



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 10:32 pm BST

PDB ID : 2GSY  
Title : The 2.6A structure of Infectious Bursal Virus Derived T=1 Particles  
Authors : Garriga, D.; Querol-Audi, J.; Abaitua, F.; Saugar, I.; Pous, J.; Verdaguer, N.; Caston, J.R.; Rodriguez, J.F.  
Deposited on : 2006-04-27  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

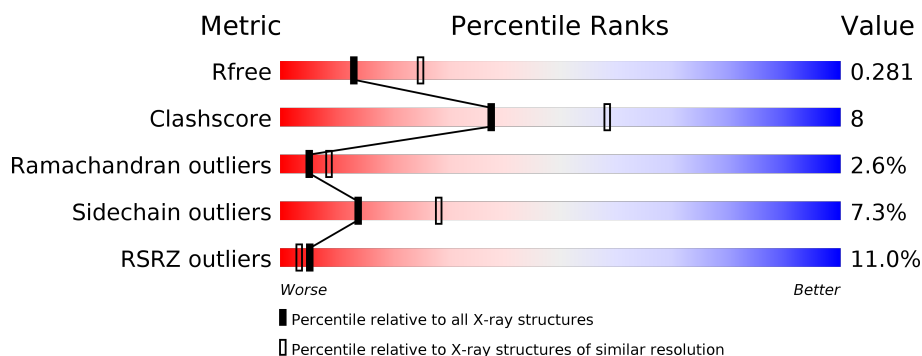
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	456	<div> <div>11%</div> <div> <div>76%</div> <div>15%</div> <div>• 6%</div> </div> </div>
1	B	456	<div> <div>12%</div> <div> <div>77%</div> <div>13%</div> <div>• 6%</div> </div> </div>
1	C	456	<div> <div>13%</div> <div> <div>77%</div> <div>14%</div> <div>• 6%</div> </div> </div>
1	D	456	<div> <div>14%</div> <div> <div>78%</div> <div>13%</div> <div>• 6%</div> </div> </div>
1	E	456	<div> <div>7%</div> <div> <div>77%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	F	456	<div> <div>13%</div> <div> <div>76%</div> <div>14%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	456	
1	H	456	
1	I	456	
1	J	456	
1	K	456	
1	L	456	
1	M	456	
1	N	456	
1	O	456	
1	P	456	
1	Q	456	
1	R	456	
1	S	456	
1	T	456	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 64447 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 polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			
1	B	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			
1	C	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			
1	D	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			
1	E	433	Total	C	N	O	S	0	0	0
			3241	2057	538	636	10			
1	F	433	Total	C	N	O	S	0	0	0
			3241	2057	538	636	10			
1	G	433	Total	C	N	O	S	0	0	0
			3241	2057	538	636	10			
1	H	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			
1	I	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			
1	J	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			
1	K	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			
1	L	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			
1	M	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			
1	N	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			
1	O	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			
1	P	430	Total	C	N	O	S	0	0	0
			3218	2041	535	632	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	429	Total	C	N	O	S	0	0	0
			3213	2038	534	631	10			
1	R	433	Total	C	N	O	S	0	0	0
			3241	2057	538	636	10			
1	S	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			
1	T	428	Total	C	N	O	S	0	0	0
			3209	2036	533	630	10			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	T	1	Total	Ca	0	0
			1	1		
2	O	1	Total	Ca	0	0
			1	1		
2	L	1	Total	Ca	0	0
			1	1		
2	S	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		
2	M	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	4	Total	O	0	0
			4	4		

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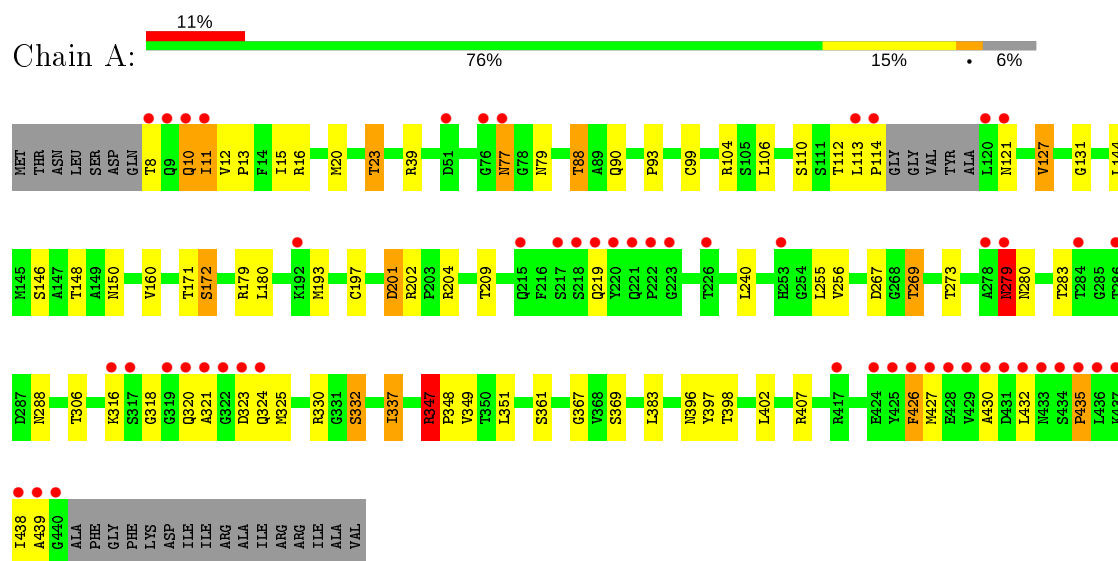
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total 2	O 2	0	0
3	D	2	Total 2	O 2	0	0
3	E	8	Total 8	O 8	0	0
3	F	4	Total 4	O 4	0	0
3	G	6	Total 6	O 6	0	0
3	H	7	Total 7	O 7	0	0
3	I	6	Total 6	O 6	0	0
3	J	1	Total 1	O 1	0	0
3	K	7	Total 7	O 7	0	0
3	L	6	Total 6	O 6	0	0
3	M	11	Total 11	O 11	0	0
3	N	5	Total 5	O 5	0	0
3	O	4	Total 4	O 4	0	0
3	P	5	Total 5	O 5	0	0
3	Q	5	Total 5	O 5	0	0
3	R	5	Total 5	O 5	0	0
3	S	7	Total 7	O 7	0	0
3	T	18	Total 18	O 18	0	0

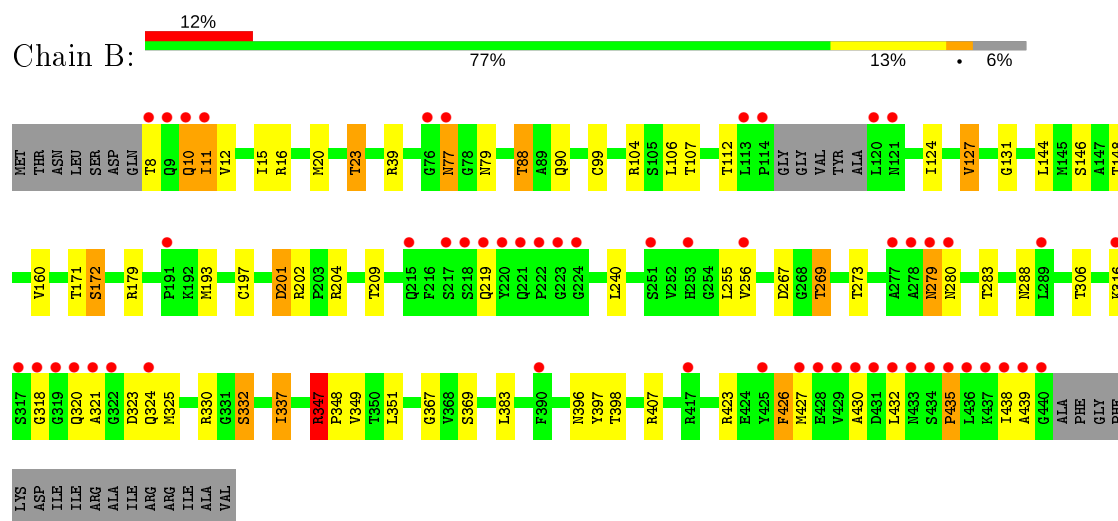
### 3 Residue-property plots [i](#)

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

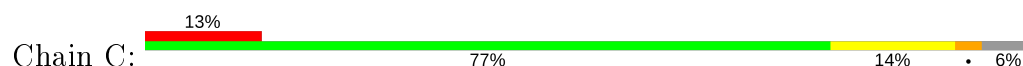
- Molecule 1: polyprotein

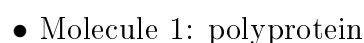


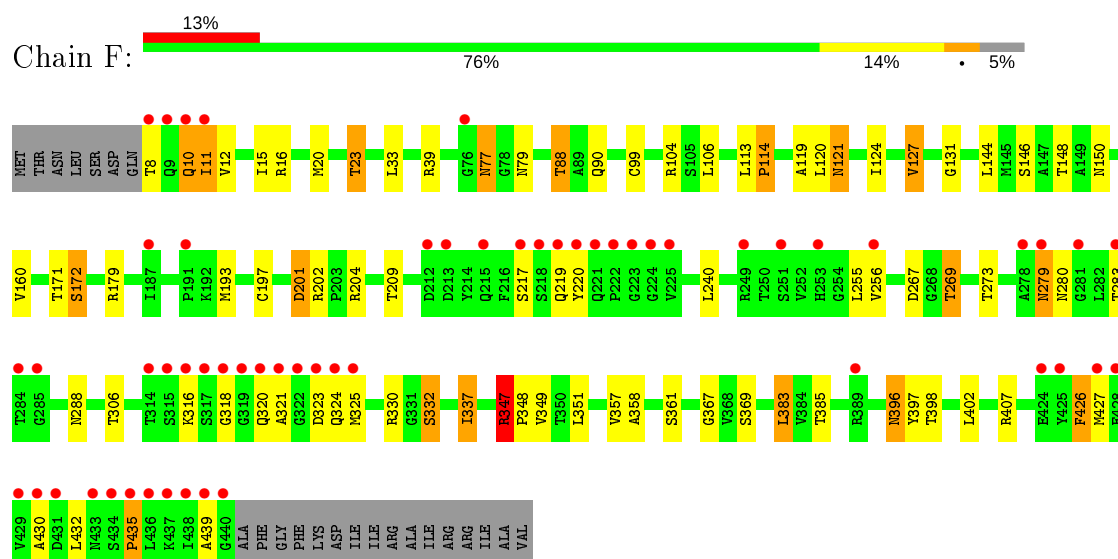
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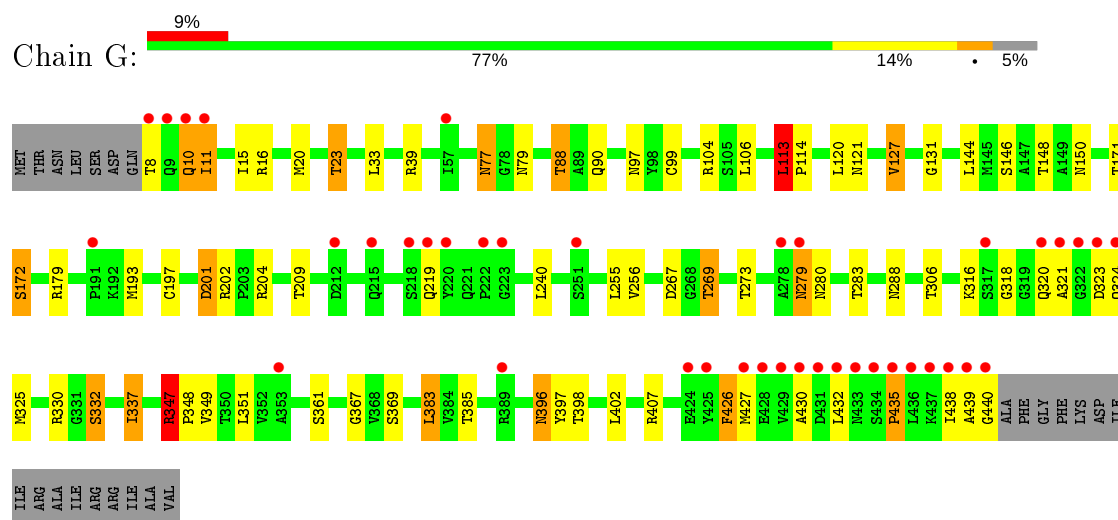
- Molecule 1: polyprotein



