



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 10:13 AM EDT

PDB ID : 4V86
Title : Structure-function Analysis of Receptor-binding in Adeno-Associated Virus Serotype 6 (AAV-6)
Authors : Xie, Q.
Deposited on : 2011-09-13
Resolution : 3.00 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

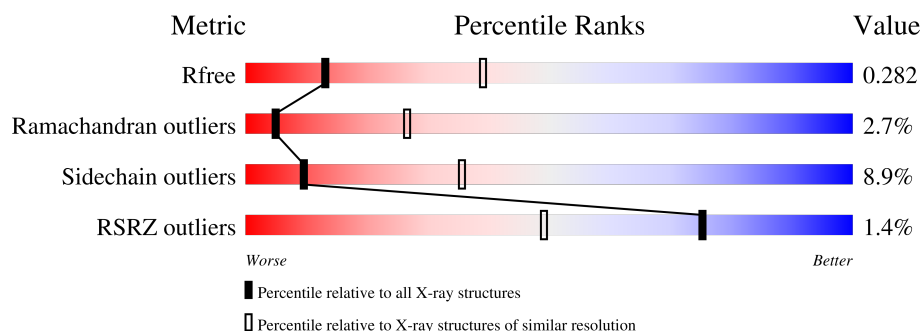
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



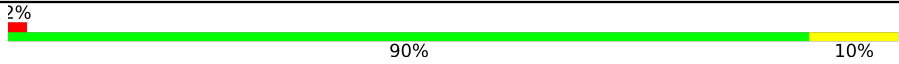
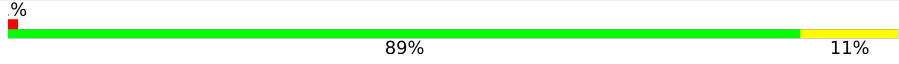
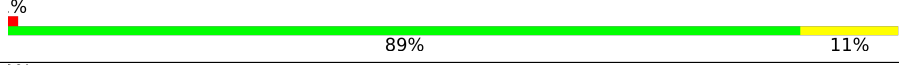
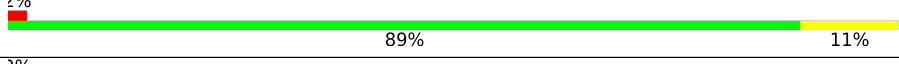
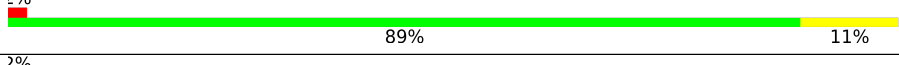
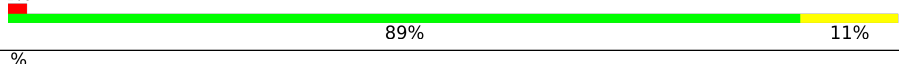
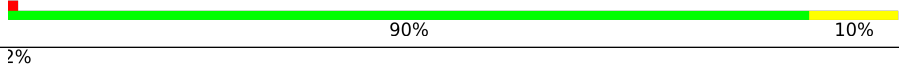
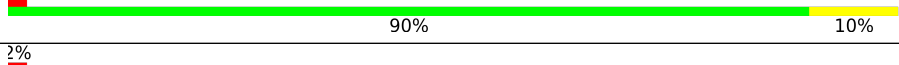
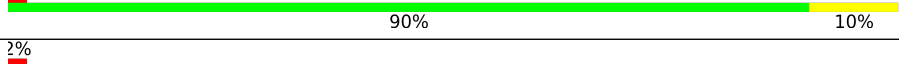
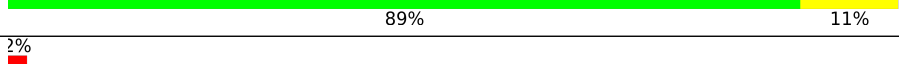
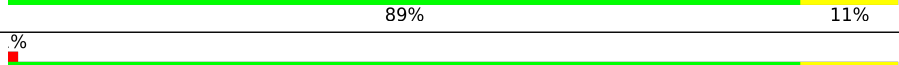
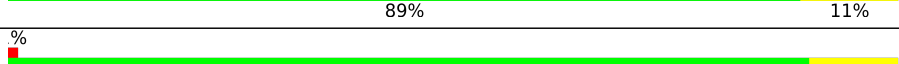
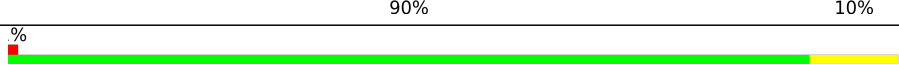
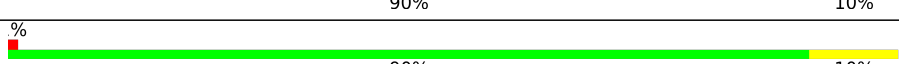
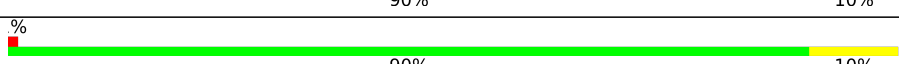
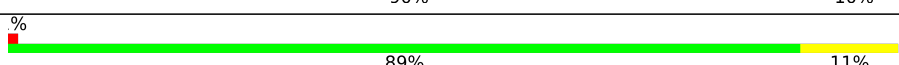
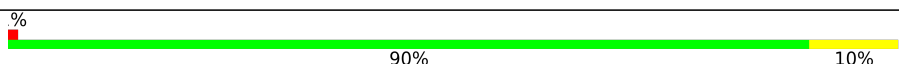
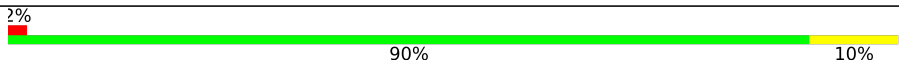
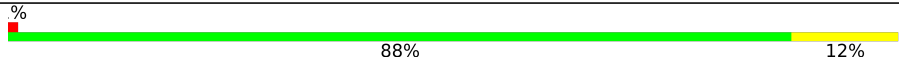
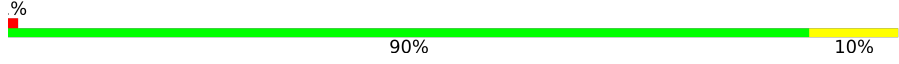
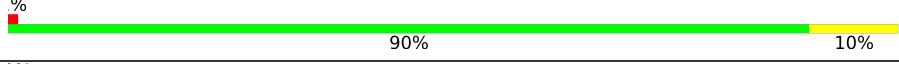
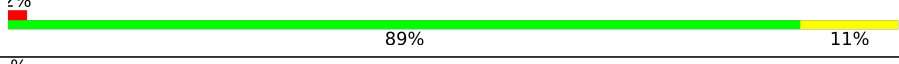
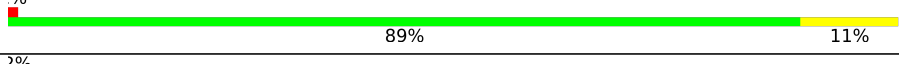
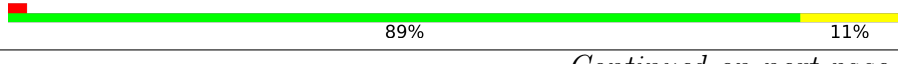

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	0	520	<div> <div>2%</div> <div>89%</div> <div>11%</div> </div>
1	1	520	<div> <div>%</div> <div>89%</div> <div>11%</div> </div>
1	2	520	<div> <div>2%</div> <div>90%</div> <div>10%</div> </div>
1	3	520	<div> <div>2%</div> <div>90%</div> <div>10%</div> </div>
1	4	520	<div> <div>%</div> <div>90%</div> <div>10%</div> </div>
1	5	520	<div> <div>%</div> <div>89%</div> <div>10%</div> </div>

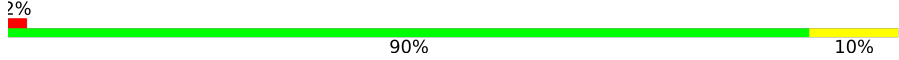
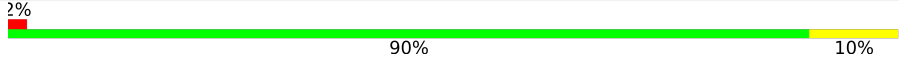


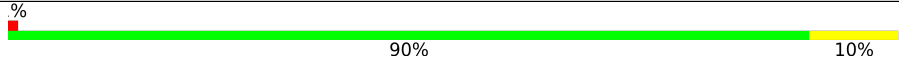
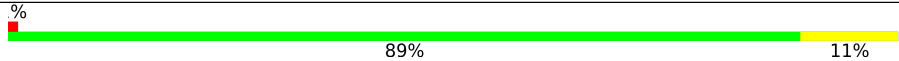
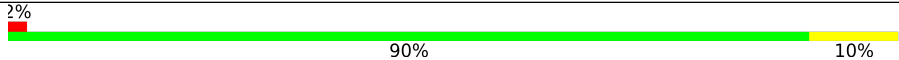
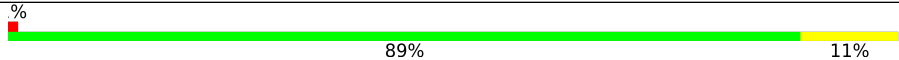
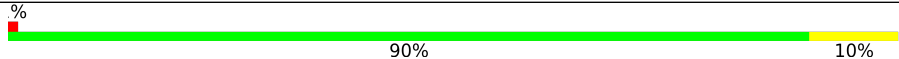
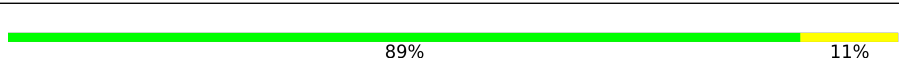
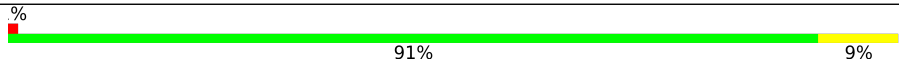
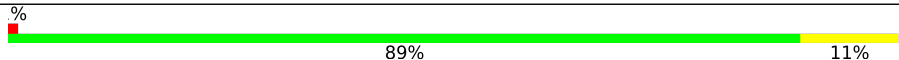


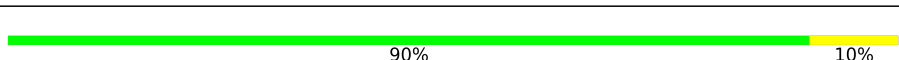
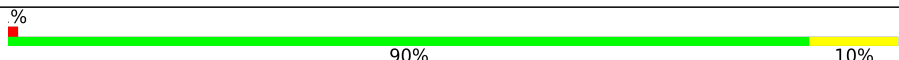
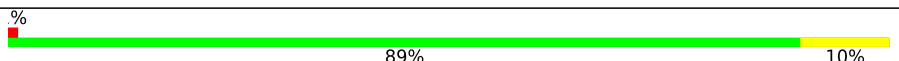
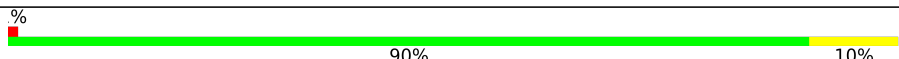
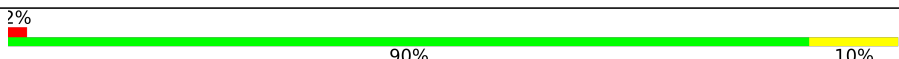

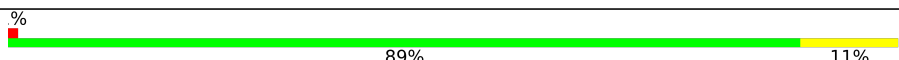
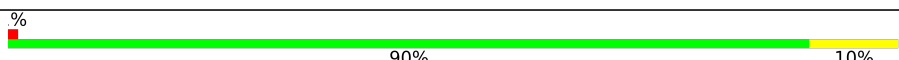
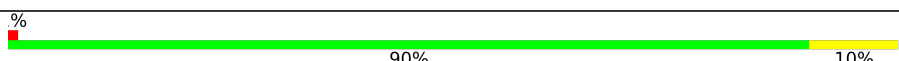
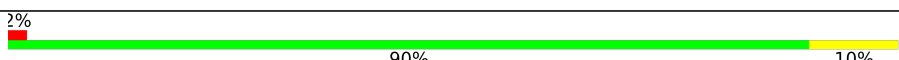
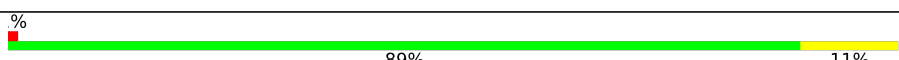
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Mol	Chain	Length	Quality of chain	
1	6	520		
1	7	520		
1	A	520		
1	B	520		
1	C	520		
1	D	520		
1	E	520		
1	F	520		
1	G	520		
1	H	520		
1	I	520		
1	J	520		
1	K	520		
1	L	520		
1	M	520		
1	N	520		
1	O	520		
1	P	520		
1	Q	520		
1	R	520		
1	S	520		
1	T	520		
1	U	520		
1	V	520		
1	W	520		

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Mol	Chain	Length	Quality of chain	
1	X	520		
1	Y	520		
1	Z	520		
1	a	520		
1	b	520		
1	c	520		
1	d	520		
1	e	520		
1	f	520		
1	g	520		
1	h	520		
1	i	520		
1	j	520		
1	k	520		
1	l	520		
1	m	520		
1	n	520		
1	o	520		
1	p	520		
1	q	520		
1	r	520		
1	s	520		
1	t	520		
1	u	520		
1	v	520		

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Mol	Chain	Length	Quality of chain	
1	w	520	<div><div></div><div>2%</div><div>89%</div><div>11%</div></div>	
1	x	520	<div><div></div><div>2%</div><div>91%</div><div>9%</div></div>	
1	y	520	<div><div></div><div>%</div><div>90%</div><div>10%</div></div>	
1	z	520	<div><div></div><div>%</div><div>89%</div><div>11%</div></div>	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 247260 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	B	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	C	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	D	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	E	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	F	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	G	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	H	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	I	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	J	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	K	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	L	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	M	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	N	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	O	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	P	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	R	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	S	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	T	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	U	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	V	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	W	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	X	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	Y	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	Z	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	a	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	b	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	c	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	d	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	e	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	f	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	g	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	h	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	i	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	j	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	k	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	l	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	m	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	n	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	o	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	p	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	q	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	r	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	s	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	t	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	u	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	v	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	w	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	x	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	y	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	z	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	0	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	1	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	2	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	3	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	4	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	5	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			

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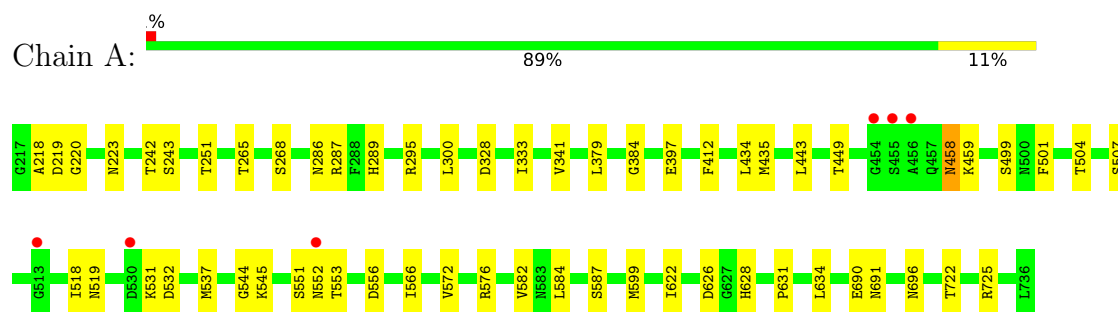
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	6	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	7	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			

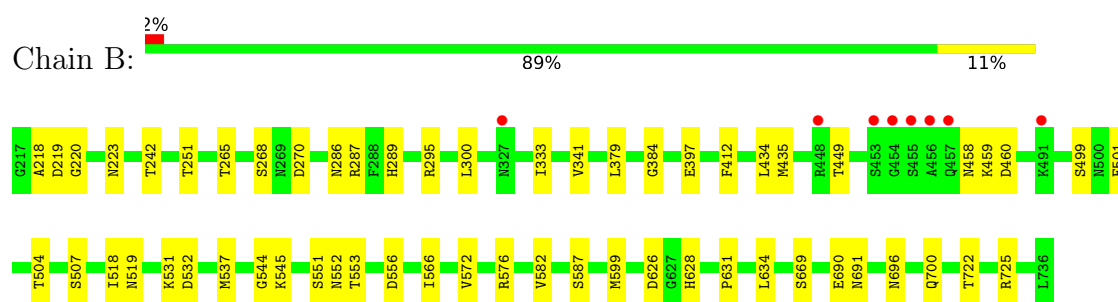
3 Residue-property plots

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

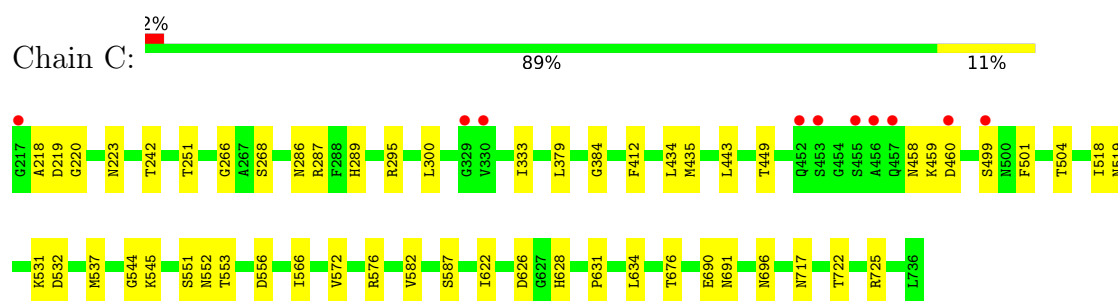
• Molecule 1: Capsid protein VP1



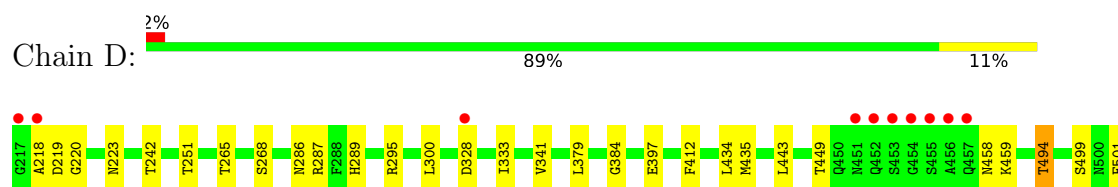
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

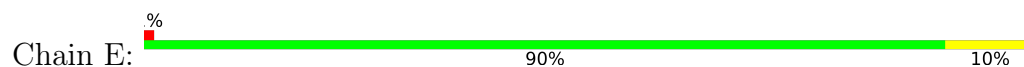


• Molecule 1: Capsid protein VP1





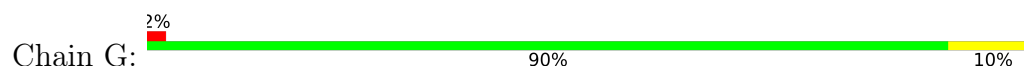
• Molecule 1: Capsid protein VP1



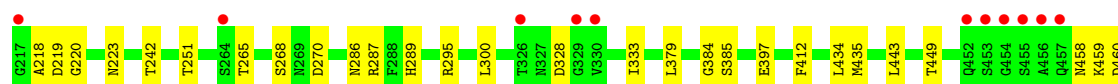
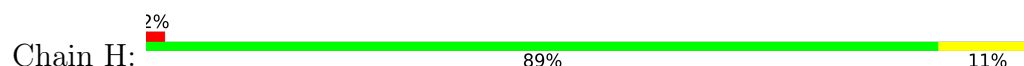
• Molecule 1: Capsid protein VP1



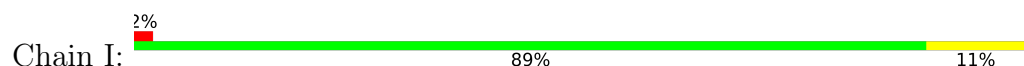
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

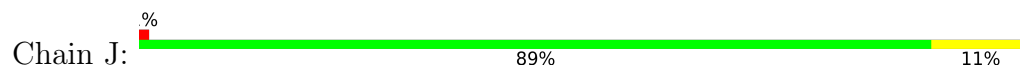


• Molecule 1: Capsid protein VP1

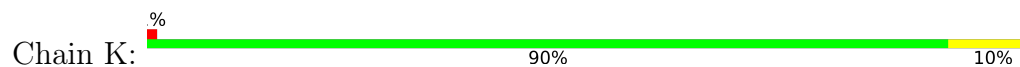




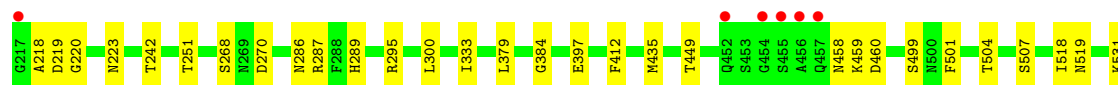
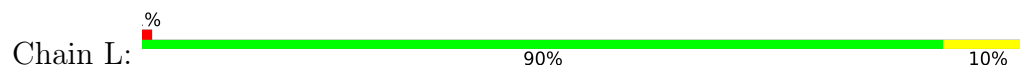
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1



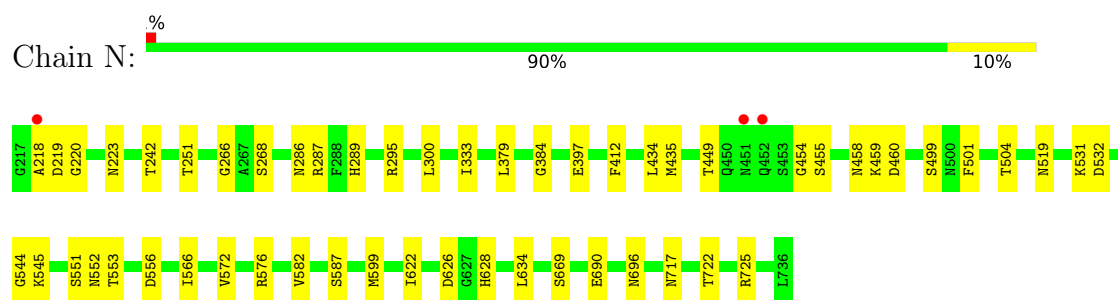
• Molecule 1: Capsid protein VP1



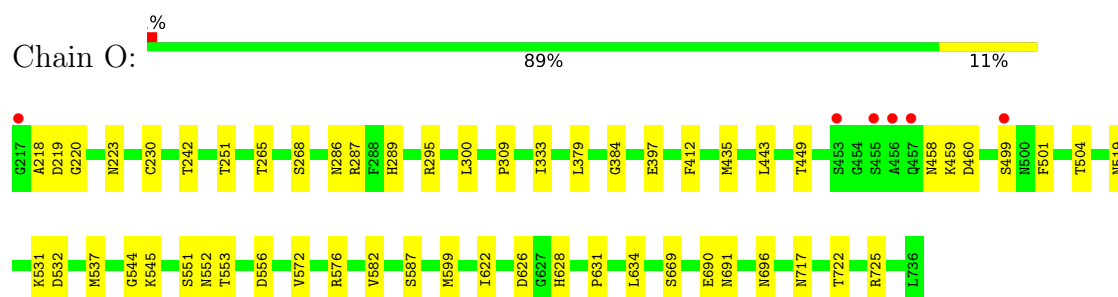
• Molecule 1: Capsid protein VP1



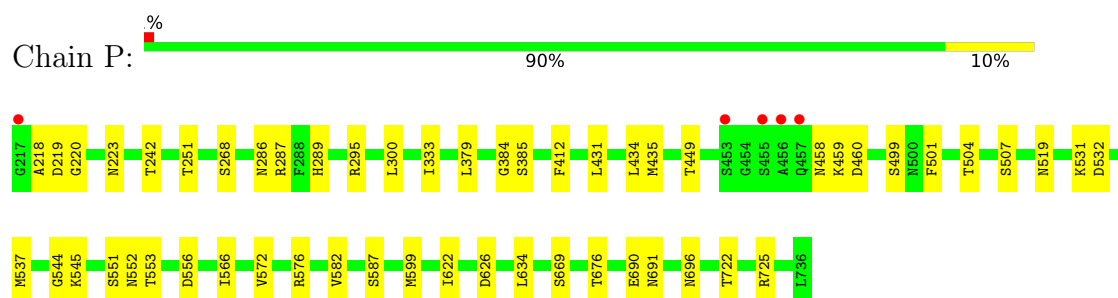
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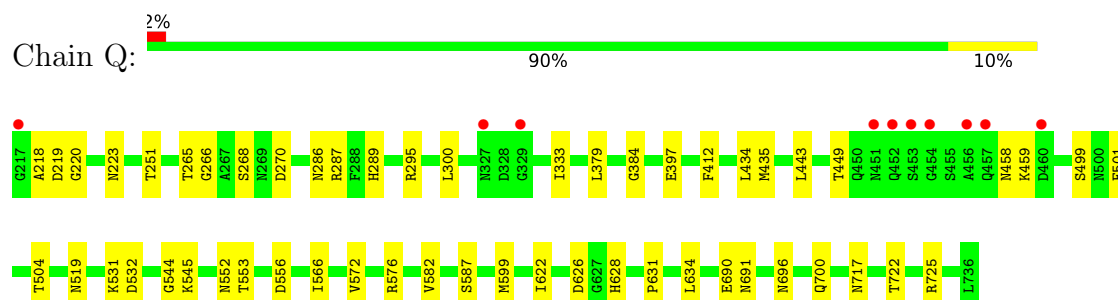
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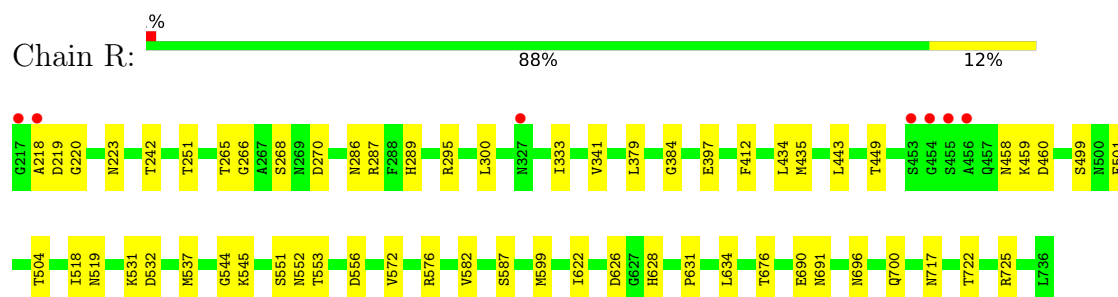
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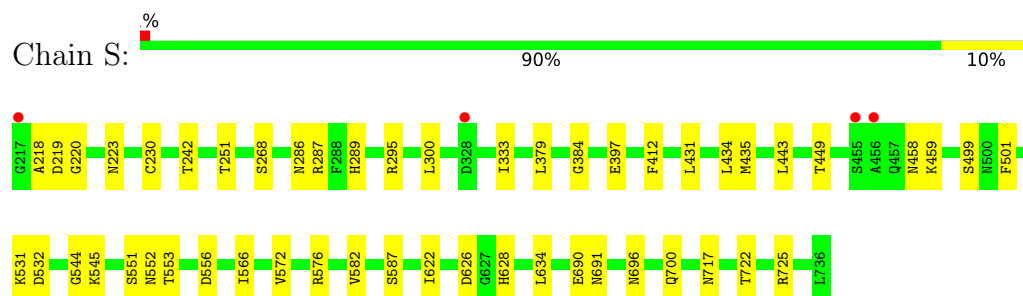
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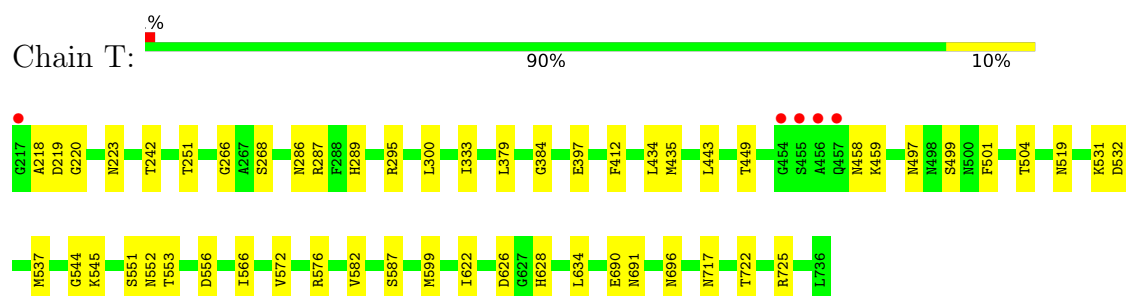
• Molecule 1: Capsid protein VP1



