



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2019 – 01:48 PM EST

PDB ID : 6E3B  
Title : STRUCTURE OF Siw14 CATALYTIC CORE  
Authors : Florio, T.; Lokareddy, R.; Cingolani, G.  
Deposited on : 2018-07-13  
Resolution : 2.50 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

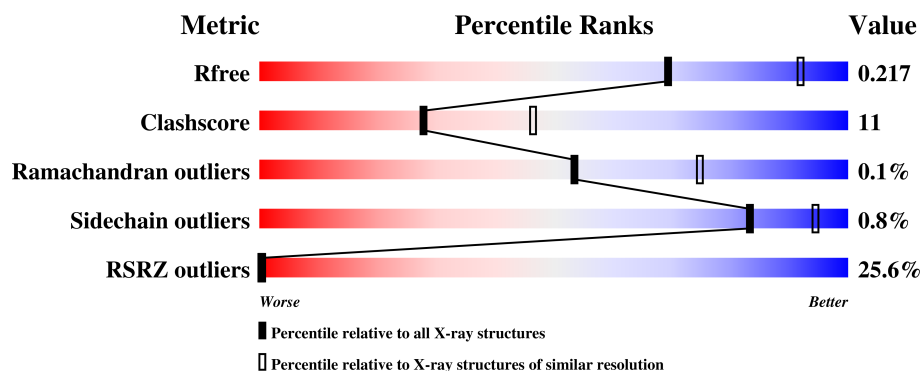
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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.



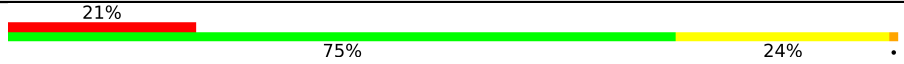
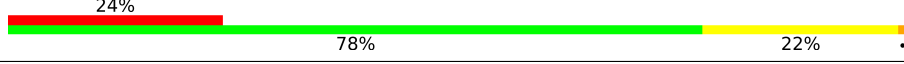




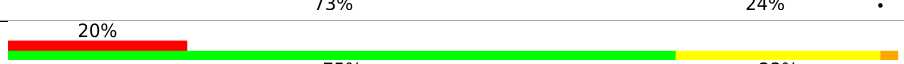
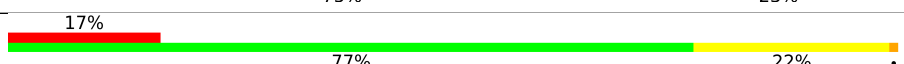
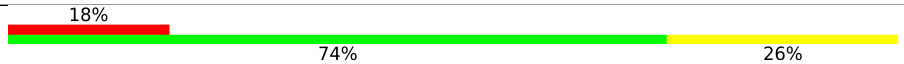
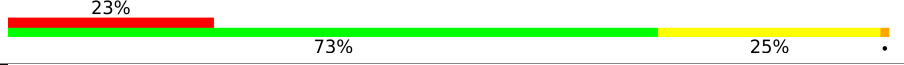
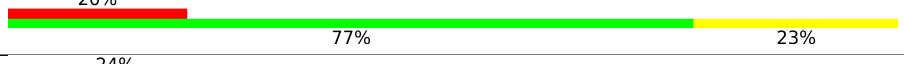



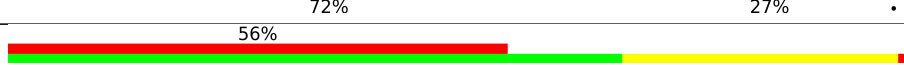
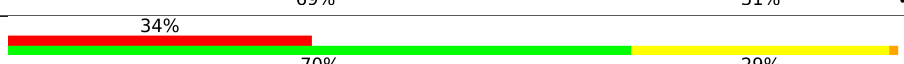
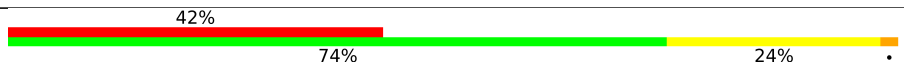

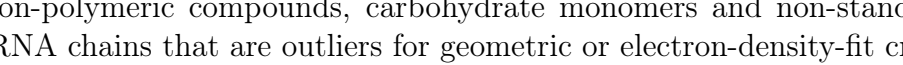
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	169	<div> <div>20%</div> <div>73%</div> <div>27%</div> <div>.</div> </div>
1	B	169	<div> <div>19%</div> <div>75%</div> <div>25%</div> <div>.</div> </div>
1	C	169	<div> <div>21%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
1	D	169	<div> <div>18%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	E	169	<div> <div>18%</div> <div>69%</div> <div>28%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	169	
1	G	169	
1	H	169	
1	I	169	
1	J	169	
1	K	169	
1	L	169	
1	M	169	
1	N	169	
1	O	169	
1	P	169	
1	Q	169	
1	R	169	
1	S	169	
1	T	169	
1	V	169	
1	W	169	
1	X	169	
1	Y	169	

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	SO4	P	301	-	-	X	-
2	SO4	W	301	-	-	X	-
2	SO4	Y	301	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34047 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 Tyrosine-protein phosphatase SIW14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			
1	B	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			
1	C	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			
1	D	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			
1	E	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			
1	F	169	Total	C	N	O	S	0	0	0
			1395	903	242	245	5			
1	G	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			
1	H	169	Total	C	N	O	S	0	0	0
			1395	903	242	245	5			
1	I	169	Total	C	N	O	S	0	0	0
			1395	903	242	245	5			
1	J	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			
1	K	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			
1	L	169	Total	C	N	O	S	0	0	0
			1395	903	242	245	5			
1	M	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			
1	N	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			
1	O	169	Total	C	N	O	S	0	0	0
			1395	903	242	245	5			
1	P	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	169	Total	C	N	O	S	0	0	0
			1395	903	242	245	5			
1	R	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			
1	S	169	Total	C	N	O	S	0	0	0
			1377	903	242	227	5			
1	T	168	Total	C	N	O	S	0	0	0
			1393	900	244	244	5			
1	V	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			
1	W	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			
1	X	169	Total	C	N	O	S	0	0	0
			1387	898	241	243	5			
1	Y	169	Total	C	N	O	S	0	0	0
			1401	906	245	245	5			

There are 24 discrepancies between the modelled and reference sequences:

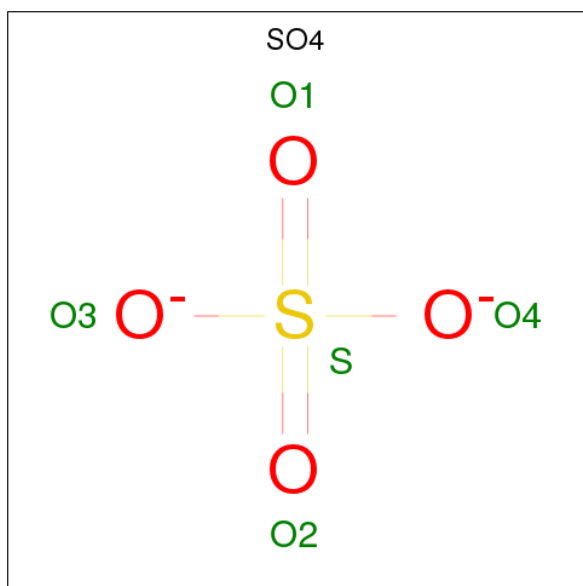
Chain	Residue	Modelled	Actual	Comment	Reference
A	214	SER	CYS	conflict	UNP P53965
B	214	SER	CYS	conflict	UNP P53965
C	214	SER	CYS	conflict	UNP P53965
D	214	SER	CYS	conflict	UNP P53965
E	214	SER	CYS	conflict	UNP P53965
F	214	SER	CYS	conflict	UNP P53965
G	214	SER	CYS	conflict	UNP P53965
H	214	SER	CYS	conflict	UNP P53965
I	214	SER	CYS	conflict	UNP P53965
J	214	SER	CYS	conflict	UNP P53965
K	214	SER	CYS	conflict	UNP P53965
L	214	SER	CYS	conflict	UNP P53965
M	214	SER	CYS	conflict	UNP P53965
N	214	SER	CYS	conflict	UNP P53965
O	214	SER	CYS	conflict	UNP P53965
P	214	SER	CYS	conflict	UNP P53965
Q	214	SER	CYS	conflict	UNP P53965
R	214	SER	CYS	conflict	UNP P53965
S	214	SER	CYS	conflict	UNP P53965
T	214	SER	CYS	conflict	UNP P53965
V	214	SER	CYS	conflict	UNP P53965
W	214	SER	CYS	conflict	UNP P53965
X	214	SER	CYS	conflict	UNP P53965

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	214	SER	CYS	conflict	UNP P53965

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	L	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	V	1	Total	O	S	0	0
			5	4	1		
2	W	1	Total	O	S	0	0
			5	4	1		
2	X	1	Total	O	S	0	0
			5	4	1		
2	Y	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	17	Total	O	0	0
			17	17		
3	C	17	Total	O	0	0
			17	17		
3	D	17	Total	O	0	0
			17	17		
3	E	13	Total	O	0	0
			13	13		
3	F	23	Total	O	0	0
			23	23		

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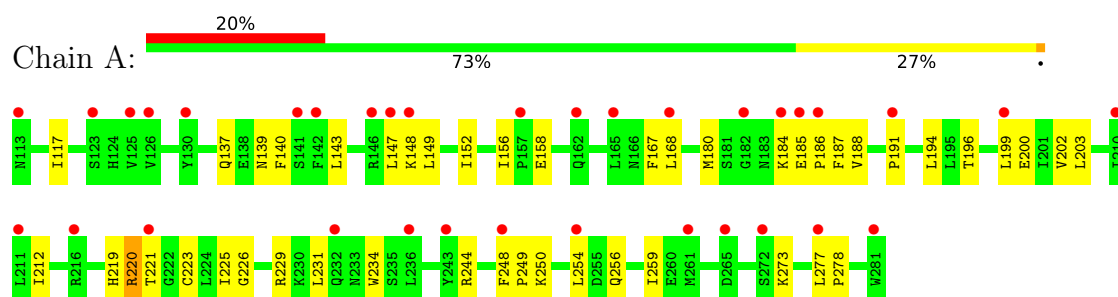
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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3	H	6	Total 6	O 6	0	0
3	I	12	Total 12	O 12	0	0
3	J	18	Total 18	O 18	0	0
3	K	17	Total 17	O 17	0	0
3	L	21	Total 21	O 21	0	0
3	M	18	Total 18	O 18	0	0
3	N	15	Total 15	O 15	0	0
3	O	18	Total 18	O 18	0	0
3	P	16	Total 16	O 16	0	0
3	Q	23	Total 23	O 23	0	0
3	R	13	Total 13	O 13	0	0
3	S	12	Total 12	O 12	0	0
3	T	17	Total 17	O 17	0	0
3	V	9	Total 9	O 9	0	0
3	W	15	Total 15	O 15	0	0
3	X	25	Total 25	O 25	0	0
3	Y	14	Total 14	O 14	0	0



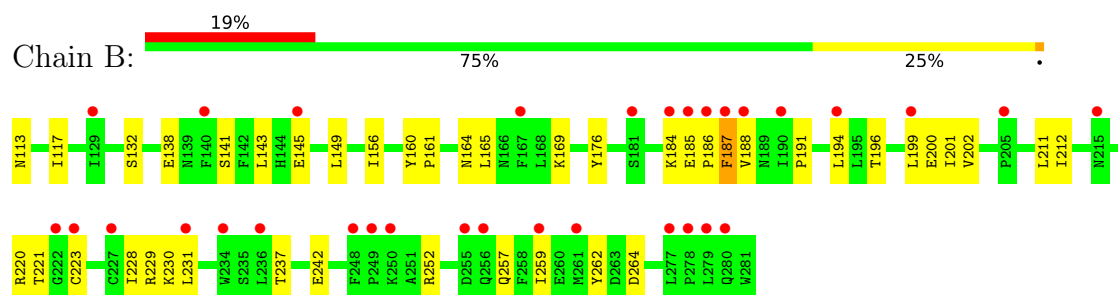
### 3 Residue-property plots

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.

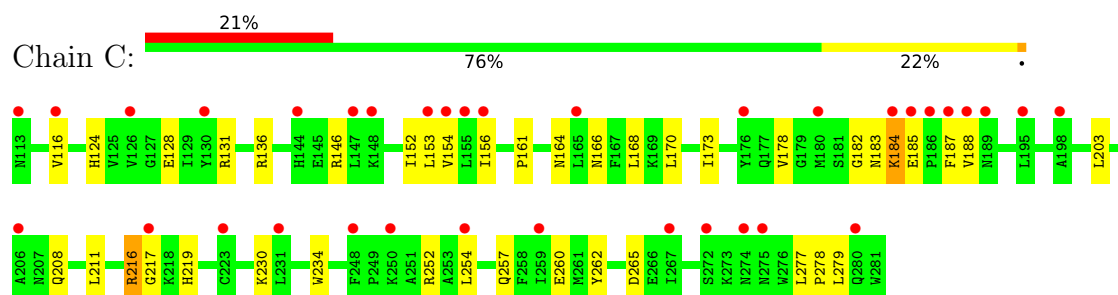
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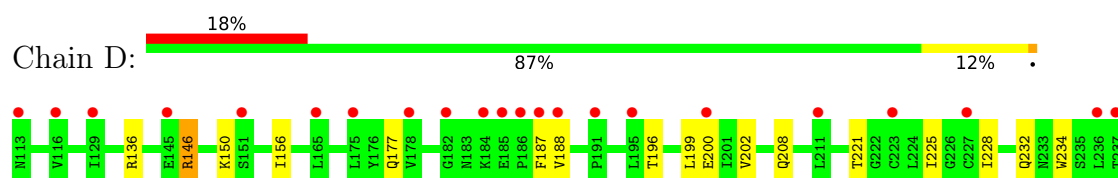
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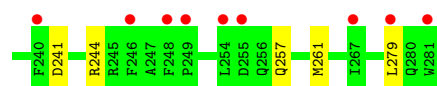


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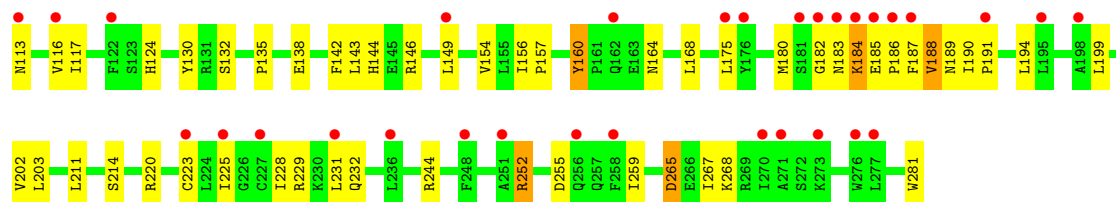


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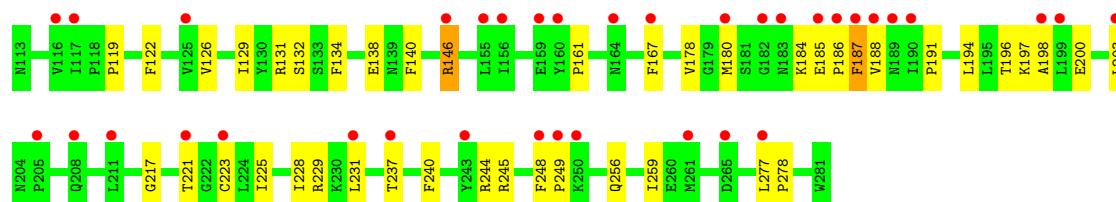
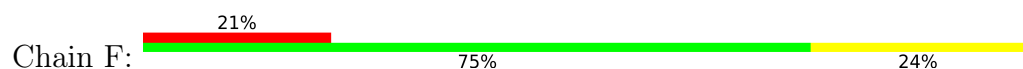




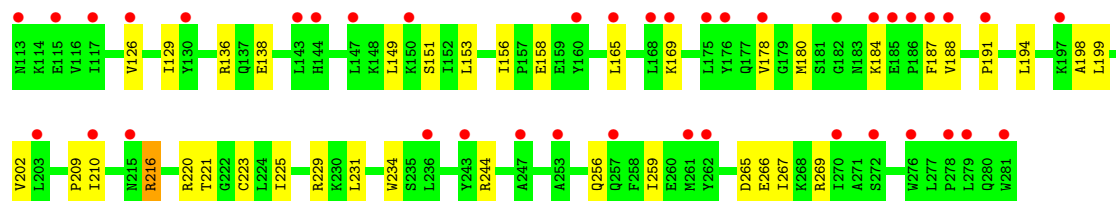
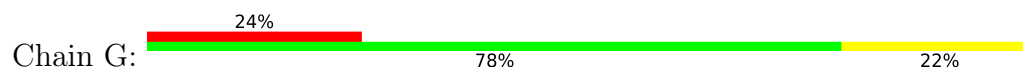
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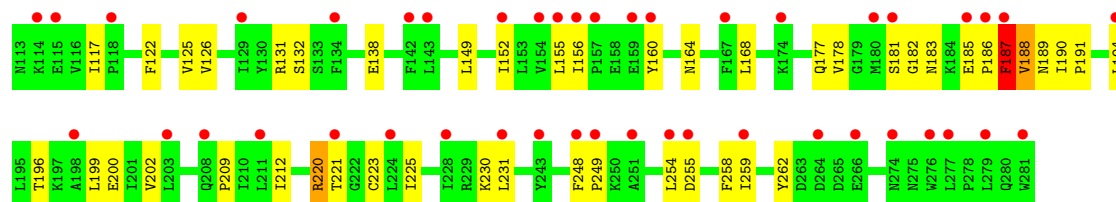
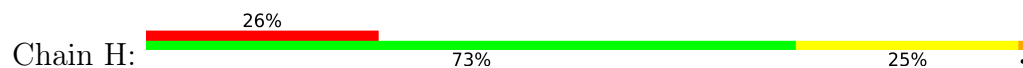
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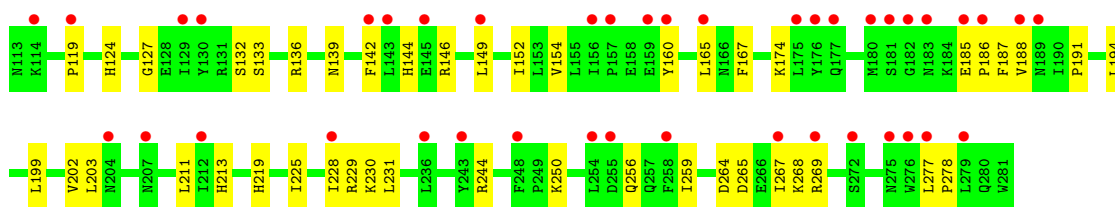