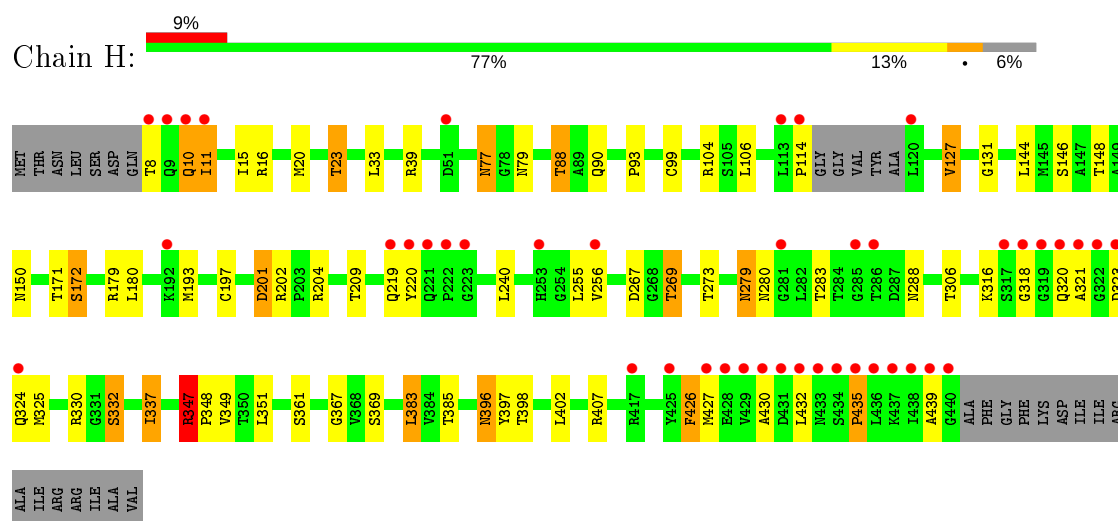




- Molecule 1: polypeptide

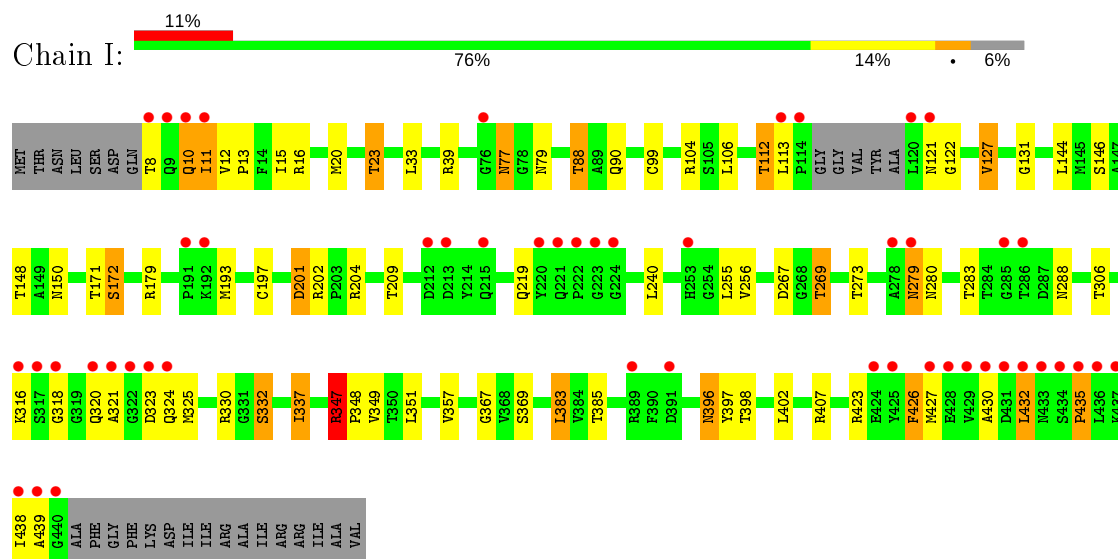


- Molecule 1: polypeptide



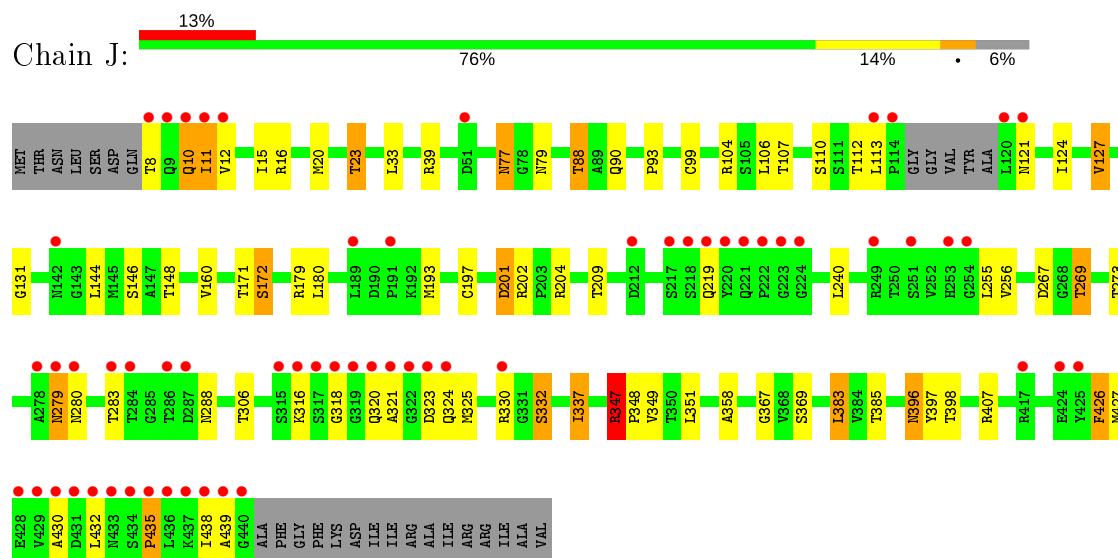
- Molecule 1: polyprotein

Chain I:



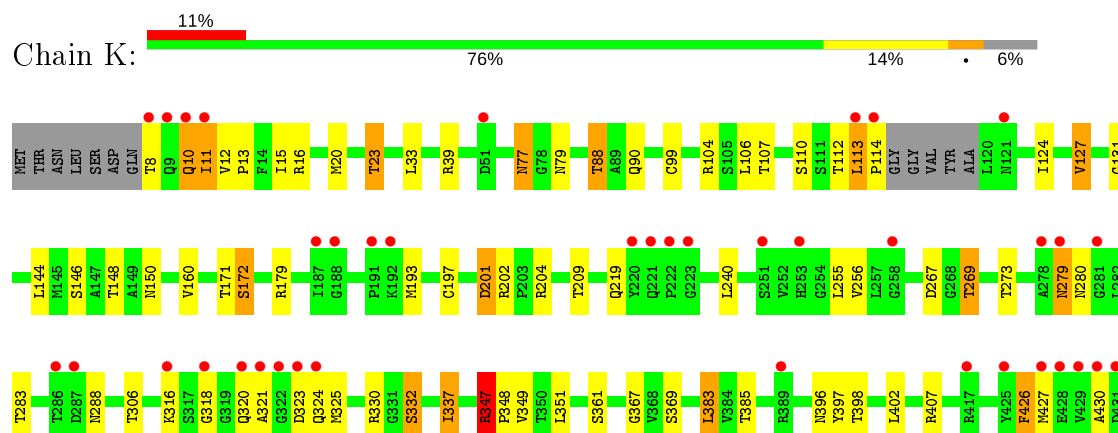
- Molecule 1: polyprotein

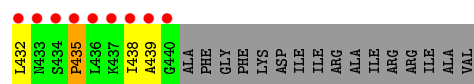
Chain J:



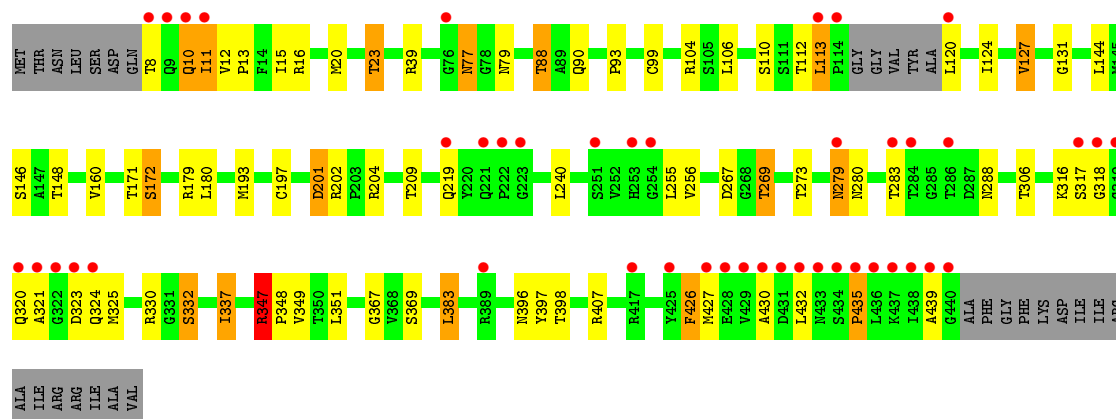
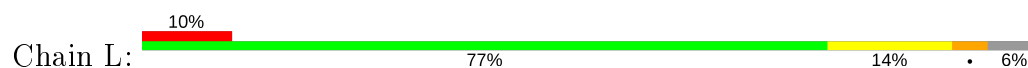
- Molecule 1: polyprotein

Chain K:

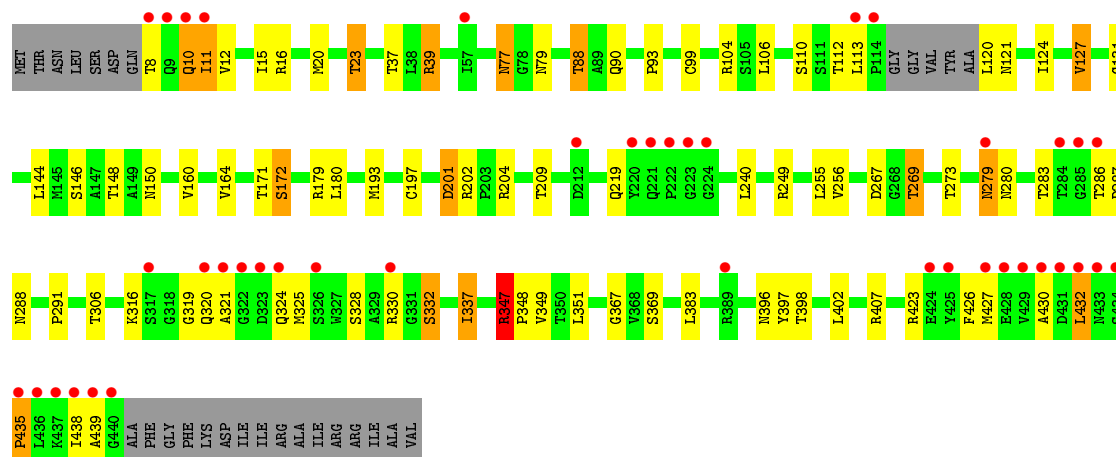
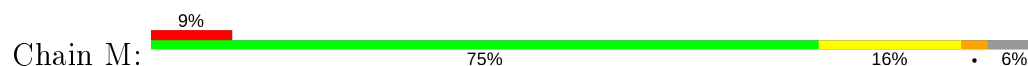




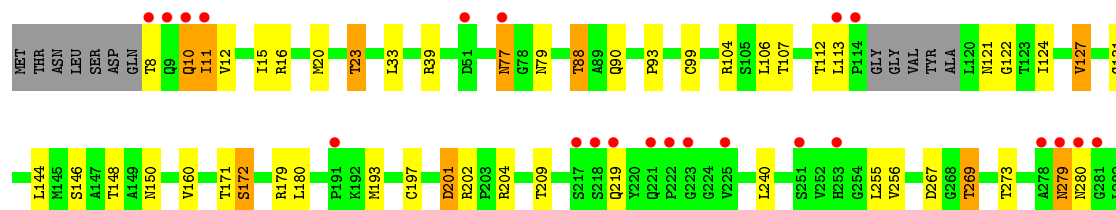
• Molecule 1: polyprotein

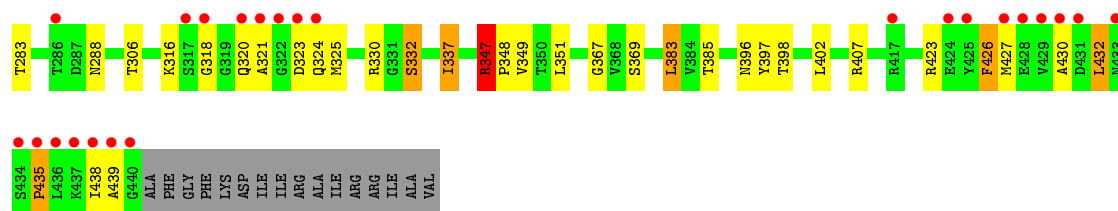


• Molecule 1: polyprotein

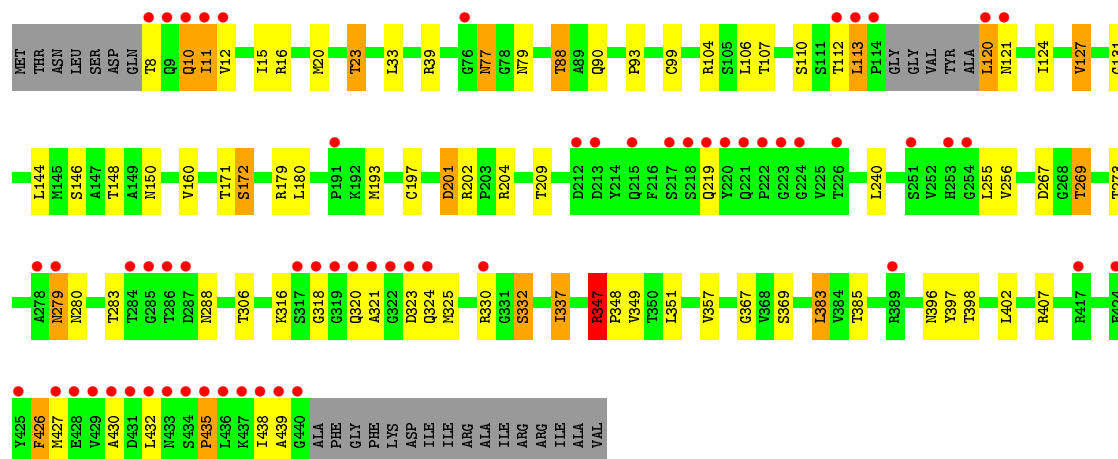
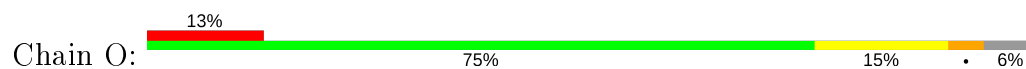


• Molecule 1: polyprotein

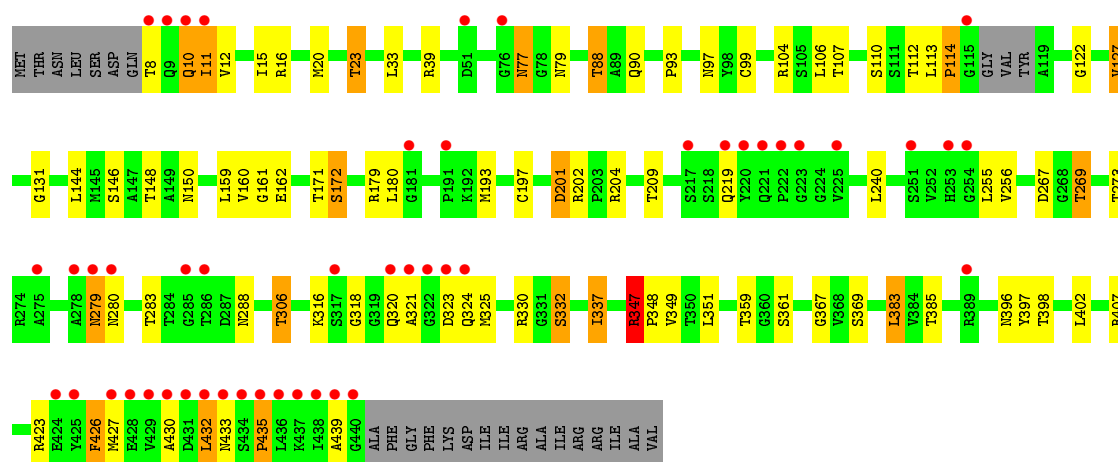
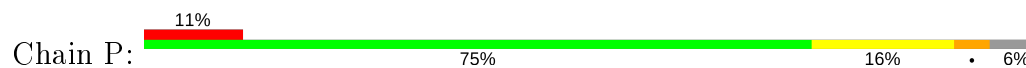