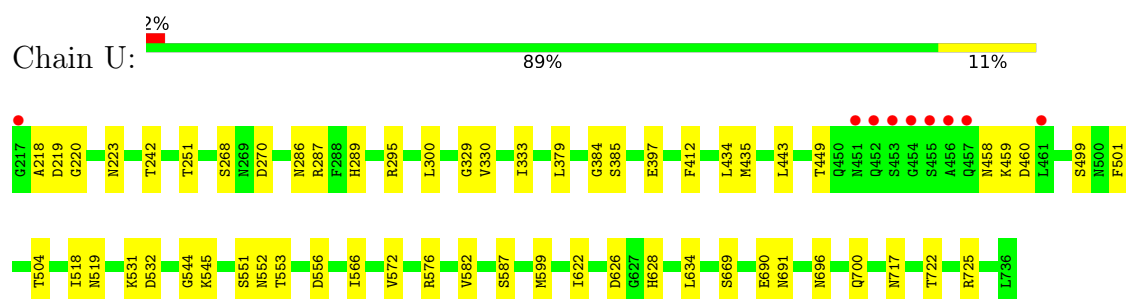
- Molecule 1: Capsid protein VP1



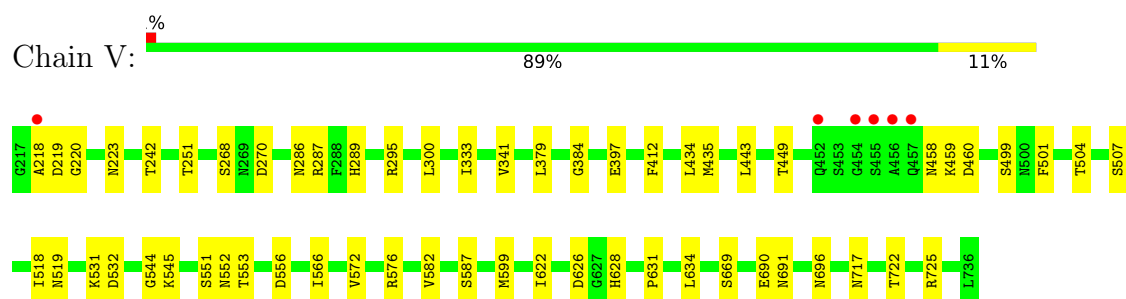
- Molecule 1: Capsid protein VP1



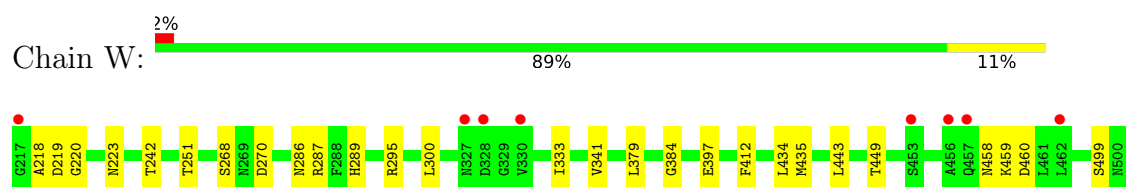
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1

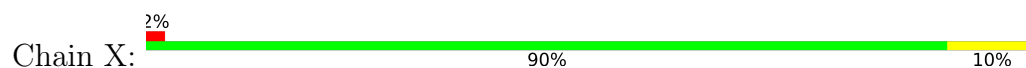


- Molecule 1: Capsid protein VP1

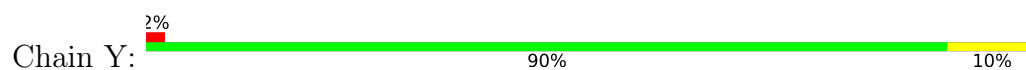




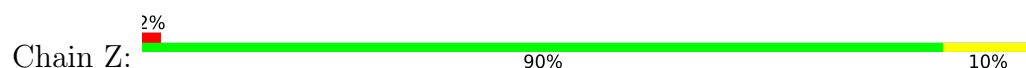
• Molecule 1: Capsid protein VP1



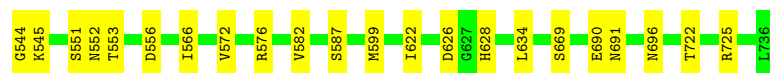
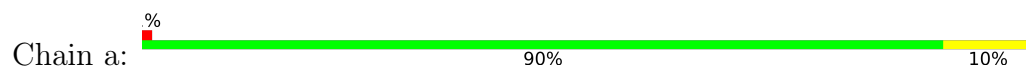
• Molecule 1: Capsid protein VP1



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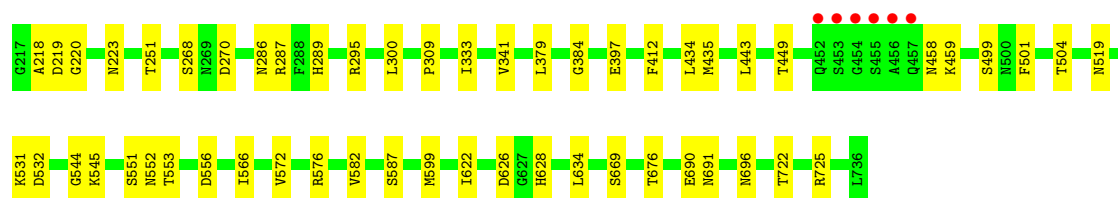


• Molecule 1: Capsid protein VP1

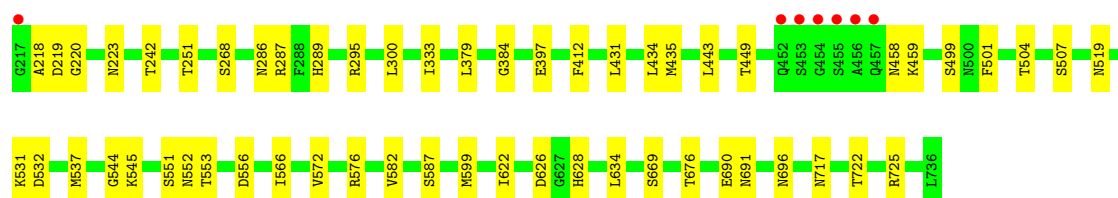
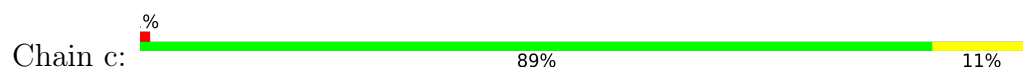


• Molecule 1: Capsid protein VP1

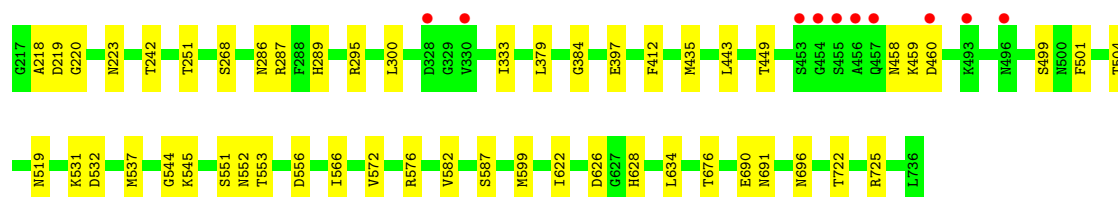
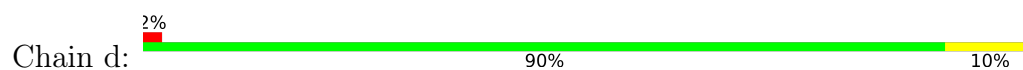




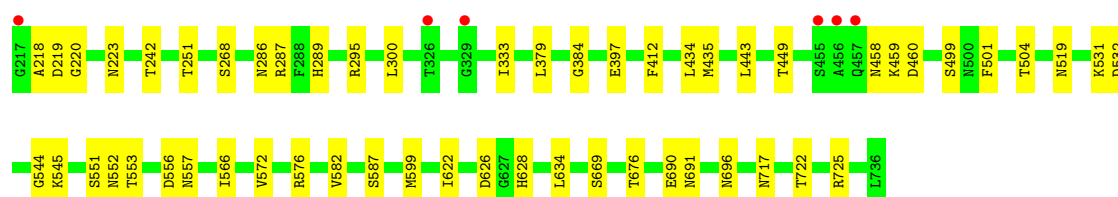
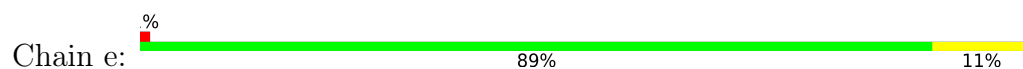
• Molecule 1: Capsid protein VP1



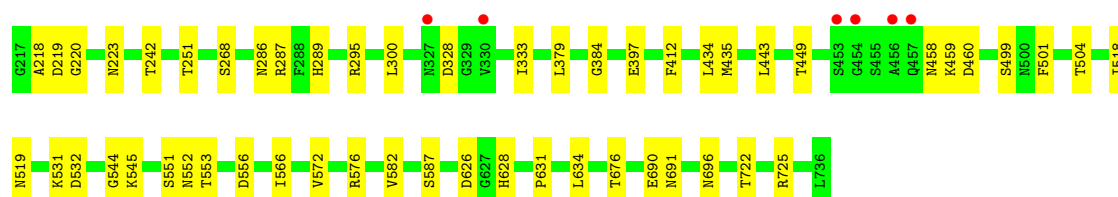
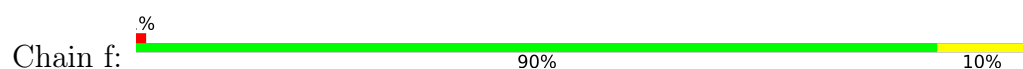
• Molecule 1: Capsid protein VP1




• Molecule 1: Capsid protein VP1

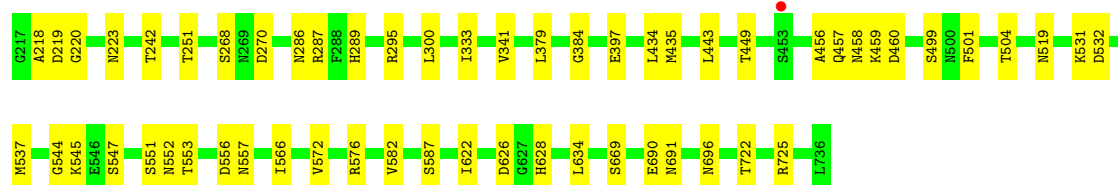


• Molecule 1: Capsid protein VP1

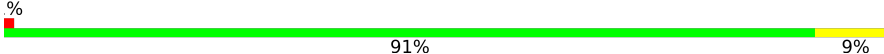


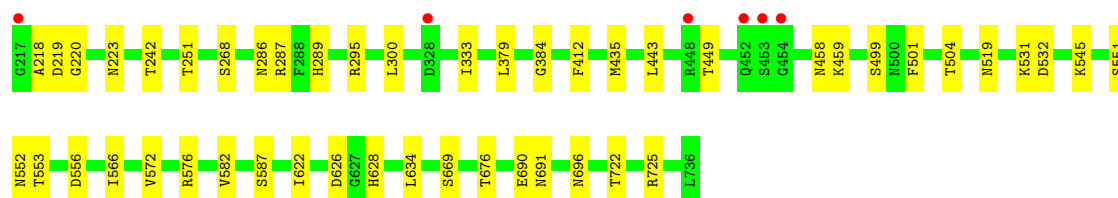
• Molecule 1: Capsid protein VP1

Chain g:  89% 11%




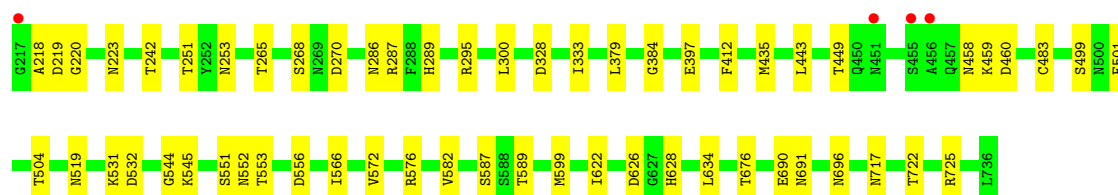
• Molecule 1: Capsid protein VP1

Chain h:  91% 9%




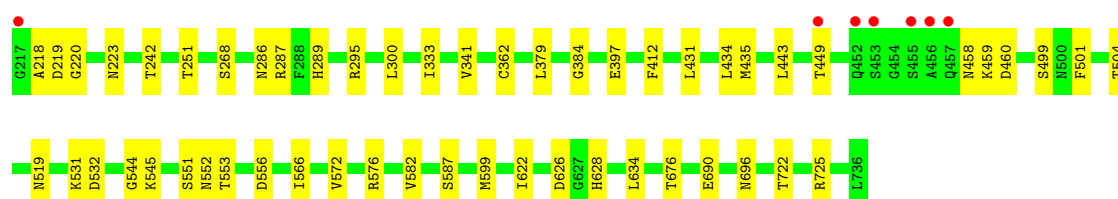
• Molecule 1: Capsid protein VP1

Chain i:  89% 11%




• Molecule 1: Capsid protein VP1

Chain j:  90% 10%



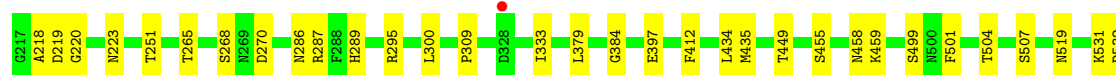
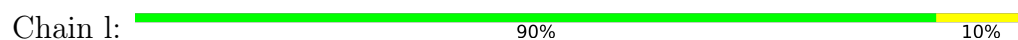
• Molecule 1: Capsid protein VP1

Chain k:  88% 12%

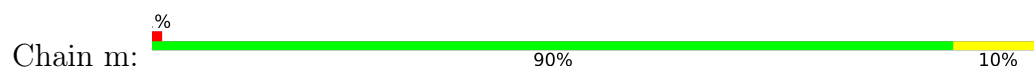




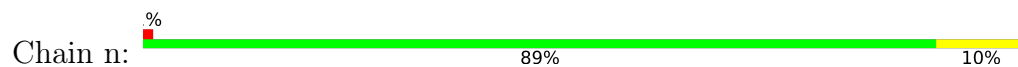
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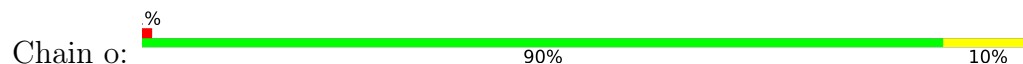
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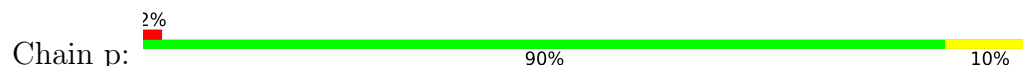
• Molecule 1: Capsid protein VP1

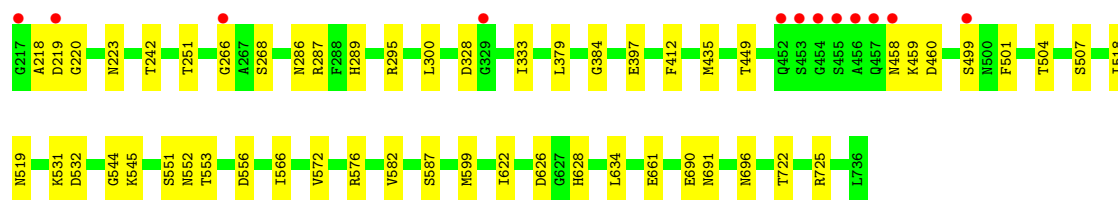


• Molecule 1: Capsid protein VP1

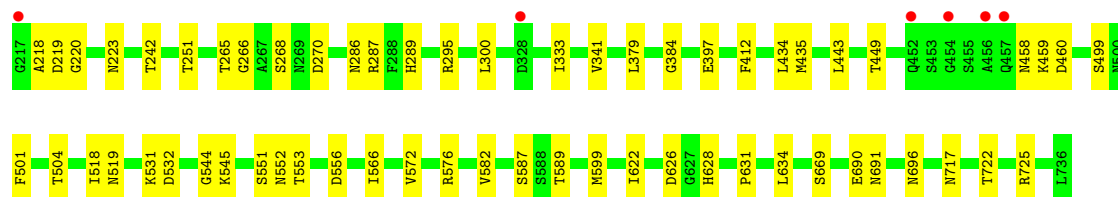
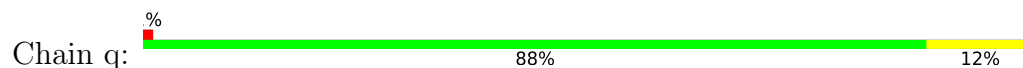


• Molecule 1: Capsid protein VP1

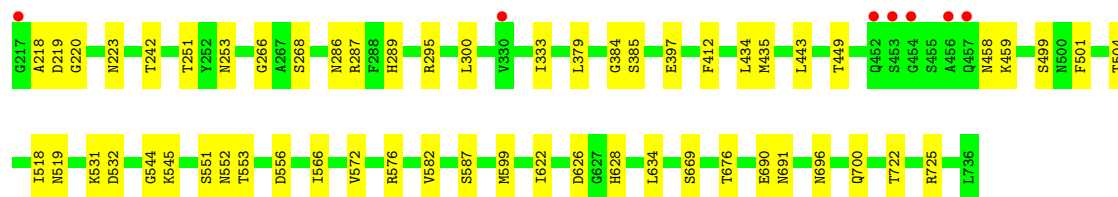
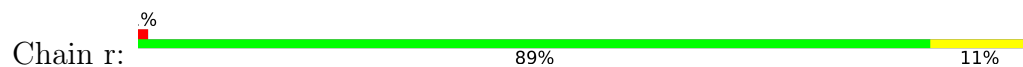




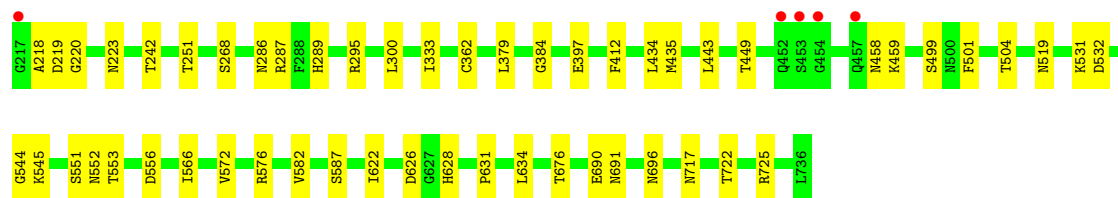
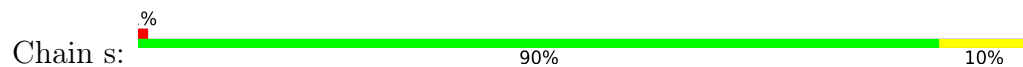
• Molecule 1: Capsid protein VP1



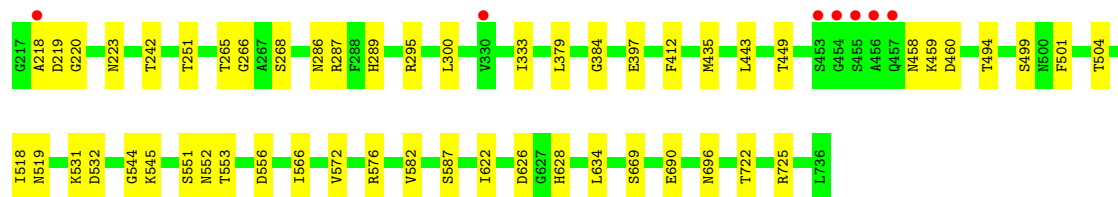
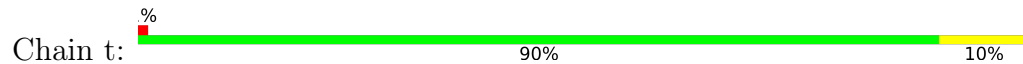
• Molecule 1: Capsid protein VP1



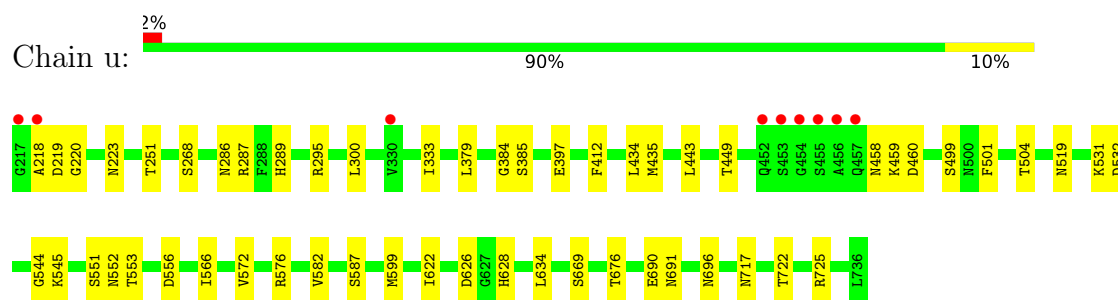
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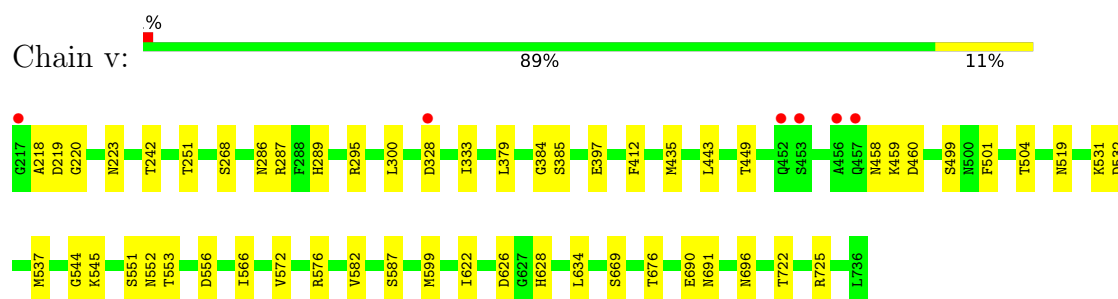
• Molecule 1: Capsid protein VP1



