2	FA1	G	148	-	7,12,12	4.29	3 (42%)	7,18,18	1.91	1 (14%)
3	GOL	H	147	-	5,5,5	0.15	0	5,5,5	0.73	0
2	FA1	H	148	-	7,12,12	4.28	3 (42%)	7,18,18	1.52	2 (28%)
3	GOL	I	147	-	5,5,5	0.29	0	5,5,5	0.36	0
2	FA1	I	148	-	7,12,12	4.56	3 (42%)	7,18,18	2.12	2 (28%)
2	FA1	J	147	-	7,12,12	3.81	2 (28%)	7,18,18	2.13	3 (42%)
2	FA1	K	147	-	7,12,12	4.14	4 (57%)	7,18,18	2.21	2 (28%)
3	GOL	L	147	-	5,5,5	0.44	0	5,5,5	0.98	0
2	FA1	L	148	-	7,12,12	4.33	4 (57%)	7,18,18	2.21	2 (28%)
2	FA1	M	147	-	7,12,12	3.76	3 (42%)	7,18,18	1.82	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FA1	N	147	-	7,12,12	5.92	6 (85%)	7,18,18	3.36	5 (71%)
3	GOL	O	147	-	5,5,5	0.55	0	5,5,5	0.84	0
2	FA1	O	148	-	7,12,12	4.52	3 (42%)	7,18,18	1.47	1 (14%)
3	GOL	P	147	-	5,5,5	0.33	0	5,5,5	0.75	0
2	FA1	P	148	-	7,12,12	4.34	3 (42%)	7,18,18	2.05	4 (57%)
3	GOL	Q	147	-	5,5,5	0.33	0	5,5,5	0.55	0
2	FA1	Q	148	-	7,12,12	4.20	5 (71%)	7,18,18	1.28	2 (28%)
2	FA1	R	147	-	7,12,12	14.56	5 (71%)	7,18,18	6.33	5 (71%)
2	FA1	S	147	-	7,12,12	3.90	2 (28%)	7,18,18	1.38	1 (14%)
3	GOL	T	147	-	5,5,5	0.23	0	5,5,5	0.64	0
2	FA1	T	148	-	7,12,12	3.87	5 (71%)	7,18,18	1.37	1 (14%)
3	GOL	U	147	-	5,5,5	0.38	0	5,5,5	0.55	0
2	FA1	U	148	-	7,12,12	4.77	3 (42%)	7,18,18	0.97	0
3	GOL	V	147	-	5,5,5	0.39	0	5,5,5	0.23	0
2	FA1	V	148	-	7,12,12	4.78	2 (28%)	7,18,18	2.28	3 (42%)
2	FA1	W	147	-	7,12,12	4.57	6 (85%)	7,18,18	1.94	3 (42%)
3	GOL	X	147	-	5,5,5	0.38	0	5,5,5	0.51	0
2	FA1	X	148	-	7,12,12	4.30	4 (57%)	7,18,18	1.77	2 (28%)

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	FA1	A	147	-	-	0/0/21/21	0/1/1/1
3	GOL	B	147	-	-	0/4/4/4	0/0/0/0
2	FA1	B	148	-	-	0/0/21/21	0/1/1/1
2	FA1	C	147	-	-	0/0/21/21	0/1/1/1
2	FA1	D	147	-	-	0/0/21/21	0/1/1/1
3	GOL	E	147	-	-	0/4/4/4	0/0/0/0
2	FA1	E	148	-	-	0/0/21/21	0/1/1/1
2	FA1	F	147	-	-	0/0/21/21	0/1/1/1
3	GOL	G	147	-	-	0/4/4/4	0/0/0/0
2	FA1	G	148	-	-	0/0/21/21	0/1/1/1
3	GOL	H	147	-	-	0/4/4/4	0/0/0/0
2	FA1	H	148	-	-	0/0/21/21	0/1/1/1
3	GOL	I	147	-	-	0/4/4/4	0/0/0/0
2	FA1	I	148	-	-	0/0/21/21	0/1/1/1
2	FA1	J	147	-	-	0/0/21/21	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FA1	K	147	-	-	0/0/21/21	0/1/1/1
3	GOL	L	147	-	-	0/4/4/4	0/0/0/0
2	FA1	L	148	-	-	0/0/21/21	0/1/1/1
2	FA1	M	147	-	-	0/0/21/21	0/1/1/1
2	FA1	N	147	-	1/1/4/6	0/0/21/21	0/1/1/1
3	GOL	O	147	-	-	0/4/4/4	0/0/0/0
2	FA1	O	148	-	-	0/0/21/21	0/1/1/1
3	GOL	P	147	-	-	0/4/4/4	0/0/0/0
2	FA1	P	148	-	-	0/0/21/21	0/1/1/1