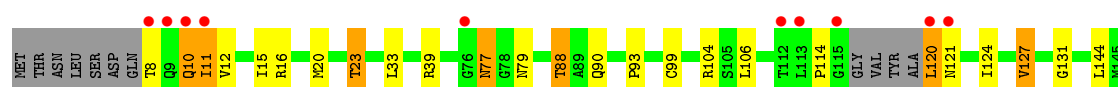
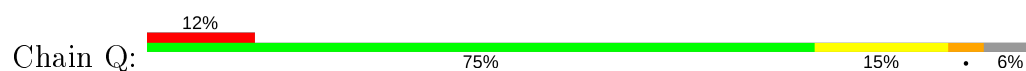
• Molecule 1: polypeptide

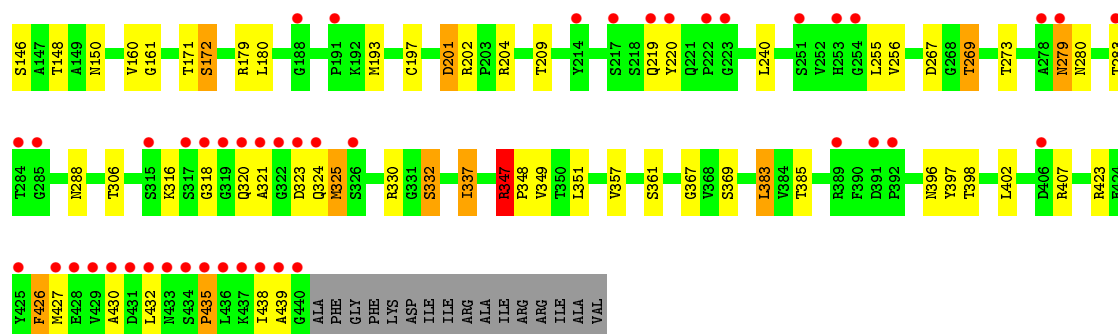


• Molecule 1: polypeptide

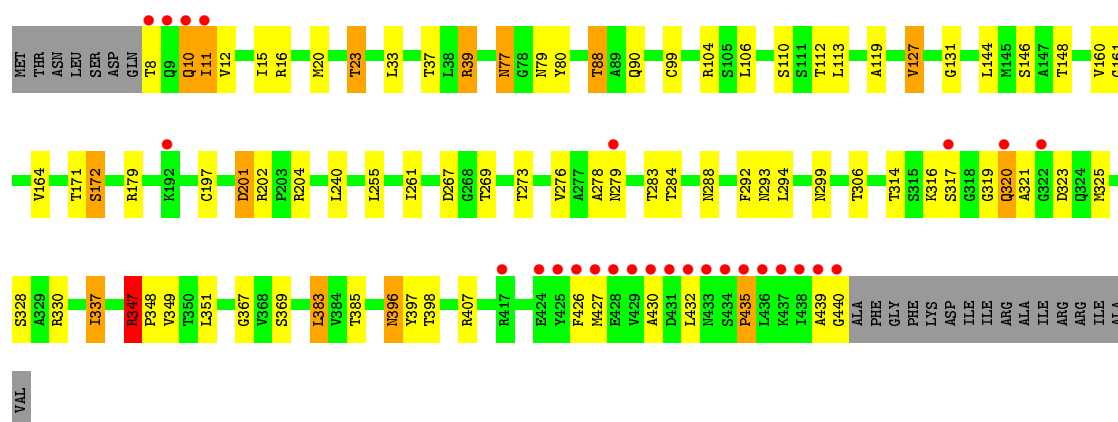


• Molecule 1: polypeptide

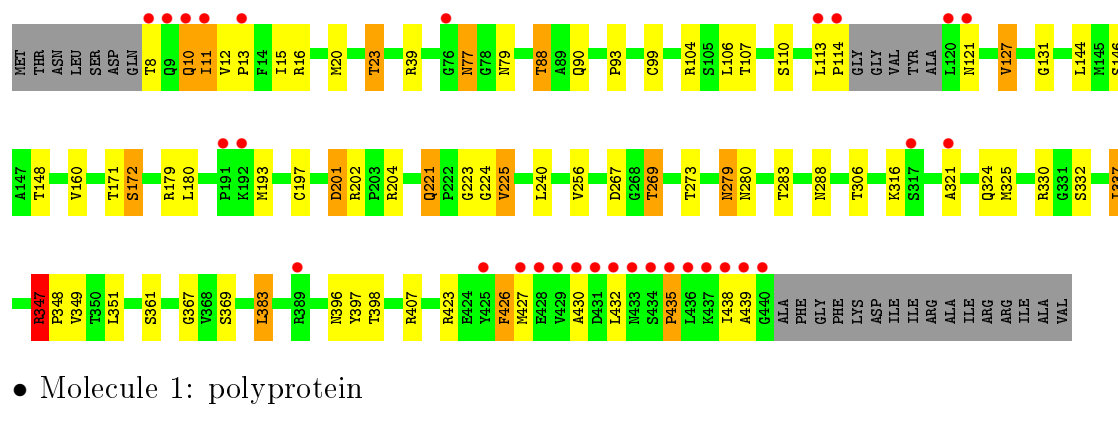
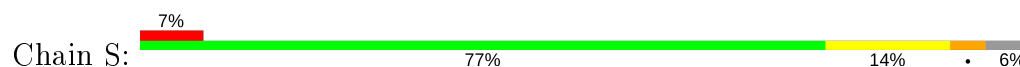




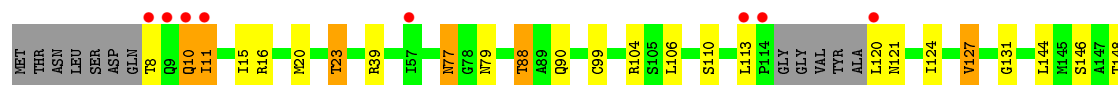
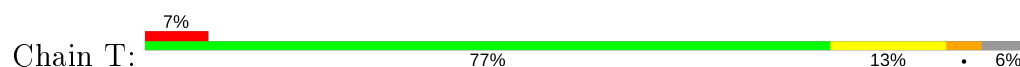
- Molecule 1: polypeptide

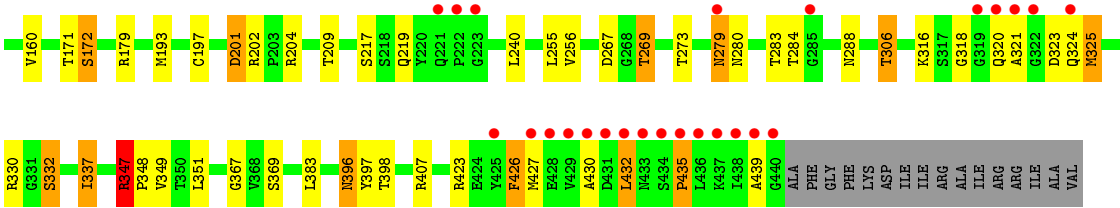


- Molecule 1: polypeptide



- Molecule 1: polypeptide





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	326.30Å 326.30Å 326.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.60 19.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.8 (19.97-2.60) 88.8 (19.93-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.19	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.254 , 0.267 0.274 , 0.281	Depositor DCC
$R_{free}$ test set	15643 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 12.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	64447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.39	0/3272	0.61	0/4471
1	B	0.39	0/3272	0.61	0/4471
1	C	0.39	0/3272	0.61	0/4471
1	D	0.38	0/3272	0.61	0/4471
1	E	0.38	0/3306	0.59	0/4519
1	F	0.39	0/3306	0.61	0/4519
1	G	0.39	0/3306	0.62	1/4519 (0.0%)
1	H	0.39	0/3272	0.61	0/4471
1	I	0.39	0/3272	0.61	0/4471
1	J	0.39	0/3272	0.61	0/4471
1	K	0.39	0/3272	0.61	0/4471
1	L	0.39	0/3272	0.61	0/4471
1	M	0.38	0/3272	0.60	0/4471
1	N	0.39	0/3272	0.61	0/4471
1	O	0.39	0/3272	0.61	0/4471
1	P	0.39	0/3281	0.61	0/4483
1	Q	0.39	0/3276	0.61	0/4476
1	R	0.38	0/3306	0.60	0/4519
1	S	0.38	0/3272	0.61	0/4471
1	T	0.40	0/3272	0.61	0/4471
All	All	0.39	0/65589	0.61	1/89629 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
1	I	0	3
1	J	0	3
1	K	0	3
1	L	0	3
1	M	0	3
1	N	0	3
1	O	0	3
1	P	0	3
1	Q	0	3
1	R	0	3
1	S	0	4
1	T	0	3
All	All	0	61

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	G	113	LEU	CA-CB-CG	5.69	128.39	115.30

There are no chirality outliers.