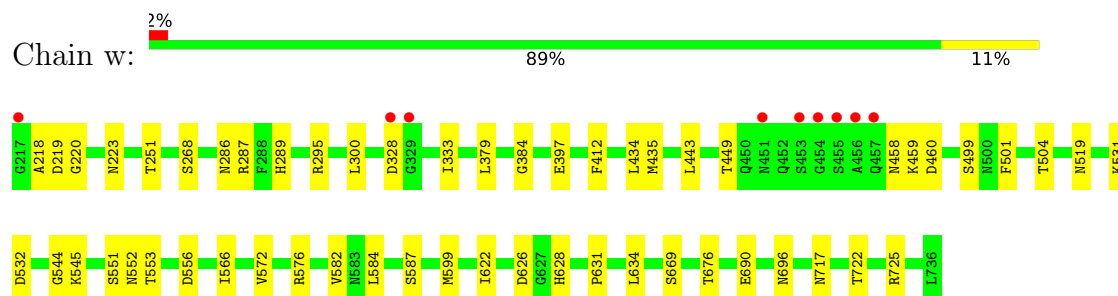
• Molecule 1: Capsid protein VP1



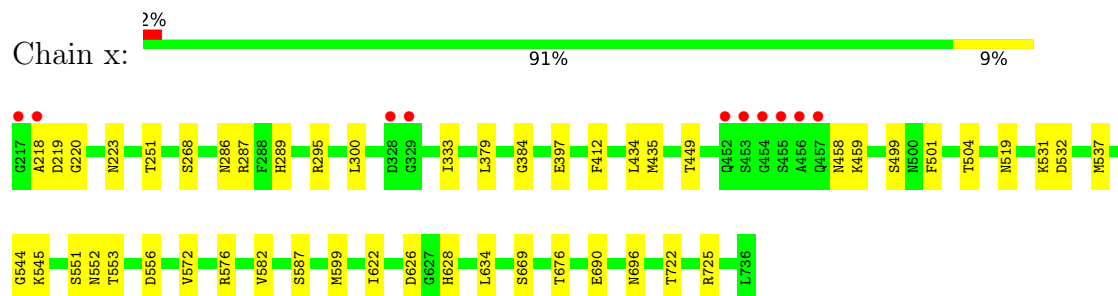
- Molecule 1: Capsid protein VP1



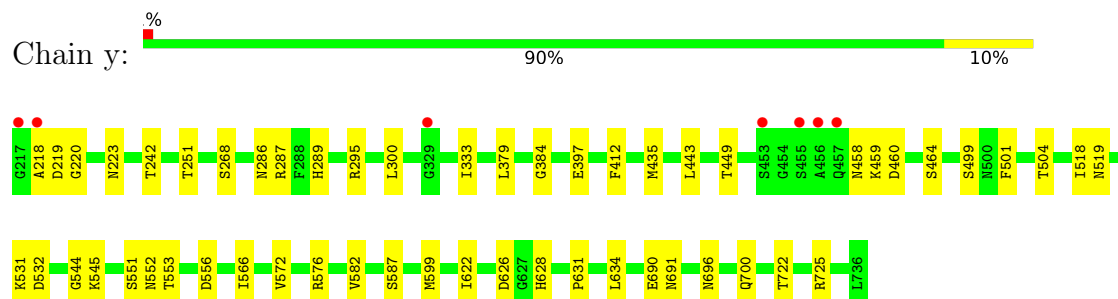
- Molecule 1: Capsid protein VP1



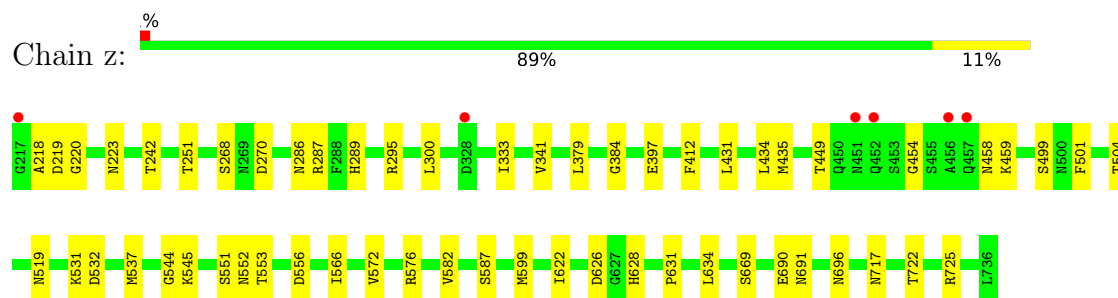
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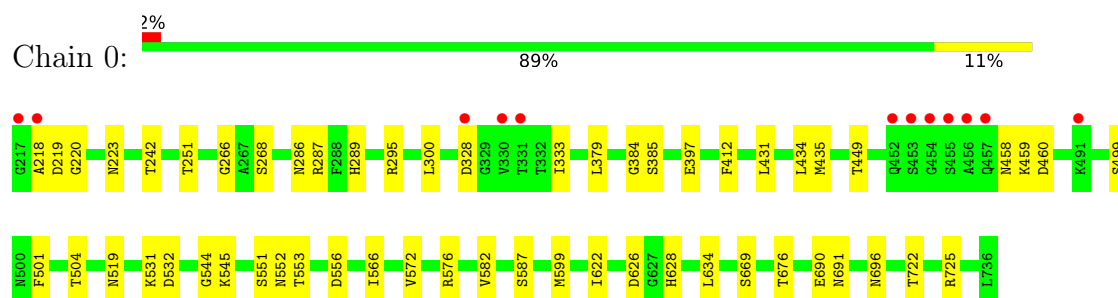
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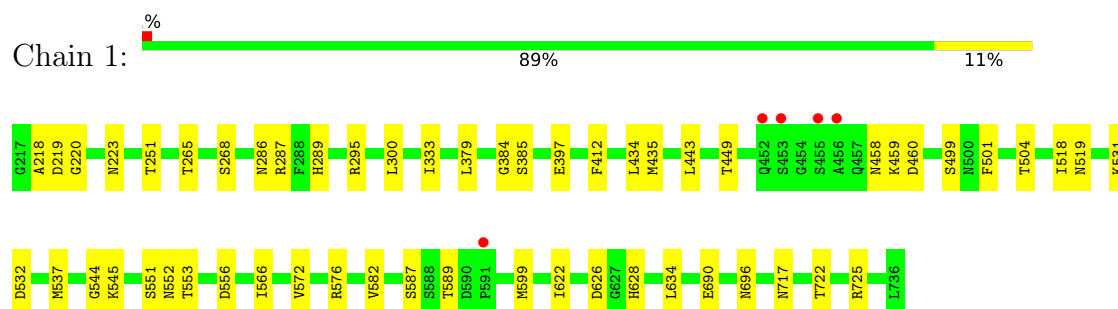
- Molecule 1: Capsid protein VP1



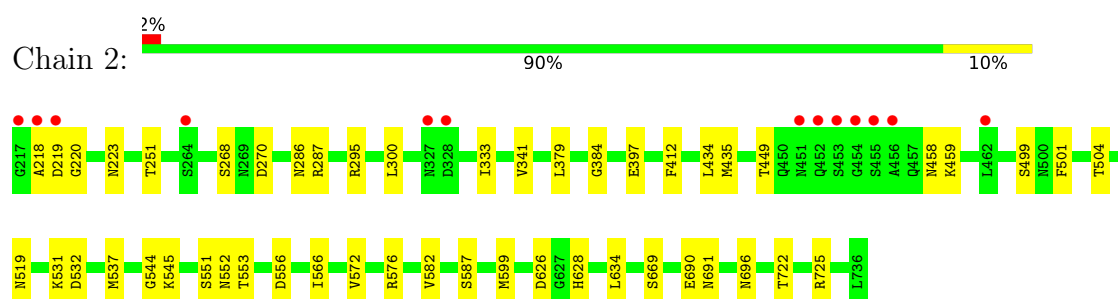
- Molecule 1: Capsid protein VP1



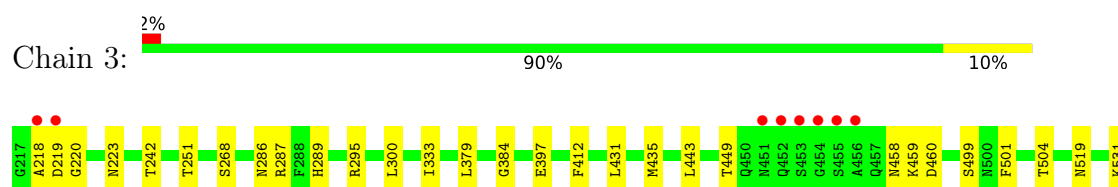
- Molecule 1: Capsid protein VP1

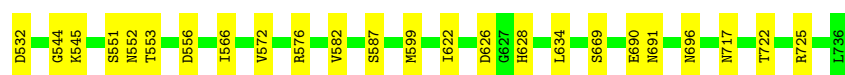


- Molecule 1: Capsid protein VP1

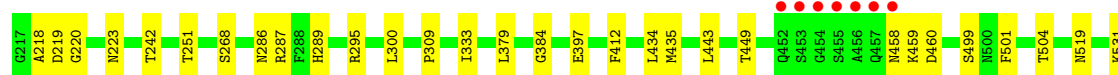
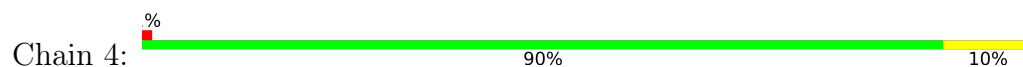


- Molecule 1: Capsid protein VP1

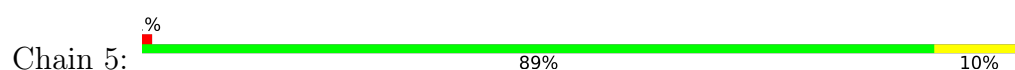




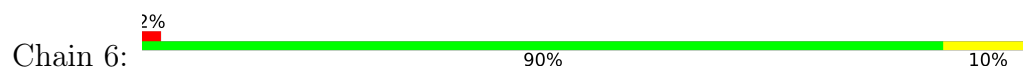
• Molecule 1: Capsid protein VP1



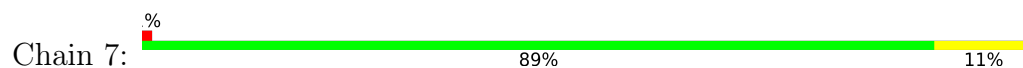
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	354.79Å 363.90Å 371.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 3.00 49.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	35.1 (49.21-3.00) 35.1 (49.21-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.251 , 0.286 0.247 , 0.282	Depositor DCC
R_{free} test set	3268 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k 0.009 for -l,-k,-h 0.023 for k,h,-l 0.008 for k,l,h 0.008 for l,h,k	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	247260	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.60	0/4247	0.63	0/5790
1	1	0.63	0/4247	0.62	0/5790
1	2	0.56	0/4247	0.62	0/5790
1	3	0.55	0/4247	0.61	0/5790
1	4	0.54	0/4247	0.60	0/5790
1	5	0.59	0/4247	0.61	0/5790
1	6	0.62	0/4247	0.62	0/5790
1	7	0.55	0/4247	0.61	0/5790
1	A	0.68	0/4247	0.65	0/5790
1	B	0.66	0/4247	0.63	0/5790
1	C	0.58	0/4247	0.62	0/5790
1	D	0.60	2/4247 (0.0%)	0.63	2/5790 (0.0%)
1	E	0.65	0/4247	0.64	0/5790
1	F	0.62	0/4247	0.64	0/5790
1	G	0.58	0/4247	0.60	0/5790
1	H	0.56	0/4247	0.61	0/5790
1	I	0.65	0/4247	0.64	0/5790
1	J	0.70	0/4247	0.65	0/5790
1	K	0.58	0/4247	0.61	0/5790
1	L	0.55	0/4247	0.60	0/5790
1	M	0.55	0/4247	0.59	0/5790
1	N	0.57	0/4247	0.60	0/5790
1	O	0.56	1/4247 (0.0%)	0.60	0/5790
1	P	0.57	0/4247	0.62	0/5790
1	Q	0.56	0/4247	0.62	0/5790
1	R	0.56	0/4247	0.61	0/5790
1	S	0.63	1/4247 (0.0%)	0.62	0/5790
1	T	0.61	0/4247	0.61	0/5790
1	U	0.62	0/4247	0.63	0/5790
1	V	0.62	0/4247	0.62	0/5790
1	W	0.69	0/4247	0.64	0/5790
1	X	0.69	0/4247	0.65	0/5790
1	Y	0.64	0/4247	0.64	0/5790
1	Z	0.59	0/4247	0.62	0/5790

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.55	0/4247	0.61	0/5790
1	b	0.57	0/4247	0.60	0/5790
1	c	0.54	0/4247	0.62	0/5790
1	d	0.55	0/4247	0.61	0/5790
1	e	0.57	0/4247	0.61	0/5790
1	f	0.52	0/4247	0.60	0/5790
1	g	0.60	0/4247	0.62	0/5790
1	h	0.59	0/4247	0.61	0/5790
1	i	0.55	1/4247 (0.0%)	0.60	0/5790
1	j	0.58	1/4247 (0.0%)	0.61	0/5790
1	k	0.59	0/4247	0.61	0/5790
1	l	0.59	0/4247	0.60	0/5790
1	m	0.66	0/4247	0.63	0/5790
1	n	0.63	1/4247 (0.0%)	0.62	0/5790
1	o	0.53	0/4247	0.60	0/5790
1	p	0.58	0/4247	0.61	0/5790
1	q	0.55	0/4247	0.61	0/5790
1	r	0.55	0/4247	0.60	0/5790
1	s	0.55	1/4247 (0.0%)	0.61	0/5790
1	t	0.55	0/4247	0.60	0/5790
1	u	0.54	0/4247	0.59	0/5790
1	v	0.55	0/4247	0.60	0/5790
1	w	0.56	0/4247	0.61	0/5790
1	x	0.55	0/4247	0.60	0/5790
1	y	0.56	0/4247	0.61	0/5790
1	z	0.56	0/4247	0.61	0/5790
All	All	0.59	8/254820 (0.0%)	0.62	2/347400 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	j	362	CYS	CB-SG	-6.32	1.71	1.82
1	s	362	CYS	CB-SG	-6.18	1.71	1.82
1	S	230	CYS	CB-SG	-6.04	1.72	1.82
1	n	483	CYS	CB-SG	-5.67	1.72	1.81
1	D	494	THR	CB-CG2	5.50	1.70	1.52
1	O	230	CYS	CB-SG	-5.44	1.73	1.81
1	D	494	THR	CA-CB	-5.10	1.40	1.53
1	i	483	CYS	CB-SG	-5.08	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	494	THR	CA-CB-CG2	-5.89	104.15	112.40
1	D	494	THR	CB-CA-C	-5.82	95.88	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	0	518/520 (100%)	466 (90%)	36 (7%)	16 (3%)	4	23
1	1	518/520 (100%)	462 (89%)	41 (8%)	15 (3%)	4	24
1	2	518/520 (100%)	463 (89%)	43 (8%)	12 (2%)	6	30
1	3	518/520 (100%)	459 (89%)	46 (9%)	13 (2%)	5	28
1	4	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	5	28
1	5	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	5	28
1	6	518/520 (100%)	464 (90%)	42 (8%)	12 (2%)	6	30
1	7	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	4	24
1	A	518/520 (100%)	460 (89%)	43 (8%)	15 (3%)	4	24
1	B	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	4	24
1	C	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	4	23
1	D	518/520 (100%)	464 (90%)	40 (8%)	14 (3%)	5	26
1	E	518/520 (100%)	463 (89%)	41 (8%)	14 (3%)	5	26
1	F	518/520 (100%)	462 (89%)	42 (8%)	14 (3%)	5	26
1	G	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	518/520 (100%)	462 (89%)	41 (8%)	15 (3%)	4	24
1	I	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	4	24
1	J	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	4	24
1	K	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	5	28
1	L	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	4	24
1	M	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	5	28
1	N	518/520 (100%)	466 (90%)	38 (7%)	14 (3%)	5	26
1	O	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	5	26
1	P	518/520 (100%)	466 (90%)	38 (7%)	14 (3%)	5	26
1	Q	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	5	26
1	R	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	4	23
1	S	518/520 (100%)	463 (89%)	42 (8%)	13 (2%)	5	28
1	T	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	5	28
1	U	518/520 (100%)	471 (91%)	31 (6%)	16 (3%)	4	23
1	V	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	4	24
1	W	518/520 (100%)	463 (89%)	42 (8%)	13 (2%)	5	28
1	X	518/520 (100%)	461 (89%)	43 (8%)	14 (3%)	5	26
1	Y	518/520 (100%)	461 (89%)	44 (8%)	13 (2%)	5	28
1	Z	518/520 (100%)	462 (89%)	44 (8%)	12 (2%)	6	30
1	a	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	5	28
1	b	518/520 (100%)	467 (90%)	39 (8%)	12 (2%)	6	30
1	c	518/520 (100%)	465 (90%)	41 (8%)	12 (2%)	6	30
1	d	518/520 (100%)	465 (90%)	40 (8%)	13 (2%)	5	28
1	e	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	5	28
1	f	518/520 (100%)	466 (90%)	36 (7%)	16 (3%)	4	23
1	g	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	5	28
1	h	518/520 (100%)	463 (89%)	44 (8%)	11 (2%)	7	33
1	i	518/520 (100%)	466 (90%)	37 (7%)	15 (3%)	4	24
1	j	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	5	28
1	k	518/520 (100%)	465 (90%)	37 (7%)	16 (3%)	4	23
1	l	518/520 (100%)	468 (90%)	38 (7%)	12 (2%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	m	518/520 (100%)	468 (90%)	37 (7%)	13 (2%)	5	28
1	n	518/520 (100%)	469 (90%)	36 (7%)	13 (2%)	5	28
1	o	518/520 (100%)	464 (90%)	40 (8%)	14 (3%)	5	26
1	p	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	4	23
1	q	518/520 (100%)	464 (90%)	38 (7%)	16 (3%)	4	23
1	r	518/520 (100%)	464 (90%)	38 (7%)	16 (3%)	4	23
1	s	518/520 (100%)	465 (90%)	40 (8%)	13 (2%)	5	28
1	t	518/520 (100%)	463 (89%)	40 (8%)	15 (3%)	4	24
1	u	518/520 (100%)	467 (90%)	37 (7%)	14 (3%)	5	26
1	v	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	4	24
1	w	518/520 (100%)	465 (90%)	38 (7%)	15 (3%)	4	24
1	x	518/520 (100%)	465 (90%)	41 (8%)	12 (2%)	6	30
1	y	518/520 (100%)	468 (90%)	35 (7%)	15 (3%)	4	24
1	z	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	5	28
All	All	31080/31200 (100%)	27915 (90%)	2328 (8%)	837 (3%)	5	26

All (837) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	LYS
1	A	519	ASN
1	A	531	LYS
1	A	545	LYS
1	B	459	LYS
1	B	519	ASN
1	B	531	LYS
1	C	459	LYS
1	C	519	ASN
1	C	531	LYS
1	C	553	THR
1	D	459	LYS
1	D	519	ASN
1	D	531	LYS
1	D	553	THR
1	E	459	LYS
1	E	519	ASN
1	E	531	LYS

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Mol	Chain	Res	Type
1	E	545	LYS
1	F	519	ASN
1	F	531	LYS
1	F	545	LYS
1	F	553	THR
1	G	459	LYS
1	G	519	ASN
1	G	531	LYS
1	G	545	LYS
1	H	459	LYS
1	H	519	ASN
1	H	531	LYS
1	H	553	THR
1	I	384	GLY
1	I	459	LYS
1	I	519	ASN
1	I	531	LYS
1	I	545	LYS
1	I	553	THR
1	J	459	LYS
1	J	519	ASN
1	J	531	LYS
1	J	553	THR
1	K	459	LYS
1	K	519	ASN
1	K	531	LYS
1	K	552	ASN
1	K	553	THR
1	L	459	LYS
1	L	519	ASN
1	L	531	LYS
1	M	459	LYS
1	M	519	ASN
1	M	531	LYS
1	N	459	LYS
1	N	519	ASN
1	N	531	LYS
1	N	553	THR
1	O	459	LYS
1	O	519	ASN
1	O	531	LYS
1	O	545	LYS

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Mol	Chain	Res	Type
1	O	553	THR
1	P	459	LYS
1	P	519	ASN
1	P	531	LYS
1	P	545	LYS
1	P	553	THR
1	Q	268	SER
1	Q	459	LYS
1	Q	519	ASN
1	Q	531	LYS
1	R	268	SER
1	R	459	LYS
1	R	519	ASN
1	R	531	LYS
1	R	545	LYS
1	S	459	LYS
1	S	519	ASN
1	S	531	LYS
1	S	545	LYS
1	T	459	LYS
1	T	519	ASN
1	T	531	LYS
1	T	545	LYS
1	U	384	GLY
1	U	459	LYS
1	U	519	ASN
1	U	531	LYS
1	U	545	LYS
1	V	459	LYS
1	V	519	ASN
1	V	531	LYS
1	V	553	THR
1	W	384	GLY
1	W	459	LYS
1	W	519	ASN
1	W	531	LYS
1	X	459	LYS
1	X	519	ASN
1	X	531	LYS
1	X	553	THR
1	Y	459	LYS
1	Y	519	ASN

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Mol	Chain	Res	Type
1	Y	531	LYS
1	Y	545	LYS
1	Y	553	THR
1	Z	459	LYS
1	Z	519	ASN
1	Z	531	LYS
1	Z	552	ASN
1	a	459	LYS
1	a	519	ASN
1	a	531	LYS
1	a	553	THR
1	b	459	LYS
1	b	519	ASN
1	b	531	LYS
1	b	545	LYS
1	b	553	THR
1	c	519	ASN
1	c	531	LYS
1	c	545	LYS
1	d	459	LYS
1	d	519	ASN
1	d	531	LYS
1	d	545	LYS
1	d	553	THR
1	e	459	LYS
1	e	519	ASN
1	e	531	LYS
1	e	545	LYS
1	e	553	THR
1	f	459	LYS
1	f	519	ASN
1	f	531	LYS
1	g	459	LYS
1	g	519	ASN
1	g	531	LYS
1	g	552	ASN
1	h	459	LYS
1	h	519	ASN
1	h	531	LYS
1	h	553	THR
1	i	459	LYS
1	i	519	ASN

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Mol	Chain	Res	Type
1	i	531	LYS
1	i	545	LYS
1	i	553	THR
1	j	268	SER
1	j	459	LYS
1	j	519	ASN
1	j	531	LYS
1	k	384	GLY
1	k	459	LYS
1	k	519	ASN
1	k	531	LYS
1	l	459	LYS
1	l	519	ASN
1	l	531	LYS
1	l	553	THR
1	m	459	LYS
1	m	519	ASN
1	m	531	LYS
1	m	553	THR
1	n	459	LYS
1	n	519	ASN
1	n	531	LYS
1	n	545	LYS
1	n	553	THR
1	o	459	LYS
1	o	519	ASN
1	o	531	LYS
1	o	553	THR
1	p	459	LYS
1	p	519	ASN
1	p	531	LYS
1	p	553	THR
1	q	459	LYS
1	q	519	ASN
1	q	531	LYS
1	q	553	THR
1	r	459	LYS
1	r	519	ASN
1	r	531	LYS
1	r	545	LYS
1	r	553	THR
1	s	459	LYS

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Mol	Chain	Res	Type
1	s	519	ASN
1	s	531	LYS
1	s	545	LYS
1	s	553	THR
1	t	459	LYS
1	t	519	ASN
1	t	531	LYS
1	t	553	THR
1	u	459	LYS
1	u	519	ASN
1	u	531	LYS
1	u	545	LYS
1	v	459	LYS
1	v	519	ASN
1	v	531	LYS
1	v	553	THR
1	w	459	LYS
1	w	519	ASN
1	w	531	LYS
1	w	545	LYS
1	x	459	LYS
1	x	519	ASN
1	x	531	LYS
1	x	545	LYS
1	x	553	THR
1	y	459	LYS
1	y	519	ASN
1	y	531	LYS
1	z	459	LYS
1	z	519	ASN
1	z	531	LYS
1	z	553	THR
1	0	459	LYS
1	0	519	ASN
1	0	531	LYS
1	0	545	LYS
1	0	553	THR
1	1	459	LYS
1	1	519	ASN
1	1	531	LYS
1	1	545	LYS
1	1	553	THR

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Mol	Chain	Res	Type
1	2	459	LYS
1	2	519	ASN
1	2	531	LYS
1	3	459	LYS
1	3	519	ASN
1	3	531	LYS
1	3	545	LYS
1	3	553	THR
1	4	459	LYS
1	4	519	ASN
1	4	531	LYS
1	5	459	LYS
1	5	519	ASN
1	5	531	LYS
1	5	545	LYS
1	6	459	LYS
1	6	519	ASN
1	6	531	LYS
1	6	545	LYS
1	7	459	LYS
1	7	519	ASN
1	7	531	LYS
1	7	553	THR
1	A	220	GLY
1	A	268	SER
1	A	384	GLY
1	A	499	SER
1	A	544	GLY
1	A	552	ASN
1	A	553	THR
1	B	220	GLY
1	B	268	SER
1	B	384	GLY
1	B	544	GLY
1	B	552	ASN
1	B	553	THR
1	C	220	GLY
1	C	268	SER
1	C	384	GLY
1	C	544	GLY
1	C	545	LYS
1	D	220	GLY

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Mol	Chain	Res	Type
1	D	268	SER
1	D	384	GLY
1	D	544	GLY
1	D	545	LYS
1	D	552	ASN
1	E	220	GLY
1	E	268	SER
1	E	384	GLY
1	E	544	GLY
1	E	552	ASN
1	E	553	THR
1	F	220	GLY
1	F	268	SER
1	F	384	GLY
1	F	459	LYS
1	F	499	SER
1	F	544	GLY
1	F	552	ASN
1	G	220	GLY
1	G	268	SER
1	G	384	GLY
1	G	544	GLY
1	G	552	ASN
1	G	553	THR
1	H	220	GLY
1	H	268	SER
1	H	384	GLY
1	H	499	SER
1	H	544	GLY
1	H	545	LYS
1	I	220	GLY
1	I	268	SER
1	I	544	GLY
1	I	552	ASN
1	J	220	GLY
1	J	268	SER
1	J	384	GLY
1	J	544	GLY
1	J	545	LYS
1	J	552	ASN
1	K	220	GLY
1	K	268	SER

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Mol	Chain	Res	Type
1	K	384	GLY
1	K	544	GLY
1	K	545	LYS
1	L	220	GLY
1	L	268	SER
1	L	384	GLY
1	L	545	LYS
1	L	552	ASN
1	L	553	THR
1	M	220	GLY
1	M	268	SER
1	M	384	GLY
1	M	545	LYS
1	M	552	ASN
1	M	553	THR
1	N	220	GLY
1	N	268	SER
1	N	384	GLY
1	N	499	SER
1	N	545	LYS
1	N	552	ASN
1	O	220	GLY
1	O	268	SER
1	O	384	GLY
1	O	552	ASN
1	P	220	GLY
1	P	268	SER
1	P	384	GLY
1	P	544	GLY
1	P	552	ASN
1	Q	220	GLY
1	Q	384	GLY
1	Q	499	SER
1	Q	545	LYS
1	Q	552	ASN
1	Q	553	THR
1	R	220	GLY
1	R	384	GLY
1	R	552	ASN
1	R	553	THR
1	S	220	GLY
1	S	268	SER

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Mol	Chain	Res	Type
1	S	384	GLY
1	S	552	ASN
1	S	553	THR
1	T	220	GLY
1	T	268	SER
1	T	384	GLY
1	T	544	GLY
1	T	552	ASN
1	T	553	THR
1	U	220	GLY
1	U	268	SER
1	U	499	SER
1	U	544	GLY
1	U	552	ASN
1	U	553	THR
1	V	220	GLY
1	V	268	SER
1	V	384	GLY
1	V	499	SER
1	V	544	GLY
1	V	545	LYS
1	V	552	ASN
1	W	220	GLY
1	W	268	SER
1	W	499	SER
1	W	544	GLY
1	W	545	LYS
1	W	552	ASN
1	W	553	THR
1	X	220	GLY
1	X	268	SER
1	X	384	GLY
1	X	545	LYS
1	X	552	ASN
1	Y	220	GLY
1	Y	268	SER
1	Y	384	GLY
1	Y	499	SER
1	Y	544	GLY
1	Z	220	GLY
1	Z	268	SER
1	Z	384	GLY

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Mol	Chain	Res	Type
1	Z	553	THR
1	a	220	GLY
1	a	268	SER
1	a	384	GLY
1	a	545	LYS
1	a	552	ASN
1	b	220	GLY
1	b	268	SER
1	b	384	GLY
1	b	544	GLY
1	c	220	GLY
1	c	268	SER
1	c	384	GLY
1	c	459	LYS
1	c	544	GLY
1	c	552	ASN
1	c	553	THR
1	d	220	GLY
1	d	268	SER
1	d	384	GLY
1	d	544	GLY
1	d	552	ASN
1	e	220	GLY
1	e	268	SER
1	e	384	GLY
1	e	544	GLY
1	f	220	GLY
1	f	268	SER
1	f	384	GLY
1	f	545	LYS
1	f	552	ASN
1	f	553	THR
1	g	220	GLY
1	g	268	SER
1	g	384	GLY
1	g	544	GLY
1	g	545	LYS
1	g	553	THR
1	h	220	GLY
1	h	268	SER
1	h	384	GLY
1	h	545	LYS