3	GOL	Q	147	-	-	0/4/4/4	0/0/0/0
2	FA1	Q	148	-	-	0/0/21/21	0/1/1/1
2	FA1	R	147	-	-	0/0/21/21	0/1/1/1
2	FA1	S	147	-	-	0/0/21/21	0/1/1/1
3	GOL	T	147	-	-	0/4/4/4	0/0/0/0
2	FA1	T	148	-	-	0/0/21/21	0/1/1/1
3	GOL	U	147	-	-	0/4/4/4	0/0/0/0
2	FA1	U	148	-	-	0/0/21/21	0/1/1/1
3	GOL	V	147	-	-	0/4/4/4	0/0/0/0
2	FA1	V	148	-	-	0/0/21/21	0/1/1/1
2	FA1	W	147	-	-	0/0/21/21	0/1/1/1
3	GOL	X	147	-	-	0/4/4/4	0/0/0/0
2	FA1	X	148	-	-	0/0/21/21	0/1/1/1

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	147	FA1	C1-C6	-12.74	1.40	1.50
2	D	147	FA1	C1-C6	-12.15	1.40	1.50
2	R	147	FA1	C1-C6	-11.14	1.41	1.50
2	V	148	FA1	C1-C6	-10.60	1.41	1.50
2	A	147	FA1	C1-C6	-10.25	1.42	1.50
2	I	148	FA1	C1-C6	-10.17	1.42	1.50
2	O	148	FA1	C1-C6	-10.03	1.42	1.50
2	U	148	FA1	C1-C6	-10.02	1.42	1.50
2	G	148	FA1	C1-C6	-9.98	1.42	1.50
2	P	148	FA1	C1-C6	-9.91	1.42	1.50
2	B	148	FA1	C1-C6	-9.75	1.42	1.50
2	E	148	FA1	C1-C6	-9.61	1.42	1.50
2	F	147	FA1	C1-C6	-9.53	1.42	1.50
2	H	148	FA1	C1-C6	-9.31	1.42	1.50
2	C	147	FA1	C1-C6	-8.89	1.43	1.50
2	W	147	FA1	C1-C6	-8.78	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	148	FA1	C1-C6	-8.76	1.43	1.50
2	L	148	FA1	C1-C6	-8.69	1.43	1.50
2	Q	148	FA1	C1-C6	-8.68	1.43	1.50
2	S	147	FA1	C1-C6	-8.54	1.43	1.50
2	J	147	FA1	C1-C6	-8.36	1.43	1.50
2	T	148	FA1	C1-C6	-7.69	1.44	1.50
2	K	147	FA1	C1-C6	-7.63	1.44	1.50
2	M	147	FA1	C1-C6	-7.54	1.44	1.50
2	R	147	FA1	C2-C3	-3.58	1.47	1.53
2	P	148	FA1	O4-C4	-3.13	1.37	1.43
2	Q	148	FA1	O3-C3	-2.59	1.37	1.43
2	W	147	FA1	C2-C3	-2.39	1.49	1.53
2	N	147	FA1	C4-C5	-2.30	1.45	1.50
2	N	147	FA1	O3-C3	2.05	1.48	1.43
2	W	147	FA1	C4-C5	2.11	1.54	1.50
2	D	147	FA1	C2-C3	2.17	1.56	1.53
2	D	147	FA1	O30-C1	2.19	1.46	1.43
2	B	148	FA1	C2-C3	2.23	1.56	1.53
2	W	147	FA1	O30-C1	2.29	1.47	1.43
2	H	148	FA1	C4-C5	2.43	1.55	1.50
2	Q	148	FA1	O4-C4	2.46	1.48	1.43
2	X	148	FA1	O30-C1	2.46	1.47	1.43
2	B	148	FA1	C4-C5	2.48	1.55	1.50
2	N	147	FA1	O30-C1	2.49	1.47	1.43
2	L	148	FA1	C4-C5	2.56	1.55	1.50
2	K	147	FA1	C4-C5	2.58	1.55	1.50
2	W	147	FA1	O3-C3	2.67	1.49	1.43
2	O	148	FA1	C2-C3	2.67	1.57	1.53
2	M	147	FA1	C4-C5	2.71	1.55	1.50
2	A	147	FA1	O30-C1	2.79	1.47	1.43
2	Q	148	FA1	C4-C5	2.87	1.55	1.50
2	T	148	FA1	C4-C5	2.89	1.55	1.50
2	D	147	FA1	C4-C5	2.99	1.56	1.50
2	T	148	FA1	C2-C3	2.99	1.57	1.53
2	G	148	FA1	O30-C1	3.04	1.48	1.43
2	I	148	FA1	C4-C5	3.20	1.56	1.50
2	U	148	FA1	C4-C5	3.24	1.56	1.50
2	T	148	FA1	C5-C6	3.42	1.38	1.32
2	K	147	FA1	O30-C1	3.43	1.49	1.43