All (61) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLN	Peptide
1	A	430	ALA	Peptide
1	A	435	PRO	Peptide
1	B	10	GLN	Peptide
1	B	430	ALA	Peptide
1	B	435	PRO	Peptide
1	C	10	GLN	Peptide
1	C	430	ALA	Peptide
1	C	435	PRO	Peptide
1	D	10	GLN	Peptide
1	D	430	ALA	Peptide
1	D	435	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	E	10	GLN	Peptide
1	E	430	ALA	Peptide
1	E	435	PRO	Peptide
1	F	10	GLN	Peptide
1	F	430	ALA	Peptide
1	F	435	PRO	Peptide
1	G	10	GLN	Peptide
1	G	430	ALA	Peptide
1	G	435	PRO	Peptide
1	H	10	GLN	Peptide
1	H	430	ALA	Peptide
1	H	435	PRO	Peptide
1	I	10	GLN	Peptide
1	I	430	ALA	Peptide
1	I	435	PRO	Peptide
1	J	10	GLN	Peptide
1	J	430	ALA	Peptide
1	J	435	PRO	Peptide
1	K	10	GLN	Peptide
1	K	430	ALA	Peptide
1	K	435	PRO	Peptide
1	L	10	GLN	Peptide
1	L	430	ALA	Peptide
1	L	435	PRO	Peptide
1	M	10	GLN	Peptide
1	M	430	ALA	Peptide
1	M	435	PRO	Peptide
1	N	10	GLN	Peptide
1	N	430	ALA	Peptide
1	N	435	PRO	Peptide
1	O	10	GLN	Peptide
1	O	430	ALA	Peptide
1	O	435	PRO	Peptide
1	P	10	GLN	Peptide
1	P	430	ALA	Peptide
1	P	435	PRO	Peptide
1	Q	10	GLN	Peptide
1	Q	430	ALA	Peptide
1	Q	435	PRO	Peptide
1	R	10	GLN	Peptide
1	R	430	ALA	Peptide
1	R	435	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	S	10	GLN	Peptide
1	S	223	GLY	Peptide
1	S	430	ALA	Peptide
1	S	435	PRO	Peptide
1	T	10	GLN	Peptide
1	T	430	ALA	Peptide
1	T	435	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3209	0	3191	48	0
1	B	3209	0	3191	46	0
1	C	3209	0	3191	50	0
1	D	3209	0	3191	44	1
1	E	3241	0	3221	54	1
1	F	3241	0	3221	55	1
1	G	3241	0	3221	53	0
1	H	3209	0	3191	49	0
1	I	3209	0	3191	55	0
1	J	3209	0	3191	49	0
1	K	3209	0	3191	55	0
1	L	3209	0	3191	48	1
1	M	3209	0	3191	55	0
1	N	3209	0	3191	55	0
1	O	3209	0	3191	54	0
1	P	3218	0	3199	63	0
1	Q	3213	0	3194	57	0
1	R	3241	0	3221	63	0
1	S	3209	0	3191	49	0
1	T	3209	0	3191	51	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	O	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
3	A	2	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	8	0	0	0	0
3	F	4	0	0	0	0
3	G	6	0	0	0	0
3	H	7	0	0	0	0
3	I	6	0	0	0	0
3	J	1	0	0	0	0
3	K	7	0	0	0	0
3	L	6	0	0	0	0
3	M	11	0	0	0	0
3	N	5	0	0	0	0
3	O	4	0	0	0	0
3	P	5	0	0	1	0
3	Q	5	0	0	0	0
3	R	5	0	0	0	0
3	S	7	0	0	0	0
3	T	18	0	0	1	0
All	All	64447	0	63951	990	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (990) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:110:SER:HB3	1:R:160:VAL:HG12	1.43	0.97
1:M:286:THR:HG21	1:R:279:ASN:HB2	1.44	0.96
1:R:204:ARG:HB3	1:R:337:ILE:HD13	1.56	0.88
1:G:204:ARG:HD2	1:G:337:ILE:HD11	1.56	0.87
1:P:150:ASN:HD21	1:Q:385:THR:H	1.20	0.87
1:H:204:ARG:HD2	1:H:337:ILE:HD11	1.57	0.87
1:D:204:ARG:HD2	1:D:337:ILE:HD11	1.56	0.87
1:L:204:ARG:HD2	1:L:337:ILE:HD11	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:110:SER:HB3	1:R:160:VAL:CG1	2.04	0.87
1:A:204:ARG:HD2	1:A:337:ILE:HD11	1.56	0.86
1:B:204:ARG:HD2	1:B:337:ILE:HD11	1.57	0.86
1:C:204:ARG:HD2	1:C:337:ILE:HD11	1.57	0.86
1:F:204:ARG:HD2	1:F:337:ILE:HD11	1.56	0.86
1:P:204:ARG:HD2	1:P:337:ILE:HD11	1.57	0.86
1:E:204:ARG:HD2	1:E:337:ILE:HD11	1.54	0.86
1:N:204:ARG:HD2	1:N:337:ILE:HD11	1.57	0.86
1:I:204:ARG:HD2	1:I:337:ILE:HD11	1.57	0.86
1:S:204:ARG:HD2	1:S:337:ILE:HD11	1.57	0.85
1:M:204:ARG:HD2	1:M:337:ILE:HD11	1.56	0.85
1:T:204:ARG:HD2	1:T:337:ILE:HD11	1.57	0.85
1:O:204:ARG:HD2	1:O:337:ILE:HD11	1.57	0.85
1:R:204:ARG:HB3	1:R:337:ILE:CD1	2.07	0.85
1:S:221:GLN:HB3	1:S:224:GLY:HA3	1.57	0.85
1:K:204:ARG:HD2	1:K:337:ILE:HD11	1.56	0.85
1:J:204:ARG:HD2	1:J:337:ILE:HD11	1.57	0.84
1:Q:204:ARG:HD2	1:Q:337:ILE:HD11	1.57	0.83
1:G:385:THR:H	1:N:150:ASN:HD21	1.25	0.82
1:F:385:THR:H	1:I:150:ASN:HD21	1.27	0.81
1:F:150:ASN:HD21	1:K:385:THR:H	1.26	0.81
1:C:150:ASN:HD21	1:J:385:THR:H	1.29	0.81
1:G:150:ASN:HD21	1:H:385:THR:H	1.29	0.80
1:E:88:THR:HG22	1:E:90:GLN:O	1.82	0.80
1:O:150:ASN:HD21	1:P:385:THR:H	1.31	0.79
1:P:88:THR:HG22	1:P:90:GLN:O	1.83	0.79
1:N:88:THR:HG22	1:N:90:GLN:O	1.83	0.79
1:D:88:THR:HG22	1:D:90:GLN:O	1.83	0.79
1:R:88:THR:HG22	1:R:90:GLN:O	1.83	0.79
1:T:88:THR:HG22	1:T:90:GLN:O	1.83	0.79
1:I:88:THR:HG22	1:I:90:GLN:O	1.83	0.79
1:B:88:THR:HG22	1:B:90:GLN:O	1.83	0.78
1:O:385:THR:H	1:Q:150:ASN:HD21	1.28	0.78
1:P:306:THR:HG22	3:P:720:HOH:O	1.82	0.78
1:F:88:THR:HG22	1:F:90:GLN:O	1.83	0.78
1:G:88:THR:HG22	1:G:90:GLN:O	1.83	0.78
1:A:88:THR:HG22	1:A:90:GLN:O	1.83	0.78
1:H:88:THR:HG22	1:H:90:GLN:O	1.84	0.78
1:J:88:THR:HG22	1:J:90:GLN:O	1.83	0.78
1:R:347:ARG:HB3	1:R:348:PRO:HD3	1.66	0.78
1:A:150:ASN:HD21	1:E:385:THR:H	1.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:THR:HG22	1:C:90:GLN:O	1.83	0.78
1:K:88:THR:HG22	1:K:90:GLN:O	1.83	0.78
1:Q:88:THR:HG22	1:Q:90:GLN:O	1.83	0.78
1:H:150:ASN:HD21	1:N:385:THR:H	1.31	0.77
1:P:20:MET:O	1:P:23:THR:HB	1.85	0.77
1:E:20:MET:O	1:E:23:THR:HB	1.84	0.77
1:K:20:MET:O	1:K:23:THR:HB	1.85	0.77
1:L:88:THR:HG22	1:L:90:GLN:O	1.84	0.77
1:O:20:MET:O	1:O:23:THR:HB	1.85	0.77
1:S:88:THR:HG22	1:S:90:GLN:O	1.85	0.77
1:G:20:MET:O	1:G:23:THR:HB	1.85	0.77
1:J:20:MET:O	1:J:23:THR:HB	1.85	0.77
1:S:316:LYS:HB2	1:S:325:MET:HE2	1.65	0.77
1:C:20:MET:O	1:C:23:THR:HB	1.85	0.77
1:L:20:MET:O	1:L:23:THR:HB	1.85	0.77
1:A:20:MET:O	1:A:23:THR:HB	1.85	0.77
1:O:88:THR:HG22	1:O:90:GLN:O	1.83	0.77
1:B:20:MET:O	1:B:23:THR:HB	1.85	0.76
1:I:20:MET:O	1:I:23:THR:HB	1.85	0.76
1:F:20:MET:O	1:F:23:THR:HB	1.84	0.76
1:M:88:THR:HG22	1:M:90:GLN:O	1.86	0.76
1:D:20:MET:O	1:D:23:THR:HB	1.85	0.76
1:H:20:MET:O	1:H:23:THR:HB	1.85	0.76
1:I:385:THR:H	1:K:150:ASN:HD21	1.34	0.76
1:Q:20:MET:O	1:Q:23:THR:HB	1.85	0.76
1:T:20:MET:O	1:T:23:THR:HB	1.85	0.76
1:H:347:ARG:HB3	1:H:348:PRO:HD3	1.68	0.76
1:J:347:ARG:HB3	1:J:348:PRO:HD3	1.68	0.76
1:N:347:ARG:HB3	1:N:348:PRO:HD3	1.68	0.75
1:O:347:ARG:HB3	1:O:348:PRO:HD3	1.68	0.75
1:G:347:ARG:HB3	1:G:348:PRO:HD3	1.68	0.75
1:N:20:MET:O	1:N:23:THR:HB	1.85	0.75
1:A:347:ARG:HB3	1:A:348:PRO:HD3	1.68	0.75
1:T:347:ARG:HB3	1:T:348:PRO:HD3	1.69	0.75
1:M:20:MET:O	1:M:23:THR:HB	1.86	0.75
1:S:20:MET:O	1:S:23:THR:HB	1.87	0.75
1:K:347:ARG:HB3	1:K:348:PRO:HD3	1.69	0.75
1:S:347:ARG:HB3	1:S:348:PRO:HD3	1.68	0.74
1:L:347:ARG:HB3	1:L:348:PRO:HD3	1.68	0.74
1:E:347:ARG:HB3	1:E:348:PRO:HD3	1.69	0.74
1:F:347:ARG:HB3	1:F:348:PRO:HD3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:THR:HG21	1:P:161:GLY:H	1.53	0.74
1:M:347:ARG:HB3	1:M:348:PRO:HD3	1.68	0.74
1:Q:347:ARG:HB3	1:Q:348:PRO:HD3	1.68	0.74
1:C:347:ARG:HB3	1:C:348:PRO:HD3	1.68	0.74
1:B:347:ARG:HB3	1:B:348:PRO:HD3	1.69	0.74
1:D:347:ARG:HB3	1:D:348:PRO:HD3	1.68	0.74
1:I:347:ARG:HB3	1:I:348:PRO:HD3	1.69	0.74
1:R:20:MET:O	1:R:23:THR:HB	1.87	0.73
1:P:347:ARG:HB3	1:P:348:PRO:HD3	1.69	0.73
1:P:110:SER:HB3	1:P:160:VAL:HG12	1.71	0.72
1:M:150:ASN:HD21	1:R:385:THR:H	1.36	0.72
1:M:255:LEU:HD23	1:M:316:LYS:HG3	1.69	0.72
1:E:323:ASP:O	1:E:324:GLN:HB2	1.90	0.71
1:D:16:ARG:HG2	1:D:23:THR:HG21	1.75	0.69
1:F:16:ARG:HG2	1:F:23:THR:HG21	1.74	0.69
1:L:16:ARG:HG2	1:L:23:THR:HG21	1.74	0.69
1:S:16:ARG:HG2	1:S:23:THR:HG21	1.74	0.69
1:H:11:ILE:HD11	1:H:16:ARG:HD2	1.75	0.69
1:H:16:ARG:HG2	1:H:23:THR:HG21	1.75	0.69
1:K:11:ILE:HD11	1:K:16:ARG:HD2	1.75	0.69
1:C:11:ILE:HD11	1:C:16:ARG:HD2	1.75	0.69
1:J:16:ARG:HG2	1:J:23:THR:HG21	1.74	0.69
1:J:11:ILE:HD11	1:J:16:ARG:HD2	1.75	0.69
1:K:16:ARG:HG2	1:K:23:THR:HG21	1.75	0.69
1:G:11:ILE:HD11	1:G:16:ARG:HD2	1.75	0.69
1:T:11:ILE:HD11	1:T:16:ARG:HD2	1.75	0.69
1:B:16:ARG:HG2	1:B:23:THR:HG21	1.75	0.69
1:D:11:ILE:HD11	1:D:16:ARG:HD2	1.75	0.69
1:H:383:LEU:HD22	1:R:383:LEU:HD22	1.75	0.69
1:L:11:ILE:HD11	1:L:16:ARG:HD2	1.75	0.69
1:M:16:ARG:HG2	1:M:23:THR:HG21	1.75	0.68
1:B:11:ILE:HD11	1:B:16:ARG:HD2	1.75	0.68
1:E:112:THR:HG23	1:P:159:LEU:HB3	1.74	0.68
1:M:104:ARG:HD3	1:M:369:SER:OG	1.94	0.68
1:P:11:ILE:HD11	1:P:16:ARG:HD2	1.75	0.68
1:P:16:ARG:HG2	1:P:23:THR:HG21	1.75	0.68
1:A:16:ARG:HG2	1:A:23:THR:HG21	1.75	0.68
1:D:267:ASP:OD1	1:D:269:THR:HB	1.94	0.68
1:I:16:ARG:HG2	1:I:23:THR:HG21	1.75	0.68
1:S:11:ILE:HD11	1:S:16:ARG:HD2	1.76	0.68
1:G:16:ARG:HG2	1:G:23:THR:HG21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASP:OD1	1:A:269:THR:HB	1.94	0.68
1:N:16:ARG:HG2	1:N:23:THR:HG21	1.75	0.68
1:O:11:ILE:HD11	1:O:16:ARG:HD2	1.75	0.68
1:Q:16:ARG:HG2	1:Q:23:THR:HG21	1.75	0.68
1:R:16:ARG:HG2	1:R:23:THR:HG21	1.76	0.67
1:O:16:ARG:HG2	1:O:23:THR:HG21	1.75	0.67
1:Q:104:ARG:HD3	1:Q:369:SER:OG	1.95	0.67
1:A:11:ILE:HD11	1:A:16:ARG:HD2	1.75	0.67
1:F:11:ILE:HD11	1:F:16:ARG:HD2	1.76	0.67