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Mol	Chain	Res	Type
1	h	552	ASN
1	i	220	GLY
1	i	268	SER
1	i	384	GLY
1	i	499	SER
1	j	220	GLY
1	j	384	GLY
1	j	544	GLY
1	j	545	LYS
1	j	552	ASN
1	j	553	THR
1	k	220	GLY
1	k	268	SER
1	k	544	GLY
1	k	545	LYS
1	k	552	ASN
1	k	553	THR
1	l	220	GLY
1	l	268	SER
1	l	384	GLY
1	l	545	LYS
1	l	552	ASN
1	m	220	GLY
1	m	268	SER
1	m	384	GLY
1	m	544	GLY
1	m	545	LYS
1	n	220	GLY
1	n	268	SER
1	n	384	GLY
1	n	499	SER
1	o	220	GLY
1	o	268	SER
1	o	384	GLY
1	o	544	GLY
1	o	545	LYS
1	o	552	ASN
1	p	220	GLY
1	p	268	SER
1	p	384	GLY
1	p	544	GLY
1	p	545	LYS

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Mol	Chain	Res	Type
1	p	552	ASN
1	q	220	GLY
1	q	268	SER
1	q	384	GLY
1	q	545	LYS
1	q	552	ASN
1	r	220	GLY
1	r	268	SER
1	r	384	GLY
1	r	544	GLY
1	r	552	ASN
1	s	220	GLY
1	s	268	SER
1	s	384	GLY
1	s	499	SER
1	s	544	GLY
1	s	552	ASN
1	t	220	GLY
1	t	268	SER
1	t	384	GLY
1	t	545	LYS
1	t	552	ASN
1	u	220	GLY
1	u	268	SER
1	u	384	GLY
1	u	544	GLY
1	u	553	THR
1	v	220	GLY
1	v	268	SER
1	v	384	GLY
1	v	544	GLY
1	v	545	LYS
1	v	552	ASN
1	w	220	GLY
1	w	268	SER
1	w	384	GLY
1	w	544	GLY
1	w	552	ASN
1	w	553	THR
1	x	220	GLY
1	x	268	SER
1	x	384	GLY

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Mol	Chain	Res	Type
1	x	544	GLY
1	x	552	ASN
1	y	220	GLY
1	y	268	SER
1	y	384	GLY
1	y	552	ASN
1	y	553	THR
1	z	220	GLY
1	z	268	SER
1	z	384	GLY
1	z	545	LYS
1	0	220	GLY
1	0	268	SER
1	0	384	GLY
1	0	552	ASN
1	1	220	GLY
1	1	268	SER
1	1	384	GLY
1	1	552	ASN
1	2	220	GLY
1	2	268	SER
1	2	384	GLY
1	2	544	GLY
1	2	545	LYS
1	2	552	ASN
1	2	553	THR
1	3	220	GLY
1	3	268	SER
1	3	384	GLY
1	3	544	GLY
1	3	552	ASN
1	4	220	GLY
1	4	268	SER
1	4	384	GLY
1	4	544	GLY
1	4	545	LYS
1	4	552	ASN
1	4	553	THR
1	5	220	GLY
1	5	268	SER
1	5	384	GLY
1	5	552	ASN

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Mol	Chain	Res	Type
1	5	553	THR
1	6	220	GLY
1	6	268	SER
1	6	384	GLY
1	6	499	SER
1	6	544	GLY
1	6	552	ASN
1	6	553	THR
1	7	220	GLY
1	7	268	SER
1	7	384	GLY
1	7	545	LYS
1	7	552	ASN
1	A	218	ALA
1	B	499	SER
1	B	545	LYS
1	C	218	ALA
1	C	499	SER
1	C	552	ASN
1	D	218	ALA
1	D	499	SER
1	E	218	ALA
1	E	499	SER
1	F	218	ALA
1	F	518	ILE
1	G	499	SER
1	H	218	ALA
1	H	552	ASN
1	I	218	ALA
1	I	499	SER
1	J	218	ALA
1	J	499	SER
1	K	218	ALA
1	L	218	ALA
1	L	499	SER
1	M	218	ALA
1	M	499	SER
1	N	218	ALA
1	N	544	GLY
1	O	218	ALA
1	P	218	ALA
1	P	460	ASP

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Mol	Chain	Res	Type
1	P	499	SER
1	Q	218	ALA
1	Q	544	GLY
1	R	218	ALA
1	R	499	SER
1	S	218	ALA
1	T	218	ALA
1	U	218	ALA
1	V	218	ALA
1	W	218	ALA
1	X	218	ALA
1	X	499	SER
1	Y	218	ALA
1	Y	552	ASN
1	Z	218	ALA
1	Z	545	LYS
1	a	218	ALA
1	a	499	SER
1	b	218	ALA
1	b	499	SER
1	b	552	ASN
1	c	218	ALA
1	c	499	SER
1	d	218	ALA
1	d	499	SER
1	e	218	ALA
1	e	499	SER
1	e	552	ASN
1	f	218	ALA
1	f	499	SER
1	g	218	ALA
1	g	499	SER
1	h	218	ALA
1	h	499	SER
1	i	552	ASN
1	j	218	ALA
1	k	218	ALA
1	k	385	SER
1	k	456	ALA
1	k	499	SER
1	l	218	ALA
1	l	499	SER

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Mol	Chain	Res	Type
1	l	544	GLY
1	m	218	ALA
1	m	499	SER
1	m	552	ASN
1	n	218	ALA
1	n	544	GLY
1	n	552	ASN
1	o	218	ALA
1	o	499	SER
1	p	218	ALA
1	p	499	SER
1	q	218	ALA
1	q	499	SER
1	q	544	GLY
1	r	218	ALA
1	r	499	SER
1	s	218	ALA
1	t	218	ALA
1	t	499	SER
1	u	218	ALA
1	u	499	SER
1	u	552	ASN
1	v	218	ALA
1	v	499	SER
1	w	218	ALA
1	w	499	SER
1	x	218	ALA
1	x	499	SER
1	y	499	SER
1	y	545	LYS
1	z	218	ALA
1	z	499	SER
1	z	544	GLY
1	z	552	ASN
1	0	218	ALA
1	0	499	SER
1	1	218	ALA
1	1	499	SER
1	1	544	GLY
1	2	218	ALA
1	2	499	SER
1	3	218	ALA

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Mol	Chain	Res	Type
1	3	499	SER
1	4	218	ALA
1	4	499	SER
1	5	218	ALA
1	5	499	SER
1	5	544	GLY
1	6	218	ALA
1	7	218	ALA
1	7	499	SER
1	7	544	GLY
1	A	328	ASP
1	A	518	ILE
1	B	218	ALA
1	G	218	ALA
1	G	385	SER
1	H	460	ASP
1	K	499	SER
1	O	499	SER
1	O	544	GLY
1	P	385	SER
1	S	499	SER
1	S	544	GLY
1	T	499	SER
1	X	385	SER
1	Z	499	SER
1	a	460	ASP
1	f	544	GLY
1	i	218	ALA
1	j	499	SER
1	n	460	ASP
1	o	460	ASP
1	p	460	ASP
1	r	253	ASN
1	v	328	ASP
1	y	218	ALA
1	5	460	ASP
1	7	460	ASP
1	B	460	ASP
1	C	460	ASP
1	E	460	ASP
1	G	460	ASP
1	I	460	ASP

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Mol	Chain	Res	Type
1	J	460	ASP
1	L	460	ASP
1	L	544	GLY
1	M	460	ASP
1	M	544	GLY
1	O	460	ASP
1	R	460	ASP
1	R	544	GLY
1	U	460	ASP
1	U	518	ILE
1	X	460	ASP
1	Z	544	GLY
1	d	460	ASP
1	f	328	ASP
1	g	460	ASP
1	i	253	ASN
1	i	328	ASP
1	i	460	ASP
1	j	460	ASP
1	k	460	ASP
1	q	460	ASP
1	t	460	ASP
1	v	385	SER
1	w	460	ASP
1	y	460	ASP
1	y	544	GLY
1	0	328	ASP
1	0	385	SER
1	0	460	ASP
1	1	385	SER
1	3	460	ASP
1	D	328	ASP
1	H	328	ASP
1	H	385	SER
1	I	328	ASP
1	I	385	SER
1	J	385	SER
1	K	460	ASP
1	N	266	GLY
1	N	460	ASP
1	U	330	VAL
1	U	385	SER

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Mol	Chain	Res	Type
1	V	460	ASP
1	W	460	ASP
1	e	460	ASP
1	f	460	ASP
1	m	460	ASP
1	p	266	GLY
1	p	328	ASP
1	r	385	SER
1	u	385	SER
1	u	460	ASP
1	v	460	ASP
1	w	328	ASP
1	1	460	ASP
1	4	460	ASP
1	7	385	SER
1	C	631	PRO
1	D	518	ILE
1	L	631	PRO
1	R	266	GLY
1	p	518	ILE
1	q	518	ILE
1	t	266	GLY
1	z	631	PRO
1	0	544	GLY
1	C	266	GLY
1	V	631	PRO
1	f	518	ILE
1	t	544	GLY
1	y	518	ILE
1	A	631	PRO
1	B	518	ILE
1	B	631	PRO
1	E	518	ILE
1	J	631	PRO
1	L	518	ILE
1	O	631	PRO
1	X	544	GLY
1	i	544	GLY
1	q	266	GLY
1	q	631	PRO
1	r	266	GLY
1	r	518	ILE

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Mol	Chain	Res	Type
1	w	631	PRO
1	0	266	GLY
1	7	631	PRO
1	F	631	PRO
1	Q	631	PRO
1	R	631	PRO
1	S	518	ILE
1	V	518	ILE
1	f	631	PRO
1	k	518	ILE
1	o	631	PRO
1	s	631	PRO
1	y	631	PRO
1	C	518	ILE
1	Q	266	GLY
1	R	518	ILE
1	T	266	GLY
1	Y	631	PRO
1	a	544	GLY
1	t	518	ILE
1	1	518	ILE

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	0	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	1	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	2	452/452 (100%)	414 (92%)	38 (8%)	11	38
1	3	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	4	452/452 (100%)	413 (91%)	39 (9%)	10	37
1	5	452/452 (100%)	411 (91%)	41 (9%)	9	34
1	6	452/452 (100%)	414 (92%)	38 (8%)	11	38
1	7	452/452 (100%)	412 (91%)	40 (9%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	452/452 (100%)	408 (90%)	44 (10%)	8	31
1	B	452/452 (100%)	409 (90%)	43 (10%)	8	32
1	C	452/452 (100%)	413 (91%)	39 (9%)	10	37
1	D	452/452 (100%)	411 (91%)	41 (9%)	9	34
1	E	452/452 (100%)	413 (91%)	39 (9%)	10	37
1	F	452/452 (100%)	413 (91%)	39 (9%)	10	37
1	G	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	H	452/452 (100%)	411 (91%)	41 (9%)	9	34
1	I	452/452 (100%)	410 (91%)	42 (9%)	9	33
1	J	452/452 (100%)	411 (91%)	41 (9%)	9	34
1	K	452/452 (100%)	415 (92%)	37 (8%)	11	39
1	L	452/452 (100%)	413 (91%)	39 (9%)	10	37
1	M	452/452 (100%)	413 (91%)	39 (9%)	10	37
1	N	452/452 (100%)	414 (92%)	38 (8%)	11	38
1	O	452/452 (100%)	411 (91%)	41 (9%)	9	34
1	P	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	Q	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	R	452/452 (100%)	408 (90%)	44 (10%)	8	31
1	S	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	T	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	U	452/452 (100%)	410 (91%)	42 (9%)	9	33
1	V	452/452 (100%)	409 (90%)	43 (10%)	8	32
1	W	452/452 (100%)	410 (91%)	42 (9%)	9	33
1	X	452/452 (100%)	415 (92%)	37 (8%)	11	39
1	Y	452/452 (100%)	413 (91%)	39 (9%)	10	37
1	Z	452/452 (100%)	413 (91%)	39 (9%)	10	37
1	a	452/452 (100%)	414 (92%)	38 (8%)	11	38
1	b	452/452 (100%)	410 (91%)	42 (9%)	9	33
1	c	452/452 (100%)	408 (90%)	44 (10%)	8	31
1	d	452/452 (100%)	413 (91%)	39 (9%)	10	37
1	e	452/452 (100%)	410 (91%)	42 (9%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	f	452/452 (100%)	415 (92%)	37 (8%)	11	39
1	g	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	h	452/452 (100%)	415 (92%)	37 (8%)	11	39
1	i	452/452 (100%)	410 (91%)	42 (9%)	9	33
1	j	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	k	452/452 (100%)	408 (90%)	44 (10%)	8	31
1	l	452/452 (100%)	413 (91%)	39 (9%)	10	37
1	m	452/452 (100%)	414 (92%)	38 (8%)	11	38
1	n	452/452 (100%)	411 (91%)	41 (9%)	9	34
1	o	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	p	452/452 (100%)	415 (92%)	37 (8%)	11	39
1	q	452/452 (100%)	408 (90%)	44 (10%)	8	31
1	r	452/452 (100%)	411 (91%)	41 (9%)	9	34
1	s	452/452 (100%)	413 (91%)	39 (9%)	10	37
1	t	452/452 (100%)	415 (92%)	37 (8%)	11	39
1	u	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	v	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	w	452/452 (100%)	412 (91%)	40 (9%)	10	36
1	x	452/452 (100%)	415 (92%)	37 (8%)	11	39
1	y	452/452 (100%)	413 (91%)	39 (9%)	10	37
1	z	452/452 (100%)	409 (90%)	43 (10%)	8	32
All	All	27120/27120 (100%)	24715 (91%)	2405 (9%)	9	35

All (2405) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	ASP
1	A	223	ASN
1	A	242	THR
1	A	243	SER
1	A	251	THR
1	A	265	THR
1	A	286	ASN
1	A	287	ARG
1	A	289	HIS

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Mol	Chain	Res	Type
1	A	295	ARG
1	A	300	LEU
1	A	333	ILE
1	A	341	VAL
1	A	379	LEU
1	A	397	GLU
1	A	412	PHE
1	A	434	LEU
1	A	435	MET
1	A	443	LEU
1	A	449	THR
1	A	458	ASN
1	A	501	PHE
1	A	504	THR
1	A	507	SER
1	A	532	ASP
1	A	537	MET
1	A	551	SER
1	A	556	ASP
1	A	566	ILE
1	A	572	VAL
1	A	576	ARG
1	A	582	VAL
1	A	584	LEU
1	A	587	SER
1	A	599	MET
1	A	622	ILE
1	A	626	ASP
1	A	628	HIS
1	A	634	LEU
1	A	690	GLU
1	A	691	ASN
1	A	696	ASN
1	A	722	THR
1	A	725	ARG
1	B	219	ASP
1	B	223	ASN
1	B	242	THR
1	B	251	THR
1	B	265	THR
1	B	270	ASP
1	B	286	ASN

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Mol	Chain	Res	Type
1	B	287	ARG
1	B	289	HIS
1	B	295	ARG
1	B	300	LEU
1	B	333	ILE
1	B	341	VAL
1	B	379	LEU
1	B	397	GLU
1	B	412	PHE
1	B	434	LEU
1	B	435	MET
1	B	449	THR
1	B	458	ASN
1	B	501	PHE
1	B	504	THR
1	B	507	SER
1	B	532	ASP
1	B	537	MET
1	B	551	SER
1	B	556	ASP
1	B	566	ILE
1	B	572	VAL
1	B	576	ARG
1	B	582	VAL
1	B	587	SER
1	B	599	MET
1	B	626	ASP
1	B	628	HIS
1	B	634	LEU
1	B	669	SER
1	B	690	GLU
1	B	691	ASN
1	B	696	ASN
1	B	700	GLN
1	B	722	THR
1	B	725	ARG
1	C	219	ASP
1	C	223	ASN
1	C	242	THR
1	C	251	THR
1	C	286	ASN
1	C	287	ARG

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Mol	Chain	Res	Type
1	C	289	HIS
1	C	295	ARG
1	C	300	LEU
1	C	333	ILE
1	C	379	LEU
1	C	412	PHE
1	C	434	LEU
1	C	435	MET
1	C	443	LEU
1	C	449	THR
1	C	458	ASN
1	C	501	PHE
1	C	504	THR
1	C	532	ASP
1	C	537	MET
1	C	551	SER
1	C	556	ASP
1	C	566	ILE
1	C	572	VAL
1	C	576	ARG
1	C	582	VAL
1	C	587	SER
1	C	622	ILE
1	C	626	ASP
1	C	628	HIS
1	C	634	LEU
1	C	676	THR
1	C	690	GLU
1	C	691	ASN
1	C	696	ASN
1	C	717	ASN
1	C	722	THR
1	C	725	ARG
1	D	219	ASP
1	D	223	ASN
1	D	242	THR
1	D	251	THR
1	D	265	THR
1	D	286	ASN
1	D	287	ARG
1	D	289	HIS
1	D	295	ARG

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Mol	Chain	Res	Type
1	D	300	LEU
1	D	333	ILE
1	D	341	VAL
1	D	379	LEU
1	D	397	GLU
1	D	412	PHE
1	D	434	LEU
1	D	435	MET
1	D	443	LEU
1	D	449	THR
1	D	458	ASN
1	D	501	PHE
1	D	504	THR
1	D	532	ASP
1	D	537	MET
1	D	551	SER
1	D	556	ASP
1	D	566	ILE
1	D	572	VAL
1	D	576	ARG
1	D	582	VAL
1	D	587	SER
1	D	599	MET
1	D	622	ILE
1	D	626	ASP
1	D	628	HIS
1	D	634	LEU
1	D	690	GLU
1	D	696	ASN
1	D	717	ASN
1	D	722	THR
1	D	725	ARG
1	E	219	ASP
1	E	223	ASN
1	E	242	THR
1	E	251	THR
1	E	286	ASN
1	E	287	ARG
1	E	289	HIS
1	E	295	ARG
1	E	300	LEU
1	E	333	ILE

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Mol	Chain	Res	Type
1	E	379	LEU
1	E	397	GLU
1	E	412	PHE
1	E	435	MET
1	E	443	LEU
1	E	449	THR
1	E	458	ASN
1	E	501	PHE
1	E	504	THR
1	E	507	SER
1	E	532	ASP
1	E	537	MET
1	E	551	SER
1	E	556	ASP
1	E	566	ILE
1	E	572	VAL
1	E	576	ARG
1	E	582	VAL
1	E	587	SER
1	E	599	MET
1	E	622	ILE
1	E	626	ASP
1	E	628	HIS
1	E	634	LEU
1	E	690	GLU
1	E	691	ASN
1	E	696	ASN
1	E	722	THR
1	E	725	ARG
1	F	219	ASP
1	F	223	ASN
1	F	242	THR
1	F	251	THR
1	F	286	ASN
1	F	287	ARG
1	F	289	HIS
1	F	295	ARG
1	F	300	LEU
1	F	333	ILE
1	F	341	VAL
1	F	379	LEU
1	F	397	GLU

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Mol	Chain	Res	Type
1	F	412	PHE
1	F	434	LEU
1	F	435	MET
1	F	443	LEU
1	F	449	THR
1	F	458	ASN
1	F	501	PHE
1	F	504	THR
1	F	532	ASP
1	F	551	SER
1	F	556	ASP
1	F	566	ILE
1	F	572	VAL
1	F	576	ARG
1	F	582	VAL
1	F	587	SER
1	F	622	ILE
1	F	626	ASP
1	F	628	HIS
1	F	634	LEU
1	F	676	THR
1	F	690	GLU
1	F	691	ASN
1	F	696	ASN
1	F	722	THR
1	F	725	ARG
1	G	219	ASP
1	G	223	ASN
1	G	242	THR
1	G	251	THR
1	G	286	ASN
1	G	287	ARG
1	G	289	HIS
1	G	295	ARG
1	G	300	LEU
1	G	333	ILE
1	G	379	LEU
1	G	397	GLU
1	G	412	PHE
1	G	434	LEU
1	G	435	MET
1	G	443	LEU

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Mol	Chain	Res	Type
1	G	449	THR
1	G	458	ASN
1	G	501	PHE
1	G	504	THR
1	G	532	ASP
1	G	537	MET
1	G	551	SER
1	G	556	ASP
1	G	566	ILE
1	G	572	VAL
1	G	576	ARG
1	G	582	VAL
1	G	587	SER
1	G	599	MET
1	G	622	ILE
1	G	626	ASP
1	G	628	HIS
1	G	634	LEU
1	G	676	THR
1	G	690	GLU
1	G	691	ASN
1	G	696	ASN
1	G	722	THR
1	G	725	ARG
1	H	219	ASP
1	H	223	ASN
1	H	242	THR
1	H	251	THR
1	H	265	THR
1	H	270	ASP
1	H	286	ASN
1	H	287	ARG
1	H	289	HIS
1	H	295	ARG
1	H	300	LEU
1	H	333	ILE
1	H	379	LEU
1	H	397	GLU
1	H	412	PHE
1	H	434	LEU
1	H	435	MET
1	H	443	LEU

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Mol	Chain	Res	Type
1	H	449	THR
1	H	458	ASN
1	H	501	PHE
1	H	504	THR
1	H	532	ASP
1	H	551	SER
1	H	556	ASP
1	H	566	ILE
1	H	572	VAL
1	H	576	ARG
1	H	582	VAL
1	H	587	SER
1	H	599	MET
1	H	622	ILE
1	H	626	ASP
1	H	628	HIS
1	H	634	LEU
1	H	690	GLU
1	H	691	ASN
1	H	696	ASN
1	H	717	ASN
1	H	722	THR
1	H	725	ARG
1	I	219	ASP
1	I	223	ASN
1	I	242	THR
1	I	251	THR
1	I	270	ASP
1	I	286	ASN
1	I	287	ARG
1	I	289	HIS
1	I	295	ARG
1	I	300	LEU
1	I	333	ILE
1	I	341	VAL
1	I	379	LEU
1	I	397	GLU
1	I	412	PHE
1	I	434	LEU
1	I	435	MET
1	I	443	LEU
1	I	449	THR

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Mol	Chain	Res	Type
1	I	458	ASN
1	I	501	PHE
1	I	504	THR
1	I	507	SER
1	I	532	ASP
1	I	537	MET
1	I	551	SER
1	I	556	ASP
1	I	566	ILE
1	I	572	VAL
1	I	576	ARG
1	I	582	VAL
1	I	587	SER
1	I	599	MET
1	I	622	ILE
1	I	626	ASP
1	I	628	HIS
1	I	634	LEU
1	I	690	GLU
1	I	696	ASN
1	I	717	ASN
1	I	722	THR
1	I	725	ARG
1	J	219	ASP
1	J	223	ASN
1	J	242	THR
1	J	251	THR
1	J	265	THR
1	J	270	ASP
1	J	286	ASN
1	J	287	ARG
1	J	289	HIS
1	J	295	ARG
1	J	300	LEU
1	J	333	ILE
1	J	341	VAL
1	J	379	LEU
1	J	397	GLU
1	J	412	PHE
1	J	434	LEU
1	J	435	MET
1	J	443	LEU

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Mol	Chain	Res	Type
1	J	449	THR
1	J	458	ASN
1	J	501	PHE
1	J	504	THR
1	J	532	ASP
1	J	551	SER
1	J	556	ASP
1	J	566	ILE
1	J	572	VAL
1	J	576	ARG
1	J	582	VAL
1	J	587	SER
1	J	599	MET
1	J	622	ILE
1	J	626	ASP
1	J	628	HIS
1	J	634	LEU
1	J	690	GLU
1	J	691	ASN
1	J	696	ASN
1	J	722	THR
1	J	725	ARG
1	K	219	ASP
1	K	223	ASN
1	K	242	THR
1	K	251	THR
1	K	286	ASN
1	K	287	ARG
1	K	289	HIS
1	K	295	ARG
1	K	300	LEU
1	K	333	ILE
1	K	379	LEU
1	K	397	GLU
1	K	412	PHE
1	K	435	MET
1	K	443	LEU
1	K	449	THR
1	K	458	ASN
1	K	501	PHE
1	K	504	THR
1	K	532	ASP

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Mol	Chain	Res	Type
1	K	551	SER
1	K	556	ASP
1	K	566	ILE
1	K	572	VAL
1	K	576	ARG
1	K	582	VAL
1	K	587	SER
1	K	626	ASP
1	K	628	HIS
1	K	634	LEU
1	K	669	SER
1	K	676	THR
1	K	690	GLU
1	K	691	ASN
1	K	696	ASN
1	K	722	THR
1	K	725	ARG
1	L	219	ASP
1	L	223	ASN
1	L	242	THR
1	L	251	THR
1	L	270	ASP
1	L	286	ASN
1	L	287	ARG
1	L	289	HIS
1	L	295	ARG
1	L	300	LEU
1	L	333	ILE
1	L	379	LEU
1	L	397	GLU
1	L	412	PHE
1	L	435	MET
1	L	449	THR
1	L	458	ASN
1	L	501	PHE
1	L	504	THR
1	L	507	SER
1	L	532	ASP
1	L	551	SER
1	L	556	ASP
1	L	566	ILE
1	L	572	VAL

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Mol	Chain	Res	Type
1	L	576	ARG
1	L	582	VAL
1	L	587	SER
1	L	599	MET
1	L	622	ILE
1	L	626	ASP
1	L	628	HIS
1	L	634	LEU
1	L	690	GLU
1	L	696	ASN
1	L	700	GLN
1	L	717	ASN
1	L	722	THR
1	L	725	ARG
1	M	219	ASP
1	M	223	ASN
1	M	251	THR
1	M	270	ASP
1	M	286	ASN
1	M	287	ARG
1	M	289	HIS
1	M	295	ARG
1	M	300	LEU
1	M	333	ILE
1	M	379	LEU
1	M	397	GLU
1	M	412	PHE
1	M	434	LEU
1	M	435	MET
1	M	449	THR
1	M	458	ASN
1	M	501	PHE
1	M	504	THR
1	M	532	ASP
1	M	537	MET
1	M	551	SER
1	M	556	ASP
1	M	566	ILE
1	M	572	VAL
1	M	576	ARG
1	M	582	VAL
1	M	587	SER

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Mol	Chain	Res	Type
1	M	599	MET
1	M	626	ASP
1	M	628	HIS
1	M	634	LEU
1	M	669	SER
1	M	676	THR
1	M	690	GLU
1	M	696	ASN
1	M	717	ASN
1	M	722	THR
1	M	725	ARG
1	N	219	ASP
1	N	223	ASN
1	N	242	THR
1	N	251	THR
1	N	286	ASN
1	N	287	ARG
1	N	289	HIS
1	N	295	ARG
1	N	300	LEU
1	N	333	ILE
1	N	379	LEU
1	N	397	GLU
1	N	412	PHE
1	N	434	LEU
1	N	435	MET
1	N	449	THR
1	N	458	ASN
1	N	501	PHE
1	N	504	THR
1	N	532	ASP
1	N	551	SER
1	N	556	ASP
1	N	566	ILE
1	N	572	VAL
1	N	576	ARG
1	N	582	VAL
1	N	587	SER
1	N	599	MET
1	N	622	ILE
1	N	626	ASP
1	N	628	HIS