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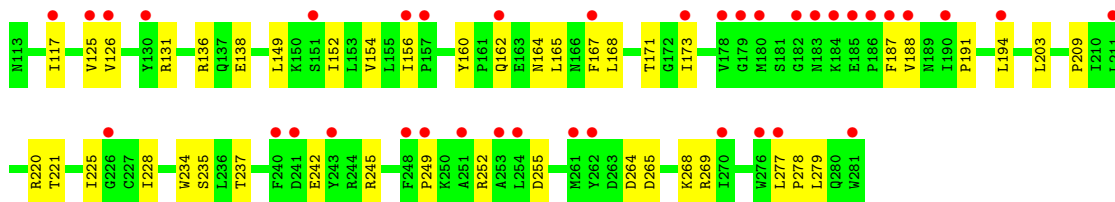
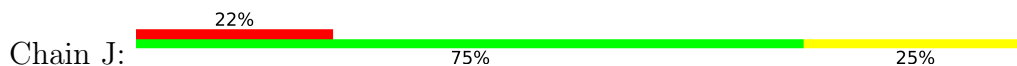


- Molecule 1: Tyrosine-protein phosphatase SIW14

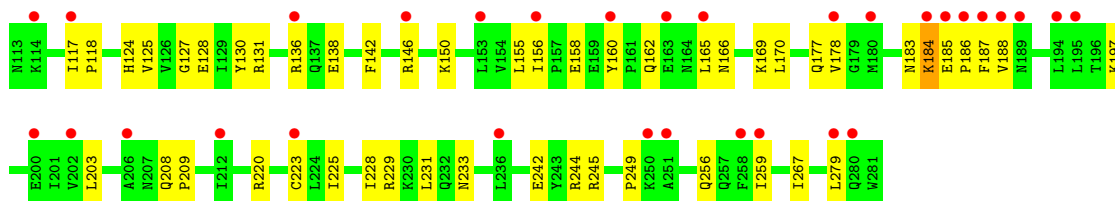




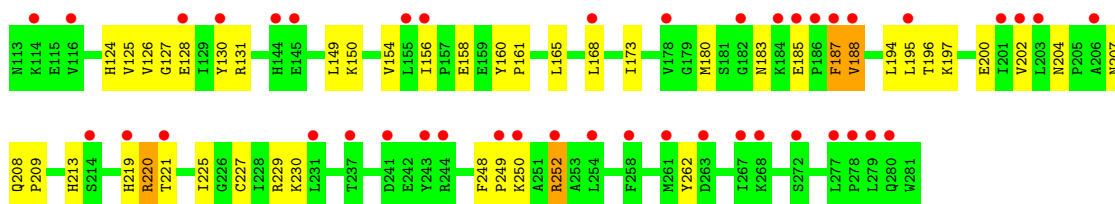
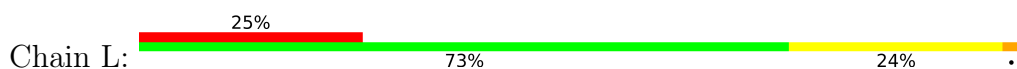
• Molecule 1: Tyrosine-protein phosphatase SIW14



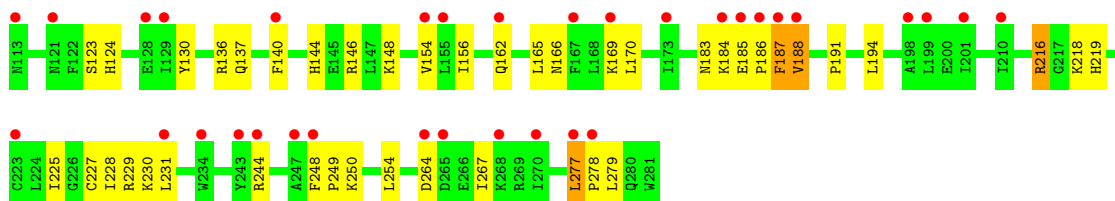
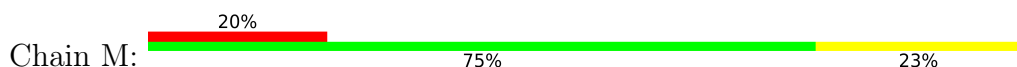
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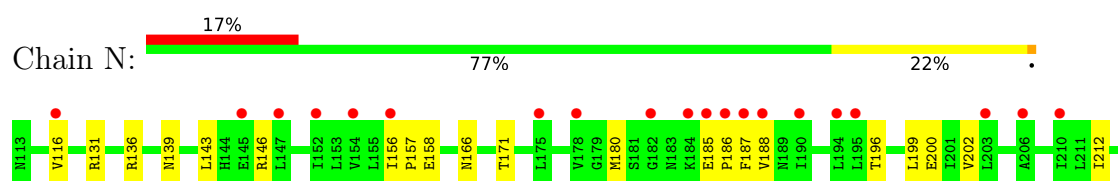
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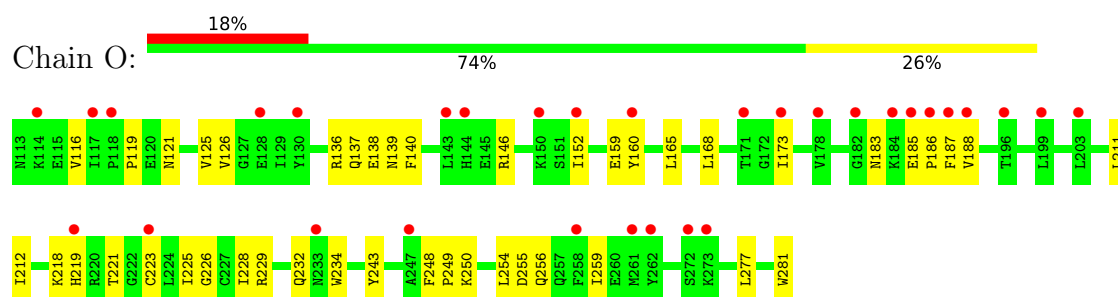
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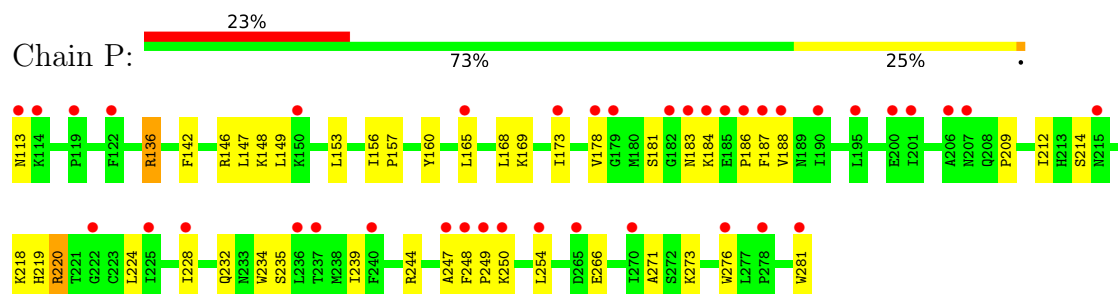
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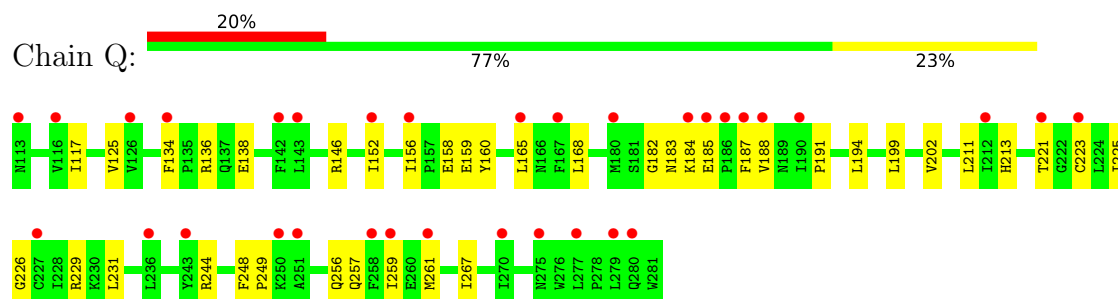
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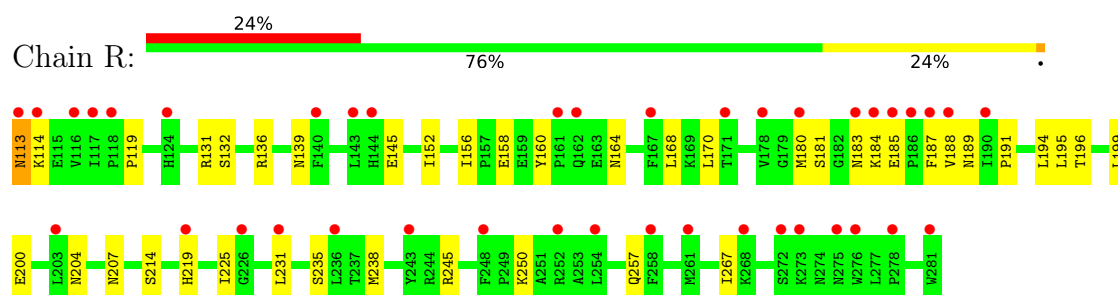
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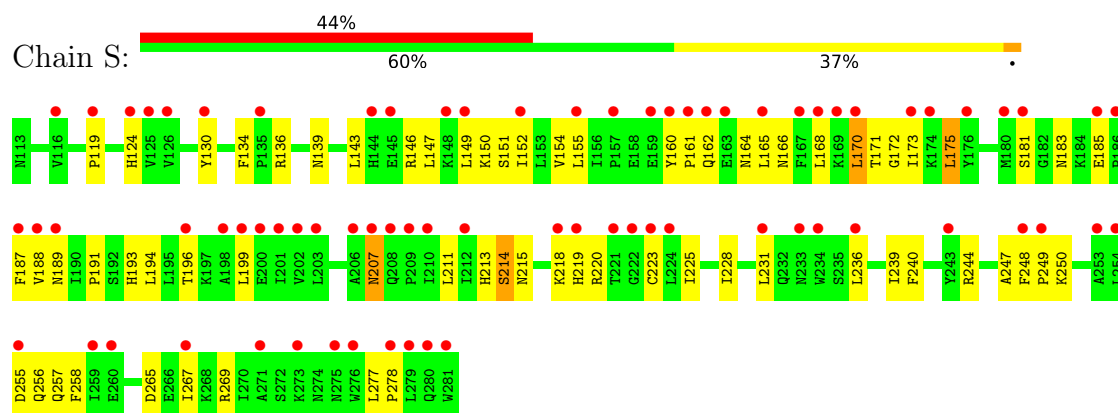
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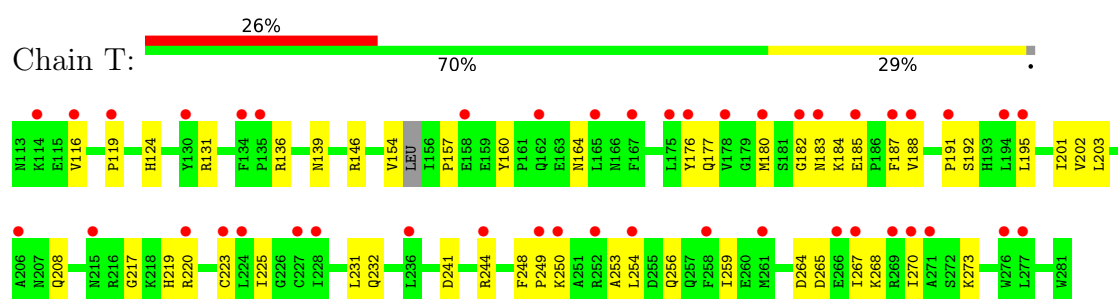
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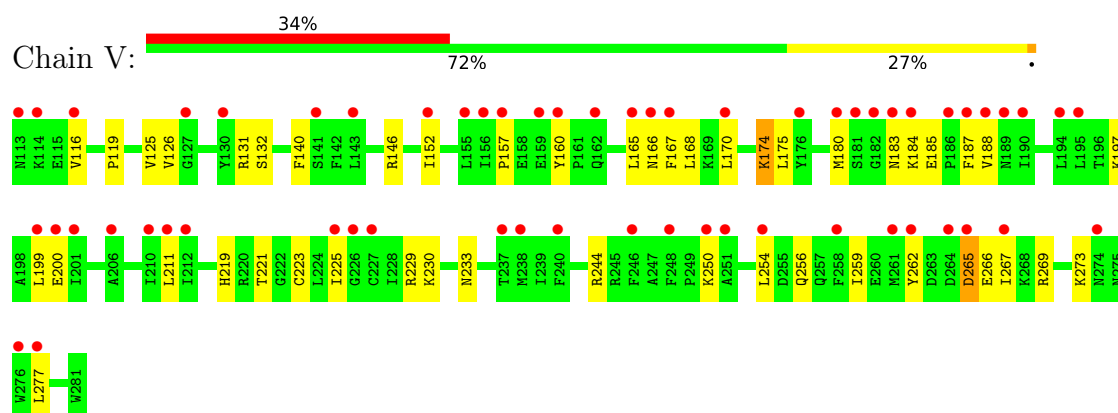
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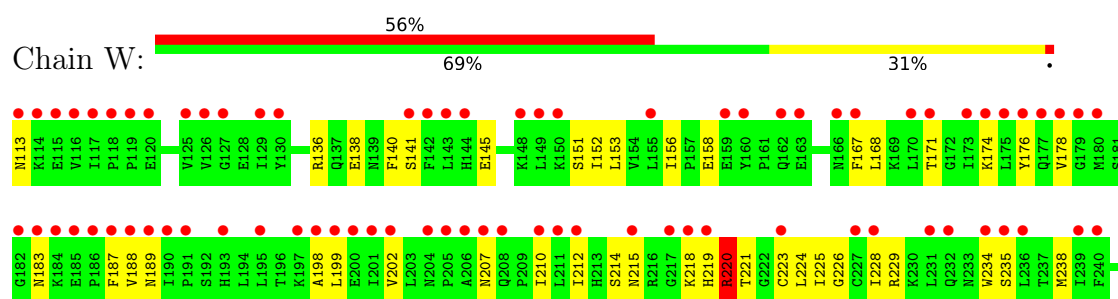
• Molecule 1: Tyrosine-protein phosphatase SIW14

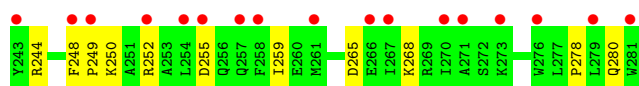


• Molecule 1: Tyrosine-protein phosphatase SIW14

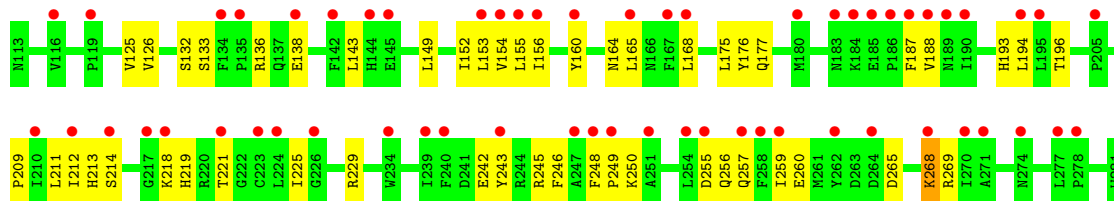


• Molecule 1: Tyrosine-protein phosphatase SIW14

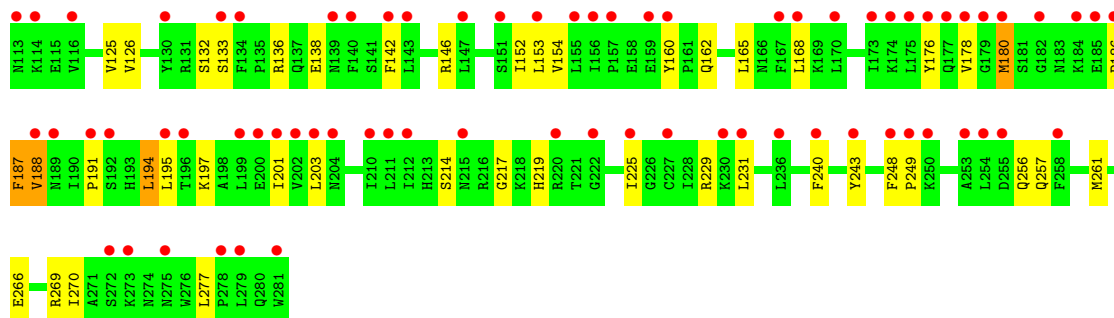
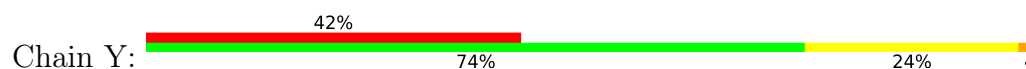




- Molecule 1: Tyrosine-protein phosphatase SIW14



- Molecule 1: Tyrosine-protein phosphatase SIW14



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.47Å 160.49Å 360.57Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	14.99 – 2.50 39.79 – 2.49	Depositor EDS
% Data completeness (in resolution range)	90.4 (14.99-2.50) 83.1 (39.79-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.01	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.62 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.230 , 0.246 0.211 , 0.217	Depositor DCC
$R_{free}$ test set	2019 reflections (1.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 24.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.336 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.357 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.290 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.340 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.329 for h,-k,-l	Xtriage
Reported twinning fraction	0.450 for h,-k,-l	Depositor
Outliers	1 of 166746 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	34047	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.20% 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: SO4

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	0.27	0/1437	0.49	0/1943
1	B	0.30	0/1437	0.53	1/1943 (0.1%)
1	C	0.28	0/1437	0.49	0/1943
1	D	0.28	0/1437	0.49	0/1943
1	E	0.34	0/1437	0.59	1/1943 (0.1%)
1	F	0.35	0/1431	0.57	3/1936 (0.2%)
1	G	0.30	0/1437	0.51	0/1943
1	H	0.31	0/1431	0.58	2/1936 (0.1%)
1	I	0.31	0/1431	0.52	0/1936
1	J	0.29	0/1437	0.50	0/1943
1	K	0.31	0/1437	0.58	1/1943 (0.1%)
1	L	0.32	0/1431	0.57	2/1936 (0.1%)
1	M	0.29	0/1437	0.56	3/1943 (0.2%)
1	N	0.28	0/1437	0.50	0/1943
1	O	0.28	0/1431	0.49	0/1936
1	P	0.27	0/1437	0.51	0/1943
1	Q	0.29	0/1431	0.53	0/1936
1	R	0.31	0/1437	0.57	1/1943 (0.1%)
1	S	0.30	0/1413	0.52	1/1900 (0.1%)
1	T	0.29	0/1428	0.54	0/1929
1	V	0.33	0/1437	0.62	2/1943 (0.1%)
1	W	0.33	0/1437	0.59	1/1943 (0.1%)
1	X	0.28	0/1423	0.52	0/1927
1	Y	0.31	0/1437	0.59	3/1943 (0.2%)
All	All	0.30	0/34405	0.54	21/46517 (0.0%)