1:I:11:ILE:HD11	1:I:16:ARG:HD2	1.75	0.67
1:C:16:ARG:HG2	1:C:23:THR:HG21	1.75	0.67
1:R:104:ARG:HD3	1:R:369:SER:OG	1.95	0.67
1:G:104:ARG:HD3	1:G:369:SER:OG	1.95	0.67
1:Q:11:ILE:HD11	1:Q:16:ARG:HD2	1.75	0.67
1:T:267:ASP:OD1	1:T:269:THR:HB	1.95	0.67
1:H:267:ASP:OD1	1:H:269:THR:HB	1.95	0.67
1:M:11:ILE:HD11	1:M:16:ARG:HD2	1.75	0.67
1:T:131:GLY:O	1:T:347:ARG:O	2.13	0.67
1:J:267:ASP:OD1	1:J:269:THR:HB	1.95	0.67
1:N:11:ILE:HD11	1:N:16:ARG:HD2	1.75	0.67
1:T:16:ARG:HG2	1:T:23:THR:HG21	1.75	0.67
1:K:267:ASP:OD1	1:K:269:THR:HB	1.95	0.67
1:P:104:ARG:HD3	1:P:369:SER:OG	1.95	0.67
1:J:131:GLY:O	1:J:347:ARG:O	2.13	0.67
1:S:131:GLY:O	1:S:347:ARG:O	2.13	0.67
1:N:104:ARG:HD3	1:N:369:SER:OG	1.95	0.66
1:B:267:ASP:OD1	1:B:269:THR:HB	1.95	0.66
1:C:267:ASP:OD1	1:C:269:THR:HB	1.95	0.66
1:L:267:ASP:OD1	1:L:269:THR:HB	1.95	0.66
1:R:11:ILE:HD11	1:R:16:ARG:HD2	1.76	0.66
1:R:349:VAL:HG12	1:R:351:LEU:HD12	1.77	0.66
1:T:104:ARG:HD3	1:T:369:SER:OG	1.95	0.66
1:K:104:ARG:HD3	1:K:369:SER:OG	1.95	0.66
1:N:267:ASP:OD1	1:N:269:THR:HB	1.95	0.66
1:S:267:ASP:OD1	1:S:269:THR:HB	1.95	0.66
1:A:104:ARG:HD3	1:A:369:SER:OG	1.96	0.66
1:F:131:GLY:O	1:F:347:ARG:O	2.14	0.66
1:G:267:ASP:OD1	1:G:269:THR:HB	1.95	0.66
1:H:283:THR:H	1:H:288:ASN:HD21	1.44	0.66
1:J:104:ARG:HD3	1:J:369:SER:OG	1.96	0.66
1:N:131:GLY:O	1:N:347:ARG:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:283:THR:H	1:Q:288:ASN:HD21	1.44	0.66
1:C:104:ARG:HD3	1:C:369:SER:OG	1.95	0.66
1:G:283:THR:H	1:G:288:ASN:HD21	1.43	0.66
1:O:283:THR:H	1:O:288:ASN:HD21	1.44	0.66
1:Q:131:GLY:O	1:Q:347:ARG:O	2.14	0.66
1:Q:267:ASP:OD1	1:Q:269:THR:HB	1.96	0.66
1:C:283:THR:H	1:C:288:ASN:HD21	1.44	0.66
1:G:131:GLY:O	1:G:347:ARG:O	2.13	0.66
1:H:104:ARG:HD3	1:H:369:SER:OG	1.96	0.66
1:K:283:THR:H	1:K:288:ASN:HD21	1.44	0.66
1:L:104:ARG:HD3	1:L:369:SER:OG	1.96	0.66
1:D:131:GLY:O	1:D:347:ARG:O	2.14	0.66
1:F:283:THR:H	1:F:288:ASN:HD21	1.44	0.66
1:L:110:SER:HB3	1:L:160:VAL:HG12	1.78	0.66
1:N:112:THR:HG22	1:N:113:LEU:H	1.61	0.66
1:O:267:ASP:OD1	1:O:269:THR:HB	1.95	0.66
1:T:110:SER:HB3	1:T:160:VAL:HG12	1.78	0.66
1:B:131:GLY:O	1:B:347:ARG:O	2.14	0.66
1:L:349:VAL:HG12	1:L:351:LEU:HD12	1.78	0.66
1:C:131:GLY:O	1:C:347:ARG:O	2.14	0.65
1:I:131:GLY:O	1:I:347:ARG:O	2.13	0.65
1:P:267:ASP:OD1	1:P:269:THR:HB	1.95	0.65
1:P:349:VAL:HG12	1:P:351:LEU:HD12	1.78	0.65
1:I:104:ARG:HD3	1:I:369:SER:OG	1.95	0.65
1:P:283:THR:H	1:P:288:ASN:HD21	1.44	0.65
1:C:349:VAL:HG12	1:C:351:LEU:HD12	1.78	0.65
1:F:267:ASP:OD1	1:F:269:THR:HB	1.95	0.65
1:B:349:VAL:HG12	1:B:351:LEU:HD12	1.78	0.65
1:I:267:ASP:OD1	1:I:269:THR:HB	1.95	0.65
1:P:131:GLY:O	1:P:347:ARG:O	2.13	0.65
1:F:104:ARG:HD3	1:F:369:SER:OG	1.96	0.65
1:E:131:GLY:O	1:E:347:ARG:O	2.15	0.65
1:F:349:VAL:HG12	1:F:351:LEU:HD12	1.79	0.65
1:O:349:VAL:HG12	1:O:351:LEU:HD12	1.78	0.65
1:O:104:ARG:HD3	1:O:369:SER:OG	1.96	0.65
1:D:104:ARG:HD3	1:D:369:SER:OG	1.96	0.65
1:D:283:THR:H	1:D:288:ASN:HD21	1.44	0.65
1:J:349:VAL:HG12	1:J:351:LEU:HD12	1.79	0.65
1:L:131:GLY:O	1:L:347:ARG:O	2.14	0.65
1:I:283:THR:H	1:I:288:ASN:HD21	1.44	0.65
1:M:267:ASP:OD1	1:M:269:THR:HB	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:349:VAL:HG12	1:M:351:LEU:HD12	1.79	0.65
1:Q:349:VAL:HG12	1:Q:351:LEU:HD12	1.78	0.64
1:B:104:ARG:HD3	1:B:369:SER:OG	1.95	0.64
1:E:267:ASP:OD1	1:E:269:THR:HB	1.97	0.64
1:E:349:VAL:HG12	1:E:351:LEU:HD12	1.79	0.64
1:D:349:VAL:HG12	1:D:351:LEU:HD12	1.79	0.64
1:E:11:ILE:HD11	1:E:16:ARG:HD2	1.78	0.64
1:H:131:GLY:O	1:H:347:ARG:O	2.14	0.64
1:J:283:THR:H	1:J:288:ASN:HD21	1.44	0.64
1:L:283:THR:H	1:L:288:ASN:HD21	1.44	0.64
1:S:283:THR:H	1:S:288:ASN:HD21	1.46	0.64
1:E:16:ARG:HG2	1:E:23:THR:HG21	1.77	0.64
1:H:349:VAL:HG12	1:H:351:LEU:HD12	1.78	0.64
1:K:131:GLY:O	1:K:347:ARG:O	2.14	0.64
1:M:283:THR:H	1:M:288:ASN:HD21	1.46	0.64
1:R:316:LYS:HB2	1:R:325:MET:HE3	1.80	0.64
1:A:131:GLY:O	1:A:347:ARG:O	2.15	0.64
1:B:283:THR:H	1:B:288:ASN:HD21	1.44	0.64
1:E:104:ARG:HD3	1:E:369:SER:OG	1.98	0.64
1:T:349:VAL:HG12	1:T:351:LEU:HD12	1.79	0.64
1:O:131:GLY:O	1:O:347:ARG:O	2.14	0.64
1:T:283:THR:H	1:T:288:ASN:HD21	1.44	0.64
1:G:349:VAL:HG12	1:G:351:LEU:HD12	1.78	0.64
1:I:349:VAL:HG12	1:I:351:LEU:HD12	1.78	0.64
1:N:349:VAL:HG12	1:N:351:LEU:HD12	1.78	0.64
1:K:349:VAL:HG12	1:K:351:LEU:HD12	1.79	0.64
1:M:179:ARG:HD3	1:M:197:CYS:HB3	1.78	0.64
1:I:383:LEU:HD22	1:N:383:LEU:HD22	1.79	0.64
1:N:283:THR:H	1:N:288:ASN:HD21	1.44	0.63
1:A:349:VAL:HG12	1:A:351:LEU:HD12	1.79	0.63
1:A:283:THR:H	1:A:288:ASN:HD21	1.44	0.63
1:E:179:ARG:HD3	1:E:197:CYS:HB3	1.79	0.63
1:R:276:VAL:HG11	1:R:292:PHE:CD2	2.33	0.63
1:S:349:VAL:HG12	1:S:351:LEU:HD12	1.79	0.63
1:S:104:ARG:HD3	1:S:369:SER:OG	1.99	0.63
1:R:179:ARG:HD3	1:R:197:CYS:HB3	1.81	0.62
1:P:150:ASN:HD21	1:Q:385:THR:N	1.94	0.62
1:I:121:ASN:HB3	1:I:357:VAL:HA	1.80	0.62
1:G:179:ARG:HD3	1:G:197:CYS:HB3	1.82	0.62
1:N:179:ARG:HD3	1:N:197:CYS:HB3	1.82	0.62
1:S:121:ASN:O	1:S:160:VAL:HB	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:179:ARG:HD3	1:I:197:CYS:HB3	1.82	0.61
1:O:179:ARG:HD3	1:O:197:CYS:HB3	1.82	0.61
1:R:131:GLY:O	1:R:347:ARG:O	2.18	0.61
1:E:283:THR:H	1:E:288:ASN:HD21	1.45	0.61
1:E:314:THR:HG22	1:E:325:MET:HE1	1.82	0.61
1:K:383:LEU:HD22	1:P:383:LEU:HD22	1.82	0.61
1:Q:179:ARG:HD3	1:Q:197:CYS:HB3	1.82	0.61
1:C:179:ARG:HD3	1:C:197:CYS:HB3	1.82	0.61
1:J:383:LEU:HD22	1:O:383:LEU:HD22	1.82	0.61
1:F:179:ARG:HD3	1:F:197:CYS:HB3	1.83	0.61
1:M:131:GLY:O	1:M:347:ARG:O	2.18	0.61
1:E:112:THR:CG2	1:P:161:GLY:H	2.14	0.60
1:T:179:ARG:HD3	1:T:197:CYS:HB3	1.83	0.60
1:J:179:ARG:HD3	1:J:197:CYS:HB3	1.83	0.60
1:H:179:ARG:HD3	1:H:197:CYS:HB3	1.82	0.60
1:L:179:ARG:HD3	1:L:197:CYS:HB3	1.83	0.60
1:B:179:ARG:HD3	1:B:197:CYS:HB3	1.82	0.60
1:D:179:ARG:HD3	1:D:197:CYS:HB3	1.83	0.60
1:P:179:ARG:HD3	1:P:197:CYS:HB3	1.82	0.60
1:A:179:ARG:HD3	1:A:197:CYS:HB3	1.83	0.60
1:T:306:THR:HG22	3:T:705:HOH:O	2.01	0.59
1:S:179:ARG:HD3	1:S:197:CYS:HB3	1.83	0.59
1:C:110:SER:HB3	1:C:160:VAL:HG12	1.84	0.59
1:K:179:ARG:HD3	1:K:197:CYS:HB3	1.83	0.59
1:K:110:SER:HB3	1:K:160:VAL:HG12	1.85	0.59
1:R:283:THR:H	1:R:288:ASN:HD21	1.50	0.58
1:N:88:THR:CG2	1:N:90:GLN:O	2.51	0.58
1:O:88:THR:CG2	1:O:90:GLN:O	2.52	0.58
1:T:110:SER:HB3	1:T:160:VAL:CG1	2.34	0.58
1:I:88:THR:CG2	1:I:90:GLN:O	2.52	0.58
1:C:88:THR:CG2	1:C:90:GLN:O	2.52	0.58
1:D:88:THR:CG2	1:D:90:GLN:O	2.51	0.58
1:J:88:THR:CG2	1:J:90:GLN:O	2.52	0.58
1:T:88:THR:CG2	1:T:90:GLN:O	2.52	0.58
1:A:121:ASN:O	1:A:160:VAL:HB	2.04	0.58
1:A:255:LEU:HD23	1:A:316:LYS:HG3	1.86	0.58
1:I:255:LEU:HD23	1:I:316:LYS:HG3	1.86	0.58
1:N:255:LEU:HD23	1:N:316:LYS:HG3	1.86	0.58
1:G:121:ASN:HB3	1:R:112:THR:HA	1.85	0.58
1:K:255:LEU:HD23	1:K:316:LYS:HG3	1.86	0.57
1:K:88:THR:CG2	1:K:90:GLN:O	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:255:LEU:HD23	1:L:316:LYS:HG3	1.85	0.57
1:B:255:LEU:HD23	1:B:316:LYS:HG3	1.86	0.57
1:P:255:LEU:HD23	1:P:316:LYS:HG3	1.87	0.57
1:F:255:LEU:HD23	1:F:316:LYS:HG3	1.87	0.57
1:C:255:LEU:HD23	1:C:316:LYS:HG3	1.86	0.57
1:M:15:ILE:HG13	1:M:397:TYR:HD2	1.70	0.57
1:T:15:ILE:HG13	1:T:397:TYR:HD2	1.70	0.57
1:B:15:ILE:HG13	1:B:397:TYR:HD2	1.70	0.57
1:D:255:LEU:HD23	1:D:316:LYS:HG3	1.86	0.57
1:S:15:ILE:HG13	1:S:397:TYR:HD2	1.70	0.57
1:E:383:LEU:HD22	1:Q:383:LEU:HD22	1.87	0.57
1:G:255:LEU:HD23	1:G:316:LYS:HG3	1.86	0.57
1:H:255:LEU:HD23	1:H:316:LYS:HG3	1.86	0.57
1:G:385:THR:N	1:N:150:ASN:HD21	2.00	0.57
1:F:88:THR:CG2	1:F:90:GLN:O	2.52	0.57
1:O:255:LEU:HD23	1:O:316:LYS:HG3	1.87	0.57
1:J:15:ILE:HG13	1:J:397:TYR:HD2	1.70	0.56
1:Q:15:ILE:HG13	1:Q:397:TYR:HD2	1.70	0.56
1:R:15:ILE:HG13	1:R:397:TYR:HD2	1.70	0.56
1:L:15:ILE:HG13	1:L:397:TYR:HD2	1.70	0.56
1:G:88:THR:CG2	1:G:90:GLN:O	2.52	0.56
1:M:316:LYS:HE2	1:M:319:GLY:H	1.70	0.56
1:P:15:ILE:HG13	1:P:397:TYR:HD2	1.70	0.56
1:Q:114:PRO:HD3	1:Q:361:SER:HB3	1.88	0.56
1:Q:88:THR:CG2	1:Q:90:GLN:O	2.52	0.56
1:E:15:ILE:HG13	1:E:397:TYR:HD2	1.70	0.56
1:P:88:THR:CG2	1:P:90:GLN:O	2.51	0.56
1:R:319:GLY:C	1:R:320:GLN:HG2	2.26	0.56
1:R:88:THR:CG2	1:R:90:GLN:O	2.52	0.56
1:F:15:ILE:HG13	1:F:397:TYR:HD2	1.70	0.56
1:H:15:ILE:HG13	1:H:397:TYR:HD2	1.70	0.56
1:K:15:ILE:HG13	1:K:397:TYR:HD2	1.70	0.56
1:F:383:LEU:HD22	1:S:383:LEU:HD22	1.88	0.56
1:E:112:THR:CG2	1:P:159:LEU:HB3	2.36	0.56
1:G:15:ILE:HG13	1:G:397:TYR:HD2	1.70	0.56
1:H:88:THR:CG2	1:H:90:GLN:O	2.53	0.56
1:C:121:ASN:O	1:C:160:VAL:HB	2.05	0.56
1:Q:255:LEU:HD23	1:Q:316:LYS:HG3	1.86	0.56
1:L:88:THR:CG2	1:L:90:GLN:O	2.52	0.56
1:P:11:ILE:CD1	1:P:16:ARG:HD2	2.36	0.56