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Mol	Chain	Res	Type
1	N	634	LEU
1	N	669	SER
1	N	690	GLU
1	N	696	ASN
1	N	717	ASN
1	N	722	THR
1	N	725	ARG
1	O	219	ASP
1	O	223	ASN
1	O	242	THR
1	O	251	THR
1	O	265	THR
1	O	286	ASN
1	O	287	ARG
1	O	289	HIS
1	O	295	ARG
1	O	300	LEU
1	O	309	PRO
1	O	333	ILE
1	O	379	LEU
1	O	397	GLU
1	O	412	PHE
1	O	435	MET
1	O	443	LEU
1	O	449	THR
1	O	458	ASN
1	O	501	PHE
1	O	504	THR
1	O	532	ASP
1	O	537	MET
1	O	551	SER
1	O	556	ASP
1	O	572	VAL
1	O	576	ARG
1	O	582	VAL
1	O	587	SER
1	O	599	MET
1	O	622	ILE
1	O	626	ASP
1	O	628	HIS
1	O	634	LEU
1	O	669	SER

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Mol	Chain	Res	Type
1	O	690	GLU
1	O	691	ASN
1	O	696	ASN
1	O	717	ASN
1	O	722	THR
1	O	725	ARG
1	P	219	ASP
1	P	223	ASN
1	P	242	THR
1	P	251	THR
1	P	286	ASN
1	P	287	ARG
1	P	289	HIS
1	P	295	ARG
1	P	300	LEU
1	P	333	ILE
1	P	379	LEU
1	P	412	PHE
1	P	431	LEU
1	P	434	LEU
1	P	435	MET
1	P	449	THR
1	P	458	ASN
1	P	501	PHE
1	P	504	THR
1	P	507	SER
1	P	532	ASP
1	P	537	MET
1	P	551	SER
1	P	556	ASP
1	P	566	ILE
1	P	572	VAL
1	P	576	ARG
1	P	582	VAL
1	P	587	SER
1	P	599	MET
1	P	622	ILE
1	P	626	ASP
1	P	634	LEU
1	P	669	SER
1	P	676	THR
1	P	690	GLU

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Mol	Chain	Res	Type
1	P	691	ASN
1	P	696	ASN
1	P	722	THR
1	P	725	ARG
1	Q	219	ASP
1	Q	223	ASN
1	Q	251	THR
1	Q	265	THR
1	Q	270	ASP
1	Q	286	ASN
1	Q	287	ARG
1	Q	289	HIS
1	Q	295	ARG
1	Q	300	LEU
1	Q	333	ILE
1	Q	379	LEU
1	Q	397	GLU
1	Q	412	PHE
1	Q	434	LEU
1	Q	435	MET
1	Q	443	LEU
1	Q	449	THR
1	Q	458	ASN
1	Q	501	PHE
1	Q	504	THR
1	Q	532	ASP
1	Q	556	ASP
1	Q	566	ILE
1	Q	572	VAL
1	Q	576	ARG
1	Q	582	VAL
1	Q	587	SER
1	Q	599	MET
1	Q	622	ILE
1	Q	626	ASP
1	Q	628	HIS
1	Q	634	LEU
1	Q	690	GLU
1	Q	691	ASN
1	Q	696	ASN
1	Q	700	GLN
1	Q	717	ASN

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Mol	Chain	Res	Type
1	Q	722	THR
1	Q	725	ARG
1	R	219	ASP
1	R	223	ASN
1	R	242	THR
1	R	251	THR
1	R	265	THR
1	R	270	ASP
1	R	286	ASN
1	R	287	ARG
1	R	289	HIS
1	R	295	ARG
1	R	300	LEU
1	R	333	ILE
1	R	341	VAL
1	R	379	LEU
1	R	397	GLU
1	R	412	PHE
1	R	434	LEU
1	R	435	MET
1	R	443	LEU
1	R	449	THR
1	R	458	ASN
1	R	501	PHE
1	R	504	THR
1	R	532	ASP
1	R	537	MET
1	R	551	SER
1	R	556	ASP
1	R	572	VAL
1	R	576	ARG
1	R	582	VAL
1	R	587	SER
1	R	599	MET
1	R	622	ILE
1	R	626	ASP
1	R	628	HIS
1	R	634	LEU
1	R	676	THR
1	R	690	GLU
1	R	691	ASN
1	R	696	ASN

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Mol	Chain	Res	Type
1	R	700	GLN
1	R	717	ASN
1	R	722	THR
1	R	725	ARG
1	S	219	ASP
1	S	223	ASN
1	S	242	THR
1	S	251	THR
1	S	286	ASN
1	S	287	ARG
1	S	289	HIS
1	S	295	ARG
1	S	300	LEU
1	S	333	ILE
1	S	379	LEU
1	S	397	GLU
1	S	412	PHE
1	S	431	LEU
1	S	434	LEU
1	S	435	MET
1	S	443	LEU
1	S	449	THR
1	S	458	ASN
1	S	501	PHE
1	S	504	THR
1	S	532	ASP
1	S	551	SER
1	S	556	ASP
1	S	566	ILE
1	S	572	VAL
1	S	576	ARG
1	S	582	VAL
1	S	587	SER
1	S	622	ILE
1	S	626	ASP
1	S	628	HIS
1	S	634	LEU
1	S	690	GLU
1	S	691	ASN
1	S	696	ASN
1	S	700	GLN
1	S	717	ASN

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Mol	Chain	Res	Type
1	S	722	THR
1	S	725	ARG
1	T	219	ASP
1	T	223	ASN
1	T	242	THR
1	T	251	THR
1	T	286	ASN
1	T	287	ARG
1	T	289	HIS
1	T	295	ARG
1	T	300	LEU
1	T	333	ILE
1	T	379	LEU
1	T	397	GLU
1	T	412	PHE
1	T	434	LEU
1	T	435	MET
1	T	443	LEU
1	T	449	THR
1	T	458	ASN
1	T	501	PHE
1	T	504	THR
1	T	532	ASP
1	T	537	MET
1	T	551	SER
1	T	556	ASP
1	T	566	ILE
1	T	572	VAL
1	T	576	ARG
1	T	582	VAL
1	T	587	SER
1	T	599	MET
1	T	622	ILE
1	T	626	ASP
1	T	628	HIS
1	T	634	LEU
1	T	690	GLU
1	T	691	ASN
1	T	696	ASN
1	T	717	ASN
1	T	722	THR
1	T	725	ARG

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Mol	Chain	Res	Type
1	U	219	ASP
1	U	223	ASN
1	U	242	THR
1	U	251	THR
1	U	270	ASP
1	U	286	ASN
1	U	287	ARG
1	U	289	HIS
1	U	295	ARG
1	U	300	LEU
1	U	333	ILE
1	U	379	LEU
1	U	397	GLU
1	U	412	PHE
1	U	434	LEU
1	U	435	MET
1	U	443	LEU
1	U	449	THR
1	U	458	ASN
1	U	501	PHE
1	U	504	THR
1	U	532	ASP
1	U	551	SER
1	U	556	ASP
1	U	566	ILE
1	U	572	VAL
1	U	576	ARG
1	U	582	VAL
1	U	587	SER
1	U	599	MET
1	U	622	ILE
1	U	626	ASP
1	U	628	HIS
1	U	634	LEU
1	U	669	SER
1	U	690	GLU
1	U	691	ASN
1	U	696	ASN
1	U	700	GLN
1	U	717	ASN
1	U	722	THR
1	U	725	ARG

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Mol	Chain	Res	Type
1	V	219	ASP
1	V	223	ASN
1	V	242	THR
1	V	251	THR
1	V	270	ASP
1	V	286	ASN
1	V	287	ARG
1	V	289	HIS
1	V	295	ARG
1	V	300	LEU
1	V	333	ILE
1	V	341	VAL
1	V	379	LEU
1	V	397	GLU
1	V	412	PHE
1	V	434	LEU
1	V	435	MET
1	V	443	LEU
1	V	449	THR
1	V	458	ASN
1	V	501	PHE
1	V	504	THR
1	V	507	SER
1	V	532	ASP
1	V	551	SER
1	V	556	ASP
1	V	566	ILE
1	V	572	VAL
1	V	576	ARG
1	V	582	VAL
1	V	587	SER
1	V	599	MET
1	V	622	ILE
1	V	626	ASP
1	V	628	HIS
1	V	634	LEU
1	V	669	SER
1	V	690	GLU
1	V	691	ASN
1	V	696	ASN
1	V	717	ASN
1	V	722	THR

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Mol	Chain	Res	Type
1	V	725	ARG
1	W	219	ASP
1	W	223	ASN
1	W	242	THR
1	W	251	THR
1	W	270	ASP
1	W	286	ASN
1	W	287	ARG
1	W	289	HIS
1	W	295	ARG
1	W	300	LEU
1	W	333	ILE
1	W	341	VAL
1	W	379	LEU
1	W	397	GLU
1	W	412	PHE
1	W	434	LEU
1	W	435	MET
1	W	443	LEU
1	W	449	THR
1	W	458	ASN
1	W	501	PHE
1	W	504	THR
1	W	532	ASP
1	W	537	MET
1	W	551	SER
1	W	556	ASP
1	W	566	ILE
1	W	572	VAL
1	W	576	ARG
1	W	582	VAL
1	W	587	SER
1	W	622	ILE
1	W	626	ASP
1	W	628	HIS
1	W	634	LEU
1	W	669	SER
1	W	690	GLU
1	W	691	ASN
1	W	696	ASN
1	W	700	GLN
1	W	722	THR

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Mol	Chain	Res	Type
1	W	725	ARG
1	X	219	ASP
1	X	223	ASN
1	X	242	THR
1	X	251	THR
1	X	286	ASN
1	X	287	ARG
1	X	289	HIS
1	X	295	ARG
1	X	300	LEU
1	X	333	ILE
1	X	379	LEU
1	X	397	GLU
1	X	412	PHE
1	X	434	LEU
1	X	435	MET
1	X	443	LEU
1	X	449	THR
1	X	458	ASN
1	X	501	PHE
1	X	504	THR
1	X	532	ASP
1	X	551	SER
1	X	556	ASP
1	X	566	ILE
1	X	572	VAL
1	X	576	ARG
1	X	582	VAL
1	X	587	SER
1	X	599	MET
1	X	622	ILE
1	X	626	ASP
1	X	634	LEU
1	X	690	GLU
1	X	691	ASN
1	X	696	ASN
1	X	722	THR
1	X	725	ARG
1	Y	219	ASP
1	Y	223	ASN
1	Y	242	THR
1	Y	251	THR

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Mol	Chain	Res	Type
1	Y	265	THR
1	Y	286	ASN
1	Y	287	ARG
1	Y	295	ARG
1	Y	300	LEU
1	Y	333	ILE
1	Y	341	VAL
1	Y	379	LEU
1	Y	397	GLU
1	Y	412	PHE
1	Y	434	LEU
1	Y	435	MET
1	Y	443	LEU
1	Y	449	THR
1	Y	458	ASN
1	Y	501	PHE
1	Y	504	THR
1	Y	532	ASP
1	Y	551	SER
1	Y	556	ASP
1	Y	566	ILE
1	Y	572	VAL
1	Y	576	ARG
1	Y	582	VAL
1	Y	587	SER
1	Y	622	ILE
1	Y	626	ASP
1	Y	628	HIS
1	Y	634	LEU
1	Y	669	SER
1	Y	690	GLU
1	Y	696	ASN
1	Y	717	ASN
1	Y	722	THR
1	Y	725	ARG
1	Z	219	ASP
1	Z	223	ASN
1	Z	251	THR
1	Z	265	THR
1	Z	270	ASP
1	Z	286	ASN
1	Z	287	ARG

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Mol	Chain	Res	Type
1	Z	289	HIS
1	Z	295	ARG
1	Z	300	LEU
1	Z	333	ILE
1	Z	379	LEU
1	Z	397	GLU
1	Z	434	LEU
1	Z	435	MET
1	Z	443	LEU
1	Z	449	THR
1	Z	458	ASN
1	Z	501	PHE
1	Z	504	THR
1	Z	507	SER
1	Z	532	ASP
1	Z	551	SER
1	Z	556	ASP
1	Z	566	ILE
1	Z	572	VAL
1	Z	576	ARG
1	Z	582	VAL
1	Z	587	SER
1	Z	599	MET
1	Z	622	ILE
1	Z	626	ASP
1	Z	628	HIS
1	Z	634	LEU
1	Z	676	THR
1	Z	690	GLU
1	Z	696	ASN
1	Z	722	THR
1	Z	725	ARG
1	a	219	ASP
1	a	223	ASN
1	a	242	THR
1	a	251	THR
1	a	265	THR
1	a	286	ASN
1	a	287	ARG
1	a	289	HIS
1	a	295	ARG
1	a	300	LEU

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Mol	Chain	Res	Type
1	a	333	ILE
1	a	379	LEU
1	a	412	PHE
1	a	435	MET
1	a	443	LEU
1	a	449	THR
1	a	458	ASN
1	a	501	PHE
1	a	504	THR
1	a	532	ASP
1	a	551	SER
1	a	556	ASP
1	a	566	ILE
1	a	572	VAL
1	a	576	ARG
1	a	582	VAL
1	a	587	SER
1	a	599	MET
1	a	622	ILE
1	a	626	ASP
1	a	628	HIS
1	a	634	LEU
1	a	669	SER
1	a	690	GLU
1	a	691	ASN
1	a	696	ASN
1	a	722	THR
1	a	725	ARG
1	b	219	ASP
1	b	223	ASN
1	b	251	THR
1	b	270	ASP
1	b	286	ASN
1	b	287	ARG
1	b	289	HIS
1	b	295	ARG
1	b	300	LEU
1	b	309	PRO
1	b	333	ILE
1	b	341	VAL
1	b	379	LEU
1	b	397	GLU

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Mol	Chain	Res	Type
1	b	412	PHE
1	b	434	LEU
1	b	435	MET
1	b	443	LEU
1	b	449	THR
1	b	458	ASN
1	b	501	PHE
1	b	504	THR
1	b	532	ASP
1	b	551	SER
1	b	556	ASP
1	b	566	ILE
1	b	572	VAL
1	b	576	ARG
1	b	582	VAL
1	b	587	SER
1	b	599	MET
1	b	622	ILE
1	b	626	ASP
1	b	628	HIS
1	b	634	LEU
1	b	669	SER
1	b	676	THR
1	b	690	GLU
1	b	691	ASN
1	b	696	ASN
1	b	722	THR
1	b	725	ARG
1	c	219	ASP
1	c	223	ASN
1	c	242	THR
1	c	251	THR
1	c	286	ASN
1	c	287	ARG
1	c	289	HIS
1	c	295	ARG
1	c	300	LEU
1	c	333	ILE
1	c	379	LEU
1	c	397	GLU
1	c	412	PHE
1	c	431	LEU

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Mol	Chain	Res	Type
1	c	434	LEU
1	c	435	MET
1	c	443	LEU
1	c	449	THR
1	c	458	ASN
1	c	501	PHE
1	c	504	THR
1	c	507	SER
1	c	532	ASP
1	c	537	MET
1	c	551	SER
1	c	556	ASP
1	c	566	ILE
1	c	572	VAL
1	c	576	ARG
1	c	582	VAL
1	c	587	SER
1	c	599	MET
1	c	622	ILE
1	c	626	ASP
1	c	628	HIS
1	c	634	LEU
1	c	669	SER
1	c	676	THR
1	c	690	GLU
1	c	691	ASN
1	c	696	ASN
1	c	717	ASN
1	c	722	THR
1	c	725	ARG
1	d	219	ASP
1	d	223	ASN
1	d	242	THR
1	d	251	THR
1	d	286	ASN
1	d	287	ARG
1	d	289	HIS
1	d	295	ARG
1	d	300	LEU
1	d	333	ILE
1	d	379	LEU
1	d	397	GLU

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Mol	Chain	Res	Type
1	d	412	PHE
1	d	435	MET
1	d	443	LEU
1	d	449	THR
1	d	458	ASN
1	d	501	PHE
1	d	504	THR
1	d	532	ASP
1	d	537	MET
1	d	551	SER
1	d	556	ASP
1	d	566	ILE
1	d	572	VAL
1	d	576	ARG
1	d	582	VAL
1	d	587	SER
1	d	599	MET
1	d	622	ILE
1	d	626	ASP
1	d	628	HIS
1	d	634	LEU
1	d	676	THR
1	d	690	GLU
1	d	691	ASN
1	d	696	ASN
1	d	722	THR
1	d	725	ARG
1	e	219	ASP
1	e	223	ASN
1	e	242	THR
1	e	251	THR
1	e	286	ASN
1	e	287	ARG
1	e	289	HIS
1	e	295	ARG
1	e	300	LEU
1	e	333	ILE
1	e	379	LEU
1	e	397	GLU
1	e	412	PHE
1	e	434	LEU
1	e	435	MET

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Mol	Chain	Res	Type
1	e	443	LEU
1	e	449	THR
1	e	458	ASN
1	e	501	PHE
1	e	504	THR
1	e	532	ASP
1	e	551	SER
1	e	556	ASP
1	e	557	ASN
1	e	566	ILE
1	e	572	VAL
1	e	576	ARG
1	e	582	VAL
1	e	587	SER
1	e	599	MET
1	e	622	ILE
1	e	626	ASP
1	e	628	HIS
1	e	634	LEU
1	e	669	SER
1	e	676	THR
1	e	690	GLU
1	e	691	ASN
1	e	696	ASN
1	e	717	ASN
1	e	722	THR
1	e	725	ARG
1	f	219	ASP
1	f	223	ASN
1	f	242	THR
1	f	251	THR
1	f	286	ASN
1	f	287	ARG
1	f	289	HIS
1	f	295	ARG
1	f	300	LEU
1	f	333	ILE
1	f	379	LEU
1	f	397	GLU
1	f	412	PHE
1	f	434	LEU
1	f	435	MET

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Mol	Chain	Res	Type
1	f	443	LEU
1	f	449	THR
1	f	458	ASN
1	f	501	PHE
1	f	504	THR
1	f	532	ASP
1	f	551	SER
1	f	556	ASP
1	f	566	ILE
1	f	572	VAL
1	f	576	ARG
1	f	582	VAL
1	f	587	SER
1	f	626	ASP
1	f	628	HIS
1	f	634	LEU
1	f	676	THR
1	f	690	GLU
1	f	691	ASN
1	f	696	ASN
1	f	722	THR
1	f	725	ARG
1	g	219	ASP
1	g	223	ASN
1	g	242	THR
1	g	251	THR
1	g	270	ASP
1	g	286	ASN
1	g	287	ARG
1	g	289	HIS
1	g	295	ARG
1	g	300	LEU
1	g	333	ILE
1	g	341	VAL
1	g	379	LEU
1	g	397	GLU
1	g	434	LEU
1	g	435	MET
1	g	443	LEU
1	g	449	THR
1	g	458	ASN
1	g	501	PHE

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Mol	Chain	Res	Type
1	g	504	THR
1	g	532	ASP
1	g	537	MET
1	g	551	SER
1	g	556	ASP
1	g	566	ILE
1	g	572	VAL
1	g	576	ARG
1	g	582	VAL
1	g	587	SER
1	g	622	ILE
1	g	626	ASP
1	g	628	HIS
1	g	634	LEU
1	g	669	SER
1	g	690	GLU
1	g	691	ASN
1	g	696	ASN
1	g	722	THR
1	g	725	ARG
1	h	219	ASP
1	h	223	ASN
1	h	242	THR
1	h	251	THR
1	h	286	ASN
1	h	287	ARG
1	h	289	HIS
1	h	295	ARG
1	h	300	LEU
1	h	333	ILE
1	h	379	LEU
1	h	412	PHE
1	h	435	MET
1	h	443	LEU
1	h	449	THR
1	h	458	ASN
1	h	501	PHE
1	h	504	THR
1	h	532	ASP
1	h	551	SER
1	h	556	ASP
1	h	566	ILE

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Mol	Chain	Res	Type
1	h	572	VAL
1	h	576	ARG
1	h	582	VAL
1	h	587	SER
1	h	622	ILE
1	h	626	ASP
1	h	628	HIS
1	h	634	LEU
1	h	669	SER
1	h	676	THR
1	h	690	GLU
1	h	691	ASN
1	h	696	ASN
1	h	722	THR
1	h	725	ARG
1	i	219	ASP
1	i	223	ASN
1	i	242	THR
1	i	251	THR
1	i	265	THR
1	i	270	ASP
1	i	286	ASN
1	i	287	ARG
1	i	289	HIS
1	i	295	ARG
1	i	300	LEU
1	i	333	ILE
1	i	379	LEU
1	i	397	GLU
1	i	412	PHE
1	i	435	MET
1	i	443	LEU
1	i	449	THR
1	i	458	ASN
1	i	501	PHE
1	i	504	THR
1	i	532	ASP
1	i	551	SER
1	i	556	ASP
1	i	566	ILE
1	i	572	VAL
1	i	576	ARG

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Mol	Chain	Res	Type
1	i	582	VAL
1	i	587	SER
1	i	589	THR
1	i	599	MET
1	i	622	ILE
1	i	626	ASP
1	i	628	HIS
1	i	634	LEU
1	i	676	THR
1	i	690	GLU
1	i	691	ASN
1	i	696	ASN
1	i	717	ASN
1	i	722	THR
1	i	725	ARG
1	j	219	ASP
1	j	223	ASN
1	j	242	THR
1	j	251	THR
1	j	286	ASN
1	j	287	ARG
1	j	289	HIS
1	j	295	ARG
1	j	300	LEU
1	j	333	ILE
1	j	341	VAL
1	j	379	LEU
1	j	397	GLU
1	j	412	PHE
1	j	431	LEU
1	j	434	LEU
1	j	435	MET
1	j	443	LEU
1	j	449	THR
1	j	458	ASN
1	j	501	PHE
1	j	504	THR
1	j	532	ASP
1	j	551	SER
1	j	556	ASP
1	j	566	ILE
1	j	572	VAL

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Mol	Chain	Res	Type
1	j	576	ARG
1	j	582	VAL
1	j	587	SER
1	j	599	MET
1	j	622	ILE
1	j	626	ASP
1	j	628	HIS
1	j	634	LEU
1	j	676	THR
1	j	690	GLU
1	j	696	ASN
1	j	722	THR
1	j	725	ARG
1	k	219	ASP
1	k	223	ASN
1	k	242	THR
1	k	251	THR
1	k	270	ASP
1	k	286	ASN
1	k	287	ARG
1	k	295	ARG
1	k	300	LEU
1	k	333	ILE
1	k	341	VAL
1	k	379	LEU
1	k	397	GLU
1	k	412	PHE
1	k	431	LEU
1	k	434	LEU
1	k	435	MET
1	k	443	LEU
1	k	449	THR
1	k	458	ASN
1	k	501	PHE
1	k	504	THR
1	k	507	SER
1	k	532	ASP
1	k	551	SER
1	k	556	ASP
1	k	566	ILE
1	k	572	VAL
1	k	576	ARG

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Mol	Chain	Res	Type
1	k	582	VAL
1	k	587	SER
1	k	599	MET
1	k	622	ILE
1	k	626	ASP
1	k	628	HIS
1	k	634	LEU
1	k	676	THR
1	k	690	GLU
1	k	691	ASN
1	k	696	ASN
1	k	700	GLN
1	k	717	ASN
1	k	722	THR
1	k	725	ARG
1	l	219	ASP
1	l	223	ASN
1	l	251	THR
1	l	265	THR
1	l	270	ASP
1	l	286	ASN
1	l	287	ARG
1	l	289	HIS
1	l	295	ARG
1	l	300	LEU
1	l	309	PRO
1	l	333	ILE
1	l	379	LEU
1	l	397	GLU
1	l	412	PHE
1	l	434	LEU
1	l	435	MET
1	l	449	THR
1	l	458	ASN
1	l	501	PHE
1	l	504	THR
1	l	507	SER
1	l	532	ASP
1	l	551	SER
1	l	556	ASP
1	l	566	ILE
1	l	572	VAL

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Mol	Chain	Res	Type
1	l	576	ARG
1	l	582	VAL
1	l	587	SER
1	l	599	MET
1	l	622	ILE
1	l	626	ASP
1	l	628	HIS
1	l	634	LEU
1	l	690	GLU
1	l	696	ASN
1	l	722	THR
1	l	725	ARG
1	m	219	ASP
1	m	223	ASN
1	m	242	THR
1	m	251	THR
1	m	286	ASN
1	m	287	ARG
1	m	289	HIS
1	m	295	ARG
1	m	300	LEU
1	m	333	ILE
1	m	379	LEU
1	m	397	GLU
1	m	412	PHE
1	m	434	LEU
1	m	435	MET
1	m	449	THR
1	m	458	ASN
1	m	501	PHE
1	m	504	THR
1	m	532	ASP
1	m	551	SER
1	m	556	ASP
1	m	566	ILE
1	m	572	VAL
1	m	576	ARG
1	m	582	VAL
1	m	587	SER
1	m	622	ILE
1	m	626	ASP
1	m	628	HIS

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Mol	Chain	Res	Type
1	m	634	LEU
1	m	669	SER
1	m	676	THR
1	m	690	GLU
1	m	696	ASN
1	m	717	ASN
1	m	722	THR
1	m	725	ARG
1	n	219	ASP
1	n	223	ASN
1	n	243	SER
1	n	251	THR
1	n	265	THR
1	n	286	ASN
1	n	287	ARG
1	n	289	HIS
1	n	295	ARG
1	n	300	LEU
1	n	333	ILE
1	n	379	LEU
1	n	397	GLU
1	n	412	PHE
1	n	431	LEU
1	n	434	LEU
1	n	435	MET
1	n	443	LEU
1	n	449	THR
1	n	458	ASN
1	n	501	PHE
1	n	504	THR
1	n	532	ASP
1	n	551	SER
1	n	556	ASP
1	n	566	ILE
1	n	572	VAL
1	n	576	ARG
1	n	582	VAL
1	n	587	SER
1	n	599	MET
1	n	622	ILE
1	n	626	ASP
1	n	628	HIS