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



Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	E	0	2
1	H	0	2
1	K	0	1
1	M	0	1
1	O	0	1
1	P	0	2
1	W	0	1
1	Y	0	2
All	All	0	14

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	199	LEU	CA-CB-CG	6.75	130.83	115.30
1	H	188	VAL	N-CA-C	-6.46	93.55	111.00
1	R	113	ASN	N-CA-C	-6.11	94.51	111.00
1	F	146	ARG	CA-CB-CG	-5.83	100.58	113.40
1	L	188	VAL	N-CA-C	-5.71	95.57	111.00
1	S	170	LEU	CA-CB-CG	5.67	128.33	115.30
1	Y	180	MET	CB-CG-SD	5.57	129.11	112.40
1	K	170	LEU	CB-CG-CD1	5.55	120.44	111.00
1	M	187	PHE	C-N-CA	5.53	135.53	121.70
1	F	187	PHE	C-N-CA	5.51	135.48	121.70
1	F	146	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	M	277	LEU	CA-CB-CG	5.43	127.80	115.30
1	M	188	VAL	N-CA-C	-5.37	96.50	111.00
1	E	265	ASP	CB-CG-OD1	5.37	123.13	118.30
1	Y	188	VAL	N-CA-C	-5.34	96.59	111.00
1	B	187	PHE	C-N-CA	5.32	135.00	121.70
1	H	187	PHE	C-N-CA	5.22	134.75	121.70
1	L	187	PHE	C-N-CA	5.21	134.73	121.70
1	V	265	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	Y	277	LEU	CA-CB-CG	5.18	127.21	115.30
1	W	265	ASP	CB-CG-OD1	-5.02	113.78	118.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	186	PRO	Peptide
1	D	146	ARG	Sidechain
1	E	186	PRO	Peptide
1	E	252	ARG	Sidechain
1	H	186	PRO	Peptide
1	H	187	PHE	Peptide
1	K	186	PRO	Peptide
1	M	186	PRO	Peptide
1	O	186	PRO	Peptide
1	P	136	ARG	Sidechain
1	P	186	PRO	Peptide
1	W	220	ARG	Sidechain
1	Y	186	PRO	Peptide
1	Y	187	PHE	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	1401	0	1416	29	0
1	B	1401	0	1416	35	0
1	C	1401	0	1416	26	0
1	D	1401	0	1416	16	0
1	E	1401	0	1416	44	0
1	F	1395	0	1405	30	0
1	G	1401	0	1416	29	0
1	H	1395	0	1405	31	0
1	I	1395	0	1405	26	0
1	J	1401	0	1416	29	0
1	K	1401	0	1416	34	0
1	L	1395	0	1405	29	0
1	M	1401	0	1416	42	0
1	N	1401	0	1416	33	0
1	O	1395	0	1405	32	0
1	P	1401	0	1416	39	0
1	Q	1395	0	1405	31	0
1	R	1401	0	1416	28	0
1	S	1377	0	1405	43	0
1	T	1393	0	1404	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	1401	0	1416	37	0
1	W	1401	0	1416	47	0
1	X	1387	0	1390	30	0
1	Y	1401	0	1416	27	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	1	0
2	H	5	0	0	1	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	1	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	5	0	0	3	0
2	Q	5	0	0	0	0
2	R	5	0	0	0	0
2	S	5	0	0	0	0
2	T	5	0	0	1	0
2	V	5	0	0	0	0
2	W	5	0	0	5	0
2	X	5	0	0	0	0
2	Y	5	0	0	2	0
3	A	14	0	0	0	0
3	B	17	0	0	0	0
3	C	17	0	0	0	0
3	D	17	0	0	0	0
3	E	13	0	0	1	0
3	F	23	0	0	3	0
3	G	15	0	0	0	0
3	H	6	0	0	0	0
3	I	12	0	0	0	0
3	J	18	0	0	2	0
3	K	17	0	0	1	0
3	L	21	0	0	2	0
3	M	18	0	0	2	0
3	N	15	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	18	0	0	0	0
3	P	16	0	0	3	0
3	Q	23	0	0	1	0
3	R	13	0	0	1	0
3	S	12	0	0	0	0
3	T	17	0	0	2	0
3	V	9	0	0	1	0
3	W	15	0	0	2	0
3	X	25	0	0	0	0
3	Y	14	0	0	0	0
All	All	34047	0	33869	719	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 11.