1:I:15:ILE:HG13	1:I:397:TYR:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:15:ILE:HG13	1:N:397:TYR:HD2	1.70	0.55
1:R:347:ARG:HB3	1:R:348:PRO:CD	2.36	0.55
1:S:316:LYS:HB2	1:S:325:MET:CE	2.35	0.55
1:A:88:THR:CG2	1:A:90:GLN:O	2.52	0.55
1:B:88:THR:CG2	1:B:90:GLN:O	2.52	0.55
1:G:11:ILE:CD1	1:G:16:ARG:HD2	2.36	0.55
1:J:255:LEU:HD23	1:J:316:LYS:HG3	1.86	0.55
1:K:11:ILE:CD1	1:K:16:ARG:HD2	2.36	0.55
1:O:11:ILE:CD1	1:O:16:ARG:HD2	2.36	0.55
1:D:11:ILE:CD1	1:D:16:ARG:HD2	2.36	0.55
1:H:11:ILE:CD1	1:H:16:ARG:HD2	2.36	0.55
1:J:11:ILE:CD1	1:J:16:ARG:HD2	2.37	0.55
1:A:15:ILE:HG13	1:A:397:TYR:HD2	1.70	0.55
1:C:15:ILE:HG13	1:C:397:TYR:HD2	1.70	0.55
1:R:283:THR:H	1:R:288:ASN:ND2	2.05	0.55
1:D:15:ILE:HG13	1:D:397:TYR:HD2	1.70	0.55
1:I:11:ILE:CD1	1:I:16:ARG:HD2	2.36	0.55
1:L:11:ILE:CD1	1:L:16:ARG:HD2	2.36	0.55
1:S:347:ARG:HB3	1:S:348:PRO:CD	2.35	0.55
1:S:88:THR:CG2	1:S:90:GLN:O	2.54	0.55
1:I:112:THR:HG22	1:I:113:LEU:H	1.71	0.55
1:H:347:ARG:HB3	1:H:348:PRO:CD	2.37	0.55
1:N:11:ILE:CD1	1:N:16:ARG:HD2	2.37	0.55
1:R:276:VAL:HG11	1:R:292:PHE:CE2	2.41	0.55
1:A:11:ILE:CD1	1:A:16:ARG:HD2	2.36	0.55
1:M:11:ILE:CD1	1:M:16:ARG:HD2	2.36	0.55
1:Q:11:ILE:CD1	1:Q:16:ARG:HD2	2.37	0.55
1:Q:347:ARG:HB3	1:Q:348:PRO:CD	2.37	0.55
1:J:347:ARG:HB3	1:J:348:PRO:CD	2.37	0.55
1:N:347:ARG:HB3	1:N:348:PRO:CD	2.37	0.55
1:R:314:THR:HG22	1:R:325:MET:HE2	1.88	0.55
1:M:88:THR:CG2	1:M:90:GLN:O	2.55	0.55
1:P:402:LEU:HD12	1:Q:33:LEU:HD13	1.90	0.54
1:E:88:THR:CG2	1:E:90:GLN:O	2.52	0.54
1:F:11:ILE:CD1	1:F:16:ARG:HD2	2.37	0.54
1:P:114:PRO:HG3	1:P:359:THR:O	2.08	0.54
1:S:11:ILE:CD1	1:S:16:ARG:HD2	2.37	0.54
1:H:426:PHE:CG	1:H:427:MET:N	2.76	0.54
1:O:15:ILE:HG13	1:O:397:TYR:HD2	1.70	0.54
1:R:349:VAL:HG12	1:R:351:LEU:CD1	2.37	0.54
1:C:11:ILE:CD1	1:C:16:ARG:HD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:347:ARG:HB3	1:M:348:PRO:CD	2.37	0.54
1:R:426:PHE:CG	1:R:427:MET:N	2.76	0.54
1:B:11:ILE:CD1	1:B:16:ARG:HD2	2.37	0.54
1:I:426:PHE:CG	1:I:427:MET:N	2.76	0.54
1:J:426:PHE:CG	1:J:427:MET:N	2.76	0.54
1:N:426:PHE:CG	1:N:427:MET:N	2.76	0.54
1:O:426:PHE:CG	1:O:427:MET:N	2.76	0.54
1:C:347:ARG:HB3	1:C:348:PRO:CD	2.37	0.54
1:D:426:PHE:CG	1:D:427:MET:N	2.76	0.54
1:B:426:PHE:CG	1:B:427:MET:N	2.76	0.53
1:I:347:ARG:HB3	1:I:348:PRO:CD	2.38	0.53
1:D:347:ARG:HB3	1:D:348:PRO:CD	2.38	0.53
1:K:347:ARG:HB3	1:K:348:PRO:CD	2.38	0.53
1:Q:426:PHE:CG	1:Q:427:MET:N	2.76	0.53
1:T:426:PHE:CG	1:T:427:MET:N	2.76	0.53
1:E:171:THR:HG21	1:E:348:PRO:HG3	1.89	0.53
1:N:121:ASN:O	1:N:160:VAL:HB	2.08	0.53
1:T:11:ILE:CD1	1:T:16:ARG:HD2	2.36	0.53
1:A:426:PHE:CG	1:A:427:MET:N	2.76	0.53
1:I:349:VAL:HG12	1:I:351:LEU:CD1	2.39	0.53
1:G:426:PHE:CG	1:G:427:MET:N	2.76	0.53
1:M:15:ILE:HD11	1:M:398:THR:HA	1.90	0.53
1:S:349:VAL:HG12	1:S:351:LEU:CD1	2.38	0.53
1:A:402:LEU:HD12	1:E:33:LEU:HD13	1.88	0.53
1:G:349:VAL:HG12	1:G:351:LEU:CD1	2.39	0.53
1:L:426:PHE:CG	1:L:427:MET:N	2.76	0.53
1:M:426:PHE:CG	1:M:427:MET:N	2.76	0.53
1:R:11:ILE:CD1	1:R:16:ARG:HD2	2.37	0.53
1:S:426:PHE:CG	1:S:427:MET:N	2.77	0.53
1:D:349:VAL:HG12	1:D:351:LEU:CD1	2.39	0.53
1:F:426:PHE:CG	1:F:427:MET:N	2.76	0.53
1:G:347:ARG:HB3	1:G:348:PRO:CD	2.37	0.53
1:L:347:ARG:HB3	1:L:348:PRO:CD	2.38	0.53
1:L:349:VAL:HG12	1:L:351:LEU:CD1	2.39	0.53
1:M:171:THR:HG21	1:M:348:PRO:HG3	1.89	0.53
1:P:347:ARG:HB3	1:P:348:PRO:CD	2.37	0.53
1:E:11:ILE:CD1	1:E:16:ARG:HD2	2.39	0.53
1:E:179:ARG:CD	1:E:197:CYS:SG	2.97	0.53
1:K:396:ASN:H	1:K:396:ASN:HD22	1.57	0.53
1:L:396:ASN:H	1:L:396:ASN:HD22	1.57	0.53
1:O:171:THR:HG21	1:O:348:PRO:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:THR:HG21	1:F:348:PRO:HG3	1.91	0.53
1:K:349:VAL:HG12	1:K:351:LEU:CD1	2.39	0.53
1:K:426:PHE:CG	1:K:427:MET:N	2.77	0.53
1:M:396:ASN:HD22	1:M:396:ASN:H	1.57	0.53
1:R:110:SER:CB	1:R:160:VAL:HG12	2.29	0.53
1:S:179:ARG:CD	1:S:197:CYS:SG	2.96	0.53
1:E:396:ASN:H	1:E:396:ASN:HD22	1.57	0.53
1:N:349:VAL:HG12	1:N:351:LEU:CD1	2.39	0.53
1:T:347:ARG:HB3	1:T:348:PRO:CD	2.38	0.53
1:A:349:VAL:HG12	1:A:351:LEU:CD1	2.39	0.52
1:D:171:THR:HG21	1:D:348:PRO:HG3	1.91	0.52
1:D:396:ASN:HD22	1:D:396:ASN:H	1.57	0.52
1:L:171:THR:HG21	1:L:348:PRO:HG3	1.91	0.52
1:O:402:LEU:HD12	1:P:33:LEU:HD13	1.91	0.52
1:B:349:VAL:HG12	1:B:351:LEU:CD1	2.39	0.52
1:C:396:ASN:HD22	1:C:396:ASN:H	1.58	0.52
1:C:426:PHE:CG	1:C:427:MET:N	2.76	0.52
1:G:171:THR:HG21	1:G:348:PRO:HG3	1.91	0.52
1:H:349:VAL:HG12	1:H:351:LEU:CD1	2.39	0.52
1:I:396:ASN:HD22	1:I:396:ASN:H	1.57	0.52
1:P:396:ASN:H	1:P:396:ASN:HD22	1.58	0.52
1:A:347:ARG:HB3	1:A:348:PRO:CD	2.38	0.52
1:I:171:THR:HG21	1:I:348:PRO:HG3	1.91	0.52
1:J:396:ASN:HD22	1:J:396:ASN:H	1.58	0.52
1:C:171:THR:HG21	1:C:348:PRO:HG3	1.91	0.52
1:E:15:ILE:HD11	1:E:398:THR:HA	1.91	0.52
1:P:426:PHE:CG	1:P:427:MET:N	2.76	0.52
1:C:349:VAL:HG12	1:C:351:LEU:CD1	2.39	0.52
1:H:171:THR:HG21	1:H:348:PRO:HG3	1.92	0.52
1:F:347:ARG:HB3	1:F:348:PRO:CD	2.38	0.52
1:F:349:VAL:HG12	1:F:351:LEU:CD1	2.39	0.52
1:H:396:ASN:HD22	1:H:396:ASN:H	1.57	0.52
1:F:119:ALA:HB3	1:P:113:LEU:HD11	1.92	0.52
1:R:171:THR:HG21	1:R:348:PRO:HG3	1.90	0.52
1:G:396:ASN:H	1:G:396:ASN:HD22	1.57	0.52
1:T:349:VAL:HG12	1:T:351:LEU:CD1	2.39	0.52
1:T:396:ASN:H	1:T:396:ASN:HD22	1.57	0.52
1:A:171:THR:HG21	1:A:348:PRO:HG3	1.91	0.52
1:A:396:ASN:H	1:A:396:ASN:HD22	1.58	0.52
1:B:171:THR:HG21	1:B:348:PRO:HG3	1.91	0.52
1:C:402:LEU:HD12	1:J:33:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:349:VAL:HG12	1:M:351:LEU:CD1	2.40	0.52
1:T:171:THR:HG21	1:T:348:PRO:HG3	1.92	0.52
1:J:349:VAL:HG12	1:J:351:LEU:CD1	2.39	0.52
1:K:171:THR:HG21	1:K:348:PRO:HG3	1.91	0.52
1:P:349:VAL:HG12	1:P:351:LEU:CD1	2.39	0.52
1:R:396:ASN:H	1:R:396:ASN:HD22	1.58	0.52
1:S:171:THR:HG21	1:S:348:PRO:HG3	1.92	0.52
1:S:15:ILE:HD11	1:S:398:THR:HA	1.92	0.52
1:T:179:ARG:CD	1:T:197:CYS:SG	2.98	0.52
1:A:150:ASN:HD21	1:E:385:THR:N	2.03	0.51
1:F:396:ASN:HD22	1:F:396:ASN:H	1.57	0.51
1:N:112:THR:HG22	1:N:113:LEU:N	2.24	0.51
1:P:171:THR:HG21	1:P:348:PRO:HG3	1.91	0.51
1:B:347:ARG:HB3	1:B:348:PRO:CD	2.38	0.51
1:E:426:PHE:CG	1:E:427:MET:N	2.78	0.51
1:O:349:VAL:HG12	1:O:351:LEU:CD1	2.39	0.51
1:O:396:ASN:HD22	1:O:396:ASN:H	1.57	0.51
1:E:349:VAL:HG12	1:E:351:LEU:CD1	2.41	0.51
1:P:15:ILE:HD11	1:P:398:THR:HA	1.93	0.51
1:Q:349:VAL:HG12	1:Q:351:LEU:CD1	2.39	0.51
1:Q:396:ASN:H	1:Q:396:ASN:HD22	1.57	0.51
1:M:287:ASP:HB2	1:R:278:ALA:HB3	1.92	0.51
1:F:121:ASN:HD22	1:F:357:VAL:HA	1.76	0.51
1:J:171:THR:HG21	1:J:348:PRO:HG3	1.91	0.51
1:M:124:ILE:HG13	1:M:160:VAL:HG22	1.92	0.51
1:M:179:ARG:CD	1:M:197:CYS:SG	2.99	0.51
1:N:171:THR:HG21	1:N:348:PRO:HG3	1.91	0.51
1:T:255:LEU:HD23	1:T:316:LYS:HG3	1.93	0.51
1:R:179:ARG:CD	1:R:197:CYS:SG	2.99	0.51
1:D:15:ILE:HD11	1:D:398:THR:HA	1.93	0.51
1:G:33:LEU:HD13	1:N:402:LEU:HD12	1.93	0.51
1:G:402:LEU:HD12	1:H:33:LEU:HD13	1.92	0.51
1:N:15:ILE:HD11	1:N:398:THR:HA	1.93	0.51
1:O:385:THR:N	1:Q:150:ASN:HD21	2.04	0.51
1:I:438:ILE:HG23	1:R:440:GLY:C	2.31	0.51
1:S:179:ARG:HD2	1:S:197:CYS:SG	2.51	0.51
1:E:171:THR:O	1:E:172:SER:HB3	2.11	0.51
1:N:179:ARG:CD	1:N:197:CYS:SG	2.99	0.51
1:O:179:ARG:CD	1:O:197:CYS:SG	2.99	0.51
1:T:15:ILE:HD11	1:T:398:THR:HA	1.93	0.51
1:B:396:ASN:H	1:B:396:ASN:HD22	1.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:ILE:HD11	1:F:398:THR:HA	1.93	0.50
1:Q:179:ARG:CD	1:Q:197:CYS:SG	2.99	0.50
1:Q:15:ILE:HD11	1:Q:398:THR:HA	1.93	0.50
1:H:15:ILE:HD11	1:H:398:THR:HA	1.93	0.50
1:Q:171:THR:HG21	1:Q:348:PRO:HG3	1.91	0.50
1:R:171:THR:O	1:R:172:SER:HB3	2.11	0.50
1:D:179:ARG:CD	1:D:197:CYS:SG	2.99	0.50
1:N:396:ASN:HD22	1:N:396:ASN:H	1.58	0.50
1:M:402:LEU:HD12	1:R:33:LEU:HD13	1.94	0.50
1:O:33:LEU:HD13	1:Q:402:LEU:HD12	1.93	0.50
1:A:15:ILE:HD11	1:A:398:THR:HA	1.93	0.50
1:J:15:ILE:HD11	1:J:398:THR:HA	1.93	0.50
1:O:15:ILE:HD11	1:O:398:THR:HA	1.93	0.50
1:R:15:ILE:HD11	1:R:398:THR:HA	1.93	0.50
1:F:114:PRO:HD3	1:F:361:SER:HB3	1.93	0.50
1:F:402:LEU:HD12	1:K:33:LEU:HD13	1.93	0.50
1:K:179:ARG:CD	1:K:197:CYS:SG	3.00	0.50
1:K:114:PRO:HD3	1:K:361:SER:HB3	1.93	0.50
1:C:150:ASN:HD21	1:J:385:THR:N	2.04	0.50
1:O:347:ARG:HB3	1:O:348:PRO:CD	2.38	0.50
1:H:397:TYR:OH	1:I:432:LEU:HD13	2.11	0.50
1:B:15:ILE:HD11	1:B:398:THR:HA	1.93	0.50
1:F:179:ARG:CD	1:F:197:CYS:SG	3.00	0.50
1:I:179:ARG:CD	1:I:197:CYS:SG	3.00	0.50
1:K:15:ILE:HD11	1:K:398:THR:HA	1.93	0.50
1:L:15:ILE:HD11	1:L:398:THR:HA	1.93	0.50
1:G:15:ILE:HD11	1:G:398:THR:HA	1.93	0.49
1:F:385:THR:N	1:I:150:ASN:HD21	2.04	0.49
1:B:179:ARG:CD	1:B:197:CYS:SG	3.01	0.49