2	C	147	FA1	C4-C5	3.55	1.57	1.50
2	L	148	FA1	O30-C1	3.67	1.49	1.43
2	G	148	FA1	C5-C6	3.75	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	148	FA1	O30-C1	3.82	1.49	1.43
2	X	148	FA1	C4-C5	3.90	1.57	1.50
2	D	147	FA1	C5-C6	4.22	1.39	1.32
2	A	147	FA1	C5-C6	4.23	1.39	1.32
2	N	147	FA1	C5-C6	4.63	1.40	1.32
2	P	148	FA1	C5-C6	4.72	1.40	1.32
2	E	148	FA1	C5-C6	4.78	1.40	1.32
2	F	147	FA1	C5-C6	4.87	1.40	1.32
2	X	148	FA1	C5-C6	5.10	1.40	1.32
2	S	147	FA1	C5-C6	5.10	1.40	1.32
2	R	147	FA1	C4-C5	5.11	1.60	1.50
2	Q	148	FA1	C5-C6	5.13	1.40	1.32
2	J	147	FA1	C5-C6	5.14	1.40	1.32
2	B	148	FA1	C5-C6	5.33	1.41	1.32
2	I	148	FA1	C5-C6	5.43	1.41	1.32
2	M	147	FA1	C5-C6	5.60	1.41	1.32
2	O	148	FA1	C5-C6	5.71	1.41	1.32
2	C	147	FA1	C5-C6	5.87	1.42	1.32
2	H	148	FA1	C5-C6	5.93	1.42	1.32
2	L	148	FA1	C5-C6	5.96	1.42	1.32
2	V	148	FA1	C5-C6	6.20	1.42	1.32
2	K	147	FA1	C5-C6	6.43	1.42	1.32
2	U	148	FA1	C5-C6	6.50	1.43	1.32
2	N	147	FA1	C2-C3	6.75	1.63	1.53
2	W	147	FA1	C5-C6	6.77	1.43	1.32
2	R	147	FA1	C5-C6	20.96	1.65	1.32
2	R	147	FA1	O30-C1	29.64	1.94	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	147	FA1	O30-C1-C6	-14.48	49.98	108.29
2	R	147	FA1	C4-C5-C6	-6.70	116.15	123.36
2	N	147	FA1	O4-C4-C5	-4.73	98.91	110.00
2	L	148	FA1	C4-C5-C6	-4.45	118.57	123.36
2	N	147	FA1	O30-C1-C6	-4.38	90.65	108.29
2	V	148	FA1	C4-C5-C6	-4.30	118.73	123.36
2	K	147	FA1	C4-C5-C6	-4.29	118.74	123.36
2	I	148	FA1	C4-C5-C6	-3.95	119.11	123.36
2	E	148	FA1	C4-C5-C6	-3.94	119.11	123.36
2	M	147	FA1	C4-C5-C6	-3.49	119.60	123.36
2	R	147	FA1	C1-C6-C5	-3.34	104.18	115.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	147	FA1	O4-C4-C3	-3.29	104.20	109.73
2	F	147	FA1	C4-C5-C6	-3.22	119.90	123.36
2	X	148	FA1	C4-C5-C6	-2.68	120.47	123.36
2	P	148	FA1	C4-C5-C6	-2.58	120.58	123.36
2	C	147	FA1	C4-C5-C6	-2.56	120.60	123.36
2	J	147	FA1	O4-C4-C3	-2.55	105.45	109.73
2	B	148	FA1	C4-C5-C6	-2.47	120.70	123.36
2	P	148	FA1	O4-C4-C5	-2.44	104.28	110.00
2	N	147	FA1	C4-C5-C6	-2.38	120.80	123.36
2	R	147	FA1	O3-C3-C2	-2.13	104.81	109.92
2	H	148	FA1	O4-C4-C3	-2.13	106.16	109.73
2	D	147	FA1	C4-C5-C6	-2.10	121.10	123.36
2	A	147	FA1	C4-C5-C6	-2.01	121.20	123.36
2	W	147	FA1	C1-C6-C5	2.03	121.81	115.15
2	Q	148	FA1	O4-C4-C5	2.03	114.76	110.00
2	C	147	FA1	C1-C6-C5	2.08	121.98	115.15
2	P	148	FA1	O3-C3-C4	2.13	113.35	109.15
2	J	147	FA1	C1-C6-C5	2.19	122.35	115.15
2	H	148	FA1	C1-C6-C5	2.19	122.36	115.15