All (719) 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:V:166:ASN:O	1:V:170:LEU:HD12	1.44	1.16
1:E:244:ARG:HD3	1:M:244:ARG:HE	1.24	1.02
1:M:230:LYS:HE3	1:M:264:ASP:OD2	1.60	1.02
1:M:230:LYS:HE3	1:M:264:ASP:CG	1.85	0.97
1:M:187:PHE:HA	1:M:188:VAL:HG13	1.49	0.93
1:M:230:LYS:HE3	1:M:264:ASP:CB	1.99	0.93
1:R:187:PHE:HA	1:R:188:VAL:HG23	1.54	0.90
1:L:187:PHE:HA	1:L:188:VAL:HG23	1.54	0.90
1:V:166:ASN:O	1:V:170:LEU:CD1	2.21	0.86
1:W:153:LEU:HB3	1:W:212:ILE:HG13	1.58	0.85
1:Y:180:MET:SD	1:Y:194:LEU:HD13	2.18	0.84
1:J:265:ASP:HA	1:J:268:LYS:HD3	1.60	0.83
1:M:216:ARG:HH22	1:M:250:LYS:CD	1.92	0.82
1:M:227:CYS:SG	3:M:408:HOH:O	2.36	0.82
1:M:216:ARG:HH22	1:M:250:LYS:HD2	1.45	0.81
1:I:142:PHE:HE1	1:I:146:ARG:HH21	1.23	0.80
1:Q:187:PHE:HA	1:Q:188:VAL:HG22	1.66	0.77
1:H:117:ILE:HD13	1:H:138:GLU:HB2	1.67	0.77
1:R:187:PHE:HA	1:R:188:VAL:CG2	2.15	0.76
1:A:244:ARG:HE	1:A:256:GLN:HE22	1.31	0.76
1:W:219:HIS:NE2	1:W:250:LYS:O	2.20	0.75
1:M:230:LYS:CE	1:M:264:ASP:OD2	2.34	0.74
1:H:220:ARG:NE	2:H:301:SO4:O3	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:230:LYS:NZ	1:I:259:ILE:O	2.21	0.73
1:V:165:LEU:HA	1:V:168:LEU:HD12	1.70	0.73
1:S:219:HIS:NE2	1:S:250:LYS:O	2.22	0.72
1:B:141:SER:HA	1:B:145:GLU:OE2	1.89	0.72
1:J:268:LYS:HG2	1:J:269:ARG:N	2.03	0.72
1:K:136:ARG:NH2	1:K:138:GLU:OE2	2.23	0.72
1:I:244:ARG:HE	1:I:256:GLN:HE22	1.37	0.72
1:R:156:ILE:HG22	1:R:158:GLU:H	1.54	0.71
1:C:146:ARG:NH2	1:T:232:GLN:OE1	2.23	0.71
1:X:136:ARG:NH1	1:X:138:GLU:OE2	2.24	0.70
1:F:187:PHE:HA	1:F:188:VAL:HG13	1.74	0.70
1:I:244:ARG:NE	1:I:256:GLN:HE22	1.89	0.70
1:M:219:HIS:NE2	1:M:250:LYS:O	2.22	0.70
1:F:178:VAL:HG12	1:F:197:LYS:HE3	1.72	0.70
1:M:162:GLN:HA	1:M:165:LEU:HB2	1.74	0.70
1:K:279:LEU:O	1:P:146:ARG:NH1	2.24	0.70
1:N:250:LYS:NZ	3:N:402:HOH:O	2.25	0.69
1:E:187:PHE:HA	1:E:188:VAL:HB	1.75	0.69
1:W:223:CYS:HA	1:W:259:ILE:HD11	1.74	0.69
1:H:178:VAL:HG13	1:H:194:LEU:HD22	1.74	0.69
1:C:128:GLU:HB2	1:C:208:GLN:HB3	1.75	0.69
1:P:244:ARG:NH1	3:P:401:HOH:O	2.26	0.68
1:K:155:LEU:O	1:K:220:ARG:NH1	2.27	0.68
1:X:152:ILE:HG12	1:X:211:LEU:HB3	1.76	0.67
1:P:136:ARG:NH1	1:Q:188:VAL:O	2.24	0.67
1:W:215:ASN:HB2	1:W:220:ARG:HH22	1.59	0.67
1:V:244:ARG:HE	1:V:256:GLN:HE22	1.41	0.67
1:H:156:ILE:O	1:H:177:GLN:NE2	2.27	0.66
1:Q:156:ILE:HG22	1:Q:158:GLU:H	1.60	0.66
1:F:146:ARG:HH12	1:N:278:PRO:HB2	1.60	0.66
1:Y:266:GLU:O	1:Y:269:ARG:HG2	1.96	0.66
1:B:187:PHE:HA	1:B:188:VAL:CG2	2.26	0.65
1:V:223:CYS:HA	1:V:259:ILE:HD11	1.79	0.65
1:B:223:CYS:HA	1:B:259:ILE:HD11	1.79	0.65
1:L:219:HIS:NE2	1:L:250:LYS:O	2.24	0.65
1:R:181:SER:HB2	1:R:184:LYS:HB2	1.79	0.65
1:F:244:ARG:HE	1:F:256:GLN:HE22	1.44	0.65
1:F:196:THR:O	1:F:200:GLU:HG3	1.97	0.65
1:W:214:SER:OG	1:W:220:ARG:NH2	2.30	0.65
1:R:196:THR:O	1:R:200:GLU:HG3	1.96	0.65
1:E:252:ARG:NE	1:E:255:ASP:OD1	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:128:GLU:HG3	1:K:208:GLN:HB3	1.78	0.64
1:E:113:ASN:HD21	1:O:277:LEU:HD13	1.63	0.64
1:W:219:HIS:N	2:W:301:SO4:O4	2.31	0.64
1:X:132:SER:HB3	1:X:211:LEU:HD11	1.79	0.64
1:C:131:ARG:NH2	1:C:217:GLY:O	2.29	0.64
1:K:178:VAL:HG22	1:K:197:LYS:HE3	1.79	0.64
1:E:252:ARG:NH2	1:E:255:ASP:OD1	2.30	0.64
1:B:228:ILE:HA	1:B:231:LEU:HD12	1.79	0.63
1:Q:223:CYS:HA	1:Q:259:ILE:HD11	1.78	0.63
1:D:146:ARG:NH2	1:M:279:LEU:O	2.32	0.63
1:K:244:ARG:NH2	1:K:256:GLN:HE22	1.96	0.63
1:G:136:ARG:NH2	1:G:138:GLU:OE2	2.30	0.62
1:L:230:LYS:NZ	1:L:262:TYR:O	2.33	0.62
1:N:156:ILE:HG22	1:N:158:GLU:H	1.62	0.62
1:S:265:ASP:O	1:S:269:ARG:HG3	1.99	0.62
1:G:231:LEU:HD21	1:G:267:ILE:HG23	1.81	0.62
1:M:191:PRO:HD2	1:M:194:LEU:HD12	1.81	0.62
1:P:149:LEU:HA	1:P:209:PRO:HB2	1.82	0.62
1:A:156:ILE:HG22	1:A:158:GLU:H	1.65	0.62
1:A:277:LEU:HG	1:A:278:PRO:HA	1.82	0.61
1:N:219:HIS:NE2	1:N:250:LYS:O	2.33	0.61
1:T:187:PHE:HA	1:T:188:VAL:HG22	1.82	0.61
1:H:223:CYS:HA	1:H:259:ILE:HD11	1.81	0.61
1:P:234:TRP:HB2	1:P:239:ILE:HD11	1.82	0.61
1:A:244:ARG:NE	1:A:256:GLN:HE22	1.98	0.61
1:B:187:PHE:HA	1:B:188:VAL:HG22	1.82	0.61
1:W:252:ARG:NH2	1:W:255:ASP:OD2	2.25	0.61
1:Y:266:GLU:O	1:Y:270:ILE:HG12	2.01	0.61
1:M:136:ARG:NH2	1:N:188:VAL:O	2.33	0.61
1:S:191:PRO:HD2	1:S:194:LEU:HD12	1.83	0.60
1:V:152:ILE:HG12	1:V:211:LEU:HB3	1.82	0.60
1:S:152:ILE:HD11	1:S:175:LEU:HD12	1.83	0.60
1:T:136:ARG:NH1	1:V:188:VAL:O	2.31	0.60
1:I:277:LEU:HD12	1:I:278:PRO:HA	1.81	0.60
1:G:187:PHE:HA	1:G:188:VAL:HB	1.84	0.60
1:K:162:GLN:O	1:K:166:ASN:ND2	2.34	0.60
1:G:156:ILE:HD12	1:G:158:GLU:HB2	1.83	0.60
1:G:180:MET:HB2	1:G:220:ARG:HD2	1.82	0.60
1:G:221:THR:O	1:G:225:ILE:HG12	2.01	0.60
1:M:228:ILE:HA	1:M:231:LEU:HD12	1.82	0.60
1:W:152:ILE:HG21	1:W:168:LEU:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:PRO:HD2	1:G:194:LEU:HD12	1.84	0.60
1:M:216:ARG:HH22	1:M:250:LYS:HD3	1.66	0.60
1:K:233:ASN:ND2	1:P:113:ASN:O	2.31	0.59
1:A:254:LEU:HD22	1:C:136:ARG:HH11	1.66	0.59
1:L:160:TYR:HD2	1:L:165:LEU:HG	1.67	0.59
1:Q:244:ARG:HE	1:Q:256:GLN:HE22	1.50	0.59
1:R:219:HIS:NE2	1:R:250:LYS:O	2.34	0.59
1:C:116:VAL:HG21	1:C:146:ARG:HD3	1.85	0.59
1:Y:178:VAL:HG22	1:Y:197:LYS:HE2	1.83	0.59
1:C:230:LYS:NZ	1:C:262:TYR:O	2.31	0.58
1:B:141:SER:HB2	1:B:145:GLU:OE1	2.03	0.58
1:Y:217:GLY:N	2:Y:301:SO4:O4	2.37	0.58
1:E:183:ASN:O	1:E:184:LYS:HG2	2.04	0.58
1:E:244:ARG:HD2	3:E:407:HOH:O	2.02	0.58
1:M:124:HIS:HD1	1:M:130:TYR:HE1	1.52	0.58
1:K:156:ILE:HG22	1:K:158:GLU:H	1.68	0.58
1:B:187:PHE:HE1	1:B:252:ARG:HD2	1.69	0.58
1:W:141:SER:O	1:W:145:GLU:HB2	2.03	0.58
1:G:136:ARG:HH21	1:G:138:GLU:CD	2.07	0.57
1:R:152:ILE:HD12	1:R:168:LEU:HD21	1.85	0.57
1:H:182:GLY:HA2	1:H:220:ARG:NH1	2.19	0.57
1:K:117:ILE:HG12	1:P:235:SER:HB2	1.87	0.57
1:E:146:ARG:HH12	1:O:234:TRP:HE1	1.51	0.57
1:N:196:THR:O	1:N:200:GLU:HG3	2.04	0.57
1:B:113:ASN:HD21	1:V:277:LEU:HD11	1.70	0.57
1:M:277:LEU:HD12	1:M:278:PRO:HA	1.85	0.57
1:P:235:SER:O	1:P:239:ILE:HG12	2.04	0.57
1:W:198:ALA:O	1:W:202:VAL:HG13	2.05	0.57
1:M:230:LYS:HE3	1:M:264:ASP:HB3	1.84	0.56
1:S:277:LEU:HG	1:S:278:PRO:HA	1.86	0.56
1:I:185:GLU:HG2	1:I:186:PRO:HD2	1.87	0.56
1:D:257:GLN:NE2	1:F:138:GLU:OE1	2.37	0.56
1:K:187:PHE:HA	1:K:188:VAL:HG22	1.87	0.56
1:F:203:LEU:HD11	1:F:231:LEU:HD13	1.88	0.56
1:K:130:TYR:HH	1:P:281:TRP:HE3	1.53	0.56
1:V:187:PHE:HA	1:V:188:VAL:HB	1.86	0.56
1:Y:240:PHE:CD1	1:Y:256:GLN:HG2	2.41	0.56
1:C:188:VAL:HG12	1:C:254:LEU:HD13	1.88	0.56
1:J:152:ILE:HD12	1:J:168:LEU:HD21	1.86	0.56
1:T:202:VAL:O	1:T:208:GLN:NE2	2.35	0.56
1:A:244:ARG:NH2	1:T:241:ASP:OD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:191:PRO:HD2	1:Y:194:LEU:HD21	1.86	0.56
1:J:187:PHE:HA	1:J:188:VAL:HB	1.88	0.56
1:S:214:SER:OG	1:S:215:ASN:N	2.37	0.56
1:V:166:ASN:C	1:V:170:LEU:HD12	2.23	0.56
1:B:230:LYS:NZ	1:B:262:TYR:O	2.39	0.56
1:Q:199:LEU:HA	1:Q:202:VAL:HG22	1.87	0.56
1:C:166:ASN:O	1:C:170:LEU:HD23	2.06	0.56
1:A:187:PHE:HA	1:A:188:VAL:HB	1.88	0.55
1:K:223:CYS:HA	1:K:259:ILE:HD11	1.89	0.55
1:N:271:ALA:CB	1:N:277:LEU:CD2	2.84	0.55
1:T:184:LYS:NZ	3:T:401:HOH:O	2.22	0.55
1:X:265:ASP:OD2	1:X:269:ARG:NH2	2.40	0.55
1:N:187:PHE:HA	1:N:188:VAL:HB	1.88	0.55
1:I:225:ILE:HD13	1:I:228:ILE:HD12	1.88	0.55
1:T:219:HIS:NE2	1:T:250:LYS:O	2.40	0.55
1:E:214:SER:HB2	1:E:220:ARG:HH11	1.71	0.55
1:G:153:LEU:HD11	1:G:178:VAL:HG23	1.87	0.55
1:B:191:PRO:HD2	1:B:194:LEU:HD12	1.88	0.55
1:G:199:LEU:HA	1:G:202:VAL:HG22	1.89	0.55
1:A:152:ILE:HD11	1:A:168:LEU:HD11	1.89	0.55
1:Y:152:ILE:HD12	1:Y:168:LEU:HD21	1.89	0.55
1:H:181:SER:H	1:H:190:ILE:HD11	1.72	0.54
1:N:185:GLU:HG2	1:N:186:PRO:HD2	1.88	0.54
1:W:234:TRP:NE1	3:W:402:HOH:O	2.33	0.54
1:H:200:GLU:OE2	1:L:197:LYS:NZ	2.40	0.54
1:L:131:ARG:HD2	1:L:225:ILE:HD13	1.90	0.54
1:K:150:LYS:HG2	1:K:209:PRO:HD2	1.90	0.54
1:R:114:LYS:NZ	1:R:145:GLU:OE1	2.35	0.54
1:E:117:ILE:HD12	1:E:138:GLU:HB2	1.89	0.54
1:E:252:ARG:CZ	1:E:255:ASP:OD1	2.56	0.54
1:I:152:ILE:HD13	1:I:211:LEU:HB3	1.89	0.54
1:A:219:HIS:N	2:A:301:SO4:O4	2.34	0.54
1:O:152:ILE:HD13	1:O:211:LEU:HB3	1.88	0.54
1:S:151:SER:OG	1:S:207:ASN:O	2.25	0.54
1:E:231:LEU:HD21	1:E:267:ILE:HG23	1.89	0.54
1:L:149:LEU:HA	1:L:209:PRO:HB2	1.90	0.54
1:T:253:ALA:HA	1:T:256:GLN:OE1	2.08	0.54
1:O:187:PHE:HA	1:O:188:VAL:HB	1.90	0.54
1:N:166:ASN:OD1	1:R:114:LYS:NZ	2.41	0.54
1:D:156:ILE:O	1:D:177:GLN:NE2	2.40	0.54
1:L:202:VAL:O	1:L:208:GLN:NE2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:188:VAL:O	1:R:136:ARG:NH1	2.34	0.53
1:R:180:MET:HG3	1:R:194:LEU:HD23	1.90	0.53
1:F:277:LEU:HD12	1:F:278:PRO:HA	1.90	0.53
1:L:127:GLY:HA3	3:L:401:HOH:O	2.09	0.53
1:X:194:LEU:HD12	1:X:194:LEU:H	1.73	0.53
1:I:219:HIS:NE2	1:I:250:LYS:O	2.41	0.53
1:K:242:GLU:HG3	1:K:245:ARG:NH2	2.24	0.53
1:M:188:VAL:O	1:O:136:ARG:NH1	2.39	0.53
1:R:160:TYR:CE2	1:R:164:ASN:HB3	2.44	0.53
1:Y:136:ARG:NH1	1:Y:138:GLU:OE2	2.40	0.53
1:L:180:MET:HG2	1:L:194:LEU:HD13	1.90	0.53
1:T:157:PRO:HD3	1:T:180:MET:O	2.08	0.53
1:J:191:PRO:HD2	1:J:194:LEU:HD12	1.91	0.53
1:G:156:ILE:HG22	1:G:220:ARG:HH21	1.73	0.53
1:H:156:ILE:HD11	1:H:220:ARG:CZ	2.38	0.53
1:L:125:VAL:HG12	1:L:126:VAL:HG12	1.90	0.53
1:H:230:LYS:NZ	1:H:262:TYR:O	2.29	0.53
1:Q:134:PHE:HD1	1:Q:213:HIS:CE1	2.27	0.53
1:S:248:PHE:CG	1:S:249:PRO:HA	2.44	0.53
1:D:232:GLN:HG2	1:D:279:LEU:HD12	1.91	0.53
1:E:252:ARG:HH21	1:E:255:ASP:CG	2.11	0.53
1:O:159:GLU:OE1	1:P:273:LYS:HE2	2.08	0.53
1:S:134:PHE:CZ	1:S:161:PRO:HG2	2.44	0.53
1:E:160:TYR:CE2	1:E:164:ASN:HB3	2.44	0.53
1:H:212:ILE:HG22	1:H:221:THR:HG23	1.90	0.53
1:I:119:PRO:HG3	1:I:139:ASN:HB3	1.90	0.53
1:F:178:VAL:HG21	1:F:198:ALA:HB2	1.91	0.53
1:Q:136:ARG:HB2	1:Q:138:GLU:OE1	2.09	0.53
1:A:234:TRP:HE1	1:S:146:ARG:HH12	1.55	0.52
1:Q:187:PHE:HA	1:Q:188:VAL:CG2	2.39	0.52
1:A:219:HIS:NE2	1:A:250:LYS:O	2.36	0.52
1:G:266:GLU:HA	1:G:269:ARG:HE	1.75	0.52
1:N:271:ALA:HB1	1:N:277:LEU:HD22	1.91	0.52
1:B:264:ASP:N	1:B:264:ASP:OD1	2.38	0.52
1:L:168:LEU:HD22	1:L:173:ILE:HB	1.91	0.52
1:J:149:LEU:HA	1:J:209:PRO:HB2	1.90	0.52
1:M:154:VAL:HG22	1:M:156:ILE:HG12	1.92	0.52
1:M:216:ARG:HH21	1:M:219:HIS:CE1	2.28	0.52
1:P:187:PHE:HA	1:P:188:VAL:HB	1.91	0.52
1:T:270:ILE:HA	1:T:273:LYS:HG2	1.92	0.52
1:B:187:PHE:CE1	1:B:252:ARG:HD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ASN:O	1:V:233:ASN:ND2	2.40	0.52
1:A:117:ILE:HG21	1:B:257:GLN:HE22	1.73	0.52
1:Y:142:PHE:HE1	1:Y:146:ARG:HH21	1.57	0.52
1:L:248:PHE:CD1	1:L:249:PRO:HA	2.44	0.51
1:O:243:TYR:OH	1:O:255:ASP:OD2	2.22	0.51
1:S:134:PHE:HZ	1:S:161:PRO:HG2	1.75	0.51
1:Y:214:SER:OG	2:Y:301:SO4:O4	2.22	0.51
1:C:183:ASN:C	1:C:185:GLU:H	2.14	0.51
1:E:244:ARG:HD3	1:M:244:ARG:NE	2.07	0.51
1:J:167:PHE:O	1:J:171:THR:HG22	2.10	0.51
1:O:125:VAL:O	1:O:229:ARG:NH2	2.41	0.51
1:S:181:SER:OG	1:S:189:ASN:O	2.27	0.51
1:T:264:ASP:OD1	1:T:264:ASP:N	2.39	0.51
1:V:131:ARG:HG2	1:V:132:SER:N	2.24	0.51
1:W:268:LYS:HB2	1:W:268:LYS:NZ	2.25	0.51
1:D:228:ILE:HG22	1:D:232:GLN:HE21	1.75	0.51
1:F:180:MET:HG2	1:F:194:LEU:HD13	1.91	0.51
1:J:131:ARG:HD2	1:J:225:ILE:HD13	1.91	0.51
1:J:171:THR:HG23	1:J:173:ILE:H	1.74	0.51
1:S:165:LEU:HA	1:S:168:LEU:HD12	1.92	0.51
1:W:187:PHE:HA	1:W:188:VAL:HB	1.92	0.51
1:B:141:SER:O	1:B:145:GLU:OE2	2.28	0.51
1:H:183:ASN:C	1:H:185:GLU:H	2.13	0.51
1:E:244:ARG:CD	1:M:244:ARG:HE	2.08	0.51
1:S:255:ASP:HA	1:S:258:PHE:CD2	2.46	0.51
1:T:154:VAL:HG23	1:T:177:GLN:HG3	1.93	0.51
1:M:166:ASN:O	1:M:170:LEU:HG	2.10	0.51
1:F:146:ARG:NH2	1:N:279:LEU:O	2.44	0.51
1:T:231:LEU:HD21	1:T:267:ILE:HG23	1.92	0.51
1:Y:180:MET:HG3	1:Y:194:LEU:HD22	1.92	0.51
1:A:212:ILE:HG22	1:A:221:THR:HG23	1.93	0.51
1:B:176:TYR:HB3	1:B:201:ILE:HD13	1.93	0.51
1:W:214:SER:OG	1:W:215:ASN:N	2.44	0.51
1:D:261:MET:HE1	3:F:406:HOH:O	2.10	0.51
1:E:146:ARG:NH2	1:O:232:GLN:OE1	2.44	0.51
1:S:136:ARG:NH1	1:T:188:VAL:H	2.08	0.51
1:X:168:LEU:HD12	1:X:175:LEU:HD12	1.92	0.51
1:J:221:THR:HG22	1:J:225:ILE:HD12	1.93	0.51
1:R:156:ILE:HD11	1:R:214:SER:HA	1.92	0.51
1:S:162:GLN:O	1:S:165:LEU:HG	2.09	0.51
1:W:215:ASN:HB2	1:W:220:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:225:ILE:O	1:W:229:ARG:HG2	2.11	0.51
1:W:235:SER:HB3	1:W:238:MET:HG2	1.93	0.51
1:E:223:CYS:HA	1:E:259:ILE:HD11	1.93	0.50
1:L:128:GLU:N	3:L:401:HOH:O	2.22	0.50
1:V:160:TYR:HD2	1:V:165:LEU:HG	1.75	0.50
1:V:131:ARG:HG3	1:V:221:THR:HG21	1.92	0.50
1:E:168:LEU:HD13	1:E:175:LEU:HB2	1.93	0.50
1:F:131:ARG:NH2	1:F:217:GLY:O	2.34	0.50
1:G:188:VAL:O	1:I:136:ARG:NH1	2.44	0.50
1:W:219:HIS:HB3	1:W:252:ARG:NH2	2.26	0.50
1:E:228:ILE:HA	1:E:231:LEU:HD12	1.93	0.50
1:N:248:PHE:CD1	1:N:249:PRO:HA	2.46	0.50
1:V:225:ILE:O	1:V:229:ARG:HG2	2.11	0.50
1:C:152:ILE:HD12	1:C:168:LEU:HD21	1.93	0.50
1:N:271:ALA:HB3	1:N:277:LEU:CD2	2.41	0.50
1:P:248:PHE:CD1	1:P:249:PRO:HA	2.46	0.50
1:S:187:PHE:HA	1:S:188:VAL:HG22	1.92	0.50
1:T:191:PRO:HA	3:T:403:HOH:O	2.11	0.50
1:J:136:ARG:NH1	1:K:188:VAL:O	2.45	0.50
1:A:244:ARG:HD3	1:T:244:ARG:CZ	2.42	0.50
1:V:269:ARG:O	1:V:273:LYS:HG2	2.12	0.50
1:L:124:HIS:HD2	1:L:130:TYR:CZ	2.29	0.50
1:V:165:LEU:HD23	1:V:168:LEU:HD12	1.93	0.50
1:E:191:PRO:HD2	1:E:194:LEU:HD12	1.93	0.50
1:H:189:ASN:OD1	1:H:258:PHE:HZ	1.95	0.50
1:K:184:LYS:O	1:K:185:GLU:HG2	2.12	0.50
1:T:160:TYR:CE2	1:T:164:ASN:HB3	2.47	0.50
1:W:229:ARG:HD2	1:W:234:TRP:CE3	2.47	0.50
1:S:244:ARG:HE	1:S:256:GLN:HE22	1.59	0.49
1:V:174:LYS:HA	1:V:174:LYS:HE2	1.93	0.49
1:B:184:LYS:O	1:B:185:GLU:HG3	2.11	0.49
1:N:271:ALA:HB1	1:N:277:LEU:CD2	2.42	0.49
1:S:240:PHE:CD1	1:S:256:GLN:HG2	2.47	0.49
1:P:266:GLU:HB3	3:P:410:HOH:O	2.11	0.49
1:E:228:ILE:HG22	1:E:232:GLN:HE21	1.78	0.49
1:W:156:ILE:HG22	1:W:158:GLU:H	1.78	0.49
1:Y:125:VAL:HG12	1:Y:126:VAL:HG12	1.94	0.49
1:B:196:THR:O	1:B:200:GLU:HG3	2.12	0.49
1:C:188:VAL:HG21	1:C:252:ARG:HH12	1.78	0.49
1:M:144:HIS:O	1:M:148:LYS:HA	2.13	0.49
1:R:188:VAL:HG12	1:R:189:ASN:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:191:PRO:HD2	1:R:194:LEU:HD22	1.93	0.49
1:K:146:ARG:NH1	1:P:234:TRP:HE1	2.10	0.49
1:L:220:ARG:NE	2:L:301:SO4:O2	2.33	0.49
1:W:249:PRO:HG3	1:X:249:PRO:HB2	1.94	0.49
1:P:156:ILE:HG13	1:P:157:PRO:HD2	1.95	0.49
1:T:192:SER:HA	1:T:195:LEU:HD12	1.94	0.49
1:X:187:PHE:HA	1:X:188:VAL:CG1	2.42	0.49
1:P:160:TYR:HD2	1:P:165:LEU:HG	1.78	0.49
1:B:156:ILE:HG22	1:B:220:ARG:NH2	2.28	0.49
1:I:187:PHE:HA	1:I:188:VAL:HB	1.95	0.49
1:M:166:ASN:ND2	3:M:403:HOH:O	2.46	0.49
1:R:245:ARG:NH2	3:R:402:HOH:O	2.44	0.49
1:S:119:PRO:HD3	1:S:139:ASN:HB3	1.95	0.49
1:E:116:VAL:HG22	1:E:142:PHE:HB2	1.95	0.48
1:A:196:THR:O	1:A:200:GLU:HG3	2.14	0.48
1:G:244:ARG:CZ	1:G:256:GLN:HE22	2.26	0.48
1:H:125:VAL:HG12	1:H:126:VAL:HG12	1.95	0.48
1:N:223:CYS:HA	1:N:259:ILE:HD11	1.94	0.48
1:X:125:VAL:HG12	1:X:126:VAL:HG12	1.94	0.48
1:C:203:LEU:HD22	1:C:279:LEU:HD21	1.94	0.48
1:J:154:VAL:HG22	1:J:156:ILE:HG12	1.95	0.48
1:O:212:ILE:HG22	1:O:221:THR:HG23	1.95	0.48
1:B:160:TYR:CE2	1:B:164:ASN:HB3	2.48	0.48
1:D:221:THR:HG22	1:D:225:ILE:HD12	1.95	0.48
1:G:229:ARG:HD2	1:G:234:TRP:CZ3	2.47	0.48
1:W:199:LEU:HA	1:W:202:VAL:HG22	1.94	0.48
1:A:184:LYS:O	1:A:185:GLU:HG2	2.13	0.48
1:D:136:ARG:NH1	1:E:188:VAL:O	2.46	0.48
1:Q:134:PHE:CD1	1:Q:213:HIS:CE1	3.02	0.48
1:S:183:ASN:C	1:S:185:GLU:H	2.16	0.48
1:S:248:PHE:CD1	1:S:249:PRO:HA	2.49	0.48
1:T:116:VAL:HG21	1:T:146:ARG:HH11	1.79	0.48
1:I:144:HIS:HB2	1:I:167:PHE:HZ	1.79	0.48
1:K:131:ARG:HD2	1:K:225:ILE:HG13	1.95	0.48
1:O:219:HIS:NE2	1:O:250:LYS:O	2.45	0.48
1:Q:191:PRO:HD2	1:Q:194:LEU:HD12	1.95	0.48
1:V:183:ASN:O	1:V:185:GLU:N	2.47	0.48
1:M:218:LYS:NZ	1:M:248:PHE:O	2.43	0.48
1:Q:231:LEU:HD21	1:Q:267:ILE:HG23	1.95	0.48
1:W:278:PRO:O	1:W:280:GLN:NE2	2.47	0.48
1:X:143:LEU:HB3	1:X:149:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:LEU:HD12	1:C:279:LEU:HD12	1.96	0.48
1:H:122:PHE:HD1	1:H:132:SER:HB3	1.79	0.48
1:N:216:ARG:HH22	1:N:250:LYS:NZ	2.12	0.48
1:P:153:LEU:HD11	1:P:178:VAL:HG23	1.96	0.48
1:P:214:SER:OG	2:P:301:SO4:S	2.66	0.48
1:V:166:ASN:C	1:V:170:LEU:CD1	2.82	0.48
1:H:160:TYR:CE2	1:H:164:ASN:HB3	2.49	0.47
1:D:244:ARG:NE	1:N:244:ARG:HD3	2.29	0.47
1:P:248:PHE:CG	1:P:249:PRO:HA	2.49	0.47
1:V:244:ARG:HE	1:V:256:GLN:NE2	2.11	0.47
1:A:199:LEU:HA	1:A:202:VAL:HG22	1.96	0.47
1:C:187:PHE:HA	1:C:188:VAL:HB	1.96	0.47
1:L:195:LEU:HD13	1:L:227:CYS:SG	2.54	0.47
1:W:244:ARG:HB3	1:W:248:PHE:CZ	2.49	0.47
1:J:203:LEU:HD22	1:J:279:LEU:HD21	1.96	0.47
1:W:174:LYS:HD3	1:W:176:TYR:CZ	2.49	0.47
1:W:221:THR:O	1:W:225:ILE:HG12	2.13	0.47
1:X:132:SER:OG	1:X:133:SER:N	2.46	0.47
1:B:132:SER:HB3	1:B:211:LEU:HD11	1.97	0.47
1:C:153:LEU:HD11	1:C:178:VAL:HG23	1.97	0.47
1:N:116:VAL:HG11	1:N:146:ARG:HD3	1.95	0.47
1:P:214:SER:OG	2:P:301:SO4:O1	2.32	0.47
1:V:174:LYS:HA	1:V:174:LYS:CE	2.44	0.47
1:J:162:GLN:HA	1:J:165:LEU:HB2	1.96	0.47
1:K:160:TYR:HD2	1:K:165:LEU:HB2	1.79	0.47
1:O:136:ARG:NE	1:O:138:GLU:OE2	2.48	0.47
1:V:160:TYR:CE2	1:V:168:LEU:HD11	2.49	0.47
1:W:167:PHE:O	1:W:171:THR:OG1	2.20	0.47
1:G:266:GLU:HG3	1:G:269:ARG:HH21	1.79	0.47
1:K:225:ILE:O	1:K:229:ARG:HG2	2.14	0.47
1:W:225:ILE:HD13	1:W:228:ILE:HD12	1.97	0.47
1:M:230:LYS:CE	1:M:264:ASP:HB3	2.45	0.47
1:O:116:VAL:HG21	1:O:146:ARG:HH11	1.80	0.47
1:G:149:LEU:HA	1:G:209:PRO:HB2	1.97	0.47
1:T:223:CYS:HA	1:T:259:ILE:HD11	1.97	0.47
1:V:116:VAL:HG11	1:V:146:ARG:HD3	1.96	0.47
1:O:188:VAL:HG12	1:O:254:LEU:HD13	1.97	0.47
1:P:271:ALA:HB1	1:P:276:TRP:HB2	1.96	0.47
1:T:248:PHE:CD1	1:T:249:PRO:HA	2.49	0.47
1:B:141:SER:CB	1:B:145:GLU:OE1	2.63	0.47
1:P:228:ILE:O	1:P:232:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:220:ARG:NE	2:P:301:SO4:O3	2.36	0.47
1:X:155:LEU:HD12	1:X:214:SER:HB3	1.97	0.47
1:Y:225:ILE:O	1:Y:229:ARG:HG2	2.14	0.47
1:G:156:ILE:HG22	1:G:220:ARG:NH2	2.28	0.46
1:H:196:THR:O	1:H:200:GLU:HG3	2.14	0.46
1:K:125:VAL:HG22	1:K:131:ARG:HG3	1.96	0.46
1:N:212:ILE:HG22	1:N:221:THR:HG23	1.96	0.46
1:P:219:HIS:NE2	1:P:250:LYS:O	2.47	0.46
1:B:237:THR:HG21	1:S:257:GLN:HG3	1.97	0.46
1:F:223:CYS:HA	1:F:259:ILE:HD11	1.96	0.46
1:F:228:ILE:HA	1:F:231:LEU:HD12	1.97	0.46
1:S:155:LEU:O	1:S:220:ARG:NH1	2.47	0.46
1:S:160:TYR:CE2	1:S:164:ASN:HB3	2.50	0.46
1:E:143:LEU:HB3	1:E:149:LEU:HD12	1.97	0.46
1:I:231:LEU:HD21	1:I:267:ILE:HG23	1.96	0.46
1:J:225:ILE:HA	1:J:228:ILE:HD12	1.96	0.46
1:X:160:TYR:CE2	1:X:164:ASN:HB3	2.50	0.46
1:E:116:VAL:HG11	1:E:146:ARG:HH11	1.81	0.46
1:H:131:ARG:HG3	1:H:221:THR:HG21	1.96	0.46
1:Q:248:PHE:CD1	1:Q:249:PRO:HA	2.50	0.46
1:V:219:HIS:NE2	1:V:250:LYS:O	2.43	0.46
1:X:153:LEU:HA	1:X:176:TYR:O	2.14	0.46
1:Y:132:SER:OG	1:Y:133:SER:N	2.48	0.46
1:B:165:LEU:HB3	1:B:169:LYS:NZ	2.31	0.46
1:G:165:LEU:HD23	1:G:169:LYS:HE2	1.97	0.46
1:H:223:CYS:HB2	1:H:255:ASP:OD2	2.15	0.46
1:L:196:THR:O	1:L:200:GLU:HG3	2.15	0.46
1:M:165:LEU:HB3	1:M:169:LYS:NZ	2.30	0.46
1:M:225:ILE:O	1:M:229:ARG:HG2	2.15	0.46
1:Q:221:THR:O	1:Q:225:ILE:HG12	2.16	0.46
1:T:265:ASP:HA	1:T:268:LYS:HG2	1.97	0.46
1:E:183:ASN:C	1:E:185:GLU:H	2.18	0.46
1:Q:184:LYS:O	1:Q:185:GLU:CG	2.63	0.46
1:Y:176:TYR:HB3	1:Y:201:ILE:HD13	1.98	0.46
1:H:221:THR:HG22	1:H:225:ILE:HD12	1.98	0.46
1:N:226:GLY:HA3	1:N:259:ILE:HD13	1.97	0.46
1:C:152:ILE:HG12	1:C:211:LEU:HB3	1.98	0.46
1:E:154:VAL:HG22	1:E:156:ILE:HG12	1.96	0.46
1:L:154:VAL:HG12	1:L:213:HIS:CE1	2.51	0.46
1:M:254:LEU:H	1:M:254:LEU:HD12	1.81	0.46
1:K:183:ASN:C	1:K:185:GLU:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:221:THR:O	1:O:225:ILE:HG12	2.15	0.46
1:Y:257:GLN:O	1:Y:261:MET:HG2	2.16	0.46
1:N:171:THR:HG22	1:R:170:LEU:HG	1.98	0.46
1:O:183:ASN:C	1:O:185:GLU:H	2.18	0.46
1:P:136:ARG:NH1	1:Q:188:VAL:H	2.14	0.46
1:T:131:ARG:HD2	1:T:225:ILE:HD13	1.98	0.46
1:B:199:LEU:HA	1:B:202:VAL:HG22	1.98	0.45
1:Q:152:ILE:HG12	1:Q:211:LEU:HB3	1.98	0.45
1:S:207:ASN:N	1:S:207:ASN:HD22	2.13	0.45
1:T:217:GLY:N	2:T:301:SO4:O2	2.49	0.45
1:W:188:VAL:HG22	1:W:189:ASN:N	2.31	0.45
1:G:151:SER:O	1:G:210:ILE:HA	2.16	0.45
1:H:199:LEU:HA	1:H:202:VAL:HG22	1.99	0.45
1:I:185:GLU:HG2	1:I:186:PRO:CD	2.47	0.45
1:I:199:LEU:HA	1:I:202:VAL:HG22	1.98	0.45
1:M:137:GLN:HA	1:M:140:PHE:CE2	2.51	0.45
1:Q:160:TYR:HD2	1:Q:165:LEU:HG	1.81	0.45
1:S:193:HIS:O	1:S:196:THR:HG22	2.16	0.45
1:S:244:ARG:NE	1:S:256:GLN:HE22	2.13	0.45
1:W:153:LEU:HD11	1:W:178:VAL:HG22	1.97	0.45
1:A:180:MET:O	1:A:220:ARG:NH1	2.49	0.45
1:R:183:ASN:O	1:R:185:GLU:N	2.50	0.45
1:V:230:LYS:NZ	1:V:259:ILE:O	2.47	0.45
1:X:160:TYR:HB3	1:X:165:LEU:HD21	1.99	0.45
1:Y:219:HIS:HA	1:Y:243:TYR:OH	2.15	0.45
1:I:203:LEU:HD11	1:I:231:LEU:HD13	1.99	0.45
1:F:140:PHE:HB3	1:F:167:PHE:CZ	2.51	0.45
1:I:160:TYR:HD2	1:I:165:LEU:HG	1.81	0.45
1:J:234:TRP:HE1	1:Q:146:ARG:HH12	1.63	0.45
1:P:165:LEU:O	1:P:169:LYS:HG3	2.17	0.45
1:Y:194:LEU:HD12	1:Y:195:LEU:N	2.31	0.45
1:F:184:LYS:NZ	3:F:404:HOH:O	2.49	0.45
1:D:241:ASP:OD1	1:N:244:ARG:NH2	2.50	0.45
1:O:226:GLY:HA3	1:O:259:ILE:HD13	1.99	0.45
1:J:237:THR:HG21	1:R:257:GLN:HA	1.97	0.45
1:V:140:PHE:HB3	1:V:167:PHE:CZ	2.52	0.45
1:H:187:PHE:HA	1:H:188:VAL:HB	1.99	0.45
1:S:124:HIS:HD2	1:S:130:TYR:CE1	2.34	0.45
1:M:216:ARG:NH2	1:M:250:LYS:HD2	2.23	0.45
1:M:230:LYS:HD2	1:M:264:ASP:HB3	1.99	0.45
1:N:136:ARG:NH1	1:O:188:VAL:O	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:202:VAL:HG23	1:T:203:LEU:HD12	1.99	0.45
1:Y:162:GLN:NE2	1:Y:165:LEU:HD23	2.32	0.45
1:Y:178:VAL:CG1	1:Y:180:MET:HE2	2.47	0.45
1:H:152:ILE:HD12	1:H:168:LEU:HD21	1.99	0.45
1:J:235:SER:HB3	1:Q:117:ILE:HG12	1.99	0.45
1:N:157:PRO:HD3	1:N:180:MET:O	2.17	0.45
1:F:237:THR:HG23	1:O:256:GLN:HB2	1.98	0.45
1:X:212:ILE:HG22	1:X:221:THR:HG23	1.98	0.45
1:Y:248:PHE:CD1	1:Y:249:PRO:HA	2.52	0.45
1:D:150:LYS:HD3	1:D:208:GLN:O	2.16	0.45
1:F:126:VAL:HG13	1:F:129:ILE:HD12	1.99	0.45
1:G:136:ARG:NH1	1:H:254:LEU:HD11	2.32	0.45
1:N:221:THR:HG22	1:N:225:ILE:HD12	1.98	0.45
1:J:160:TYR:CE2	1:J:164:ASN:HB3	2.52	0.44
1:L:219:HIS:CD2	1:L:252:ARG:HD3	2.52	0.44
1:P:147:LEU:HB3	1:P:149:LEU:HG	1.98	0.44
1:T:182:GLY:HA2	1:T:220:ARG:NH1	2.31	0.44
1:V:197:LYS:HA	1:V:200:GLU:HG2	2.00	0.44
1:W:140:PHE:HB3	1:W:167:PHE:CE1	2.52	0.44
1:G:136:ARG:NH1	1:H:189:ASN:OD1	2.43	0.44
1:J:162:GLN:NE2	1:J:165:LEU:HD22	2.31	0.44
1:B:169:LYS:O	1:E:144:HIS:HE1	2.01	0.44
1:L:156:ILE:HG22	1:L:158:GLU:H	1.82	0.44
1:V:185:GLU:OE1	1:V:188:VAL:HA	2.18	0.44
1:X:248:PHE:CD1	1:X:249:PRO:HA	2.53	0.44
1:E:132:SER:HB3	1:E:211:LEU:HD11	1.99	0.44
1:F:184:LYS:HE2	1:F:184:LYS:HB2	1.87	0.44
1:H:131:ARG:HE	1:H:225:ILE:HD13	1.81	0.44
1:L:221:THR:HG22	1:L:225:ILE:HD12	1.99	0.44
1:S:225:ILE:HA	1:S:228:ILE:HD12	1.99	0.44
1:X:256:GLN:HA	1:X:259:ILE:HD12	2.00	0.44
1:D:199:LEU:HA	1:D:202:VAL:HG22	2.00	0.44
1:D:196:THR:O	1:D:200:GLU:HG3	2.17	0.44
1:G:153:LEU:HD21	1:G:198:ALA:HB1	1.99	0.44
1:J:265:ASP:OD2	3:J:401:HOH:O	2.21	0.44
1:O:125:VAL:HG12	1:O:126:VAL:HG12	2.00	0.44
1:O:225:ILE:HD13	1:O:228:ILE:HD12	1.99	0.44
1:S:199:LEU:HD12	1:S:231:LEU:HD11	1.99	0.44
1:C:146:ARG:HH12	1:T:232:GLN:HB3	1.82	0.44
1:E:229:ARG:HH11	1:E:232:GLN:HE22	1.66	0.44
1:H:155:LEU:C	1:H:156:ILE:HG12	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:125:VAL:HG23	1:J:126:VAL:H	1.82	0.44
1:K:146:ARG:HH22	1:P:232:GLN:CD	2.20	0.44
1:M:184:LYS:O	1:M:185:GLU:HG3	2.17	0.44
1:O:121:ASN:OD1	1:O:218:LYS:NZ	2.43	0.44
1:P:148:LYS:HD3	3:P:405:HOH:O	2.18	0.44
1:P:212:ILE:HG21	1:P:224:LEU:HD23	2.00	0.44
1:C:277:LEU:HD12	1:C:278:PRO:HA	2.00	0.44
1:F:185:GLU:HG3	1:F:186:PRO:HD2	1.98	0.44
1:I:124:HIS:NE2	1:I:127:GLY:O	2.48	0.44
1:Q:182:GLY:HA2	3:Q:408:HOH:O	2.18	0.44
1:R:119:PRO:HB2	1:R:132:SER:HB2	2.00	0.44
1:W:183:ASN:HA	1:W:188:VAL:CG2	2.47	0.44
1:F:221:THR:HG22	1:F:225:ILE:HD12	2.00	0.44
1:F:248:PHE:CG	1:F:249:PRO:HA	2.53	0.44
1:J:249:PRO:HG3	1:K:249:PRO:HB2	2.00	0.44
1:K:231:LEU:HD21	1:K:267:ILE:HG23	1.99	0.44
1:Q:248:PHE:CG	1:Q:249:PRO:HA	2.52	0.44
1:D:187:PHE:HA	1:D:188:VAL:HB	2.00	0.43
1:E:135:PRO:HB3	1:E:143:LEU:HD11	2.00	0.43
1:H:248:PHE:CD1	1:H:249:PRO:HA	2.53	0.43
1:I:132:SER:OG	1:I:133:SER:N	2.51	0.43
1:K:118:PRO:HB3	1:K:142:PHE:CE2	2.53	0.43
1:W:183:ASN:HA	1:W:188:VAL:HG21	2.00	0.43
1:X:218:LYS:NZ	1:X:246:PHE:O	2.50	0.43
1:W:188:VAL:O	1:Y:136:ARG:NH2	2.51	0.43
1:Y:154:VAL:HG21	1:Y:160:TYR:CE1	2.53	0.43
1:A:139:ASN:O	1:A:143:LEU:HG	2.17	0.43
1:E:265:ASP:HA	1:E:268:LYS:HG2	2.01	0.43
1:M:248:PHE:CG	1:M:249:PRO:HA	2.53	0.43
1:X:154:VAL:HG22	1:X:213:HIS:NE2	2.33	0.43
1:C:154:VAL:HG22	1:C:156:ILE:HG12	1.99	0.43
1:E:225:ILE:O	1:E:229:ARG:HG2	2.18	0.43
1:N:199:LEU:HA	1:N:202:VAL:HG22	2.00	0.43
1:P:146:ARG:HE	1:P:146:ARG:HA	1.83	0.43
1:R:119:PRO:HG3	1:R:139:ASN:HB3	2.00	0.43
1:F:134:PHE:HZ	1:F:161:PRO:HG2	1.83	0.43
1:Q:136:ARG:NH1	1:R:188:VAL:O	2.52	0.43
1:R:195:LEU:O	1:R:199:LEU:HG	2.18	0.43
1:V:266:GLU:HG2	1:V:267:ILE:N	2.33	0.43
1:B:143:LEU:HB3	1:B:149:LEU:HD12	1.99	0.43
1:N:264:ASP:OD1	1:N:264:ASP:N	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:204:ASN:HB3	1:R:207:ASN:HD22	1.83	0.43
1:R:231:LEU:HD21	1:R:267:ILE:HG23	2.00	0.43
1:S:154:VAL:HG22	1:S:213:HIS:CE1	2.54	0.43
1:T:187:PHE:HA	1:T:188:VAL:CG2	2.48	0.43
1:E:199:LEU:HA	1:E:202:VAL:HG22	2.01	0.43
1:E:265:ASP:HA	1:E:268:LYS:HE2	2.01	0.43
1:Q:183:ASN:C	1:Q:185:GLU:H	2.22	0.43
1:S:154:VAL:HG22	1:S:213:HIS:NE2	2.34	0.43
1:E:182:GLY:HA2	1:E:220:ARG:HH21	1.83	0.43
1:F:119:PRO:HB2	1:F:132:SER:HB2	2.00	0.43
1:S:218:LYS:HB3	1:S:247:ALA:HA	2.00	0.43
1:W:136:ARG:NH1	1:W:138:GLU:OE2	2.51	0.43
1:X:149:LEU:HA	1:X:209:PRO:HB2	1.99	0.43
1:X:193:HIS:O	1:X:196:THR:HG22	2.18	0.43
1:G:225:ILE:O	1:G:229:ARG:HG2	2.19	0.43
1:G:244:ARG:NE	1:G:256:GLN:HE22	2.17	0.43
1:Q:125:VAL:HG11	1:Q:225:ILE:HD12	2.01	0.43
1:B:229:ARG:NH2	1:B:242:GLU:OE2	2.49	0.43
1:C:257:GLN:HA	1:C:260:GLU:HG2	2.00	0.43
1:G:126:VAL:HG13	1:G:129:ILE:HD12	2.00	0.43
1:I:264:ASP:O	1:I:268:LYS:HG3	2.19	0.43
1:P:218:LYS:HG2	1:P:247:ALA:HA	2.01	0.43
1:Q:158:GLU:HG2	1:Q:159:GLU:N	2.33	0.43
1:F:245:ARG:HD3	3:F:405:HOH:O	2.17	0.42
1:G:265:ASP:O	1:G:269:ARG:HG3	2.19	0.42
1:I:265:ASP:O	1:I:269:ARG:HG3	2.19	0.42
1:J:264:ASP:O	1:J:268:LYS:HB3	2.19	0.42
1:A:147:LEU:HD23	1:A:149:LEU:HD21	2.00	0.42
1:I:154:VAL:HG13	1:I:213:HIS:CE1	2.53	0.42
1:W:219:HIS:N	2:W:301:SO4:S	2.92	0.42
1:B:160:TYR:HA	1:B:161:PRO:HD3	1.93	0.42
1:L:225:ILE:O	1:L:229:ARG:HG2	2.20	0.42
1:O:137:GLN:HA	1:O:140:PHE:CD2	2.54	0.42
1:T:183:ASN:C	1:T:185:GLU:H	2.22	0.42
1:T:188:VAL:HG23	1:T:254:LEU:HD12	2.02	0.42
1:V:157:PRO:HD3	1:V:180:MET:O	2.19	0.42
1:C:161:PRO:HB2	1:C:164:ASN:HD22	1.84	0.42
1:H:255:ASP:O	1:H:259:ILE:HG12	2.20	0.42
1:K:203:LEU:HD11	1:K:231:LEU:HD13	2.01	0.42
1:L:183:ASN:O	1:L:185:GLU:N	2.52	0.42
1:N:244:ARG:NE	1:N:256:GLN:HE22	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLU:OE1	1:A:186:PRO:HD2	2.19	0.42
1:E:146:ARG:HE	1:O:281:TRP:HE1	1.67	0.42
1:F:191:PRO:HD2	1:F:194:LEU:HD12	2.01	0.42
1:J:125:VAL:HG12	3:J:413:HOH:O	2.19	0.42
1:O:168:LEU:HD22	1:O:173:ILE:HB	2.01	0.42
1:R:181:SER:CB	1:R:184:LYS:HB2	2.48	0.42
1:B:141:SER:CA	1:B:145:GLU:OE2	2.63	0.42
1:X:242:GLU:HG3	1:X:245:ARG:NH2	2.34	0.42
1:E:157:PRO:HD3	1:E:180:MET:O	2.19	0.42
1:G:216:ARG:NH2	2:G:301:SO4:O3	2.48	0.42
1:I:225:ILE:O	1:I:229:ARG:HG2	2.19	0.42
1:K:225:ILE:HD13	1:K:228:ILE:HD12	2.02	0.42
1:W:215:ASN:H	1:W:220:ARG:HH21	1.67	0.42
1:W:218:LYS:N	2:W:301:SO4:S	2.93	0.42
1:W:252:ARG:HH21	1:W:255:ASP:CG	2.17	0.42
1:A:137:GLN:HA	1:A:140:PHE:CE2	2.55	0.42
1:B:185:GLU:O	1:B:187:PHE:N	2.53	0.42
1:J:242:GLU:HG3	1:J:245:ARG:NH2	2.34	0.42
1:M:165:LEU:O	1:M:169:LYS:HG3	2.20	0.42
1:M:183:ASN:HA	1:M:188:VAL:HG12	2.02	0.42
1:N:139:ASN:O	1:N:143:LEU:HG	2.20	0.42
1:S:168:LEU:O	1:S:172:GLY:N	2.49	0.42
1:F:225:ILE:HA	1:F:228:ILE:HD12	2.02	0.42
1:W:214:SER:HB3	2:W:301:SO4:O2	2.19	0.42
1:X:156:ILE:O	1:X:177:GLN:NE2	2.53	0.42
1:X:243:TYR:OH	1:X:255:ASP:OD2	2.36	0.42
1:B:212:ILE:HG22	1:B:221:THR:HG23	2.02	0.42
1:C:182:GLY:H	1:C:184:LYS:NZ	2.18	0.42
1:L:160:TYR:HA	1:L:161:PRO:HD3	1.96	0.42
1:O:248:PHE:CG	1:O:249:PRO:HA	2.54	0.42
1:P:254:LEU:HA	1:P:254:LEU:HD13	1.87	0.42
1:S:150:LYS:C	1:S:173:ILE:HG23	2.40	0.42
1:A:223:CYS:HA	1:A:259:ILE:HD11	2.02	0.41
1:Q:152:ILE:HD12	1:Q:168:LEU:HD21	2.02	0.41
1:V:119:PRO:HB2	1:V:132:SER:HB2	2.02	0.41
1:W:113:ASN:N	3:W:404:HOH:O	2.52	0.41
1:W:212:ILE:HG21	1:W:224:LEU:HD23	2.01	0.41
1:C:216:ARG:HH11	1:C:219:HIS:HE1	1.68	0.41
1:I:191:PRO:HD2	1:I:194:LEU:HD12	2.02	0.41
1:K:169:LYS:HD3	1:K:169:LYS:HA	1.86	0.41
1:M:231:LEU:HD21	1:M:267:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:199:LEU:HB3	1:S:267:ILE:HG12	2.01	0.41
1:W:167:PHE:CE1	1:W:171:THR:HG21	2.55	0.41
1:X:265:ASP:O	1:X:268:LYS:HG3	2.19	0.41
1:L:204:ASN:HB3	1:L:207:ASN:HD22	1.84	0.41
1:D:234:TRP:HE1	1:M:146:ARG:HH12	1.67	0.41
1:R:131:ARG:HD2	1:R:225:ILE:HD13	2.01	0.41
1:S:160:TYR:HA	1:S:161:PRO:HD3	1.96	0.41
1:S:236:LEU:HD12	1:S:239:ILE:HD12	2.02	0.41
1:T:119:PRO:HG3	1:T:139:ASN:HB3	2.03	0.41
1:A:226:GLY:HA3	1:A:259:ILE:HD13	2.02	0.41
1:J:252:ARG:HH21	1:J:255:ASP:CG	2.22	0.41
1:Q:225:ILE:O	1:Q:229:ARG:HG2	2.21	0.41
1:T:154:VAL:HG11	1:T:160:TYR:CE1	2.55	0.41
1:W:151:SER:O	1:W:210:ILE:HA	2.20	0.41
1:X:219:HIS:NE2	1:X:250:LYS:O	2.49	0.41
1:X:257:GLN:O	1:X:260:GLU:HG3	2.20	0.41
1:A:203:LEU:HD11	1:A:231:LEU:HD13	2.02	0.41
1:A:248:PHE:CD1	1:A:249:PRO:HA	2.56	0.41
1:O:225:ILE:O	1:O:229:ARG:HG2	2.20	0.41
1:S:143:LEU:HD23	1:S:147:LEU:HD12	2.02	0.41
1:W:220:ARG:N	2:W:301:SO4:O1	2.41	0.41
1:D:146:ARG:HD2	1:D:146:ARG:HA	1.83	0.41
1:G:223:CYS:HA	1:G:259:ILE:HD11	2.03	0.41
1:O:223:CYS:HA	1:O:259:ILE:HD11	2.01	0.41
1:K:146:ARG:HG2	1:P:281:TRP:CD1	2.56	0.41
1:Q:226:GLY:HA3	1:Q:259:ILE:HD13	2.02	0.41
1:X:225:ILE:O	1:X:229:ARG:HG2	2.20	0.41
1:Y:203:LEU:HD11	1:Y:231:LEU:HD12	2.02	0.41
1:E:189:ASN:OD1	1:E:190:ILE:N	2.54	0.41
1:I:149:LEU:HD13	1:I:152:ILE:HD11	2.02	0.41
1:N:263:ASP:O	3:N:401:HOH:O	2.22	0.41
1:A:225:ILE:O	1:A:229:ARG:HG2	2.20	0.41
1:C:124:HIS:HB3	1:T:124:HIS:HB3	2.02	0.41
1:C:168:LEU:HD22	1:C:173:ILE:HB	2.02	0.41
1:F:240:PHE:CD1	1:F:256:GLN:HG2	2.56	0.41
1:J:277:LEU:HG	1:J:278:PRO:HA	2.03	0.41
1:K:124:HIS:HE1	1:K:127:GLY:O	2.04	0.41
1:M:230:LYS:CD	1:M:264:ASP:HB3	2.51	0.41
1:N:185:GLU:HG2	1:N:186:PRO:CD	2.51	0.41
1:P:183:ASN:HA	1:P:188:VAL:HG23	2.03	0.41
1:S:255:ASP:HA	1:S:258:PHE:HD2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:HIS:HA	1:E:130:TYR:HD1	1.86	0.41
1:V:125:VAL:HG12	1:V:126:VAL:HG12	2.03	0.41
1:A:191:PRO:HD2	1:A:194:LEU:HD12	2.01	0.41
1:F:225:ILE:O	1:F:229:ARG:HG2	2.21	0.41
1:H:149:LEU:HA	1:H:209:PRO:HB2	2.02	0.41
3:K:411:HOH:O	1:P:142:PHE:HE1	2.03	0.41
1:S:166:ASN:O	1:S:170:LEU:HD13	2.21	0.41
1:S:149:LEU:HD13	1:S:211:LEU:HB2	2.02	0.41
1:B:117:ILE:HD12	1:B:138:GLU:HB2	2.04	0.40
1:F:122:PHE:HA	1:F:131:ARG:O	2.21	0.40
1:H:190:ILE:HA	1:H:191:PRO:HD3	1.89	0.40
1:P:168:LEU:HD22	1:P:173:ILE:HB	2.03	0.40
1:K:244:ARG:CZ	1:Q:244:ARG:HD2	2.51	0.40
1:R:235:SER:OG	1:R:238:MET:HG2	2.20	0.40
1:Y:153:LEU:HD11	1:Y:178:VAL:HG23	2.03	0.40
1:K:156:ILE:O	1:K:177:GLN:NE2	2.49	0.40
1:L:150:LYS:HG3	1:L:209:PRO:HD2	2.03	0.40
1:L:187:PHE:CA	1:L:188:VAL:HG23	2.38	0.40
1:N:131:ARG:HG3	1:N:221:THR:HG21	2.03	0.40
1:T:176:TYR:HB3	1:T:201:ILE:HD13	2.03	0.40
1:V:254:LEU:HG	3:V:408:HOH:O	2.20	0.40
1:E:281:TRP:HE1	1:O:146:ARG:NH2	2.19	0.40
1:J:117:ILE:HD12	1:J:138:GLU:HB2	2.03	0.40
1:Q:257:GLN:HG2	1:Q:261:MET:HE2	2.03	0.40
1:X:149:LEU:HD23	1:X:209:PRO:HB2	2.04	0.40
1:L:124:HIS:HD2	1:L:130:TYR:CE1	2.39	0.40
1:O:119:PRO:HG3	1:O:139:ASN:HB3	2.03	0.40
1:C:234:TRP:HA	1:T:116:VAL:O	2.21	0.40
1:T:136:ARG:NH1	1:V:188:VAL:H	2.19	0.40
1:B:113:ASN:ND2	1:V:277:LEU:HD11	2.34	0.40
1:W:207:ASN:O	1:W:210:ILE:HB	2.22	0.40
1:W:226:GLY:HA3	1:W:259:ILE:HD13	2.03	0.40
1:A:140:PHE:HB3	1:A:167:PHE:CZ	2.57	0.40
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.88	0.40
1:E:203:LEU:HD11	1:E:231:LEU:HD13	2.02	0.40
1:O:160:TYR:HD2	1:O:165:LEU:HG	1.86	0.40
1:E:146:ARG:HH21	1:O:281:TRP:HE1	1.70	0.40
1:P:181:SER:OG	1:P:184:LYS:HB2	2.21	0.40
1:V:230:LYS:NZ	1:V:262:TYR:HB3	2.37	0.40
1:Y:187:PHE:HA	1:Y:188:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	167/169 (99%)	158 (95%)	9 (5%)	0	100	100
1	B	167/169 (99%)	156 (93%)	11 (7%)	0	100	100
1	C	167/169 (99%)	156 (93%)	10 (6%)	1 (1%)	27	46
1	D	167/169 (99%)	157 (94%)	10 (6%)	0	100	100
1	E	167/169 (99%)	155 (93%)	10 (6%)	2 (1%)	14	26
1	F	167/169 (99%)	159 (95%)	8 (5%)	0	100	100
1	G	167/169 (99%)	157 (94%)	10 (6%)	0	100	100
1	H	167/169 (99%)	158 (95%)	9 (5%)	0	100	100
1	I	167/169 (99%)	157 (94%)	10 (6%)	0	100	100
1	J	167/169 (99%)	158 (95%)	9 (5%)	0	100	100
1	K	167/169 (99%)	157 (94%)	10 (6%)	0	100	100
1	L	167/169 (99%)	155 (93%)	12 (7%)	0	100	100
1	M	167/169 (99%)	156 (93%)	11 (7%)	0	100	100
1	N	167/169 (99%)	157 (94%)	10 (6%)	0	100	100
1	O	167/169 (99%)	157 (94%)	10 (6%)	0	100	100
1	P	167/169 (99%)	155 (93%)	12 (7%)	0	100	100
1	Q	167/169 (99%)	157 (94%)	10 (6%)	0	100	100
1	R	167/169 (99%)	158 (95%)	9 (5%)	0	100	100
1	S	167/169 (99%)	157 (94%)	10 (6%)	0	100	100
1	T	164/169 (97%)	153 (93%)	11 (7%)	0	100	100
1	V	167/169 (99%)	157 (94%)	9 (5%)	1 (1%)	27	46
1	W	167/169 (99%)	156 (93%)	11 (7%)	0	100	100
1	X	167/169 (99%)	156 (93%)	11 (7%)	0	100	100
1	Y	167/169 (99%)	156 (93%)	11 (7%)	0	100	100
All	All	4005/4056 (99%)	3758 (94%)	243 (6%)	4 (0%)	53	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	184	LYS
1	C	184	LYS
1	E	184	LYS
1	E	188	VAL