1:K:171:THR:O	1:K:172:SER:HB3	2.12	0.49
1:L:179:ARG:CD	1:L:197:CYS:SG	3.00	0.49
1:T:110:SER:CB	1:T:160:VAL:HG12	2.41	0.49
1:C:15:ILE:HD11	1:C:398:THR:HA	1.93	0.49
1:F:150:ASN:HD21	1:K:385:THR:N	2.02	0.49
1:I:15:ILE:HD11	1:I:398:THR:HA	1.93	0.49
1:C:179:ARG:CD	1:C:197:CYS:SG	3.01	0.49
1:A:179:ARG:CD	1:A:197:CYS:SG	3.00	0.49
1:O:121:ASN:O	1:O:160:VAL:HB	2.12	0.49
1:R:204:ARG:HB3	1:R:337:ILE:HD11	1.89	0.49
1:F:171:THR:O	1:F:172:SER:HB3	2.13	0.49
1:J:179:ARG:CD	1:J:197:CYS:SG	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:179:ARG:CD	1:P:197:CYS:SG	3.01	0.49
1:H:171:THR:O	1:H:172:SER:HB3	2.13	0.49
1:I:256:VAL:HG13	1:I:280:ASN:H	1.78	0.49
1:J:171:THR:O	1:J:172:SER:HB3	2.13	0.49
1:N:171:THR:O	1:N:172:SER:HB3	2.13	0.49
1:A:171:THR:O	1:A:172:SER:HB3	2.13	0.49
1:E:347:ARG:HB3	1:E:348:PRO:CD	2.39	0.49
1:I:171:THR:O	1:I:172:SER:HB3	2.13	0.49
1:J:256:VAL:HG13	1:J:280:ASN:H	1.78	0.49
1:R:80:TYR:O	1:R:267:ASP:HB2	2.12	0.49
1:E:316:LYS:O	1:E:317:SER:HB3	2.12	0.48
1:E:204:ARG:HB3	1:E:337:ILE:CD1	2.43	0.48
1:G:383:LEU:HD22	1:L:383:LEU:HD22	1.94	0.48
1:H:179:ARG:CD	1:H:197:CYS:SG	3.01	0.48
1:Q:171:THR:O	1:Q:172:SER:HB3	2.13	0.48
1:Q:179:ARG:HD2	1:Q:197:CYS:SG	2.53	0.48
1:G:179:ARG:CD	1:G:197:CYS:SG	3.01	0.48
1:D:179:ARG:HD2	1:D:197:CYS:SG	2.53	0.48
1:Q:120:LEU:HD21	1:Q:161:GLY:H	1.78	0.48
1:T:124:ILE:HG13	1:T:160:VAL:HG22	1.95	0.48
1:G:171:THR:O	1:G:172:SER:HB3	2.13	0.48
1:H:114:PRO:HD3	1:H:361:SER:HB3	1.94	0.48
1:O:110:SER:HB3	1:O:160:VAL:HG12	1.95	0.48
1:D:171:THR:O	1:D:172:SER:HB3	2.13	0.48
1:G:256:VAL:HG13	1:G:280:ASN:H	1.78	0.48
1:K:256:VAL:HG13	1:K:280:ASN:H	1.79	0.48
1:L:171:THR:O	1:L:172:SER:HB3	2.13	0.48
1:N:179:ARG:HD2	1:N:197:CYS:SG	2.53	0.48
1:Q:124:ILE:HG13	1:Q:160:VAL:HG22	1.95	0.48
1:B:256:VAL:HG13	1:B:280:ASN:H	1.79	0.48
1:D:256:VAL:HG13	1:D:280:ASN:H	1.78	0.48
1:G:150:ASN:HD21	1:H:385:THR:N	2.04	0.48
1:T:179:ARG:HD2	1:T:197:CYS:SG	2.53	0.48
1:C:171:THR:O	1:C:172:SER:HB3	2.13	0.48
1:O:179:ARG:HD2	1:O:197:CYS:SG	2.54	0.48
1:A:256:VAL:HG13	1:A:280:ASN:H	1.78	0.48
1:L:110:SER:HB3	1:L:160:VAL:CG1	2.42	0.48
1:O:121:ASN:HB3	1:O:357:VAL:HG13	1.96	0.48
1:P:171:THR:O	1:P:172:SER:HB3	2.13	0.48
1:T:121:ASN:O	1:T:160:VAL:HB	2.14	0.48
1:B:171:THR:O	1:B:172:SER:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:179:ARG:HD2	1:K:197:CYS:SG	2.54	0.48
1:P:256:VAL:HG13	1:P:280:ASN:H	1.79	0.48
1:A:110:SER:HB3	1:A:160:VAL:HG12	1.95	0.48
1:M:204:ARG:HB3	1:M:337:ILE:CD1	2.44	0.48
1:T:256:VAL:HG13	1:T:280:ASN:H	1.78	0.48
1:C:256:VAL:HG13	1:C:280:ASN:H	1.78	0.47
1:H:402:LEU:HD12	1:N:33:LEU:HD13	1.96	0.47
1:F:33:LEU:HD13	1:I:402:LEU:HD12	1.96	0.47
1:O:171:THR:O	1:O:172:SER:HB3	2.13	0.47
1:L:396:ASN:HD22	1:L:396:ASN:N	2.12	0.47
1:O:396:ASN:HD22	1:O:396:ASN:N	2.13	0.47
1:S:171:THR:O	1:S:172:SER:HB3	2.13	0.47
1:L:124:ILE:HG13	1:L:160:VAL:HG22	1.96	0.47
1:F:179:ARG:HD2	1:F:197:CYS:SG	2.54	0.47
1:H:256:VAL:HG13	1:H:280:ASN:H	1.79	0.47
1:I:179:ARG:HD2	1:I:197:CYS:SG	2.55	0.47
1:K:110:SER:HB3	1:K:160:VAL:CG1	2.44	0.47
1:M:179:ARG:HD2	1:M:197:CYS:SG	2.55	0.47
1:O:204:ARG:HB3	1:O:337:ILE:CD1	2.44	0.47
1:C:396:ASN:HD22	1:C:396:ASN:N	2.13	0.47
1:E:179:ARG:HD2	1:E:197:CYS:SG	2.54	0.47
1:E:256:VAL:HG13	1:E:280:ASN:H	1.79	0.47
1:M:8:THR:HG22	1:M:11:ILE:HG22	1.97	0.47
1:G:114:PRO:HD3	1:G:361:SER:HB3	1.96	0.47
1:L:204:ARG:HB3	1:L:337:ILE:CD1	2.45	0.47
1:P:204:ARG:HB3	1:P:337:ILE:CD1	2.45	0.47
1:A:179:ARG:HD2	1:A:197:CYS:SG	2.55	0.47
1:F:256:VAL:HG13	1:F:280:ASN:H	1.79	0.47
1:F:204:ARG:HB3	1:F:337:ILE:CD1	2.44	0.47
1:H:396:ASN:N	1:H:396:ASN:HD22	2.12	0.47
1:J:396:ASN:HD22	1:J:396:ASN:N	2.13	0.47
1:L:179:ARG:HD2	1:L:197:CYS:SG	2.54	0.47
1:S:396:ASN:HD22	1:S:396:ASN:H	1.62	0.47
1:D:396:ASN:HD22	1:D:396:ASN:N	2.12	0.47
1:J:204:ARG:HB3	1:J:337:ILE:CD1	2.44	0.47
1:K:396:ASN:N	1:K:396:ASN:HD22	2.12	0.47
1:N:396:ASN:N	1:N:396:ASN:HD22	2.13	0.47
1:Q:204:ARG:HB3	1:Q:337:ILE:CD1	2.44	0.47
1:Q:8:THR:HG22	1:Q:11:ILE:HG22	1.97	0.47
1:R:179:ARG:HD2	1:R:197:CYS:SG	2.54	0.47
1:B:204:ARG:HB3	1:B:337:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:THR:HG22	1:D:11:ILE:HG22	1.97	0.47
1:I:8:THR:HG22	1:I:11:ILE:HG22	1.97	0.47
1:M:106:LEU:HD23	1:M:367:GLY:HA3	1.97	0.47
1:K:397:TYR:OH	1:N:432:LEU:HD13	2.14	0.47
1:O:256:VAL:HG13	1:O:280:ASN:H	1.79	0.47
1:T:204:ARG:HB3	1:T:337:ILE:CD1	2.45	0.47
1:A:396:ASN:HD22	1:A:396:ASN:N	2.13	0.47
1:K:204:ARG:HB3	1:K:337:ILE:CD1	2.45	0.47
1:N:204:ARG:HB3	1:N:337:ILE:CD1	2.45	0.47
1:T:396:ASN:N	1:T:396:ASN:HD22	2.13	0.47
1:A:204:ARG:HB3	1:A:337:ILE:CD1	2.45	0.46
1:B:124:ILE:HG13	1:B:160:VAL:HG22	1.96	0.46
1:C:204:ARG:HB3	1:C:337:ILE:CD1	2.45	0.46
1:L:256:VAL:HG13	1:L:280:ASN:H	1.78	0.46
1:M:171:THR:O	1:M:172:SER:HB3	2.15	0.46
1:P:179:ARG:HD2	1:P:197:CYS:SG	2.55	0.46
1:B:179:ARG:HD2	1:B:197:CYS:SG	2.55	0.46
1:B:396:ASN:N	1:B:396:ASN:HD22	2.13	0.46
1:F:8:THR:HG22	1:F:11:ILE:HG22	1.97	0.46
1:F:396:ASN:HD22	1:F:396:ASN:N	2.12	0.46
1:G:8:THR:HG22	1:G:11:ILE:HG22	1.97	0.46
1:I:396:ASN:HD22	1:I:396:ASN:N	2.13	0.46
1:N:256:VAL:HG13	1:N:280:ASN:H	1.79	0.46
1:Q:256:VAL:HG13	1:Q:280:ASN:H	1.79	0.46
1:G:204:ARG:HB3	1:G:337:ILE:CD1	2.45	0.46
1:I:204:ARG:HB3	1:I:337:ILE:CD1	2.45	0.46
1:J:121:ASN:HD21	1:J:358:ALA:H	1.62	0.46
1:P:122:GLY:C	1:P:160:VAL:HG23	2.36	0.46
1:T:8:THR:HG22	1:T:11:ILE:HG22	1.98	0.46
1:J:179:ARG:HD2	1:J:197:CYS:SG	2.55	0.46
1:D:204:ARG:HB3	1:D:337:ILE:CD1	2.45	0.46
1:G:179:ARG:HD2	1:G:197:CYS:SG	2.56	0.46
1:G:396:ASN:N	1:G:396:ASN:HD22	2.13	0.46
1:H:8:THR:HG22	1:H:11:ILE:HG22	1.97	0.46
1:K:8:THR:HG22	1:K:11:ILE:HG22	1.97	0.46
1:T:171:THR:O	1:T:172:SER:HB3	2.14	0.46
1:N:8:THR:HG22	1:N:11:ILE:HG22	1.97	0.46
1:P:396:ASN:HD22	1:P:396:ASN:N	2.13	0.46
1:P:8:THR:HG22	1:P:11:ILE:HG22	1.98	0.46
1:Q:396:ASN:N	1:Q:396:ASN:HD22	2.13	0.46
1:A:8:THR:HG22	1:A:11:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:THR:HG22	1:C:11:ILE:HG22	1.97	0.46
1:H:204:ARG:HB3	1:H:337:ILE:CD1	2.45	0.46
1:M:396:ASN:N	1:M:396:ASN:HD22	2.13	0.46
1:N:124:ILE:HG13	1:N:160:VAL:HG22	1.98	0.46
1:C:179:ARG:HD2	1:C:197:CYS:SG	2.55	0.46
1:Q:121:ASN:HB3	1:Q:357:VAL:HG13	1.98	0.46
1:E:396:ASN:HD22	1:E:396:ASN:N	2.14	0.46
1:N:106:LEU:HD23	1:N:367:GLY:HA3	1.98	0.46
1:Q:106:LEU:HD23	1:Q:367:GLY:HA3	1.98	0.46
1:R:396:ASN:N	1:R:396:ASN:HD22	2.13	0.46
1:E:106:LEU:HD23	1:E:367:GLY:HA3	1.98	0.46
1:L:8:THR:HG22	1:L:11:ILE:HG22	1.98	0.46
1:R:77:ASN:HD21	1:R:79:ASN:HB2	1.80	0.46
1:S:256:VAL:HG13	1:S:280:ASN:H	1.81	0.46
1:I:106:LEU:HD23	1:I:367:GLY:HA3	1.98	0.45
1:O:106:LEU:HD23	1:O:367:GLY:HA3	1.98	0.45
1:H:179:ARG:HD2	1:H:197:CYS:SG	2.56	0.45
1:K:106:LEU:HD23	1:K:367:GLY:HA3	1.97	0.45
1:N:11:ILE:HB	1:N:12:VAL:H	1.64	0.45
1:G:15:ILE:HD13	1:G:15:ILE:HA	1.86	0.45
1:H:150:ASN:HD21	1:N:385:THR:N	2.07	0.45
1:C:120:LEU:HG	1:O:113:LEU:HD21	1.99	0.45
1:B:8:THR:HG22	1:B:11:ILE:HG22	1.97	0.45
1:O:11:ILE:HB	1:O:12:VAL:H	1.64	0.45
1:O:8:THR:HG22	1:O:11:ILE:HG22	1.97	0.45
1:B:77:ASN:HD21	1:B:79:ASN:HB2	1.82	0.45
1:I:15:ILE:HD13	1:I:15:ILE:HA	1.86	0.45
1:M:209:THR:HA	1:M:332:SER:HB3	1.99	0.45
1:M:256:VAL:HG13	1:M:280:ASN:H	1.80	0.45
1:R:8:THR:HG22	1:R:11:ILE:HG22	1.98	0.45
1:S:204:ARG:HB3	1:S:337:ILE:CD1	2.47	0.45
1:A:106:LEU:HD23	1:A:367:GLY:HA3	1.98	0.45
1:D:106:LEU:HD23	1:D:367:GLY:HA3	1.98	0.45
1:O:77:ASN:HD21	1:O:79:ASN:HB2	1.82	0.45
1:R:255:LEU:HD22	1:R:325:MET:HE2	1.99	0.45
1:S:15:ILE:HG13	1:S:397:TYR:CD2	2.51	0.45
1:F:124:ILE:HG13	1:F:160:VAL:HG22	1.99	0.45
1:F:77:ASN:HD21	1:F:79:ASN:HB2	1.82	0.45
1:J:8:THR:HG22	1:J:11:ILE:HG22	1.97	0.45
1:M:77:ASN:HD21	1:M:79:ASN:HB2	1.82	0.45
1:P:77:ASN:HD21	1:P:79:ASN:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:106:LEU:HD23	1:T:367:GLY:HA3	1.99	0.45
1:N:77:ASN:HD21	1:N:79:ASN:HB2	1.82	0.45
1:Q:77:ASN:HD21	1:Q:79:ASN:HB2	1.82	0.45
1:R:119:ALA:HB1	1:R:161:GLY:HA3	1.99	0.45
1:S:106:LEU:HD23	1:S:367:GLY:HA3	1.99	0.45
1:S:8:THR:HG22	1:S:11:ILE:HG22	1.99	0.45
1:D:15:ILE:HG13	1:D:397:TYR:CD2	2.52	0.44
1:E:204:ARG:HB3	1:E:337:ILE:HD11	1.99	0.44
1:F:106:LEU:HD23	1:F:367:GLY:HA3	1.99	0.44
1:G:106:LEU:HD23	1:G:367:GLY:HA3	1.99	0.44
1:L:106:LEU:HD23	1:L:367:GLY:HA3	1.98	0.44
1:M:127:VAL:HG22	1:M:144:LEU:HB3	1.99	0.44
1:G:120:LEU:HD23	1:R:113:LEU:HD12	1.98	0.44
1:I:127:VAL:HG22	1:I:144:LEU:HB3	1.99	0.44
1:B:106:LEU:HD23	1:B:367:GLY:HA3	1.98	0.44
1:C:438:ILE:HG23	1:G:440:GLY:C	2.37	0.44
1:I:77:ASN:HD21	1:I:79:ASN:HB2	1.82	0.44
1:C:110:SER:HB3	1:C:160:VAL:CG1	2.46	0.44