2	Q	148	FA1	C1-C6-C5	2.24	122.51	115.15
2	V	148	FA1	O4-C4-C3	2.28	113.57	109.73
2	R	147	FA1	O4-C4-C5	2.33	115.46	110.00
2	X	148	FA1	C1-C6-C5	2.54	123.50	115.15
2	W	147	FA1	O3-C3-C4	2.56	114.20	109.15
2	S	147	FA1	C1-C6-C5	2.56	123.58	115.15
2	O	148	FA1	C1-C6-C5	2.58	123.63	115.15
2	T	148	FA1	C1-C6-C5	2.70	124.03	115.15
2	E	148	FA1	C1-C6-C5	2.71	124.05	115.15
2	M	147	FA1	C1-C6-C5	2.85	124.52	115.15
2	A	147	FA1	C1-C6-C5	3.01	125.05	115.15
2	F	147	FA1	C1-C6-C5	3.02	125.09	115.15
2	B	148	FA1	C1-C6-C5	3.04	125.14	115.15
2	P	148	FA1	C1-C6-C5	3.05	125.19	115.15
2	I	148	FA1	C1-C6-C5	3.17	125.56	115.15
2	G	148	FA1	C1-C6-C5	3.22	125.73	115.15
2	L	148	FA1	C1-C6-C5	3.25	125.83	115.15
2	D	147	FA1	C1-C6-C5	3.34	126.12	115.15
2	V	148	FA1	C1-C6-C5	3.50	126.66	115.15
2	K	147	FA1	C1-C6-C5	3.50	126.67	115.15
2	N	147	FA1	C1-C6-C5	3.79	127.60	115.15
2	N	147	FA1	O3-C3-C2	3.99	119.50	109.92
2	J	147	FA1	O4-C4-C5	4.35	120.19	110.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	N	147	FA1	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	148	FA1	1	0
3	E	147	GOL	1	0
3	G	147	GOL	1	0
2	N	147	FA1	2	0
3	O	147	GOL	2	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	141/147 (95%)	-0.45	0  	18, 29, 50, 63	3 (2%)
1	B	141/147 (95%)	-0.57	0  	18, 26, 38, 51	3 (2%)
1	C	139/147 (94%)	-0.44	1 (0%)  	19, 28, 53, 72	5 (3%)
1	D	141/147 (95%)	-0.35	1 (0%)  	18, 29, 54, 65	5 (3%)
1	E	141/147 (95%)	-0.35	2 (1%)  	19, 29, 53, 69	4 (2%)
1	F	137/147 (93%)	-0.42	0  	18, 28, 46, 70	3 (2%)
1	G	141/147 (95%)	-0.37	0  	19, 26, 47, 67	1 (0%)
1	H	141/147 (95%)	-0.46	0  	17, 25, 39, 59	5 (3%)
1	I	141/147 (95%)	-0.34	2 (1%)  	17, 26, 51, 68	5 (3%)
1	J	141/147 (95%)	-0.39	2 (1%)  	13, 19, 43, 61	4 (2%)
1	K	141/147 (95%)	-0.36	1 (0%)  	19, 29, 55, 70	4 (2%)
1	L	141/147 (95%)	-0.44	0  	11, 21, 38, 59	8 (5%)
1	M	141/147 (95%)	-0.39	1 (0%)  	15, 21, 46, 62	8 (5%)
1	N	141/147 (95%)	-0.38	1 (0%)  	18, 29, 51, 65	7 (4%)
1	O	141/147 (95%)	-0.40	1 (0%)  	14, 25, 49, 68	7 (4%)
1	P	141/147 (95%)	-0.39	0  	19, 27, 43, 58	9 (6%)
1	Q	141/147 (95%)	-0.43	0  	15, 22, 41, 63	9 (6%)
1	R	141/147 (95%)	-0.31	1 (0%)  	18, 27, 57, 65	8 (5%)
1	S	141/147 (95%)	-0.38	2 (1%)  	15, 23, 45, 68	1 (0%)
1	T	141/147 (95%)	-0.55	0  	16, 24, 36, 58	8 (5%)
1	U	141/147 (95%)	-0.32	2 (1%)  	20, 30, 53, 67	8 (5%)
1	V	141/147 (95%)	-0.36	1 (0%)  	18, 29, 55, 67	8 (5%)
1	W	141/147 (95%)	-0.45	3 (2%)  	15, 23, 49, 72	8 (5%)