### 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	156/156 (100%)	153 (98%)	3 (2%)	60	83
1	B	156/156 (100%)	156 (100%)	0	100	100
1	C	156/156 (100%)	154 (99%)	2 (1%)	71	89
1	D	156/156 (100%)	156 (100%)	0	100	100
1	E	156/156 (100%)	155 (99%)	1 (1%)	87	96
1	F	155/156 (99%)	155 (100%)	0	100	100
1	G	156/156 (100%)	154 (99%)	2 (1%)	71	89
1	H	155/156 (99%)	153 (99%)	2 (1%)	71	89
1	I	155/156 (99%)	154 (99%)	1 (1%)	87	96
1	J	156/156 (100%)	155 (99%)	1 (1%)	87	96
1	K	156/156 (100%)	155 (99%)	1 (1%)	87	96
1	L	155/156 (99%)	153 (99%)	2 (1%)	71	89
1	M	156/156 (100%)	154 (99%)	2 (1%)	71	89
1	N	156/156 (100%)	155 (99%)	1 (1%)	87	96
1	O	155/156 (99%)	155 (100%)	0	100	100
1	P	156/156 (100%)	155 (99%)	1 (1%)	87	96
1	Q	155/156 (99%)	155 (100%)	0	100	100
1	R	156/156 (100%)	155 (99%)	1 (1%)	87	96
1	S	155/156 (99%)	150 (97%)	5 (3%)	42	69
1	T	155/156 (99%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	156/156 (100%)	153 (98%)	3 (2%)	60	83
1	W	156/156 (100%)	155 (99%)	1 (1%)	87	96
1	X	153/156 (98%)	152 (99%)	1 (1%)	85	95
1	Y	156/156 (100%)	155 (99%)	1 (1%)	87	96
All	All	3733/3744 (100%)	3702 (99%)	31 (1%)	83	94