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Mol	Chain	Res	Type
1	n	634	LEU
1	n	676	THR
1	n	690	GLU
1	n	696	ASN
1	n	717	ASN
1	n	722	THR
1	n	725	ARG
1	o	219	ASP
1	o	223	ASN
1	o	242	THR
1	o	251	THR
1	o	265	THR
1	o	270	ASP
1	o	286	ASN
1	o	287	ARG
1	o	289	HIS
1	o	295	ARG
1	o	300	LEU
1	o	333	ILE
1	o	341	VAL
1	o	379	LEU
1	o	397	GLU
1	o	412	PHE
1	o	435	MET
1	o	449	THR
1	o	458	ASN
1	o	501	PHE
1	o	504	THR
1	o	507	SER
1	o	532	ASP
1	o	551	SER
1	o	556	ASP
1	o	566	ILE
1	o	572	VAL
1	o	576	ARG
1	o	582	VAL
1	o	587	SER
1	o	599	MET
1	o	622	ILE
1	o	626	ASP
1	o	628	HIS
1	o	634	LEU

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Mol	Chain	Res	Type
1	o	690	GLU
1	o	691	ASN
1	o	696	ASN
1	o	722	THR
1	o	725	ARG
1	p	219	ASP
1	p	223	ASN
1	p	242	THR
1	p	251	THR
1	p	286	ASN
1	p	287	ARG
1	p	289	HIS
1	p	295	ARG
1	p	300	LEU
1	p	333	ILE
1	p	379	LEU
1	p	397	GLU
1	p	412	PHE
1	p	435	MET
1	p	449	THR
1	p	458	ASN
1	p	501	PHE
1	p	504	THR
1	p	507	SER
1	p	532	ASP
1	p	551	SER
1	p	556	ASP
1	p	566	ILE
1	p	572	VAL
1	p	576	ARG
1	p	582	VAL
1	p	587	SER
1	p	599	MET
1	p	622	ILE
1	p	626	ASP
1	p	628	HIS
1	p	634	LEU
1	p	690	GLU
1	p	691	ASN
1	p	696	ASN
1	p	722	THR
1	p	725	ARG

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Mol	Chain	Res	Type
1	q	219	ASP
1	q	223	ASN
1	q	242	THR
1	q	251	THR
1	q	265	THR
1	q	270	ASP
1	q	286	ASN
1	q	287	ARG
1	q	289	HIS
1	q	295	ARG
1	q	300	LEU
1	q	333	ILE
1	q	341	VAL
1	q	379	LEU
1	q	397	GLU
1	q	412	PHE
1	q	434	LEU
1	q	435	MET
1	q	443	LEU
1	q	449	THR
1	q	458	ASN
1	q	501	PHE
1	q	504	THR
1	q	532	ASP
1	q	551	SER
1	q	556	ASP
1	q	566	ILE
1	q	572	VAL
1	q	576	ARG
1	q	582	VAL
1	q	587	SER
1	q	589	THR
1	q	599	MET
1	q	622	ILE
1	q	626	ASP
1	q	628	HIS
1	q	634	LEU
1	q	669	SER
1	q	690	GLU
1	q	691	ASN
1	q	696	ASN
1	q	717	ASN

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Mol	Chain	Res	Type
1	q	722	THR
1	q	725	ARG
1	r	219	ASP
1	r	223	ASN
1	r	242	THR
1	r	251	THR
1	r	286	ASN
1	r	287	ARG
1	r	289	HIS
1	r	295	ARG
1	r	300	LEU
1	r	333	ILE
1	r	379	LEU
1	r	397	GLU
1	r	412	PHE
1	r	434	LEU
1	r	435	MET
1	r	443	LEU
1	r	449	THR
1	r	458	ASN
1	r	501	PHE
1	r	504	THR
1	r	532	ASP
1	r	551	SER
1	r	556	ASP
1	r	566	ILE
1	r	572	VAL
1	r	576	ARG
1	r	582	VAL
1	r	587	SER
1	r	599	MET
1	r	622	ILE
1	r	626	ASP
1	r	628	HIS
1	r	634	LEU
1	r	669	SER
1	r	676	THR
1	r	690	GLU
1	r	691	ASN
1	r	696	ASN
1	r	700	GLN
1	r	722	THR

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Mol	Chain	Res	Type
1	r	725	ARG
1	s	219	ASP
1	s	223	ASN
1	s	242	THR
1	s	251	THR
1	s	286	ASN
1	s	287	ARG
1	s	289	HIS
1	s	295	ARG
1	s	300	LEU
1	s	333	ILE
1	s	379	LEU
1	s	397	GLU
1	s	412	PHE
1	s	434	LEU
1	s	435	MET
1	s	443	LEU
1	s	449	THR
1	s	458	ASN
1	s	501	PHE
1	s	504	THR
1	s	532	ASP
1	s	551	SER
1	s	556	ASP
1	s	566	ILE
1	s	572	VAL
1	s	576	ARG
1	s	582	VAL
1	s	587	SER
1	s	622	ILE
1	s	626	ASP
1	s	628	HIS
1	s	634	LEU
1	s	676	THR
1	s	690	GLU
1	s	691	ASN
1	s	696	ASN
1	s	717	ASN
1	s	722	THR
1	s	725	ARG
1	t	219	ASP
1	t	223	ASN

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Mol	Chain	Res	Type
1	t	242	THR
1	t	251	THR
1	t	265	THR
1	t	286	ASN
1	t	287	ARG
1	t	289	HIS
1	t	295	ARG
1	t	300	LEU
1	t	333	ILE
1	t	379	LEU
1	t	397	GLU
1	t	412	PHE
1	t	435	MET
1	t	443	LEU
1	t	449	THR
1	t	458	ASN
1	t	501	PHE
1	t	504	THR
1	t	532	ASP
1	t	551	SER
1	t	556	ASP
1	t	566	ILE
1	t	572	VAL
1	t	576	ARG
1	t	582	VAL
1	t	587	SER
1	t	622	ILE
1	t	626	ASP
1	t	628	HIS
1	t	634	LEU
1	t	669	SER
1	t	690	GLU
1	t	696	ASN
1	t	722	THR
1	t	725	ARG
1	u	219	ASP
1	u	223	ASN
1	u	251	THR
1	u	286	ASN
1	u	287	ARG
1	u	289	HIS
1	u	295	ARG

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Mol	Chain	Res	Type
1	u	300	LEU
1	u	333	ILE
1	u	379	LEU
1	u	397	GLU
1	u	412	PHE
1	u	434	LEU
1	u	435	MET
1	u	443	LEU
1	u	449	THR
1	u	458	ASN
1	u	501	PHE
1	u	504	THR
1	u	532	ASP
1	u	551	SER
1	u	556	ASP
1	u	566	ILE
1	u	572	VAL
1	u	576	ARG
1	u	582	VAL
1	u	587	SER
1	u	599	MET
1	u	622	ILE
1	u	626	ASP
1	u	628	HIS
1	u	634	LEU
1	u	669	SER
1	u	676	THR
1	u	690	GLU
1	u	691	ASN
1	u	696	ASN
1	u	717	ASN
1	u	722	THR
1	u	725	ARG
1	v	219	ASP
1	v	223	ASN
1	v	242	THR
1	v	251	THR
1	v	286	ASN
1	v	287	ARG
1	v	289	HIS
1	v	295	ARG
1	v	300	LEU

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Mol	Chain	Res	Type
1	v	333	ILE
1	v	379	LEU
1	v	397	GLU
1	v	412	PHE
1	v	435	MET
1	v	443	LEU
1	v	449	THR
1	v	458	ASN
1	v	501	PHE
1	v	504	THR
1	v	532	ASP
1	v	537	MET
1	v	551	SER
1	v	556	ASP
1	v	566	ILE
1	v	572	VAL
1	v	576	ARG
1	v	582	VAL
1	v	587	SER
1	v	599	MET
1	v	622	ILE
1	v	626	ASP
1	v	628	HIS
1	v	634	LEU
1	v	669	SER
1	v	676	THR
1	v	690	GLU
1	v	691	ASN
1	v	696	ASN
1	v	722	THR
1	v	725	ARG
1	w	219	ASP
1	w	223	ASN
1	w	251	THR
1	w	286	ASN
1	w	287	ARG
1	w	289	HIS
1	w	295	ARG
1	w	300	LEU
1	w	333	ILE
1	w	379	LEU
1	w	397	GLU

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Mol	Chain	Res	Type
1	w	412	PHE
1	w	434	LEU
1	w	435	MET
1	w	443	LEU
1	w	449	THR
1	w	458	ASN
1	w	501	PHE
1	w	504	THR
1	w	532	ASP
1	w	551	SER
1	w	556	ASP
1	w	566	ILE
1	w	572	VAL
1	w	576	ARG
1	w	582	VAL
1	w	584	LEU
1	w	587	SER
1	w	599	MET
1	w	622	ILE
1	w	626	ASP
1	w	628	HIS
1	w	634	LEU
1	w	669	SER
1	w	676	THR
1	w	690	GLU
1	w	696	ASN
1	w	717	ASN
1	w	722	THR
1	w	725	ARG
1	x	219	ASP
1	x	223	ASN
1	x	251	THR
1	x	286	ASN
1	x	287	ARG
1	x	289	HIS
1	x	295	ARG
1	x	300	LEU
1	x	333	ILE
1	x	379	LEU
1	x	397	GLU
1	x	412	PHE
1	x	434	LEU

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Mol	Chain	Res	Type
1	x	435	MET
1	x	449	THR
1	x	458	ASN
1	x	501	PHE
1	x	504	THR
1	x	532	ASP
1	x	537	MET
1	x	551	SER
1	x	556	ASP
1	x	572	VAL
1	x	576	ARG
1	x	582	VAL
1	x	587	SER
1	x	599	MET
1	x	622	ILE
1	x	626	ASP
1	x	628	HIS
1	x	634	LEU
1	x	669	SER
1	x	676	THR
1	x	690	GLU
1	x	696	ASN
1	x	722	THR
1	x	725	ARG
1	y	219	ASP
1	y	223	ASN
1	y	242	THR
1	y	251	THR
1	y	286	ASN
1	y	287	ARG
1	y	289	HIS
1	y	295	ARG
1	y	300	LEU
1	y	333	ILE
1	y	379	LEU
1	y	397	GLU
1	y	412	PHE
1	y	435	MET
1	y	443	LEU
1	y	449	THR
1	y	458	ASN
1	y	464	SER

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Mol	Chain	Res	Type
1	y	501	PHE
1	y	504	THR
1	y	532	ASP
1	y	551	SER
1	y	556	ASP
1	y	566	ILE
1	y	572	VAL
1	y	576	ARG
1	y	582	VAL
1	y	587	SER
1	y	599	MET
1	y	622	ILE
1	y	626	ASP
1	y	628	HIS
1	y	634	LEU
1	y	690	GLU
1	y	691	ASN
1	y	696	ASN
1	y	700	GLN
1	y	722	THR
1	y	725	ARG
1	z	219	ASP
1	z	223	ASN
1	z	242	THR
1	z	251	THR
1	z	270	ASP
1	z	286	ASN
1	z	287	ARG
1	z	289	HIS
1	z	295	ARG
1	z	300	LEU
1	z	333	ILE
1	z	341	VAL
1	z	379	LEU
1	z	397	GLU
1	z	412	PHE
1	z	431	LEU
1	z	434	LEU
1	z	435	MET
1	z	449	THR
1	z	458	ASN
1	z	501	PHE

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Mol	Chain	Res	Type
1	z	504	THR
1	z	532	ASP
1	z	537	MET
1	z	551	SER
1	z	556	ASP
1	z	566	ILE
1	z	572	VAL
1	z	576	ARG
1	z	582	VAL
1	z	587	SER
1	z	599	MET
1	z	622	ILE
1	z	626	ASP
1	z	628	HIS
1	z	634	LEU
1	z	669	SER
1	z	690	GLU
1	z	691	ASN
1	z	696	ASN
1	z	717	ASN
1	z	722	THR
1	z	725	ARG
1	0	219	ASP
1	0	223	ASN
1	0	242	THR
1	0	251	THR
1	0	286	ASN
1	0	287	ARG
1	0	289	HIS
1	0	295	ARG
1	0	300	LEU
1	0	333	ILE
1	0	379	LEU
1	0	397	GLU
1	0	412	PHE
1	0	431	LEU
1	0	434	LEU
1	0	435	MET
1	0	449	THR
1	0	458	ASN
1	0	501	PHE
1	0	504	THR

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Mol	Chain	Res	Type
1	0	532	ASP
1	0	551	SER
1	0	556	ASP
1	0	566	ILE
1	0	572	VAL
1	0	576	ARG
1	0	582	VAL
1	0	587	SER
1	0	599	MET
1	0	622	ILE
1	0	626	ASP
1	0	628	HIS
1	0	634	LEU
1	0	669	SER
1	0	676	THR
1	0	690	GLU
1	0	691	ASN
1	0	696	ASN
1	0	722	THR
1	0	725	ARG
1	1	219	ASP
1	1	223	ASN
1	1	251	THR
1	1	265	THR
1	1	286	ASN
1	1	287	ARG
1	1	289	HIS
1	1	295	ARG
1	1	300	LEU
1	1	333	ILE
1	1	379	LEU
1	1	397	GLU
1	1	412	PHE
1	1	434	LEU
1	1	435	MET
1	1	443	LEU
1	1	449	THR
1	1	458	ASN
1	1	501	PHE
1	1	504	THR
1	1	532	ASP
1	1	537	MET

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Mol	Chain	Res	Type
1	1	551	SER
1	1	556	ASP
1	1	566	ILE
1	1	572	VAL
1	1	576	ARG
1	1	582	VAL
1	1	587	SER
1	1	589	THR
1	1	599	MET
1	1	622	ILE
1	1	626	ASP
1	1	628	HIS
1	1	634	LEU
1	1	690	GLU
1	1	696	ASN
1	1	717	ASN
1	1	722	THR
1	1	725	ARG
1	2	219	ASP
1	2	223	ASN
1	2	251	THR
1	2	270	ASP
1	2	286	ASN
1	2	287	ARG
1	2	295	ARG
1	2	300	LEU
1	2	333	ILE
1	2	341	VAL
1	2	379	LEU
1	2	397	GLU
1	2	412	PHE
1	2	434	LEU
1	2	435	MET
1	2	449	THR
1	2	458	ASN
1	2	501	PHE
1	2	504	THR
1	2	532	ASP
1	2	537	MET
1	2	551	SER
1	2	556	ASP
1	2	566	ILE

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Mol	Chain	Res	Type
1	2	572	VAL
1	2	576	ARG
1	2	582	VAL
1	2	587	SER
1	2	599	MET
1	2	626	ASP
1	2	628	HIS
1	2	634	LEU
1	2	669	SER
1	2	690	GLU
1	2	691	ASN
1	2	696	ASN
1	2	722	THR
1	2	725	ARG
1	3	219	ASP
1	3	223	ASN
1	3	242	THR
1	3	251	THR
1	3	286	ASN
1	3	287	ARG
1	3	289	HIS
1	3	295	ARG
1	3	300	LEU
1	3	333	ILE
1	3	379	LEU
1	3	397	GLU
1	3	412	PHE
1	3	431	LEU
1	3	435	MET
1	3	443	LEU
1	3	449	THR
1	3	458	ASN
1	3	501	PHE
1	3	504	THR
1	3	532	ASP
1	3	551	SER
1	3	556	ASP
1	3	566	ILE
1	3	572	VAL
1	3	576	ARG
1	3	582	VAL
1	3	587	SER

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Mol	Chain	Res	Type
1	3	599	MET
1	3	622	ILE
1	3	626	ASP
1	3	628	HIS
1	3	634	LEU
1	3	669	SER
1	3	690	GLU
1	3	691	ASN
1	3	696	ASN
1	3	717	ASN
1	3	722	THR
1	3	725	ARG
1	4	219	ASP
1	4	223	ASN
1	4	242	THR
1	4	251	THR
1	4	286	ASN
1	4	287	ARG
1	4	289	HIS
1	4	295	ARG
1	4	300	LEU
1	4	309	PRO
1	4	333	ILE
1	4	379	LEU
1	4	397	GLU
1	4	412	PHE
1	4	434	LEU
1	4	435	MET
1	4	443	LEU
1	4	449	THR
1	4	458	ASN
1	4	501	PHE
1	4	504	THR
1	4	532	ASP
1	4	551	SER
1	4	556	ASP
1	4	566	ILE
1	4	572	VAL
1	4	576	ARG
1	4	582	VAL
1	4	587	SER
1	4	622	ILE

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Mol	Chain	Res	Type
1	4	626	ASP
1	4	628	HIS
1	4	634	LEU
1	4	669	SER
1	4	690	GLU
1	4	691	ASN
1	4	696	ASN
1	4	722	THR
1	4	725	ARG
1	5	219	ASP
1	5	223	ASN
1	5	242	THR
1	5	251	THR
1	5	270	ASP
1	5	286	ASN
1	5	287	ARG
1	5	289	HIS
1	5	295	ARG
1	5	300	LEU
1	5	333	ILE
1	5	341	VAL
1	5	379	LEU
1	5	397	GLU
1	5	412	PHE
1	5	434	LEU
1	5	435	MET
1	5	443	LEU
1	5	449	THR
1	5	458	ASN
1	5	501	PHE
1	5	504	THR
1	5	507	SER
1	5	532	ASP
1	5	551	SER
1	5	556	ASP
1	5	566	ILE
1	5	572	VAL
1	5	576	ARG
1	5	582	VAL
1	5	587	SER
1	5	599	MET
1	5	622	ILE

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Mol	Chain	Res	Type
1	5	626	ASP
1	5	628	HIS
1	5	634	LEU
1	5	690	GLU
1	5	696	ASN
1	5	717	ASN
1	5	722	THR
1	5	725	ARG
1	6	219	ASP
1	6	223	ASN
1	6	251	THR
1	6	270	ASP
1	6	286	ASN
1	6	287	ARG
1	6	289	HIS
1	6	295	ARG
1	6	300	LEU
1	6	333	ILE
1	6	379	LEU
1	6	397	GLU
1	6	412	PHE
1	6	434	LEU
1	6	435	MET
1	6	449	THR
1	6	458	ASN
1	6	501	PHE
1	6	504	THR
1	6	532	ASP
1	6	551	SER
1	6	556	ASP
1	6	566	ILE
1	6	572	VAL
1	6	576	ARG
1	6	582	VAL
1	6	587	SER
1	6	599	MET
1	6	626	ASP
1	6	628	HIS
1	6	634	LEU
1	6	676	THR
1	6	690	GLU
1	6	691	ASN

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Mol	Chain	Res	Type
1	6	696	ASN
1	6	717	ASN
1	6	722	THR
1	6	725	ARG
1	7	219	ASP
1	7	223	ASN
1	7	242	THR
1	7	251	THR
1	7	286	ASN
1	7	287	ARG
1	7	289	HIS
1	7	295	ARG
1	7	300	LEU
1	7	333	ILE
1	7	379	LEU
1	7	397	GLU
1	7	412	PHE
1	7	431	LEU
1	7	435	MET
1	7	449	THR
1	7	458	ASN
1	7	501	PHE
1	7	504	THR
1	7	507	SER
1	7	532	ASP
1	7	551	SER
1	7	556	ASP
1	7	566	ILE
1	7	572	VAL
1	7	576	ARG
1	7	582	VAL
1	7	587	SER
1	7	599	MET
1	7	622	ILE
1	7	626	ASP
1	7	628	HIS
1	7	634	LEU
1	7	669	SER
1	7	690	GLU
1	7	696	ASN
1	7	700	GLN
1	7	717	ASN

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Mol	Chain	Res	Type
1	7	722	THR
1	7	725	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1634) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	255	HIS
1	A	259	GLN
1	A	272	HIS
1	A	286	ASN
1	A	302	ASN
1	A	320	GLN
1	A	335	ASN
1	A	375	GLN
1	A	382	ASN
1	A	383	ASN
1	A	386	GLN
1	A	408	ASN
1	A	458	ASN
1	A	486	GLN
1	A	487	GLN
1	A	497	ASN
1	A	498	ASN
1	A	512	ASN
1	A	519	ASN
1	A	557	ASN
1	A	608	GLN
1	A	624	HIS
1	A	630	HIS
1	A	691	ASN
1	A	696	ASN
1	A	717	ASN
1	B	253	ASN
1	B	255	HIS
1	B	259	GLN
1	B	272	HIS
1	B	286	ASN
1	B	302	ASN
1	B	320	GLN
1	B	335	ASN
1	B	350	GLN

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Mol	Chain	Res	Type
1	B	360	GLN
1	B	375	GLN
1	B	382	ASN
1	B	386	GLN
1	B	408	ASN
1	B	458	ASN
1	B	486	GLN
1	B	487	GLN
1	B	497	ASN
1	B	498	ASN
1	B	512	ASN
1	B	519	ASN
1	B	557	ASN
1	B	608	GLN
1	B	624	HIS
1	B	630	HIS
1	B	691	ASN
1	B	696	ASN
1	B	717	ASN
1	C	253	ASN
1	C	255	HIS
1	C	259	GLN
1	C	272	HIS
1	C	286	ASN
1	C	302	ASN
1	C	320	GLN
1	C	335	ASN
1	C	360	GLN
1	C	375	GLN
1	C	382	ASN
1	C	383	ASN
1	C	386	GLN
1	C	408	ASN
1	C	458	ASN
1	C	486	GLN
1	C	487	GLN
1	C	497	ASN
1	C	498	ASN
1	C	512	ASN
1	C	519	ASN
1	C	557	ASN
1	C	608	GLN

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Mol	Chain	Res	Type
1	C	624	HIS
1	C	630	HIS
1	C	691	ASN
1	C	696	ASN
1	C	717	ASN
1	D	255	HIS
1	D	259	GLN
1	D	272	HIS
1	D	286	ASN
1	D	302	ASN
1	D	320	GLN
1	D	335	ASN
1	D	350	GLN
1	D	375	GLN
1	D	382	ASN
1	D	386	GLN
1	D	408	ASN
1	D	458	ASN
1	D	486	GLN
1	D	487	GLN
1	D	497	ASN
1	D	498	ASN
1	D	512	ASN
1	D	519	ASN
1	D	557	ASN
1	D	608	GLN
1	D	624	HIS
1	D	630	HIS
1	D	691	ASN
1	D	696	ASN
1	D	717	ASN
1	E	255	HIS
1	E	259	GLN
1	E	272	HIS
1	E	286	ASN
1	E	302	ASN
1	E	320	GLN
1	E	335	ASN
1	E	382	ASN
1	E	383	ASN
1	E	386	GLN
1	E	408	ASN

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Mol	Chain	Res	Type
1	E	427	HIS
1	E	458	ASN
1	E	486	GLN
1	E	487	GLN
1	E	497	ASN
1	E	498	ASN
1	E	512	ASN
1	E	519	ASN
1	E	557	ASN
1	E	608	GLN
1	E	624	HIS
1	E	630	HIS
1	E	691	ASN
1	E	696	ASN
1	E	717	ASN
1	F	253	ASN
1	F	255	HIS
1	F	259	GLN
1	F	272	HIS
1	F	286	ASN
1	F	302	ASN
1	F	320	GLN
1	F	335	ASN
1	F	375	GLN
1	F	382	ASN
1	F	386	GLN
1	F	408	ASN
1	F	427	HIS
1	F	458	ASN
1	F	486	GLN
1	F	487	GLN
1	F	497	ASN
1	F	498	ASN
1	F	512	ASN
1	F	519	ASN
1	F	557	ASN
1	F	608	GLN
1	F	624	HIS
1	F	630	HIS
1	F	691	ASN
1	F	696	ASN
1	F	717	ASN

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Mol	Chain	Res	Type
1	G	255	HIS
1	G	259	GLN
1	G	272	HIS
1	G	286	ASN
1	G	302	ASN
1	G	320	GLN
1	G	335	ASN
1	G	360	GLN
1	G	382	ASN
1	G	386	GLN
1	G	408	ASN
1	G	458	ASN
1	G	486	GLN
1	G	487	GLN
1	G	497	ASN
1	G	498	ASN
1	G	512	ASN
1	G	519	ASN
1	G	557	ASN
1	G	608	GLN
1	G	624	HIS
1	G	630	HIS
1	G	691	ASN
1	G	696	ASN
1	G	717	ASN
1	H	253	ASN
1	H	255	HIS
1	H	259	GLN
1	H	272	HIS
1	H	286	ASN
1	H	302	ASN
1	H	320	GLN
1	H	335	ASN
1	H	360	GLN
1	H	375	GLN
1	H	382	ASN
1	H	383	ASN
1	H	386	GLN
1	H	408	ASN
1	H	427	HIS
1	H	458	ASN
1	H	486	GLN

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Mol	Chain	Res	Type
1	H	487	GLN
1	H	497	ASN
1	H	498	ASN
1	H	512	ASN
1	H	519	ASN
1	H	557	ASN
1	H	608	GLN
1	H	624	HIS
1	H	630	HIS
1	H	691	ASN
1	H	696	ASN
1	H	717	ASN
1	I	255	HIS
1	I	272	HIS
1	I	286	ASN
1	I	302	ASN
1	I	320	GLN
1	I	335	ASN
1	I	360	GLN
1	I	382	ASN
1	I	386	GLN
1	I	408	ASN
1	I	427	HIS
1	I	458	ASN
1	I	486	GLN
1	I	487	GLN
1	I	497	ASN
1	I	498	ASN
1	I	512	ASN
1	I	519	ASN
1	I	557	ASN
1	I	608	GLN
1	I	624	HIS
1	I	630	HIS
1	I	691	ASN
1	I	696	ASN
1	I	717	ASN
1	J	253	ASN
1	J	255	HIS
1	J	259	GLN
1	J	272	HIS
1	J	286	ASN

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Mol	Chain	Res	Type
1	J	302	ASN
1	J	320	GLN
1	J	335	ASN
1	J	360	GLN
1	J	375	GLN
1	J	382	ASN
1	J	383	ASN
1	J	386	GLN
1	J	408	ASN
1	J	458	ASN
1	J	486	GLN
1	J	487	GLN
1	J	497	ASN
1	J	498	ASN
1	J	512	ASN
1	J	519	ASN
1	J	557	ASN
1	J	608	GLN
1	J	624	HIS
1	J	630	HIS
1	J	673	GLN
1	J	691	ASN
1	J	696	ASN
1	J	717	ASN
1	K	253	ASN
1	K	255	HIS
1	K	259	GLN
1	K	272	HIS
1	K	286	ASN
1	K	302	ASN
1	K	320	GLN
1	K	335	ASN
1	K	375	GLN
1	K	382	ASN
1	K	383	ASN
1	K	386	GLN
1	K	408	ASN
1	K	427	HIS
1	K	458	ASN
1	K	486	GLN
1	K	487	GLN
1	K	497	ASN

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Mol	Chain	Res	Type
1	K	498	ASN
1	K	512	ASN
1	K	519	ASN
1	K	557	ASN
1	K	608	GLN
1	K	624	HIS
1	K	630	HIS
1	K	691	ASN
1	K	696	ASN
1	K	717	ASN
1	L	253	ASN
1	L	255	HIS
1	L	259	GLN
1	L	272	HIS
1	L	286	ASN
1	L	302	ASN
1	L	320	GLN
1	L	335	ASN
1	L	375	GLN
1	L	382	ASN
1	L	386	GLN
1	L	408	ASN
1	L	427	HIS
1	L	458	ASN
1	L	486	GLN
1	L	487	GLN
1	L	497	ASN
1	L	498	ASN
1	L	512	ASN
1	L	519	ASN
1	L	557	ASN
1	L	608	GLN
1	L	624	HIS
1	L	630	HIS
1	L	691	ASN
1	L	696	ASN
1	L	717	ASN
1	M	253	ASN
1	M	255	HIS
1	M	259	GLN
1	M	272	HIS
1	M	286	ASN