1	X	137/147 (93%)	-0.44	1 (0%)  	17, 27, 47, 58	8 (5%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3374/3528 (95%)	-0.41	22 (0%) 89 89	11, 26, 51, 72	139 (4%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	23	VAL	3.9
1	J	23	VAL	3.5
1	W	22	ALA	3.0
1	D	23	VAL	2.9
1	V	3	LEU	2.7
1	E	23	VAL	2.6
1	O	19	ARG	2.6
1	I	23	VAL	2.6
1	W	23	VAL	2.5
1	N	23	VAL	2.4
1	E	3	LEU	2.4
1	J	19	ARG	2.2
1	U	19	ARG	2.2
1	I	19	ARG	2.2
1	R	22	ALA	2.2
1	U	3	LEU	2.2
1	K	23	VAL	2.1
1	M	22	ALA	2.1
1	S	3	LEU	2.1
1	W	21	PRO	2.1
1	X	3	LEU	2.1
1	C	19	ARG	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	P	147	6/6	0.90	0.17	3.00	42,46,47,49	0
3	GOL	V	147	6/6	0.85	0.23	2.36	74,75,75,75	0
3	GOL	L	147	6/6	0.88	0.14	2.22	53,54,56,58	0
2	FA1	O	148	12/12	0.98	0.11	2.10	21,24,26,29	0
3	GOL	E	147	6/6	0.88	0.21	2.08	58,59,61,61	0
2	FA1	T	148	12/12	0.95	0.12	1.76	21,22,25,27	0
3	GOL	H	147	6/6	0.90	0.13	1.71	41,46,48,49	0
2	FA1	Q	148	12/12	0.98	0.10	1.56	18,22,30,30	0
2	FA1	N	147	12/12	0.94	0.12	1.53	22,26,29,31	0
2	FA1	B	148	12/12	0.97	0.10	1.51	21,24,26,28	0
3	GOL	T	147	6/6	0.95	0.10	1.25	40,40,42,42	0
2	FA1	R	147	12/12	0.92	0.11	0.83	28,33,35,35	0
3	GOL	O	147	6/6	0.85	0.20	0.81	49,53,55,56	0
2	FA1	E	148	12/12	0.97	0.11	0.70	21,27,28,32	0
2	FA1	A	147	12/12	0.97	0.10	0.67	23,24,26,31	0
2	FA1	M	147	12/12	0.97	0.11	0.57	18,21,27,28	0
2	FA1	V	148	12/12	0.97	0.11	0.49	26,29,32,35	0
3	GOL	B	147	6/6	0.95	0.10	0.38	31,39,43,43	0
2	FA1	J	147	12/12	0.98	0.10	0.36	16,19,23,26	0
2	FA1	W	147	12/12	0.97	0.11	0.34	21,23,26,26	0
2	FA1	U	148	12/12	0.97	0.09	0.29	23,32,34,35	0
2	FA1	D	147	12/12	0.98	0.10	0.29	22,27,29,30	0
2	FA1	C	147	12/12	0.96	0.10	0.28	26,28,31,34	0
2	FA1	S	147	12/12	0.97	0.10	0.27	22,24,25,26	0
3	GOL	X	147	6/6	0.89	0.12	0.19	51,56,56,58	0
2	FA1	G	148	12/12	0.98	0.10	0.12	20,26,31,34	0
2	FA1	F	147	12/12	0.97	0.09	0.01	26,30,34,34	0
2	FA1	K	147	12/12	0.97	0.10	-0.02	24,31,34,35	0
2	FA1	P	148	12/12	0.98	0.09	-0.08	23,24,27,27	0
3	GOL	U	147	6/6	0.93	0.13	-0.14	56,60,61,61	0
3	GOL	I	147	6/6	0.81	0.15	-0.15	69,73,73,74	0
2	FA1	X	148	12/12	0.97	0.09	-0.55	26,30,31,34	0
3	GOL	G	147	6/6	0.96	0.11	-0.69	48,51,53,54	0
2	FA1	I	148	12/12	0.97	0.08	-0.74	22,29,32,34	0
3	GOL	Q	147	6/6	0.94	0.09	-1.06	61,63,63,64	0
2	FA1	H	148	12/12	0.98	0.08	-1.15	18,23,25,27	0
2	FA1	L	148	12/12	0.98	0.08	-1.45	16,22,25,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.