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

Mol	Chain	Res	Type
1	A	148	LYS
1	A	220	ARG
1	A	273	LYS
1	C	216	ARG
1	C	265	ASP
1	E	160	TYR
1	G	184	LYS
1	G	216	ARG
1	H	220	ARG
1	H	231	LEU
1	I	174	LYS
1	J	220	ARG
1	K	184	LYS
1	L	220	ARG
1	L	252	ARG
1	M	123	SER
1	M	216	ARG
1	N	216	ARG
1	P	220	ARG
1	R	113	ASN
1	S	171	THR
1	S	175	LEU
1	S	207	ASN
1	S	214	SER
1	S	223	CYS
1	V	174	LYS
1	V	175	LEU
1	V	265	ASP
1	W	220	ARG
1	X	268	LYS
1	Y	194	LEU



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	B	257	GLN
1	B	280	GLN
1	E	144	HIS
1	F	183	ASN
1	F	256	GLN
1	G	137	GLN
1	I	256	GLN
1	J	162	GLN
1	K	166	ASN
1	K	256	GLN
1	N	113	ASN
1	N	256	GLN
1	O	162	GLN
1	O	166	ASN
1	O	177	GLN
1	Q	213	HIS
1	W	189	ASN
1	Y	162	GLN

### 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](#)

24 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	SO4	A	301	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	B	301	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	C	301	-	4,4,4	0.19	0	6,6,6	0.08	0
2	SO4	D	301	-	4,4,4	0.17	0	6,6,6	0.08	0
2	SO4	E	301	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	F	301	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	G	301	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	H	301	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	I	301	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	J	301	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	K	301	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	L	301	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	M	301	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	N	301	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	O	301	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	P	301	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	Q	301	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	R	301	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	S	301	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	T	301	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	V	301	-	4,4,4	0.17	0	6,6,6	0.12	0
2	SO4	W	301	-	4,4,4	0.11	0	6,6,6	0.39	0
2	SO4	X	301	-	4,4,4	0.17	0	6,6,6	0.08	0
2	SO4	Y	301	-	4,4,4	0.17	0	6,6,6	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	B	301	-	-	0/0/0/0	0/0/0/0
2	SO4	C	301	-	-	0/0/0/0	0/0/0/0
2	SO4	D	301	-	-	0/0/0/0	0/0/0/0
2	SO4	E	301	-	-	0/0/0/0	0/0/0/0
2	SO4	F	301	-	-	0/0/0/0	0/0/0/0
2	SO4	G	301	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	H	301	-	-	0/0/0/0	0/0/0/0
2	SO4	I	301	-	-	0/0/0/0	0/0/0/0
2	SO4	J	301	-	-	0/0/0/0	0/0/0/0
2	SO4	K	301	-	-	0/0/0/0	0/0/0/0
2	SO4	L	301	-	-	0/0/0/0	0/0/0/0
2	SO4	M	301	-	-	0/0/0/0	0/0/0/0
2	SO4	N	301	-	-	0/0/0/0	0/0/0/0
2	SO4	O	301	-	-	0/0/0/0	0/0/0/0
2	SO4	P	301	-	-	0/0/0/0	0/0/0/0
2	SO4	Q	301	-	-	0/0/0/0	0/0/0/0
2	SO4	R	301	-	-	0/0/0/0	0/0/0/0
2	SO4	S	301	-	-	0/0/0/0	0/0/0/0
2	SO4	T	301	-	-	0/0/0/0	0/0/0/0
2	SO4	V	301	-	-	0/0/0/0	0/0/0/0
2	SO4	W	301	-	-	0/0/0/0	0/0/0/0
2	SO4	X	301	-	-	0/0/0/0	0/0/0/0
2	SO4	Y	301	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	SO4	1	0
2	G	301	SO4	1	0
2	H	301	SO4	1	0
2	L	301	SO4	1	0
2	P	301	SO4	3	0
2	T	301	SO4	1	0
2	W	301	SO4	5	0
2	Y	301	SO4	2	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	169/169 (100%)	1.28	34 (20%) 1 1	34, 52, 69, 84	0
1	B	169/169 (100%)	1.28	32 (18%) 1 1	32, 47, 70, 92	0
1	C	169/169 (100%)	1.31	35 (20%) 1 0	27, 46, 77, 107	0
1	D	169/169 (100%)	1.20	31 (18%) 1 1	29, 48, 70, 100	0
1	E	169/169 (100%)	1.26	31 (18%) 1 1	34, 45, 75, 103	0
1	F	169/169 (100%)	1.44	36 (21%) 1 0	36, 48, 70, 99	0
1	G	169/169 (100%)	1.47	40 (23%) 0 0	35, 53, 75, 97	0
1	H	169/169 (100%)	1.47	44 (26%) 0 0	44, 55, 76, 99	0
1	I	169/169 (100%)	1.43	41 (24%) 0 0	42, 54, 80, 94	0
1	J	169/169 (100%)	1.42	38 (22%) 0 0	35, 50, 81, 108	0
1	K	169/169 (100%)	1.49	31 (18%) 1 1	40, 53, 79, 110	0
1	L	169/169 (100%)	1.41	43 (25%) 0 0	39, 53, 67, 81	0
1	M	169/169 (100%)	1.26	33 (19%) 1 1	38, 50, 74, 87	0
1	N	169/169 (100%)	1.23	29 (17%) 1 1	35, 48, 66, 102	0
1	O	169/169 (100%)	1.26	31 (18%) 1 1	35, 48, 70, 83	0
1	P	169/169 (100%)	1.45	39 (23%) 0 0	37, 52, 72, 107	0
1	Q	169/169 (100%)	1.41	33 (19%) 1 1	33, 47, 78, 124	0
1	R	169/169 (100%)	1.35	40 (23%) 0 0	32, 47, 72, 110	0
1	S	169/169 (100%)	1.90	74 (43%) 0 0	42, 69, 92, 100	0
1	T	168/169 (99%)	1.61	44 (26%) 0 0	34, 57, 86, 102	0
1	V	169/169 (100%)	1.84	58 (34%) 0 0	33, 57, 95, 126	0
1	W	169/169 (100%)	2.68	94 (55%) 0 0	50, 72, 112, 131	0
1	X	169/169 (100%)	1.92	58 (34%) 0 0	36, 63, 115, 154	0
1	Y	169/169 (100%)	1.97	71 (42%) 0 0	33, 63, 84, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4055/4056 (99%)	1.51	1040 (25%) 0 0	27, 52, 84, 154	0