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Mol	Chain	Res	Type
1	M	302	ASN
1	M	320	GLN
1	M	335	ASN
1	M	375	GLN
1	M	382	ASN
1	M	383	ASN
1	M	386	GLN
1	M	408	ASN
1	M	427	HIS
1	M	458	ASN
1	M	486	GLN
1	M	487	GLN
1	M	497	ASN
1	M	498	ASN
1	M	512	ASN
1	M	519	ASN
1	M	557	ASN
1	M	608	GLN
1	M	624	HIS
1	M	630	HIS
1	M	691	ASN
1	M	696	ASN
1	M	717	ASN
1	N	255	HIS
1	N	259	GLN
1	N	272	HIS
1	N	286	ASN
1	N	302	ASN
1	N	320	GLN
1	N	335	ASN
1	N	375	GLN
1	N	382	ASN
1	N	386	GLN
1	N	408	ASN
1	N	458	ASN
1	N	486	GLN
1	N	487	GLN
1	N	497	ASN
1	N	498	ASN
1	N	512	ASN
1	N	519	ASN
1	N	557	ASN

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Mol	Chain	Res	Type
1	N	608	GLN
1	N	624	HIS
1	N	630	HIS
1	N	691	ASN
1	N	696	ASN
1	N	717	ASN
1	O	253	ASN
1	O	255	HIS
1	O	259	GLN
1	O	272	HIS
1	O	286	ASN
1	O	302	ASN
1	O	320	GLN
1	O	335	ASN
1	O	360	GLN
1	O	375	GLN
1	O	382	ASN
1	O	386	GLN
1	O	408	ASN
1	O	427	HIS
1	O	458	ASN
1	O	486	GLN
1	O	487	GLN
1	O	497	ASN
1	O	498	ASN
1	O	512	ASN
1	O	519	ASN
1	O	557	ASN
1	O	608	GLN
1	O	624	HIS
1	O	630	HIS
1	O	691	ASN
1	O	696	ASN
1	O	700	GLN
1	O	717	ASN
1	P	253	ASN
1	P	255	HIS
1	P	272	HIS
1	P	286	ASN
1	P	302	ASN
1	P	320	GLN
1	P	335	ASN

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Mol	Chain	Res	Type
1	P	375	GLN
1	P	382	ASN
1	P	386	GLN
1	P	408	ASN
1	P	427	HIS
1	P	458	ASN
1	P	486	GLN
1	P	487	GLN
1	P	497	ASN
1	P	498	ASN
1	P	512	ASN
1	P	519	ASN
1	P	557	ASN
1	P	608	GLN
1	P	624	HIS
1	P	630	HIS
1	P	691	ASN
1	P	696	ASN
1	P	717	ASN
1	Q	253	ASN
1	Q	255	HIS
1	Q	259	GLN
1	Q	272	HIS
1	Q	286	ASN
1	Q	302	ASN
1	Q	320	GLN
1	Q	335	ASN
1	Q	350	GLN
1	Q	360	GLN
1	Q	375	GLN
1	Q	382	ASN
1	Q	383	ASN
1	Q	386	GLN
1	Q	408	ASN
1	Q	427	HIS
1	Q	458	ASN
1	Q	486	GLN
1	Q	487	GLN
1	Q	497	ASN
1	Q	498	ASN
1	Q	512	ASN
1	Q	519	ASN

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Mol	Chain	Res	Type
1	Q	557	ASN
1	Q	608	GLN
1	Q	624	HIS
1	Q	630	HIS
1	Q	691	ASN
1	Q	696	ASN
1	Q	717	ASN
1	R	253	ASN
1	R	255	HIS
1	R	272	HIS
1	R	286	ASN
1	R	302	ASN
1	R	320	GLN
1	R	335	ASN
1	R	360	GLN
1	R	375	GLN
1	R	382	ASN
1	R	386	GLN
1	R	408	ASN
1	R	427	HIS
1	R	458	ASN
1	R	486	GLN
1	R	487	GLN
1	R	497	ASN
1	R	498	ASN
1	R	512	ASN
1	R	519	ASN
1	R	557	ASN
1	R	608	GLN
1	R	624	HIS
1	R	630	HIS
1	R	691	ASN
1	R	696	ASN
1	R	717	ASN
1	S	253	ASN
1	S	255	HIS
1	S	272	HIS
1	S	286	ASN
1	S	302	ASN
1	S	335	ASN
1	S	375	GLN
1	S	382	ASN

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Mol	Chain	Res	Type
1	S	383	ASN
1	S	386	GLN
1	S	408	ASN
1	S	427	HIS
1	S	458	ASN
1	S	486	GLN
1	S	487	GLN
1	S	497	ASN
1	S	498	ASN
1	S	512	ASN
1	S	519	ASN
1	S	557	ASN
1	S	608	GLN
1	S	630	HIS
1	S	691	ASN
1	S	696	ASN
1	S	717	ASN
1	T	253	ASN
1	T	255	HIS
1	T	259	GLN
1	T	272	HIS
1	T	286	ASN
1	T	302	ASN
1	T	320	GLN
1	T	335	ASN
1	T	375	GLN
1	T	382	ASN
1	T	386	GLN
1	T	408	ASN
1	T	427	HIS
1	T	458	ASN
1	T	486	GLN
1	T	487	GLN
1	T	497	ASN
1	T	498	ASN
1	T	512	ASN
1	T	519	ASN
1	T	557	ASN
1	T	608	GLN
1	T	624	HIS
1	T	630	HIS
1	T	691	ASN

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Mol	Chain	Res	Type
1	T	696	ASN
1	T	717	ASN
1	U	253	ASN
1	U	255	HIS
1	U	259	GLN
1	U	272	HIS
1	U	286	ASN
1	U	302	ASN
1	U	320	GLN
1	U	335	ASN
1	U	350	GLN
1	U	375	GLN
1	U	382	ASN
1	U	386	GLN
1	U	408	ASN
1	U	427	HIS
1	U	458	ASN
1	U	486	GLN
1	U	487	GLN
1	U	497	ASN
1	U	498	ASN
1	U	512	ASN
1	U	519	ASN
1	U	557	ASN
1	U	608	GLN
1	U	630	HIS
1	U	691	ASN
1	U	696	ASN
1	U	717	ASN
1	V	253	ASN
1	V	255	HIS
1	V	259	GLN
1	V	272	HIS
1	V	286	ASN
1	V	302	ASN
1	V	320	GLN
1	V	335	ASN
1	V	350	GLN
1	V	375	GLN
1	V	382	ASN
1	V	386	GLN
1	V	408	ASN

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Mol	Chain	Res	Type
1	V	427	HIS
1	V	458	ASN
1	V	486	GLN
1	V	487	GLN
1	V	497	ASN
1	V	498	ASN
1	V	512	ASN
1	V	519	ASN
1	V	557	ASN
1	V	608	GLN
1	V	624	HIS
1	V	630	HIS
1	V	691	ASN
1	V	696	ASN
1	V	717	ASN
1	W	253	ASN
1	W	255	HIS
1	W	272	HIS
1	W	286	ASN
1	W	302	ASN
1	W	320	GLN
1	W	335	ASN
1	W	350	GLN
1	W	360	GLN
1	W	375	GLN
1	W	382	ASN
1	W	386	GLN
1	W	408	ASN
1	W	458	ASN
1	W	486	GLN
1	W	487	GLN
1	W	497	ASN
1	W	498	ASN
1	W	512	ASN
1	W	519	ASN
1	W	557	ASN
1	W	608	GLN
1	W	691	ASN
1	W	696	ASN
1	W	717	ASN
1	X	227	ASN
1	X	253	ASN

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Mol	Chain	Res	Type
1	X	255	HIS
1	X	259	GLN
1	X	272	HIS
1	X	286	ASN
1	X	302	ASN
1	X	320	GLN
1	X	335	ASN
1	X	350	GLN
1	X	375	GLN
1	X	382	ASN
1	X	386	GLN
1	X	408	ASN
1	X	458	ASN
1	X	486	GLN
1	X	487	GLN
1	X	497	ASN
1	X	498	ASN
1	X	512	ASN
1	X	519	ASN
1	X	557	ASN
1	X	608	GLN
1	X	624	HIS
1	X	630	HIS
1	X	691	ASN
1	X	696	ASN
1	X	717	ASN
1	Y	255	HIS
1	Y	259	GLN
1	Y	272	HIS
1	Y	286	ASN
1	Y	302	ASN
1	Y	320	GLN
1	Y	335	ASN
1	Y	375	GLN
1	Y	382	ASN
1	Y	383	ASN
1	Y	386	GLN
1	Y	408	ASN
1	Y	427	HIS
1	Y	458	ASN
1	Y	486	GLN
1	Y	487	GLN

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Mol	Chain	Res	Type
1	Y	497	ASN
1	Y	498	ASN
1	Y	512	ASN
1	Y	519	ASN
1	Y	557	ASN
1	Y	608	GLN
1	Y	630	HIS
1	Y	691	ASN
1	Y	696	ASN
1	Y	717	ASN
1	Z	253	ASN
1	Z	255	HIS
1	Z	259	GLN
1	Z	272	HIS
1	Z	286	ASN
1	Z	302	ASN
1	Z	320	GLN
1	Z	335	ASN
1	Z	375	GLN
1	Z	382	ASN
1	Z	386	GLN
1	Z	408	ASN
1	Z	458	ASN
1	Z	486	GLN
1	Z	487	GLN
1	Z	497	ASN
1	Z	498	ASN
1	Z	512	ASN
1	Z	519	ASN
1	Z	557	ASN
1	Z	608	GLN
1	Z	630	HIS
1	Z	691	ASN
1	Z	696	ASN
1	Z	717	ASN
1	a	253	ASN
1	a	255	HIS
1	a	259	GLN
1	a	272	HIS
1	a	286	ASN
1	a	302	ASN
1	a	320	GLN

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Mol	Chain	Res	Type
1	a	335	ASN
1	a	360	GLN
1	a	375	GLN
1	a	382	ASN
1	a	386	GLN
1	a	408	ASN
1	a	427	HIS
1	a	458	ASN
1	a	486	GLN
1	a	487	GLN
1	a	497	ASN
1	a	498	ASN
1	a	512	ASN
1	a	519	ASN
1	a	557	ASN
1	a	608	GLN
1	a	624	HIS
1	a	630	HIS
1	a	691	ASN
1	a	696	ASN
1	a	700	GLN
1	b	259	GLN
1	b	272	HIS
1	b	286	ASN
1	b	302	ASN
1	b	320	GLN
1	b	335	ASN
1	b	360	GLN
1	b	382	ASN
1	b	386	GLN
1	b	408	ASN
1	b	427	HIS
1	b	458	ASN
1	b	486	GLN
1	b	487	GLN
1	b	497	ASN
1	b	498	ASN
1	b	512	ASN
1	b	519	ASN
1	b	557	ASN
1	b	608	GLN
1	b	624	HIS

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Mol	Chain	Res	Type
1	b	630	HIS
1	b	691	ASN
1	b	696	ASN
1	b	717	ASN
1	c	227	ASN
1	c	253	ASN
1	c	255	HIS
1	c	259	GLN
1	c	272	HIS
1	c	286	ASN
1	c	302	ASN
1	c	320	GLN
1	c	335	ASN
1	c	350	GLN
1	c	375	GLN
1	c	382	ASN
1	c	386	GLN
1	c	408	ASN
1	c	427	HIS
1	c	458	ASN
1	c	486	GLN
1	c	487	GLN
1	c	497	ASN
1	c	498	ASN
1	c	512	ASN
1	c	519	ASN
1	c	557	ASN
1	c	608	GLN
1	c	624	HIS
1	c	630	HIS
1	c	691	ASN
1	c	696	ASN
1	c	717	ASN
1	d	253	ASN
1	d	255	HIS
1	d	259	GLN
1	d	272	HIS
1	d	286	ASN
1	d	302	ASN
1	d	320	GLN
1	d	335	ASN
1	d	360	GLN

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Mol	Chain	Res	Type
1	d	375	GLN
1	d	382	ASN
1	d	386	GLN
1	d	408	ASN
1	d	427	HIS
1	d	458	ASN
1	d	486	GLN
1	d	487	GLN
1	d	497	ASN
1	d	498	ASN
1	d	512	ASN
1	d	519	ASN
1	d	557	ASN
1	d	608	GLN
1	d	630	HIS
1	d	691	ASN
1	d	696	ASN
1	d	717	ASN
1	e	253	ASN
1	e	255	HIS
1	e	259	GLN
1	e	272	HIS
1	e	286	ASN
1	e	302	ASN
1	e	320	GLN
1	e	335	ASN
1	e	360	GLN
1	e	375	GLN
1	e	383	ASN
1	e	386	GLN
1	e	408	ASN
1	e	427	HIS
1	e	458	ASN
1	e	486	GLN
1	e	487	GLN
1	e	497	ASN
1	e	498	ASN
1	e	512	ASN
1	e	519	ASN
1	e	557	ASN
1	e	608	GLN
1	e	624	HIS

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Mol	Chain	Res	Type
1	e	630	HIS
1	e	691	ASN
1	e	696	ASN
1	e	717	ASN
1	f	253	ASN
1	f	255	HIS
1	f	259	GLN
1	f	272	HIS
1	f	286	ASN
1	f	302	ASN
1	f	320	GLN
1	f	335	ASN
1	f	350	GLN
1	f	375	GLN
1	f	382	ASN
1	f	386	GLN
1	f	408	ASN
1	f	458	ASN
1	f	486	GLN
1	f	487	GLN
1	f	497	ASN
1	f	498	ASN
1	f	512	ASN
1	f	519	ASN
1	f	557	ASN
1	f	608	GLN
1	f	624	HIS
1	f	630	HIS
1	f	691	ASN
1	f	696	ASN
1	f	717	ASN
1	g	253	ASN
1	g	255	HIS
1	g	259	GLN
1	g	272	HIS
1	g	286	ASN
1	g	302	ASN
1	g	320	GLN
1	g	335	ASN
1	g	375	GLN
1	g	382	ASN
1	g	386	GLN

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Mol	Chain	Res	Type
1	g	408	ASN
1	g	427	HIS
1	g	458	ASN
1	g	486	GLN
1	g	487	GLN
1	g	497	ASN
1	g	498	ASN
1	g	512	ASN
1	g	519	ASN
1	g	557	ASN
1	g	608	GLN
1	g	630	HIS
1	g	691	ASN
1	g	696	ASN
1	g	717	ASN
1	h	253	ASN
1	h	255	HIS
1	h	259	GLN
1	h	272	HIS
1	h	286	ASN
1	h	302	ASN
1	h	320	GLN
1	h	335	ASN
1	h	375	GLN
1	h	382	ASN
1	h	383	ASN
1	h	386	GLN
1	h	408	ASN
1	h	427	HIS
1	h	458	ASN
1	h	486	GLN
1	h	487	GLN
1	h	497	ASN
1	h	498	ASN
1	h	512	ASN
1	h	519	ASN
1	h	557	ASN
1	h	608	GLN
1	h	624	HIS
1	h	630	HIS
1	h	691	ASN
1	h	696	ASN

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Mol	Chain	Res	Type
1	h	717	ASN
1	i	253	ASN
1	i	259	GLN
1	i	272	HIS
1	i	286	ASN
1	i	302	ASN
1	i	320	GLN
1	i	335	ASN
1	i	375	GLN
1	i	382	ASN
1	i	386	GLN
1	i	408	ASN
1	i	458	ASN
1	i	486	GLN
1	i	487	GLN
1	i	497	ASN
1	i	498	ASN
1	i	512	ASN
1	i	519	ASN
1	i	557	ASN
1	i	608	GLN
1	i	624	HIS
1	i	630	HIS
1	i	691	ASN
1	i	696	ASN
1	i	717	ASN
1	j	253	ASN
1	j	255	HIS
1	j	259	GLN
1	j	272	HIS
1	j	286	ASN
1	j	302	ASN
1	j	320	GLN
1	j	335	ASN
1	j	350	GLN
1	j	375	GLN
1	j	382	ASN
1	j	383	ASN
1	j	386	GLN
1	j	408	ASN
1	j	427	HIS
1	j	458	ASN

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Mol	Chain	Res	Type
1	j	486	GLN
1	j	487	GLN
1	j	497	ASN
1	j	498	ASN
1	j	512	ASN
1	j	519	ASN
1	j	557	ASN
1	j	608	GLN
1	j	624	HIS
1	j	630	HIS
1	j	691	ASN
1	j	696	ASN
1	j	717	ASN
1	k	253	ASN
1	k	255	HIS
1	k	259	GLN
1	k	272	HIS
1	k	286	ASN
1	k	302	ASN
1	k	320	GLN
1	k	335	ASN
1	k	375	GLN
1	k	382	ASN
1	k	383	ASN
1	k	386	GLN
1	k	408	ASN
1	k	458	ASN
1	k	486	GLN
1	k	487	GLN
1	k	497	ASN
1	k	498	ASN
1	k	512	ASN
1	k	519	ASN
1	k	557	ASN
1	k	608	GLN
1	k	630	HIS
1	k	691	ASN
1	k	696	ASN
1	k	717	ASN
1	l	253	ASN
1	l	255	HIS
1	l	259	GLN

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Mol	Chain	Res	Type
1	l	272	HIS
1	l	286	ASN
1	l	302	ASN
1	l	320	GLN
1	l	335	ASN
1	l	360	GLN
1	l	375	GLN
1	l	382	ASN
1	l	383	ASN
1	l	386	GLN
1	l	408	ASN
1	l	458	ASN
1	l	486	GLN
1	l	487	GLN
1	l	497	ASN
1	l	498	ASN
1	l	512	ASN
1	l	519	ASN
1	l	557	ASN
1	l	608	GLN
1	l	630	HIS
1	l	691	ASN
1	l	696	ASN
1	l	717	ASN
1	m	253	ASN
1	m	259	GLN
1	m	272	HIS
1	m	286	ASN
1	m	302	ASN
1	m	320	GLN
1	m	335	ASN
1	m	360	GLN
1	m	375	GLN
1	m	382	ASN
1	m	383	ASN
1	m	386	GLN
1	m	408	ASN
1	m	427	HIS
1	m	458	ASN
1	m	486	GLN
1	m	487	GLN
1	m	497	ASN

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Mol	Chain	Res	Type
1	m	498	ASN
1	m	512	ASN
1	m	519	ASN
1	m	557	ASN
1	m	608	GLN
1	m	624	HIS
1	m	630	HIS
1	m	691	ASN
1	m	696	ASN
1	m	717	ASN
1	n	253	ASN
1	n	255	HIS
1	n	259	GLN
1	n	272	HIS
1	n	286	ASN
1	n	302	ASN
1	n	320	GLN
1	n	335	ASN
1	n	375	GLN
1	n	382	ASN
1	n	386	GLN
1	n	408	ASN
1	n	427	HIS
1	n	458	ASN
1	n	486	GLN
1	n	487	GLN
1	n	497	ASN
1	n	498	ASN
1	n	512	ASN
1	n	519	ASN
1	n	557	ASN
1	n	608	GLN
1	n	624	HIS
1	n	630	HIS
1	n	691	ASN
1	n	696	ASN
1	n	717	ASN
1	o	255	HIS
1	o	259	GLN
1	o	272	HIS
1	o	286	ASN
1	o	302	ASN

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Mol	Chain	Res	Type
1	o	320	GLN
1	o	335	ASN
1	o	350	GLN
1	o	382	ASN
1	o	386	GLN
1	o	408	ASN
1	o	458	ASN
1	o	486	GLN
1	o	487	GLN
1	o	497	ASN
1	o	498	ASN
1	o	512	ASN
1	o	519	ASN
1	o	557	ASN
1	o	608	GLN
1	o	630	HIS
1	o	691	ASN
1	o	696	ASN
1	o	717	ASN
1	p	253	ASN
1	p	255	HIS
1	p	259	GLN
1	p	272	HIS
1	p	286	ASN
1	p	302	ASN
1	p	320	GLN
1	p	335	ASN
1	p	350	GLN
1	p	375	GLN
1	p	382	ASN
1	p	386	GLN
1	p	408	ASN
1	p	427	HIS
1	p	458	ASN
1	p	486	GLN
1	p	487	GLN
1	p	497	ASN
1	p	498	ASN
1	p	512	ASN
1	p	519	ASN
1	p	557	ASN
1	p	608	GLN

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Mol	Chain	Res	Type
1	p	624	HIS
1	p	630	HIS
1	p	691	ASN
1	p	696	ASN
1	p	717	ASN
1	q	253	ASN
1	q	255	HIS
1	q	259	GLN
1	q	272	HIS
1	q	286	ASN
1	q	302	ASN
1	q	320	GLN
1	q	335	ASN
1	q	375	GLN
1	q	382	ASN
1	q	386	GLN
1	q	408	ASN
1	q	427	HIS
1	q	458	ASN
1	q	486	GLN
1	q	487	GLN
1	q	497	ASN
1	q	498	ASN
1	q	512	ASN
1	q	519	ASN
1	q	557	ASN
1	q	608	GLN
1	q	624	HIS
1	q	630	HIS
1	q	691	ASN
1	q	696	ASN
1	q	717	ASN
1	r	253	ASN
1	r	255	HIS
1	r	259	GLN
1	r	272	HIS
1	r	286	ASN
1	r	302	ASN
1	r	320	GLN
1	r	335	ASN
1	r	375	GLN
1	r	382	ASN

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Mol	Chain	Res	Type
1	r	386	GLN
1	r	408	ASN
1	r	427	HIS
1	r	458	ASN
1	r	486	GLN
1	r	487	GLN
1	r	497	ASN
1	r	498	ASN
1	r	512	ASN
1	r	519	ASN
1	r	557	ASN
1	r	608	GLN
1	r	630	HIS
1	r	691	ASN
1	r	696	ASN
1	r	717	ASN
1	s	253	ASN
1	s	255	HIS
1	s	259	GLN
1	s	272	HIS
1	s	286	ASN
1	s	302	ASN
1	s	320	GLN
1	s	335	ASN
1	s	350	GLN
1	s	375	GLN
1	s	382	ASN
1	s	383	ASN
1	s	386	GLN
1	s	408	ASN
1	s	427	HIS
1	s	458	ASN
1	s	486	GLN
1	s	487	GLN
1	s	497	ASN
1	s	498	ASN
1	s	512	ASN
1	s	519	ASN
1	s	557	ASN
1	s	608	GLN
1	s	624	HIS
1	s	630	HIS

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Mol	Chain	Res	Type
1	s	691	ASN
1	s	696	ASN
1	s	717	ASN
1	t	253	ASN
1	t	255	HIS
1	t	259	GLN
1	t	272	HIS
1	t	286	ASN
1	t	302	ASN
1	t	320	GLN
1	t	335	ASN
1	t	350	GLN
1	t	375	GLN
1	t	382	ASN
1	t	383	ASN
1	t	386	GLN
1	t	408	ASN
1	t	458	ASN
1	t	486	GLN
1	t	487	GLN
1	t	497	ASN
1	t	498	ASN
1	t	512	ASN
1	t	519	ASN
1	t	557	ASN
1	t	608	GLN
1	t	624	HIS
1	t	630	HIS
1	t	691	ASN
1	t	696	ASN
1	t	717	ASN
1	u	253	ASN
1	u	255	HIS
1	u	259	GLN
1	u	272	HIS
1	u	286	ASN
1	u	302	ASN
1	u	335	ASN
1	u	375	GLN
1	u	382	ASN
1	u	383	ASN
1	u	386	GLN

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Mol	Chain	Res	Type
1	u	408	ASN
1	u	427	HIS
1	u	458	ASN
1	u	486	GLN
1	u	487	GLN
1	u	497	ASN
1	u	498	ASN
1	u	512	ASN
1	u	519	ASN
1	u	557	ASN
1	u	608	GLN
1	u	624	HIS
1	u	630	HIS
1	u	691	ASN
1	u	696	ASN
1	u	717	ASN
1	v	227	ASN
1	v	253	ASN
1	v	255	HIS
1	v	259	GLN
1	v	272	HIS
1	v	286	ASN
1	v	302	ASN
1	v	320	GLN
1	v	335	ASN
1	v	375	GLN
1	v	382	ASN
1	v	386	GLN
1	v	408	ASN
1	v	427	HIS
1	v	458	ASN
1	v	486	GLN
1	v	487	GLN
1	v	497	ASN
1	v	498	ASN
1	v	512	ASN
1	v	519	ASN
1	v	557	ASN
1	v	608	GLN
1	v	624	HIS
1	v	630	HIS
1	v	691	ASN

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Mol	Chain	Res	Type
1	v	696	ASN
1	v	717	ASN
1	w	253	ASN
1	w	255	HIS
1	w	259	GLN
1	w	272	HIS
1	w	286	ASN
1	w	302	ASN
1	w	320	GLN
1	w	335	ASN
1	w	360	GLN
1	w	375	GLN
1	w	382	ASN
1	w	386	GLN
1	w	408	ASN
1	w	427	HIS
1	w	458	ASN
1	w	486	GLN
1	w	487	GLN
1	w	497	ASN
1	w	498	ASN
1	w	512	ASN
1	w	519	ASN
1	w	557	ASN
1	w	608	GLN
1	w	624	HIS
1	w	630	HIS
1	w	691	ASN
1	w	696	ASN
1	w	717	ASN
1	x	253	ASN
1	x	255	HIS
1	x	259	GLN
1	x	272	HIS
1	x	286	ASN
1	x	302	ASN
1	x	320	GLN
1	x	335	ASN
1	x	360	GLN
1	x	375	GLN
1	x	382	ASN
1	x	383	ASN

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Mol	Chain	Res	Type
1	x	386	GLN
1	x	408	ASN
1	x	427	HIS
1	x	458	ASN
1	x	486	GLN
1	x	487	GLN
1	x	497	ASN
1	x	498	ASN
1	x	512	ASN
1	x	519	ASN
1	x	557	ASN
1	x	608	GLN
1	x	624	HIS
1	x	630	HIS
1	x	691	ASN
1	x	696	ASN
1	x	700	GLN
1	x	717	ASN
1	y	253	ASN
1	y	255	HIS
1	y	259	GLN
1	y	272	HIS
1	y	286	ASN
1	y	302	ASN
1	y	320	GLN
1	y	335	ASN
1	y	375	GLN
1	y	382	ASN
1	y	383	ASN
1	y	386	GLN
1	y	408	ASN
1	y	458	ASN
1	y	486	GLN
1	y	487	GLN
1	y	497	ASN
1	y	498	ASN
1	y	512	ASN
1	y	519	ASN
1	y	557	ASN
1	y	608	GLN
1	y	624	HIS
1	y	630	HIS