All (1040) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	182	GLY	24.0
1	J	186	PRO	21.1
1	W	187	PHE	15.6
1	X	185	GLU	13.2
1	F	186	PRO	11.0
1	W	175	LEU	10.8
1	X	186	PRO	10.4
1	X	184	LYS	9.5
1	E	185	GLU	9.0
1	Y	178	VAL	8.5
1	S	160	TYR	8.5
1	K	188	VAL	8.4
1	W	219	HIS	8.4
1	G	185	GLU	8.3
1	W	239	ILE	8.3
1	R	188	VAL	8.1
1	T	188	VAL	8.1
1	Y	186	PRO	8.0
1	Y	185	GLU	7.9
1	H	187	PHE	7.8
1	G	184	LYS	7.8
1	K	184	LYS	7.4
1	I	254	LEU	7.1
1	K	251	ALA	7.1
1	S	188	VAL	7.1
1	L	186	PRO	7.1
1	Q	185	GLU	7.0
1	I	279	LEU	6.9
1	K	186	PRO	6.9
1	K	187	PHE	6.8
1	Q	116	VAL	6.7
1	T	276	TRP	6.6
1	W	276	TRP	6.6
1	X	277	LEU	6.6
1	P	186	PRO	6.6
1	O	185	GLU	6.6
1	Q	187	PHE	6.5

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Mol	Chain	Res	Type	RSRZ
1	Y	196	THR	6.5
1	W	198	ALA	6.4
1	F	188	VAL	6.4
1	D	188	VAL	6.4
1	T	185	GLU	6.3
1	E	186	PRO	6.3
1	W	114	LYS	6.3
1	Y	200	GLU	6.2
1	B	187	PHE	6.2
1	V	194	LEU	6.2
1	X	214	SER	6.2
1	W	149	LEU	6.2
1	M	186	PRO	6.1
1	X	259	ILE	6.1
1	Y	195	LEU	6.1
1	T	178	VAL	6.0
1	W	173	ILE	5.9
1	G	270	ILE	5.9
1	X	167	PHE	5.8
1	X	187	PHE	5.8
1	T	266	GLU	5.7
1	W	206	ALA	5.7
1	W	185	GLU	5.7
1	Q	188	VAL	5.6
1	X	190	ILE	5.6
1	S	200	GLU	5.6
1	W	119	PRO	5.6
1	Y	275	ASN	5.6
1	W	197	LYS	5.5
1	H	277	LEU	5.5
1	Q	186	PRO	5.5
1	T	180	MET	5.5
1	G	186	PRO	5.5
1	T	254	LEU	5.5
1	V	187	PHE	5.4
1	T	195	LEU	5.4
1	F	187	PHE	5.4
1	W	143	LEU	5.4
1	W	125	VAL	5.3
1	W	188	VAL	5.3
1	W	258	PHE	5.2
1	T	270	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	V	183	ASN	5.2
1	Y	254	LEU	5.2
1	Y	180	MET	5.2
1	D	185	GLU	5.2
1	Y	179	GLY	5.1
1	W	150	LYS	5.1
1	S	161	PRO	5.1
1	P	187	PHE	5.1
1	W	178	VAL	5.1
1	W	235	SER	5.1
1	C	184	LYS	5.0
1	G	160	TYR	5.0
1	P	249	PRO	5.0
1	B	185	GLU	5.0
1	K	250	LYS	5.0
1	W	180	MET	5.0
1	S	207	ASN	5.0
1	X	258	PHE	5.0
1	T	162	GLN	5.0
1	W	231	LEU	4.9
1	T	167	PHE	4.9
1	W	115	GLU	4.9
1	X	156	ILE	4.9
1	N	188	VAL	4.9
1	H	186	PRO	4.9
1	J	173	ILE	4.9
1	F	185	GLU	4.9
1	Y	273	LYS	4.9
1	V	189	ASN	4.8
1	K	156	ILE	4.8
1	B	250	LYS	4.8
1	V	184	LYS	4.8
1	C	248	PHE	4.8
1	B	227	CYS	4.8
1	I	267	ILE	4.8
1	B	279	LEU	4.7
1	R	226	GLY	4.7
1	C	187	PHE	4.7
1	V	156	ILE	4.7
1	P	206	ALA	4.7
1	Q	184	LYS	4.7
1	B	223	CYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	R	167	PHE	4.7
1	M	277	LEU	4.7
1	S	173	ILE	4.7
1	C	185	GLU	4.6
1	Y	272	SER	4.6
1	F	237	THR	4.6
1	G	247	ALA	4.6
1	X	154	VAL	4.5
1	V	157	PRO	4.5
1	P	185	GLU	4.5
1	S	259	ILE	4.5
1	T	183	ASN	4.5
1	A	281	TRP	4.5
1	I	186	PRO	4.5
1	P	188	VAL	4.5
1	W	186	PRO	4.5
1	Y	182	GLY	4.5
1	D	236	LEU	4.4
1	C	267	ILE	4.4
1	W	211	LEU	4.4
1	M	113	ASN	4.4
1	H	228	ILE	4.4
1	W	248	PHE	4.4
1	R	185	GLU	4.4
1	V	276	TRP	4.4
1	N	184	LYS	4.3
1	K	236	LEU	4.3
1	Y	175	LEU	4.3
1	S	176	TYR	4.3
1	V	188	VAL	4.3
1	P	190	ILE	4.3
1	P	237	THR	4.3
1	W	193	HIS	4.3
1	G	165	LEU	4.3
1	W	223	CYS	4.3
1	S	152	ILE	4.3
1	M	185	GLU	4.3
1	Q	279	LEU	4.2
1	I	159	GLU	4.2
1	X	240	PHE	4.2
1	F	277	LEU	4.2
1	Y	240	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	I	185	GLU	4.2
1	W	190	ILE	4.2
1	A	186	PRO	4.2
1	W	167	PHE	4.2
1	S	165	LEU	4.2
1	V	186	PRO	4.2
1	S	267	ILE	4.2
1	S	162	GLN	4.2
1	T	277	LEU	4.2
1	W	236	LEU	4.1
1	V	261	MET	4.1
1	V	251	ALA	4.1
1	N	248	PHE	4.1
1	H	264	ASP	4.1
1	X	160	TYR	4.1
1	I	177	GLN	4.1
1	N	186	PRO	4.1
1	O	188	VAL	4.1
1	J	182	GLY	4.1
1	W	218	LYS	4.1
1	Q	190	ILE	4.1
1	O	143	LEU	4.1
1	Y	160	TYR	4.1
1	K	212	ILE	4.1
1	A	165	LEU	4.0
1	H	155	LEU	4.0
1	J	277	LEU	4.0
1	Y	230	LYS	4.0
1	W	182	GLY	4.0
1	K	117	ILE	4.0
1	Y	203	LEU	4.0
1	X	223	CYS	4.0
1	Q	261	MET	4.0
1	G	187	PHE	4.0
1	S	249	PRO	4.0
1	N	254	LEU	4.0
1	W	279	LEU	4.0
1	I	176	TYR	4.0
1	J	184	LYS	4.0
1	W	273	LYS	4.0
1	S	157	PRO	4.0
1	F	249	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	N	187	PHE	3.9
1	Y	155	LEU	3.9
1	E	276	TRP	3.9
1	O	196	THR	3.9
1	W	171	THR	3.9
1	C	126	VAL	3.9
1	H	254	LEU	3.9
1	B	234	TRP	3.9
1	D	184	LYS	3.9
1	N	182	GLY	3.9
1	I	181	SER	3.9
1	Y	116	VAL	3.9
1	T	258	PHE	3.9
1	W	228	ILE	3.9
1	H	198	ALA	3.9
1	X	180	MET	3.9
1	F	199	LEU	3.9
1	V	170	LEU	3.9
1	W	281	TRP	3.9
1	C	180	MET	3.8
1	Y	225	ILE	3.8
1	S	186	PRO	3.8
1	L	184	LYS	3.8
1	X	194	LEU	3.8
1	B	184	LYS	3.8
1	P	250	LYS	3.8
1	W	184	LYS	3.8
1	A	113	ASN	3.8
1	T	175	LEU	3.8
1	H	243	TYR	3.8
1	J	187	PHE	3.8
1	X	255	ASP	3.8
1	Y	249	PRO	3.8
1	L	268	LYS	3.8
1	W	148	LYS	3.8
1	V	258	PHE	3.7
1	L	156	ILE	3.7
1	Y	139	ASN	3.7
1	P	184	LYS	3.7
1	S	167	PHE	3.7
1	E	183	ASN	3.7
1	L	182	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	V	180	MET	3.7
1	W	160	TYR	3.7
1	K	258	PHE	3.6
1	W	240	PHE	3.6
1	C	198	ALA	3.6
1	O	186	PRO	3.6
1	S	168	LEU	3.6
1	W	271	ALA	3.6
1	F	117	ILE	3.6
1	W	183	ASN	3.6
1	K	185	GLU	3.6
1	P	240	PHE	3.6
1	W	170	LEU	3.6
1	S	218	LYS	3.6
1	S	248	PHE	3.5
1	Q	275	ASN	3.5
1	J	162	GLN	3.5
1	F	261	MET	3.5
1	B	186	PRO	3.5
1	T	187	PHE	3.5
1	Y	248	PHE	3.5
1	H	279	LEU	3.5
1	L	206	ALA	3.5
1	T	227	CYS	3.5
1	A	184	LYS	3.5
1	W	201	ILE	3.5
1	M	265	ASP	3.5
1	H	251	ALA	3.5
1	H	259	ILE	3.5
1	H	266	GLU	3.5
1	B	277	LEU	3.5
1	Q	223	CYS	3.5
1	F	155	LEU	3.5
1	I	276	TRP	3.5
1	H	185	GLU	3.5
1	M	154	VAL	3.5
1	Y	191	PRO	3.5
1	E	176	TYR	3.4
1	H	156	ILE	3.4
1	Q	212	ILE	3.4
1	V	254	LEU	3.4
1	K	200	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	146	ARG	3.4
1	O	117	ILE	3.4
1	Y	177	GLN	3.4
1	A	277	LEU	3.4
1	P	195	LEU	3.4
1	V	199	LEU	3.4
1	J	183	ASN	3.4
1	F	208	GLN	3.4
1	L	263	ASP	3.4
1	V	200	GLU	3.4
1	A	210	ILE	3.4
1	N	156	ILE	3.4
1	J	188	VAL	3.4
1	P	270	ILE	3.4
1	V	190	ILE	3.4
1	H	211	LEU	3.4
1	T	194	LEU	3.4
1	W	207	ASN	3.4
1	S	180	MET	3.4
1	G	276	TRP	3.3
1	W	261	MET	3.3
1	X	189	ASN	3.3
1	D	267	ILE	3.3
1	F	167	PHE	3.3
1	I	156	ILE	3.3
1	H	160	TYR	3.3
1	L	261	MET	3.3
1	F	250	LYS	3.3
1	S	187	PHE	3.3
1	K	178	VAL	3.3
1	B	248	PHE	3.3
1	V	165	LEU	3.3
1	A	221	THR	3.3
1	M	198	ALA	3.3
1	S	280	GLN	3.3
1	S	116	VAL	3.3
1	B	249	PRO	3.3
1	J	211	LEU	3.3
1	S	206	ALA	3.3
1	W	212	ILE	3.3
1	T	252	ARG	3.3
1	W	252	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	L	249	PRO	3.3
1	Y	278	PRO	3.3
1	N	195	LEU	3.3
1	Q	236	LEU	3.3
1	Q	277	LEU	3.3
1	P	173	ILE	3.3
1	Y	204	ASN	3.3
1	I	269	ARG	3.3
1	C	254	LEU	3.2
1	L	195	LEU	3.2
1	E	113	ASN	3.2
1	I	189	ASN	3.2
1	V	212	ILE	3.2
1	I	243	TYR	3.2
1	X	257	GLN	3.2
1	D	186	PRO	3.2
1	I	142	PHE	3.2
1	M	248	PHE	3.2
1	O	187	PHE	3.2
1	Q	167	PHE	3.2
1	V	114	LYS	3.2
1	F	198	ALA	3.2
1	V	246	PHE	3.2
1	V	248	PHE	3.2
1	W	270	ILE	3.2
1	P	183	ASN	3.2
1	P	265	ASP	3.2
1	R	248	PHE	3.2
1	G	191	PRO	3.2
1	K	195	LEU	3.2
1	H	152	ILE	3.2
1	I	258	PHE	3.2
1	W	117	ILE	3.2
1	Y	156	ILE	3.2
1	P	276	TRP	3.2
1	F	183	ASN	3.2
1	G	113	ASN	3.2
1	B	194	LEU	3.2
1	V	162	GLN	3.2
1	X	249	PRO	3.2
1	H	208	GLN	3.1
1	D	175	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	125	VAL	3.1
1	V	211	LEU	3.1
1	I	255	ASP	3.1
1	J	167	PHE	3.1
1	X	183	ASN	3.1
1	V	262	TYR	3.1
1	Y	176	TYR	3.1
1	F	182	GLY	3.1
1	E	258	PHE	3.1
1	V	267	ILE	3.1
1	K	163	GLU	3.1
1	S	273	LYS	3.1
1	J	178	VAL	3.1
1	V	237	THR	3.1
1	F	189	ASN	3.1
1	L	214	SER	3.1
1	G	117	ILE	3.1
1	J	270	ILE	3.1
1	Q	280	GLN	3.1
1	V	264	ASP	3.1
1	K	165	LEU	3.1
1	S	198	ALA	3.1
1	W	200	GLU	3.1
1	C	130	TYR	3.1
1	F	248	PHE	3.1
1	W	142	PHE	3.1
1	D	255	ASP	3.1
1	W	205	PRO	3.1
1	B	188	VAL	3.1
1	W	166	ASN	3.0
1	V	240	PHE	3.0
1	J	276	TRP	3.0
1	I	275	ASN	3.0
1	P	236	LEU	3.0
1	M	184	LYS	3.0
1	B	167	PHE	3.0
1	N	265	ASP	3.0
1	Y	192	SER	3.0
1	S	253	ALA	3.0
1	A	125	VAL	3.0
1	C	188	VAL	3.0
1	R	278	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	280	GLN	3.0
1	B	231	LEU	3.0
1	D	254	LEU	3.0
1	E	277	LEU	3.0
1	C	186	PRO	3.0
1	I	188	VAL	3.0
1	X	188	VAL	3.0
1	Y	189	ASN	3.0
1	E	187	PHE	3.0
1	J	130	TYR	3.0
1	X	271	ALA	3.0
1	S	278	PRO	3.0
1	P	222	GLY	3.0
1	W	113	ASN	3.0
1	W	126	VAL	3.0
1	F	223	CYS	3.0
1	V	238	MET	3.0
1	O	258	PHE	3.0
1	O	171	THR	3.0
1	W	163	GLU	2.9
1	W	266	GLU	2.9
1	D	187	PHE	2.9
1	H	134	PHE	2.9
1	M	268	LYS	2.9
1	G	236	LEU	2.9
1	S	119	PRO	2.9
1	S	149	LEU	2.9
1	D	113	ASN	2.9
1	A	168	LEU	2.9
1	C	275	ASN	2.9
1	F	231	LEU	2.9
1	H	221	THR	2.9
1	I	182	GLY	2.9
1	O	130	TYR	2.9
1	G	178	VAL	2.9
1	J	261	MET	2.9
1	R	261	MET	2.9
1	D	240	PHE	2.9
1	W	141	SER	2.9
1	G	169	LYS	2.9
1	W	243	TYR	2.9
1	W	202	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	151	SER	2.9
1	E	191	PRO	2.9
1	I	165	LEU	2.9
1	O	160	TYR	2.9
1	W	176	TYR	2.9
1	A	248	PHE	2.9
1	H	142	PHE	2.9
1	H	167	PHE	2.9
1	A	147	LEU	2.9
1	Y	168	LEU	2.9
1	D	151	SER	2.9
1	D	223	CYS	2.9
1	L	187	PHE	2.9
1	V	152	ILE	2.9
1	V	167	PHE	2.9
1	X	234	TRP	2.9
1	J	254	LEU	2.9
1	S	231	LEU	2.9
1	B	261	MET	2.8
1	Q	180	MET	2.8
1	E	271	ALA	2.8
1	E	149	LEU	2.8
1	L	277	LEU	2.8
1	X	168	LEU	2.8
1	P	179	GLY	2.8
1	T	176	TYR	2.8
1	P	248	PHE	2.8
1	A	141	SER	2.8
1	N	178	VAL	2.8
1	R	162	GLN	2.8
1	R	161	PRO	2.8
1	E	231	LEU	2.8
1	X	268	LYS	2.8
1	W	189	ASN	2.8
1	R	281	TRP	2.8
1	W	234	TRP	2.8
1	C	154	VAL	2.8
1	M	278	PRO	2.8
1	X	212	ILE	2.8
1	A	265	ASP	2.8
1	S	199	LEU	2.8
1	O	223	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	S	223	CYS	2.8
1	D	116	VAL	2.8
1	N	154	VAL	2.8
1	S	276	TRP	2.8
1	L	241	ASP	2.8
1	V	265	ASP	2.8
1	W	267	ILE	2.8
1	R	171	THR	2.8
1	K	194	LEU	2.8
1	X	153	LEU	2.8
1	R	118	PRO	2.8
1	S	124	HIS	2.8
1	W	191	PRO	2.8
1	E	162	GLN	2.8
1	S	130	TYR	2.8
1	I	228	ILE	2.8
1	I	236	LEU	2.8
1	M	231	LEU	2.8
1	R	254	LEU	2.8
1	W	116	VAL	2.7
1	G	130	TYR	2.7
1	R	183	ASN	2.7
1	R	184	LYS	2.7
1	D	195	LEU	2.7
1	G	279	LEU	2.7
1	I	175	LEU	2.7
1	M	155	LEU	2.7
1	L	272	SER	2.7
1	W	232	GLN	2.7
1	O	182	GLY	2.7
1	F	156	ILE	2.7
1	J	281	TRP	2.7
1	Q	259	ILE	2.7
1	L	203	LEU	2.7
1	W	174	LYS	2.7
1	Y	174	LYS	2.7
1	T	191	PRO	2.7
1	Q	156	ILE	2.7
1	Q	258	PHE	2.7
1	S	212	ILE	2.7
1	T	267	ILE	2.7
1	J	194	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	279	LEU	2.7
1	S	224	LEU	2.7
1	X	155	LEU	2.7
1	Y	153	LEU	2.7
1	Y	199	LEU	2.7
1	S	174	LYS	2.7
1	H	274	ASN	2.7
1	P	182	GLY	2.7
1	C	250	LYS	2.7
1	Q	142	PHE	2.7
1	S	234	TRP	2.7
1	O	114	LYS	2.7
1	R	178	VAL	2.7
1	C	206	ALA	2.7
1	C	272	SER	2.7
1	A	185	GLU	2.7
1	C	176	TYR	2.7
1	W	130	TYR	2.7
1	K	136	ARG	2.7
1	A	157	PRO	2.7
1	W	127	GLY	2.7
1	I	180	MET	2.7
1	D	145	GLU	2.7
1	J	185	GLU	2.7
1	S	260	GLU	2.7
1	N	190	ILE	2.7
1	R	140	PHE	2.7
1	X	270	ILE	2.7
1	C	217	GLY	2.7
1	I	183	ASN	2.7
1	V	274	ASN	2.7
1	W	217	GLY	2.7
1	W	118	PRO	2.7
1	K	180	MET	2.7
1	S	163	GLU	2.6
1	P	178	VAL	2.6
1	V	116	VAL	2.6
1	V	181	SER	2.6
1	C	144	HIS	2.6
1	F	164	ASN	2.6
1	K	259	ILE	2.6
1	N	194	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	P	215	ASN	2.6
1	R	113	ASN	2.6
1	Y	157	PRO	2.6
1	P	247	ALA	2.6
1	R	144	HIS	2.6
1	E	195	LEU	2.6
1	V	127	GLY	2.6
1	I	272	SER	2.6
1	E	116	VAL	2.6
1	L	144	HIS	2.6
1	S	196	THR	2.6
1	D	211	LEU	2.6
1	R	231	LEU	2.6
1	X	224	LEU	2.6
1	H	249	PRO	2.6
1	Q	152	ILE	2.6
1	V	210	ILE	2.6
1	I	204	ASN	2.6
1	J	253	ALA	2.6
1	Q	251	ALA	2.6
1	W	177	GLN	2.6
1	Y	184	LYS	2.6
1	Y	281	TRP	2.6
1	B	129	ILE	2.6
1	F	243	TYR	2.6
1	W	159	GLU	2.6
1	X	243	TYR	2.6
1	G	188	VAL	2.6
1	R	252	ARG	2.6
1	F	211	LEU	2.6
1	C	156	ILE	2.6
1	M	234	TRP	2.6
1	W	129	ILE	2.6
1	Y	210	ILE	2.6
1	N	145	GLU	2.6
1	Y	222	GLY	2.6
1	L	116	VAL	2.6
1	S	221	THR	2.6
1	G	168	LEU	2.6
1	G	175	LEU	2.6
1	H	118	PRO	2.6
1	H	224	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	190	ILE	2.6
1	S	189	ASN	2.6
1	I	130	TYR	2.6
1	K	160	TYR	2.6
1	L	243	TYR	2.6
1	V	160	TYR	2.6
1	N	206	ALA	2.5
1	Q	143	LEU	2.5
1	H	248	PHE	2.5
1	Y	173	ILE	2.5
1	F	180	MET	2.5
1	G	261	MET	2.5
1	N	281	TRP	2.5
1	J	262	TYR	2.5
1	H	143	LEU	2.5
1	L	202	VAL	2.5
1	M	199	LEU	2.5
1	J	248	PHE	2.5
1	Y	167	PHE	2.5
1	A	272	SER	2.5
1	K	114	LYS	2.5
1	R	114	LYS	2.5
1	R	273	LYS	2.5
1	S	209	PRO	2.5
1	L	254	LEU	2.5
1	B	255	ASP	2.5
1	R	117	ILE	2.5
1	V	113	ASN	2.5
1	Y	255	ASP	2.5
1	L	267	ILE	2.5
1	V	225	ILE	2.5
1	W	227	CYS	2.5
1	S	181	SER	2.5
1	T	244	ARG	2.5
1	X	262	TYR	2.5
1	B	236	LEU	2.5
1	Y	215	ASN	2.5
1	Y	142	PHE	2.5
1	L	221	THR	2.5
1	P	113	ASN	2.5
1	S	233	ASN	2.5
1	S	279	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	W	179	GLY	2.5
1	W	215	ASN	2.5
1	L	219	HIS	2.5
1	N	185	GLU	2.5
1	X	248	PHE	2.5
1	J	157	PRO	2.5
1	Q	227	CYS	2.5
1	C	113	ASN	2.5
1	C	231	LEU	2.5
1	N	116	VAL	2.5
1	S	281	TRP	2.5
1	W	144	HIS	2.5
1	Y	202	VAL	2.5
1	Y	236	LEU	2.5
1	A	232	GLN	2.5
1	P	200	GLU	2.5
1	M	270	ILE	2.5
1	J	179	GLY	2.5
1	S	159	GLU	2.5
1	W	120	GLU	2.5
1	S	144	HIS	2.4
1	H	231	LEU	2.4
1	L	252	ARG	2.4
1	N	203	LEU	2.4
1	O	203	LEU	2.4
1	P	114	LYS	2.4
1	S	202	VAL	2.4
1	B	278	PRO	2.4
1	K	189	ASN	2.4
1	M	128	GLU	2.4
1	V	166	ASN	2.4
1	T	114	LYS	2.4
1	O	272	SER	2.4
1	J	243	TYR	2.4
1	T	223	CYS	2.4
1	L	185	GLU	2.4
1	M	187	PHE	2.4
1	T	134	PHE	2.4
1	E	273	LYS	2.4
1	X	119	PRO	2.4
1	X	217	GLY	2.4
1	R	203	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	V	155	LEU	2.4
1	O	178	VAL	2.4
1	V	159	GLU	2.4
1	C	148	LYS	2.4
1	T	250	LYS	2.4
1	E	256	GLN	2.4
1	M	121	ASN	2.4
1	T	135	PRO	2.4
1	G	115	GLU	2.4
1	H	203	LEU	2.4
1	G	197	LYS	2.4
1	F	146	ARG	2.4
1	W	208	GLN	2.4
1	A	182	GLY	2.4
1	H	180	MET	2.4
1	S	210	ILE	2.4
1	K	223	CYS	2.4
1	G	150	LYS	2.4
1	C	155	LEU	2.4
1	Y	170	LEU	2.4
1	Y	279	LEU	2.4
1	O	233	ASN	2.4
1	W	204	ASN	2.4
1	I	129	ILE	2.4
1	E	248	PHE	2.4
1	J	240	PHE	2.4
1	V	176	TYR	2.4
1	T	249	PRO	2.4
1	T	261	MET	2.4
1	N	276	TRP	2.4
1	Y	253	ALA	2.4
1	M	244	ARG	2.4
1	A	211	LEU	2.4
1	X	165	LEU	2.4
1	Y	231	LEU	2.4
1	X	116	VAL	2.4
1	X	138	GLU	2.4
1	S	169	LYS	2.4
1	J	180	MET	2.4
1	M	243	TYR	2.4
1	H	255	ASP	2.4
1	S	255	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	Y	220	ARG	2.4
1	W	162	GLN	2.4
1	S	185	GLU	2.4
1	E	223	CYS	2.4
1	V	143	LEU	2.4
1	V	227	CYS	2.4
1	X	195	LEU	2.4
1	C	116	VAL	2.3
1	G	210	ILE	2.3
1	J	117	ILE	2.3
1	J	241	ASP	2.3
1	P	201	ILE	2.3
1	R	190	ILE	2.3
1	T	269	ARG	2.3
1	R	243	TYR	2.3
1	S	125	VAL	2.3
1	A	261	MET	2.3
1	D	129	ILE	2.3
1	D	200	GLU	2.3
1	Y	212	ILE	2.3
1	E	184	LYS	2.3
1	T	271	ALA	2.3
1	Q	221	THR	2.3
1	V	226	GLY	2.3
1	A	199	LEU	2.3
1	E	175	LEU	2.3
1	I	143	LEU	2.3
1	X	145	GLU	2.3
1	A	162	GLN	2.3
1	D	227	CYS	2.3
1	P	228	ILE	2.3
1	X	210	ILE	2.3
1	C	189	ASN	2.3
1	C	274	ASN	2.3
1	S	271	ALA	2.3
1	Y	243	TYR	2.3
1	E	182	GLY	2.3
1	G	182	GLY	2.3
1	C	147	LEU	2.3
1	G	147	LEU	2.3
1	K	153	LEU	2.3
1	O	128	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	W	255	ASP	2.3
1	L	114	LYS	2.3
1	R	180	MET	2.3
1	E	270	ILE	2.3
1	C	223	CYS	2.3
1	R	258	PHE	2.3
1	Y	258	PHE	2.3
1	T	206	ALA	2.3
1	V	206	ALA	2.3
1	G	203	LEU	2.3
1	Y	147	LEU	2.3
1	Y	250	LYS	2.3
1	O	219	HIS	2.3
1	D	191	PRO	2.3
1	L	278	PRO	2.3
1	M	188	VAL	2.3
1	B	145	GLU	2.3
1	B	259	ILE	2.3
1	D	182	GLY	2.3
1	M	129	ILE	2.3
1	C	280	GLN	2.3
1	H	194	LEU	2.3
1	L	168	LEU	2.3
1	S	219	HIS	2.3
1	B	205	PRO	2.3
1	A	216	ARG	2.3
1	M	169	LYS	2.3
1	P	207	ASN	2.3
1	Q	270	ILE	2.3
1	R	276	TRP	2.3
1	V	141	SER	2.3
1	K	206	ALA	2.3
1	L	258	PHE	2.3
1	L	130	TYR	2.3
1	O	199	LEU	2.3
1	O	262	TYR	2.3
1	Y	211	LEU	2.3
1	E	227	CYS	2.3
1	O	150	LYS	2.2
1	X	274	ASN	2.2
1	B	222	GLY	2.2
1	L	201	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	V	201	ILE	2.2
1	X	134	PHE	2.2
1	D	279	LEU	2.2
1	S	203	LEU	2.2
1	G	243	TYR	2.2
1	I	160	TYR	2.2
1	I	119	PRO	2.2
1	S	135	PRO	2.2
1	R	275	ASN	2.2
1	J	126	VAL	2.2
1	A	123	SER	2.2
1	G	272	SER	2.2
1	R	272	SER	2.2
1	B	190	ILE	2.2
1	G	144	HIS	2.2
1	Q	134	PHE	2.2
1	R	187	PHE	2.2
1	R	268	LYS	2.2
1	X	221	THR	2.2
1	P	165	LEU	2.2
1	Y	143	LEU	2.2
1	I	157	PRO	2.2
1	S	222	GLY	2.2
1	F	159	GLU	2.2
1	L	128	GLU	2.2
1	L	250	LYS	2.2
1	M	223	CYS	2.2
1	Q	126	VAL	2.2
1	M	210	ILE	2.2
1	O	144	HIS	2.2
1	T	220	ARG	2.2
1	X	251	ALA	2.2
1	G	257	GLN	2.2
1	N	147	LEU	2.2
1	R	143	LEU	2.2
1	S	236	LEU	2.2
1	W	199	LEU	2.2
1	Y	113	ASN	2.2
1	H	154	VAL	2.2
1	N	210	ILE	2.2
1	O	152	ILE	2.2
1	X	247	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	Y	227	CYS	2.2
1	D	165	LEU	2.2
1	X	226	GLY	2.2
1	A	130	TYR	2.2
1	G	281	TRP	2.2
1	K	202	VAL	2.2
1	Y	159	GLU	2.2
1	H	129	ILE	2.2
1	M	173	ILE	2.2
1	P	150	LYS	2.2
1	R	236	LEU	2.2
1	T	165	LEU	2.2
1	V	195	LEU	2.2
1	W	195	LEU	2.2
1	X	278	PRO	2.2
1	R	219	HIS	2.2
1	Q	250	LYS	2.2
1	S	126	VAL	2.2
1	J	251	ALA	2.2
1	P	278	PRO	2.2
1	R	186	PRO	2.2
1	S	170	LEU	2.2
1	H	159	GLU	2.2
1	L	145	GLU	2.2
1	H	181	SER	2.2
1	R	124	HIS	2.1
1	W	257	GLN	2.1
1	T	130	TYR	2.1
1	G	126	VAL	2.1
1	E	251	ALA	2.1
1	M	264	ASP	2.1
1	O	247	ALA	2.1
1	Y	201	ILE	2.1
1	J	249	PRO	2.1
1	L	155	LEU	2.1
1	V	277	LEU	2.1
1	W	155	LEU	2.1
1	X	254	LEU	2.1
1	X	144	HIS	2.1
1	G	176	TYR	2.1
1	S	275	ASN	2.1
1	M	247	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	T	116	VAL	2.1
1	D	237	THR	2.1
1	A	191	PRO	2.1
1	H	157	PRO	2.1
1	J	156	ILE	2.1
1	I	248	PHE	2.1
1	A	254	LEU	2.1
1	C	165	LEU	2.1
1	K	280	GLN	2.1
1	W	254	LEU	2.1
1	S	145	GLU	2.1
1	E	198	ALA	2.1
1	F	125	VAL	2.1
1	H	114	LYS	2.1
1	T	182	GLY	2.1
1	B	256	GLN	2.1
1	P	281	TRP	2.1
1	T	119	PRO	2.1
1	X	239	ILE	2.1
1	E	122	PHE	2.1
1	N	258	PHE	2.1
1	B	199	LEU	2.1
1	E	236	LEU	2.1
1	F	203	LEU	2.1
1	L	279	LEU	2.1
1	S	155	LEU	2.1
1	S	254	LEU	2.1
1	T	224	LEU	2.1
1	I	114	LYS	2.1
1	T	215	ASN	2.1
1	P	225	ILE	2.1
1	S	201	ILE	2.1
1	D	246	PHE	2.1
1	E	181	SER	2.1
1	F	265	ASP	2.1
1	T	236	LEU	2.1
1	H	174	LYS	2.1
1	V	250	LYS	2.1
1	Y	133	SER	2.1
1	F	205	PRO	2.1
1	H	115	GLU	2.1
1	L	188	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	T	158	GLU	2.1
1	X	135	PRO	2.1
1	Y	188	VAL	2.1
1	K	146	ARG	2.1
1	A	236	LEU	2.1
1	B	140	PHE	2.1
1	P	122	PHE	2.1
1	X	264	ASP	2.1
1	C	195	LEU	2.1
1	N	227	CYS	2.1
1	D	281	TRP	2.1
1	G	215	ASN	2.1
1	Q	113	ASN	2.1
1	O	261	MET	2.1
1	D	249	PRO	2.1
1	P	119	PRO	2.1
1	X	218	LYS	2.1
1	A	243	TYR	2.1
1	V	130	TYR	2.1
1	C	259	ILE	2.1
1	M	201	ILE	2.1
1	N	219	HIS	2.1
1	W	210	ILE	2.1
1	D	248	PHE	2.1
1	I	149	LEU	2.1
1	I	277	LEU	2.1
1	L	231	LEU	2.1
1	M	140	PHE	2.1
1	P	254	LEU	2.1
1	M	162	GLN	2.1
1	A	148	LYS	2.1
1	L	244	ARG	2.1
1	O	273	LYS	2.1
1	L	178	VAL	2.0
1	L	237	THR	2.0
1	B	181	SER	2.0
1	B	280	GLN	2.0
1	I	212	ILE	2.0
1	S	243	TYR	2.0
1	T	228	ILE	2.0
1	Y	151	SER	2.0
1	O	184	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	Y	114	LYS	2.0
1	G	253	ALA	2.0
1	W	249	PRO	2.0
1	A	126	VAL	2.0
1	D	178	VAL	2.0
1	F	116	VAL	2.0
1	I	145	GLU	2.0
1	R	116	VAL	2.0
1	S	208	GLN	2.0
1	C	153	LEU	2.0
1	G	143	LEU	2.0
1	G	262	TYR	2.0
1	J	190	ILE	2.0
1	J	226	GLY	2.0
1	O	173	ILE	2.0
1	S	148	LYS	2.0
1	Q	243	TYR	2.0
1	Y	130	TYR	2.0
1	X	142	PHE	2.0
1	Y	134	PHE	2.0
1	Y	140	PHE	2.0
1	H	276	TRP	2.0
1	H	281	TRP	2.0
1	O	118	PRO	2.0
1	F	221	THR	2.0
1	B	215	ASN	2.0
1	I	207	ASN	2.0
1	E	225	ILE	2.0
1	N	152	ILE	2.0
1	N	175	LEU	2.0
1	Q	165	LEU	2.0
1	A	142	PHE	2.0
1	F	160	TYR	2.0
1	M	167	PHE	2.0
1	N	260	GLU	2.0
1	G	278	PRO	2.0
1	X	205	PRO	2.0

## 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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	L	301	5/5	0.82	0.21	55,55,56,56	0
2	SO4	X	301	5/5	0.83	0.21	58,58,58,59	0
2	SO4	W	301	5/5	0.86	0.18	78,80,81,83	0
2	SO4	H	301	5/5	0.90	0.19	55,55,55,56	0
2	SO4	J	301	5/5	0.90	0.20	42,42,43,43	0
2	SO4	Q	301	5/5	0.91	0.22	51,51,51,52	0
2	SO4	F	301	5/5	0.91	0.17	42,42,42,43	0
2	SO4	N	301	5/5	0.92	0.22	47,47,47,48	0
2	SO4	B	301	5/5	0.92	0.21	49,50,50,50	0
2	SO4	E	301	5/5	0.92	0.19	32,33,33,33	0
2	SO4	G	301	5/5	0.93	0.16	62,62,62,62	0
2	SO4	O	301	5/5	0.93	0.15	46,46,46,46	0
2	SO4	Y	301	5/5	0.93	0.15	53,55,56,56	0
2	SO4	D	301	5/5	0.94	0.21	39,39,40,40	0
2	SO4	S	301	5/5	0.94	0.16	47,47,47,48	0
2	SO4	V	301	5/5	0.94	0.18	51,51,51,51	0
2	SO4	I	301	5/5	0.94	0.15	42,42,43,43	0
2	SO4	M	301	5/5	0.94	0.15	41,42,42,43	0
2	SO4	K	301	5/5	0.95	0.16	40,41,41,42	0
2	SO4	R	301	5/5	0.95	0.15	26,28,28,29	0
2	SO4	C	301	5/5	0.96	0.15	39,39,39,39	0
2	SO4	P	301	5/5	0.96	0.16	45,45,45,45	0
2	SO4	A	301	5/5	0.96	0.19	30,30,31,31	0
2	SO4	T	301	5/5	0.97	0.09	50,50,50,50	0

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

There are no such residues in this entry.