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Mol	Chain	Res	Type
1	y	691	ASN
1	y	696	ASN
1	y	700	GLN
1	y	717	ASN
1	z	227	ASN
1	z	253	ASN
1	z	255	HIS
1	z	259	GLN
1	z	272	HIS
1	z	286	ASN
1	z	302	ASN
1	z	335	ASN
1	z	375	GLN
1	z	382	ASN
1	z	386	GLN
1	z	408	ASN
1	z	458	ASN
1	z	486	GLN
1	z	487	GLN
1	z	497	ASN
1	z	498	ASN
1	z	512	ASN
1	z	519	ASN
1	z	557	ASN
1	z	608	GLN
1	z	624	HIS
1	z	630	HIS
1	z	691	ASN
1	z	696	ASN
1	z	717	ASN
1	0	253	ASN
1	0	255	HIS
1	0	259	GLN
1	0	272	HIS
1	0	286	ASN
1	0	302	ASN
1	0	318	ASN
1	0	320	GLN
1	0	335	ASN
1	0	360	GLN
1	0	375	GLN
1	0	382	ASN

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Mol	Chain	Res	Type
1	0	386	GLN
1	0	408	ASN
1	0	427	HIS
1	0	458	ASN
1	0	486	GLN
1	0	487	GLN
1	0	497	ASN
1	0	498	ASN
1	0	512	ASN
1	0	519	ASN
1	0	557	ASN
1	0	608	GLN
1	0	624	HIS
1	0	630	HIS
1	0	678	GLN
1	0	691	ASN
1	0	696	ASN
1	0	717	ASN
1	1	253	ASN
1	1	255	HIS
1	1	259	GLN
1	1	272	HIS
1	1	286	ASN
1	1	302	ASN
1	1	320	GLN
1	1	335	ASN
1	1	350	GLN
1	1	375	GLN
1	1	382	ASN
1	1	383	ASN
1	1	386	GLN
1	1	408	ASN
1	1	427	HIS
1	1	458	ASN
1	1	486	GLN
1	1	487	GLN
1	1	497	ASN
1	1	498	ASN
1	1	512	ASN
1	1	519	ASN
1	1	557	ASN
1	1	608	GLN

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Mol	Chain	Res	Type
1	1	624	HIS
1	1	630	HIS
1	1	691	ASN
1	1	696	ASN
1	1	717	ASN
1	2	253	ASN
1	2	255	HIS
1	2	259	GLN
1	2	272	HIS
1	2	286	ASN
1	2	302	ASN
1	2	320	GLN
1	2	335	ASN
1	2	375	GLN
1	2	382	ASN
1	2	383	ASN
1	2	386	GLN
1	2	408	ASN
1	2	427	HIS
1	2	458	ASN
1	2	486	GLN
1	2	487	GLN
1	2	497	ASN
1	2	498	ASN
1	2	512	ASN
1	2	519	ASN
1	2	557	ASN
1	2	608	GLN
1	2	624	HIS
1	2	630	HIS
1	2	691	ASN
1	2	696	ASN
1	2	700	GLN
1	2	717	ASN
1	3	253	ASN
1	3	259	GLN
1	3	272	HIS
1	3	286	ASN
1	3	302	ASN
1	3	320	GLN
1	3	335	ASN
1	3	375	GLN

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Mol	Chain	Res	Type
1	3	382	ASN
1	3	386	GLN
1	3	408	ASN
1	3	427	HIS
1	3	458	ASN
1	3	486	GLN
1	3	487	GLN
1	3	497	ASN
1	3	498	ASN
1	3	512	ASN
1	3	519	ASN
1	3	557	ASN
1	3	608	GLN
1	3	624	HIS
1	3	630	HIS
1	3	691	ASN
1	3	696	ASN
1	3	717	ASN
1	4	253	ASN
1	4	255	HIS
1	4	272	HIS
1	4	286	ASN
1	4	302	ASN
1	4	320	GLN
1	4	335	ASN
1	4	375	GLN
1	4	382	ASN
1	4	386	GLN
1	4	408	ASN
1	4	427	HIS
1	4	458	ASN
1	4	486	GLN
1	4	487	GLN
1	4	497	ASN
1	4	498	ASN
1	4	512	ASN
1	4	519	ASN
1	4	557	ASN
1	4	608	GLN
1	4	624	HIS
1	4	630	HIS
1	4	691	ASN

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Mol	Chain	Res	Type
1	4	696	ASN
1	4	717	ASN
1	5	253	ASN
1	5	255	HIS
1	5	259	GLN
1	5	272	HIS
1	5	286	ASN
1	5	302	ASN
1	5	320	GLN
1	5	335	ASN
1	5	350	GLN
1	5	375	GLN
1	5	382	ASN
1	5	386	GLN
1	5	408	ASN
1	5	427	HIS
1	5	458	ASN
1	5	486	GLN
1	5	487	GLN
1	5	497	ASN
1	5	498	ASN
1	5	512	ASN
1	5	519	ASN
1	5	557	ASN
1	5	608	GLN
1	5	630	HIS
1	5	691	ASN
1	5	696	ASN
1	5	717	ASN
1	6	253	ASN
1	6	255	HIS
1	6	259	GLN
1	6	272	HIS
1	6	286	ASN
1	6	302	ASN
1	6	320	GLN
1	6	335	ASN
1	6	350	GLN
1	6	375	GLN
1	6	382	ASN
1	6	386	GLN
1	6	408	ASN

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Mol	Chain	Res	Type
1	6	427	HIS
1	6	458	ASN
1	6	486	GLN
1	6	487	GLN
1	6	497	ASN
1	6	498	ASN
1	6	512	ASN
1	6	519	ASN
1	6	557	ASN
1	6	608	GLN
1	6	624	HIS
1	6	630	HIS
1	6	691	ASN
1	6	696	ASN
1	6	700	GLN
1	6	717	ASN
1	7	253	ASN
1	7	255	HIS
1	7	259	GLN
1	7	272	HIS
1	7	286	ASN
1	7	302	ASN
1	7	320	GLN
1	7	335	ASN
1	7	350	GLN
1	7	375	GLN
1	7	382	ASN
1	7	386	GLN
1	7	408	ASN
1	7	427	HIS
1	7	458	ASN
1	7	486	GLN
1	7	487	GLN
1	7	497	ASN
1	7	498	ASN
1	7	512	ASN
1	7	519	ASN
1	7	557	ASN
1	7	608	GLN
1	7	624	HIS
1	7	630	HIS
1	7	691	ASN

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Mol	Chain	Res	Type
1	7	696	ASN
1	7	717	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	0	520/520 (100%)	-0.46	12 (2%) 60 31	45, 60, 92, 141	0
1	1	520/520 (100%)	-0.43	5 (0%) 82 59	44, 61, 91, 139	0
1	2	520/520 (100%)	-0.43	13 (2%) 57 29	46, 60, 93, 141	0
1	3	520/520 (100%)	-0.50	8 (1%) 73 46	43, 59, 91, 138	0
1	4	520/520 (100%)	-0.62	7 (1%) 77 51	44, 59, 92, 140	0
1	5	520/520 (100%)	-0.52	7 (1%) 77 51	43, 57, 90, 138	0
1	6	520/520 (100%)	-0.47	8 (1%) 73 46	42, 57, 90, 139	0
1	7	520/520 (100%)	-0.58	3 (0%) 89 72	42, 58, 90, 138	0
1	A	520/520 (100%)	-0.30	6 (1%) 79 54	45, 61, 92, 139	0
1	B	520/520 (100%)	-0.44	8 (1%) 73 46	46, 61, 93, 139	0
1	C	520/520 (100%)	-0.43	10 (1%) 66 37	45, 60, 92, 140	0
1	D	520/520 (100%)	-0.43	10 (1%) 66 37	44, 61, 92, 139	0
1	E	520/520 (100%)	-0.45	4 (0%) 86 65	46, 61, 92, 139	0
1	F	520/520 (100%)	-0.36	11 (2%) 63 34	45, 61, 93, 138	0
1	G	520/520 (100%)	-0.51	8 (1%) 73 46	46, 60, 91, 140	0
1	H	520/520 (100%)	-0.47	12 (2%) 60 31	43, 60, 92, 137	0
1	I	520/520 (100%)	-0.39	8 (1%) 73 46	45, 61, 92, 139	0
1	J	520/520 (100%)	-0.34	7 (1%) 77 51	45, 62, 92, 141	0
1	K	520/520 (100%)	-0.52	7 (1%) 77 51	43, 57, 91, 139	0
1	L	520/520 (100%)	-0.57	6 (1%) 79 54	42, 58, 90, 141	0
1	M	520/520 (100%)	-0.52	5 (0%) 82 59	43, 58, 90, 138	0
1	N	520/520 (100%)	-0.59	3 (0%) 89 72	42, 58, 90, 138	0
1	O	520/520 (100%)	-0.53	6 (1%) 79 54	42, 58, 91, 141	0
1	P	520/520 (100%)	-0.53	5 (0%) 82 59	43, 58, 90, 141	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Q	520/520 (100%)	-0.46	10 (1%) 66 37	42, 59, 91, 138	0
1	R	520/520 (100%)	-0.52	7 (1%) 77 51	43, 58, 91, 139	0
1	S	520/520 (100%)	-0.53	4 (0%) 86 65	41, 57, 88, 141	0
1	T	520/520 (100%)	-0.50	5 (0%) 82 59	42, 57, 90, 140	0
1	U	520/520 (100%)	-0.47	9 (1%) 70 41	45, 60, 91, 139	0
1	V	520/520 (100%)	-0.42	6 (1%) 79 54	45, 61, 92, 140	0
1	W	520/520 (100%)	-0.36	9 (1%) 70 41	46, 61, 93, 139	0
1	X	520/520 (100%)	-0.34	12 (2%) 60 31	44, 61, 93, 141	0
1	Y	520/520 (100%)	-0.40	11 (2%) 63 34	45, 61, 92, 139	0
1	Z	520/520 (100%)	-0.46	10 (1%) 66 37	44, 60, 91, 140	0
1	a	520/520 (100%)	-0.48	7 (1%) 77 51	44, 59, 92, 139	0
1	b	520/520 (100%)	-0.56	6 (1%) 79 54	42, 58, 90, 137	0
1	c	520/520 (100%)	-0.56	7 (1%) 77 51	44, 59, 90, 141	0
1	d	520/520 (100%)	-0.51	10 (1%) 66 37	45, 60, 91, 141	0
1	e	520/520 (100%)	-0.54	6 (1%) 79 54	43, 58, 89, 141	0
1	f	520/520 (100%)	-0.52	6 (1%) 79 54	45, 59, 92, 141	0
1	g	520/520 (100%)	-0.51	1 (0%) 95 87	46, 60, 92, 134	0
1	h	520/520 (100%)	-0.49	6 (1%) 79 54	45, 60, 91, 140	0
1	i	520/520 (100%)	-0.56	4 (0%) 86 65	43, 59, 90, 138	0
1	j	520/520 (100%)	-0.53	7 (1%) 77 51	43, 58, 90, 139	0
1	k	520/520 (100%)	-0.54	3 (0%) 89 72	41, 58, 90, 135	0
1	l	520/520 (100%)	-0.55	1 (0%) 95 87	42, 57, 90, 138	0
1	m	520/520 (100%)	-0.56	7 (1%) 77 51	42, 57, 89, 138	0
1	n	520/520 (100%)	-0.51	5 (0%) 82 59	42, 57, 90, 139	0
1	o	520/520 (100%)	-0.54	5 (0%) 82 59	45, 60, 92, 139	0
1	p	520/520 (100%)	-0.44	12 (2%) 60 31	46, 60, 91, 139	0
1	q	520/520 (100%)	-0.50	6 (1%) 79 54	44, 60, 92, 139	0
1	r	520/520 (100%)	-0.57	7 (1%) 77 51	43, 58, 90, 138	0
1	s	520/520 (100%)	-0.53	5 (0%) 82 59	43, 59, 91, 139	0
1	t	520/520 (100%)	-0.53	7 (1%) 77 51	43, 59, 91, 140	0
1	u	520/520 (100%)	-0.50	9 (1%) 70 41	43, 58, 90, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	v	520/520 (100%)	-0.54	6 (1%) 79 54	42, 59, 90, 141	0
1	w	520/520 (100%)	-0.47	9 (1%) 70 41	43, 60, 92, 141	0
1	x	520/520 (100%)	-0.48	10 (1%) 66 37	44, 60, 92, 140	0
1	y	520/520 (100%)	-0.54	7 (1%) 77 51	43, 59, 90, 139	0
1	z	520/520 (100%)	-0.45	6 (1%) 79 54	44, 59, 91, 141	0
All	All	31200/31200 (100%)	-0.49	427 (1%) 75 49	41, 59, 91, 141	0

All (427) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	x	217	GLY	7.6
1	2	217	GLY	6.3
1	T	217	GLY	5.5
1	P	453	SER	5.5
1	u	217	GLY	5.2
1	s	217	GLY	5.2
1	w	456	ALA	5.1
1	U	217	GLY	5.0
1	a	217	GLY	5.0
1	0	217	GLY	4.7
1	z	217	GLY	4.7
1	C	456	ALA	4.6
1	0	218	ALA	4.6
1	C	453	SER	4.6
1	v	456	ALA	4.5
1	u	456	ALA	4.5
1	d	453	SER	4.5
1	f	456	ALA	4.5
1	J	456	ALA	4.4
1	x	456	ALA	4.4
1	S	456	ALA	4.4
1	M	217	GLY	4.4
1	h	453	SER	4.3
1	p	452	GLN	4.2
1	p	217	GLY	4.2
1	G	456	ALA	4.2
1	3	454	GLY	4.2
1	C	217	GLY	4.2
1	Q	453	SER	4.1
1	Q	456	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	y	456	ALA	4.0
1	2	218	ALA	4.0
1	2	456	ALA	4.0
1	I	217	GLY	3.9
1	K	456	ALA	3.9
1	P	456	ALA	3.9
1	X	456	ALA	3.9
1	w	455	SER	3.9
1	0	456	ALA	3.9
1	p	453	SER	3.9
1	G	453	SER	3.8
1	r	217	GLY	3.8
1	t	454	GLY	3.8
1	t	456	ALA	3.8
1	D	217	GLY	3.7
1	c	456	ALA	3.7
1	x	218	ALA	3.7
1	2	453	SER	3.7
1	Z	457	GLN	3.7
1	v	217	GLY	3.7
1	b	456	ALA	3.6
1	L	455	SER	3.6
1	6	456	ALA	3.6
1	W	217	GLY	3.6
1	P	217	GLY	3.6
1	D	456	ALA	3.6
1	Y	456	ALA	3.6
1	u	454	GLY	3.6
1	p	456	ALA	3.6
1	X	451	ASN	3.6
1	j	456	ALA	3.6
1	P	457	GLN	3.6
1	6	457	GLN	3.6
1	1	455	SER	3.6
1	r	330	VAL	3.5
1	X	457	GLN	3.5
1	N	218	ALA	3.5
1	0	455	SER	3.5
1	I	455	SER	3.5
1	X	455	SER	3.5
1	0	454	GLY	3.5
1	3	456	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	x	455	SER	3.5
1	w	457	GLN	3.5
1	K	457	GLN	3.5
1	L	217	GLY	3.5
1	p	329	GLY	3.5
1	Z	456	ALA	3.5
1	0	452	GLN	3.5
1	3	452	GLN	3.4
1	4	456	ALA	3.4
1	h	217	GLY	3.4
1	s	452	GLN	3.4
1	F	454	GLY	3.4
1	m	217	GLY	3.4
1	3	453	SER	3.4
1	J	457	GLN	3.4
1	b	452	GLN	3.4
1	n	453	SER	3.4
1	R	217	GLY	3.4
1	e	217	GLY	3.4
1	t	453	SER	3.4
1	6	452	GLN	3.4
1	T	456	ALA	3.3
1	2	219	ASP	3.3
1	p	457	GLN	3.3
1	B	453	SER	3.3
1	D	455	SER	3.3
1	n	456	ALA	3.3
1	I	452	GLN	3.3
1	B	455	SER	3.3
1	0	453	SER	3.3
1	G	217	GLY	3.3
1	t	455	SER	3.2
1	Y	452	GLN	3.2
1	6	453	SER	3.2
1	u	455	SER	3.2
1	e	456	ALA	3.2
1	j	457	GLN	3.2
1	H	454	GLY	3.2
1	a	456	ALA	3.2
1	X	452	GLN	3.2
1	Y	455	SER	3.2
1	c	217	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	456	ALA	3.1
1	q	452	GLN	3.1
1	u	218	ALA	3.1
1	j	453	SER	3.1
1	j	455	SER	3.1
1	x	453	SER	3.1
1	A	456	ALA	3.1
1	J	217	GLY	3.1
1	p	454	GLY	3.1
1	K	453	SER	3.1
1	2	451	ASN	3.1
1	r	454	GLY	3.1
1	4	454	GLY	3.1
1	r	456	ALA	3.1
1	C	452	GLN	3.0
1	4	457	GLN	3.0
1	O	456	ALA	3.0
1	w	329	GLY	3.0
1	L	457	GLN	3.0
1	x	457	GLN	3.0
1	c	453	SER	3.0
1	4	453	SER	3.0
1	d	457	GLN	3.0
1	H	453	SER	3.0
1	I	453	SER	3.0
1	7	217	GLY	3.0
1	J	453	SER	3.0
1	1	456	ALA	3.0
1	C	457	GLN	3.0
1	x	329	GLY	3.0
1	R	453	SER	3.0
1	W	456	ALA	3.0
1	w	454	GLY	2.9
1	u	453	SER	2.9
1	U	456	ALA	2.9
1	U	453	SER	2.9
1	Y	457	GLN	2.9
1	J	455	SER	2.9
1	Q	452	GLN	2.9
1	W	327	ASN	2.9
1	Z	217	GLY	2.9
1	y	217	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	329	GLY	2.9
1	5	457	GLN	2.9
1	Z	453	SER	2.9
1	S	217	GLY	2.9
1	q	328	ASP	2.9
1	i	455	SER	2.9
1	m	455	SER	2.9
1	d	456	ALA	2.9
1	v	452	GLN	2.9
1	u	330	VAL	2.9
1	p	455	SER	2.8
1	r	453	SER	2.8
1	o	456	ALA	2.8
1	p	219	ASP	2.8
1	a	453	SER	2.8
1	N	452	GLN	2.8
1	K	328	ASP	2.8
1	K	455	SER	2.8
1	C	460	ASP	2.8
1	L	456	ALA	2.8
1	I	456	ALA	2.8
1	c	452	GLN	2.8
1	w	453	SER	2.8
1	D	457	GLN	2.8
1	V	456	ALA	2.8
1	w	217	GLY	2.8
1	4	452	GLN	2.8
1	m	456	ALA	2.8
1	S	328	ASP	2.8
1	6	455	SER	2.7
1	O	499	SER	2.7
1	W	668	ALA	2.7
1	a	452	GLN	2.7
1	Y	454	GLY	2.7
1	Z	451	ASN	2.7
1	z	456	ALA	2.7
1	G	328	ASP	2.7
1	O	457	GLN	2.7
1	n	457	GLN	2.7
1	u	452	GLN	2.7
1	Y	217	GLY	2.7
1	2	454	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	452	GLN	2.7
1	y	455	SER	2.7
1	W	330	VAL	2.7
1	A	455	SER	2.7
1	K	454	GLY	2.7
1	U	455	SER	2.7
1	G	330	VAL	2.7
1	0	328	ASP	2.7
1	J	454	GLY	2.7
1	Q	457	GLN	2.7
1	m	452	GLN	2.7
1	Q	451	ASN	2.6
1	w	328	ASP	2.6
1	6	451	ASN	2.6
1	m	453	SER	2.6
1	X	328	ASP	2.6
1	w	451	ASN	2.6
1	M	329	GLY	2.6
1	U	452	GLN	2.6
1	5	454	GLY	2.6
1	f	454	GLY	2.6
1	o	457	GLN	2.6
1	3	218	ALA	2.6
1	d	454	GLY	2.6
1	Z	452	GLN	2.6
1	s	454	GLY	2.6
1	E	457	GLN	2.6
1	i	217	GLY	2.6
1	Y	552	ASN	2.6
1	a	451	ASN	2.6
1	Y	453	SER	2.6
1	1	453	SER	2.6
1	H	456	ALA	2.6
1	h	452	GLN	2.6
1	2	452	GLN	2.6
1	D	218	ALA	2.6
1	n	217	GLY	2.6
1	b	457	GLN	2.6
1	E	456	ALA	2.6
1	3	455	SER	2.6
1	U	454	GLY	2.6
1	H	452	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	328	ASP	2.5
1	a	455	SER	2.5
1	s	453	SER	2.5
1	R	218	ALA	2.5
1	7	454	GLY	2.5
1	A	454	GLY	2.5
1	d	460	ASP	2.5
1	X	454	GLY	2.5
1	0	457	GLN	2.5
1	v	457	GLN	2.5
1	x	454	GLY	2.5
1	y	218	ALA	2.5
1	X	587	SER	2.5
1	f	330	VAL	2.5
1	j	452	GLN	2.5
1	z	452	GLN	2.5
1	B	454	GLY	2.5
1	F	457	GLN	2.5
1	c	457	GLN	2.5
1	e	455	SER	2.5
1	B	327	ASN	2.5
1	i	456	ALA	2.5
1	Z	455	SER	2.5
1	b	455	SER	2.5
1	H	217	GLY	2.5
1	e	457	GLN	2.5
1	R	454	GLY	2.4
1	B	457	GLN	2.4
1	D	453	SER	2.4
1	G	455	SER	2.4
1	F	456	ALA	2.4
1	C	330	VAL	2.4
1	C	455	SER	2.4
1	R	456	ALA	2.4
1	h	448	ARG	2.4
1	b	453	SER	2.4
1	W	457	GLN	2.4
1	W	462	LEU	2.4
1	j	217	GLY	2.4
1	J	452	GLN	2.4
1	T	455	SER	2.4
1	7	328	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	V	454	GLY	2.4
1	h	328	ASP	2.4
1	K	452	GLN	2.4
1	X	453	SER	2.4
1	x	452	GLN	2.4
1	o	454	GLY	2.3
1	f	453	SER	2.3
1	D	328	ASP	2.3
1	F	455	SER	2.3
1	A	530	ASP	2.3
1	U	457	GLN	2.3
1	q	456	ALA	2.3
1	Q	217	GLY	2.3
1	l	452	GLN	2.3
1	4	458	ASN	2.3
1	m	454	GLY	2.3
1	F	589	THR	2.3
1	H	330	VAL	2.3
1	k	217	GLY	2.3
1	d	496	ASN	2.3
1	l	328	ASP	2.3
1	3	219	ASP	2.3
1	6	454	GLY	2.3
1	l	591	PRO	2.3
1	V	452	GLN	2.3
1	t	457	GLN	2.3
1	M	328	ASP	2.3
1	u	457	GLN	2.3
1	A	552	ASN	2.3
1	Z	454	GLY	2.3
1	q	217	GLY	2.3
1	5	552	ASN	2.3
1	D	452	GLN	2.3
1	H	455	SER	2.3
1	2	264	SER	2.3
1	Q	454	GLY	2.3
1	U	451	ASN	2.3
1	F	453	SER	2.3
1	f	327	ASN	2.2
1	z	328	ASP	2.2
1	5	456	ALA	2.2
1	6	217	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	461	LEU	2.2
1	Q	460	ASP	2.2
1	B	491	LYS	2.2
1	i	451	ASN	2.2
1	T	457	GLN	2.2
1	I	454	GLY	2.2
1	L	452	GLN	2.2
1	X	458	ASN	2.2
1	2	327	ASN	2.2
1	g	453	SER	2.2
1	p	499	SER	2.2
1	N	451	ASN	2.2
1	s	457	GLN	2.2
1	0	331	THR	2.2
1	E	588	SER	2.2
1	R	455	SER	2.2
1	2	455	SER	2.2
1	r	452	GLN	2.2
1	t	218	ALA	2.2
1	2	462	LEU	2.2
1	H	457	GLN	2.2
1	4	455	SER	2.2
1	W	328	ASP	2.2
1	h	454	GLY	2.2
1	p	458	ASN	2.2
1	H	264	SER	2.1
1	O	455	SER	2.1
1	a	457	GLN	2.1
1	X	460	ASP	2.1
1	2	328	ASP	2.1
1	F	217	GLY	2.1
1	Q	327	ASN	2.1
1	G	452	GLN	2.1
1	P	455	SER	2.1
1	y	453	SER	2.1
1	z	457	GLN	2.1
1	D	454	GLY	2.1
1	Z	460	ASP	2.1
1	E	458	ASN	2.1
1	3	451	ASN	2.1
1	H	329	GLY	2.1
1	W	453	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	n	455	SER	2.1
1	Z	328	ASP	2.1
1	0	491	LYS	2.1
1	V	455	SER	2.1
1	H	326	THR	2.1
1	R	327	ASN	2.1
1	F	329	GLY	2.1
1	T	454	GLY	2.1
1	C	499	SER	2.1
1	d	455	SER	2.1
1	d	493	LYS	2.1
1	j	449	THR	2.1
1	r	457	GLN	2.1
1	G	218	ALA	2.1
1	V	218	ALA	2.1
1	H	491	LYS	2.1
1	f	457	GLN	2.1
1	S	455	SER	2.1
1	k	330	VAL	2.1
1	O	217	GLY	2.1
1	Y	499	SER	2.1
1	y	457	GLN	2.1
1	e	326	THR	2.1
1	M	460	ASP	2.1
1	e	329	GLY	2.1
1	v	328	ASP	2.1
1	5	328	ASP	2.1
1	m	457	GLN	2.1
1	I	451	ASN	2.1
1	o	219	ASP	2.1
1	x	328	ASP	2.1
1	F	326	THR	2.0
1	Y	327	ASN	2.0
1	L	454	GLY	2.0
1	y	329	GLY	2.0
1	V	457	GLN	2.0
1	c	455	SER	2.0
1	d	328	ASP	2.0
1	k	328	ASP	2.0
1	d	330	VAL	2.0
1	Y	496	ASN	2.0
1	q	454	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	448	ARG	2.0
1	O	453	SER	2.0
1	o	453	SER	2.0
1	0	330	VAL	2.0
1	I	496	ASN	2.0
1	c	454	GLY	2.0
1	5	327	ASN	2.0
1	v	453	SER	2.0
1	Q	329	GLY	2.0
1	b	454	GLY	2.0
1	p	266	GLY	2.0
1	5	217	GLY	2.0
1	D	451	ASN	2.0
1	z	451	ASN	2.0
1	q	457	GLN	2.0
1	A	513	GLY	2.0
1	X	327	ASN	2.0
1	M	330	VAL	2.0
1	t	330	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.