1:C:121:ASN:HD21	1:C:358:ALA:HB3	1.82	0.44
1:C:209:THR:HA	1:C:332:SER:HB3	2.00	0.44
1:I:201:ASP:OD1	1:I:201:ASP:N	2.49	0.44
1:P:15:ILE:HA	1:P:15:ILE:HD13	1.86	0.44
1:P:106:LEU:HD23	1:P:367:GLY:HA3	1.99	0.44
1:T:113:LEU:HD22	1:T:120:LEU:HD22	2.00	0.44
1:B:127:VAL:HG22	1:B:144:LEU:HB3	2.00	0.44
1:B:209:THR:HA	1:B:332:SER:HB3	2.00	0.44
1:C:15:ILE:HG13	1:C:397:TYR:CD2	2.52	0.44
1:E:127:VAL:HG22	1:E:144:LEU:HB3	2.00	0.44
1:E:15:ILE:HG13	1:E:397:TYR:CD2	2.51	0.44
1:K:77:ASN:HD21	1:K:79:ASN:HB2	1.82	0.44
1:Q:204:ARG:HB3	1:Q:337:ILE:HD11	1.99	0.44
1:J:124:ILE:HG13	1:J:160:VAL:HG22	2.00	0.44
1:J:201:ASP:OD1	1:J:201:ASP:N	2.49	0.44
1:J:77:ASN:HD21	1:J:79:ASN:HB2	1.82	0.44
1:P:127:VAL:HG22	1:P:144:LEU:HB3	2.00	0.44
1:A:209:THR:HA	1:A:332:SER:HB3	1.99	0.44
1:A:77:ASN:HD21	1:A:79:ASN:HB2	1.82	0.44
1:F:11:ILE:HB	1:F:12:VAL:H	1.65	0.44
1:H:127:VAL:HG22	1:H:144:LEU:HB3	2.00	0.44
1:H:15:ILE:HG13	1:H:397:TYR:CD2	2.52	0.44
1:K:127:VAL:HG22	1:K:144:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:127:VAL:HG22	1:L:144:LEU:HB3	2.00	0.44
1:M:112:THR:HG22	1:M:113:LEU:N	2.33	0.44
1:R:261:ILE:HD12	1:R:276:VAL:HG21	1.99	0.44
1:A:320:GLN:N	1:A:323:ASP:OD2	2.51	0.44
1:J:106:LEU:HD23	1:J:367:GLY:HA3	1.99	0.44
1:K:320:GLN:N	1:K:323:ASP:OD2	2.51	0.44
1:O:127:VAL:HG22	1:O:144:LEU:HB3	2.00	0.44
1:Q:320:GLN:N	1:Q:323:ASP:OD2	2.51	0.44
1:T:204:ARG:HB3	1:T:337:ILE:HD11	2.00	0.44
1:B:320:GLN:N	1:B:323:ASP:OD2	2.51	0.44
1:C:112:THR:HA	1:L:120:LEU:O	2.18	0.44
1:C:204:ARG:HB3	1:C:337:ILE:HD11	2.00	0.44
1:I:15:ILE:HG13	1:I:397:TYR:CD2	2.52	0.44
1:I:385:THR:N	1:K:150:ASN:HD21	2.09	0.44
1:L:77:ASN:HD21	1:L:79:ASN:HB2	1.82	0.44
1:O:209:THR:HA	1:O:332:SER:HB3	2.00	0.44
1:T:15:ILE:HG13	1:T:397:TYR:CD2	2.52	0.44
1:A:204:ARG:HB3	1:A:337:ILE:HD11	2.00	0.43
1:D:209:THR:HA	1:D:332:SER:HB3	2.00	0.43
1:G:77:ASN:HD21	1:G:79:ASN:HB2	1.82	0.43
1:H:106:LEU:HD23	1:H:367:GLY:HA3	1.99	0.43
1:M:204:ARG:HB3	1:M:337:ILE:HD11	2.00	0.43
1:Q:11:ILE:HB	1:Q:12:VAL:H	1.64	0.43
1:Q:209:THR:HA	1:Q:332:SER:HB3	2.00	0.43
1:E:8:THR:HG22	1:E:11:ILE:HG22	1.98	0.43
1:H:209:THR:HA	1:H:332:SER:HB3	2.01	0.43
1:L:320:GLN:N	1:L:323:ASP:OD2	2.51	0.43
1:P:112:THR:O	1:P:361:SER:HB2	2.17	0.43
1:T:209:THR:HA	1:T:332:SER:HB3	2.00	0.43
1:B:201:ASP:OD1	1:B:201:ASP:N	2.50	0.43
1:B:15:ILE:HG13	1:B:397:TYR:CD2	2.52	0.43
1:D:320:GLN:N	1:D:323:ASP:OD2	2.50	0.43
1:F:15:ILE:HD13	1:F:15:ILE:HA	1.86	0.43
1:K:204:ARG:HB3	1:K:337:ILE:HD11	2.00	0.43
1:I:33:LEU:HD13	1:K:402:LEU:HD12	1.99	0.43
1:M:201:ASP:O	1:M:202:ARG:HB2	2.18	0.43
1:Q:15:ILE:HG13	1:Q:397:TYR:CD2	2.52	0.43
1:S:114:PRO:HD3	1:S:361:SER:HB3	2.00	0.43
1:C:320:GLN:N	1:C:323:ASP:OD2	2.51	0.43
1:E:171:THR:O	1:E:172:SER:CB	2.66	0.43
1:G:201:ASP:O	1:G:202:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:171:THR:O	1:J:172:SER:CB	2.66	0.43
1:K:15:ILE:HG13	1:K:397:TYR:CD2	2.51	0.43
1:S:201:ASP:O	1:S:202:ARG:HB2	2.18	0.43
1:A:114:PRO:HD3	1:A:361:SER:HB3	2.01	0.43
1:D:77:ASN:HD21	1:D:79:ASN:HB2	1.82	0.43
1:F:204:ARG:HB3	1:F:337:ILE:HD11	2.00	0.43
1:F:320:GLN:N	1:F:323:ASP:OD2	2.52	0.43
1:G:201:ASP:OD1	1:G:201:ASP:N	2.49	0.43
1:H:320:GLN:N	1:H:323:ASP:OD2	2.51	0.43
1:I:320:GLN:N	1:I:323:ASP:OD2	2.52	0.43
1:N:204:ARG:HB3	1:N:337:ILE:HD11	2.00	0.43
1:O:150:ASN:HD21	1:P:385:THR:N	2.07	0.43
1:Q:121:ASN:O	1:Q:160:VAL:HB	2.18	0.43
1:C:77:ASN:HD21	1:C:79:ASN:HB2	1.83	0.43
1:D:283:THR:H	1:D:288:ASN:ND2	2.15	0.43
1:G:171:THR:O	1:G:172:SER:CB	2.66	0.43
1:M:11:ILE:HB	1:M:12:VAL:H	1.65	0.43
1:N:320:GLN:N	1:N:323:ASP:OD2	2.51	0.43
1:O:204:ARG:HB3	1:O:337:ILE:HD11	2.00	0.43
1:T:201:ASP:O	1:T:202:ARG:HB2	2.18	0.43
1:T:77:ASN:HD21	1:T:79:ASN:HB2	1.82	0.43
1:A:127:VAL:HG22	1:A:144:LEU:HB3	2.00	0.43
1:C:106:LEU:HD23	1:C:367:GLY:HA3	1.98	0.43
1:F:209:THR:HA	1:F:332:SER:HB3	2.00	0.43
1:G:127:VAL:HG22	1:G:144:LEU:HB3	2.00	0.43
1:J:209:THR:HA	1:J:332:SER:HB3	2.00	0.43
1:M:93:PRO:HG3	1:M:180:LEU:HB3	2.00	0.43
1:N:171:THR:O	1:N:172:SER:CB	2.67	0.43
1:P:171:THR:O	1:P:172:SER:CB	2.66	0.43
1:S:93:PRO:HG3	1:S:180:LEU:HB3	2.01	0.43
1:D:201:ASP:O	1:D:202:ARG:HB2	2.19	0.43
1:F:121:ASN:ND2	1:F:358:ALA:H	2.16	0.43
1:F:201:ASP:O	1:F:202:ARG:HB2	2.19	0.43
1:H:171:THR:O	1:H:172:SER:CB	2.66	0.43
1:N:15:ILE:HG13	1:N:397:TYR:CD2	2.51	0.43
1:O:113:LEU:HD22	1:O:120:LEU:HD22	2.00	0.43
1:C:127:VAL:HG22	1:C:144:LEU:HB3	2.00	0.43
1:E:209:THR:HA	1:E:332:SER:HB3	1.99	0.43
1:F:171:THR:O	1:F:172:SER:CB	2.67	0.43
1:G:320:GLN:N	1:G:323:ASP:OD2	2.51	0.43
1:L:209:THR:HA	1:L:332:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:127:VAL:HG22	1:N:144:LEU:HB3	2.01	0.43
1:O:320:GLN:N	1:O:323:ASP:OD2	2.52	0.43
1:Q:121:ASN:HB3	1:Q:357:VAL:HA	2.01	0.43
1:S:396:ASN:HD22	1:S:396:ASN:N	2.17	0.43
1:S:77:ASN:HD21	1:S:79:ASN:HB2	1.83	0.43
1:T:127:VAL:HG22	1:T:144:LEU:HB3	1.99	0.43
1:A:15:ILE:HG13	1:A:397:TYR:CD2	2.52	0.43
1:A:171:THR:O	1:A:172:SER:CB	2.67	0.43
1:B:15:ILE:HA	1:B:15:ILE:HD13	1.86	0.43
1:B:201:ASP:O	1:B:202:ARG:HB2	2.19	0.43
1:D:124:ILE:HG13	1:D:160:VAL:HG22	2.00	0.43
1:E:11:ILE:HB	1:E:12:VAL:H	1.65	0.43
1:I:11:ILE:HB	1:I:12:VAL:H	1.65	0.43
1:I:209:THR:HA	1:I:332:SER:HB3	2.01	0.43
1:J:320:GLN:N	1:J:323:ASP:OD2	2.52	0.43
1:M:291:PRO:HB3	1:R:293:ASN:ND2	2.34	0.43
1:P:320:GLN:N	1:P:323:ASP:OD2	2.51	0.43
1:R:106:LEU:HD23	1:R:367:GLY:HA3	2.00	0.43
1:R:201:ASP:O	1:R:202:ARG:HB2	2.19	0.43
1:S:110:SER:HB3	1:S:160:VAL:CG1	2.49	0.43
1:G:204:ARG:HB3	1:G:337:ILE:HD11	2.00	0.42
1:M:15:ILE:HG13	1:M:397:TYR:CD2	2.52	0.42
1:H:77:ASN:HD21	1:H:79:ASN:HB2	1.83	0.42
1:K:171:THR:O	1:K:172:SER:CB	2.66	0.42
1:K:201:ASP:OD1	1:K:201:ASP:N	2.49	0.42
1:K:209:THR:HA	1:K:332:SER:HB3	2.00	0.42
1:P:201:ASP:O	1:P:202:ARG:HB2	2.19	0.42
1:P:204:ARG:HB3	1:P:337:ILE:HD11	2.01	0.42
1:Q:127:VAL:HG22	1:Q:144:LEU:HB3	2.00	0.42
1:S:11:ILE:HB	1:S:12:VAL:H	1.64	0.42
1:T:171:THR:O	1:T:172:SER:CB	2.67	0.42
1:A:201:ASP:O	1:A:202:ARG:HB2	2.20	0.42
1:D:127:VAL:HG22	1:D:144:LEU:HB3	2.00	0.42
1:J:201:ASP:O	1:J:202:ARG:HB2	2.19	0.42
1:M:110:SER:CB	1:M:160:VAL:HG12	2.49	0.42
1:E:116:GLY:HA2	1:P:162:GLU:HA	2.02	0.42
1:P:209:THR:HA	1:P:332:SER:HB3	2.00	0.42
1:R:11:ILE:HB	1:R:12:VAL:H	1.64	0.42
1:C:171:THR:O	1:C:172:SER:CB	2.67	0.42
1:D:171:THR:O	1:D:172:SER:CB	2.67	0.42
1:G:209:THR:HA	1:G:332:SER:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:ASP:O	1:H:202:ARG:HB2	2.19	0.42
1:J:15:ILE:HG13	1:J:397:TYR:CD2	2.52	0.42
1:K:124:ILE:HG13	1:K:160:VAL:HG22	2.02	0.42
1:M:150:ASN:HD21	1:R:385:THR:N	2.11	0.42
1:M:37:THR:OG1	1:M:39:ARG:NH1	2.53	0.42
1:J:204:ARG:HB3	1:J:337:ILE:HD11	2.00	0.42
1:L:201:ASP:N	1:L:201:ASP:OD1	2.49	0.42
1:N:15:ILE:HA	1:N:15:ILE:HD13	1.86	0.42
1:O:171:THR:O	1:O:172:SER:CB	2.67	0.42
1:P:15:ILE:HG13	1:P:397:TYR:CD2	2.52	0.42
1:B:204:ARG:HB3	1:B:337:ILE:HD11	2.01	0.42
1:F:127:VAL:HG22	1:F:144:LEU:HB3	2.00	0.42
1:L:171:THR:O	1:L:172:SER:CB	2.67	0.42
1:L:204:ARG:HB3	1:L:337:ILE:HD11	2.00	0.42
1:M:249:ARG:HB2	1:M:328:SER:HB3	2.01	0.42
1:M:20:MET:HG2	1:M:423:ARG:HG2	2.02	0.42
1:R:171:THR:O	1:R:172:SER:CB	2.67	0.42
1:R:347:ARG:HH11	1:R:347:ARG:HG2	1.85	0.42
1:T:316:LYS:HB2	1:T:325:MET:HE2	2.01	0.42
1:C:110:SER:CB	1:C:160:VAL:HG12	2.47	0.42
1:F:113:LEU:HA	1:F:114:PRO:HD3	1.83	0.42
1:S:110:SER:HB3	1:S:160:VAL:HG12	2.01	0.42
1:T:320:GLN:N	1:T:323:ASP:OD2	2.52	0.42
1:J:127:VAL:HG22	1:J:144:LEU:HB3	2.00	0.42
1:L:201:ASP:O	1:L:202:ARG:HB2	2.20	0.42
1:M:432:LEU:HD13	1:T:397:TYR:OH	2.20	0.42
1:N:209:THR:HA	1:N:332:SER:HB3	2.01	0.42
1:P:11:ILE:HB	1:P:12:VAL:H	1.65	0.42
1:P:432:LEU:HB2	1:P:433:ASN:H	1.67	0.42
1:Q:201:ASP:O	1:Q:202:ARG:HB2	2.19	0.42
1:R:37:THR:OG1	1:R:39:ARG:NH1	2.53	0.42
1:C:201:ASP:O	1:C:202:ARG:HB2	2.19	0.42
1:D:110:SER:HB3	1:D:160:VAL:HG12	2.01	0.42
1:H:204:ARG:HB3	1:H:337:ILE:HD11	2.00	0.42
1:I:171:THR:O	1:I:172:SER:CB	2.67	0.42
1:J:110:SER:HB3	1:J:160:VAL:HG12	2.01	0.42
1:L:112:THR:HG22	1:L:113:LEU:N	2.35	0.42
1:Q:171:THR:O	1:Q:172:SER:CB	2.67	0.42
1:R:127:VAL:HG22	1:R:144:LEU:HB3	2.01	0.42
1:A:93:PRO:HG3	1:A:180:LEU:HB3	2.02	0.41
1:J:11:ILE:HB	1:J:12:VAL:H	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:201:ASP:O	1:K:202:ARG:HB2	2.20	0.41
1:R:321:ALA:C	1:R:323:ASP:H	2.22	0.41
1:S:127:VAL:HG22	1:S:144:LEU:HB3	2.01	0.41
1:S:204:ARG:HB3	1:S:337:ILE:HD11	2.02	0.41
1:L:15:ILE:HG13	1:L:397:TYR:CD2	2.52	0.41
1:O:201:ASP:O	1:O:202:ARG:HB2	2.20	0.41
1:R:15:ILE:HG13	1:R:397:TYR:CD2	2.51	0.41
1:D:204:ARG:HB3	1:D:337:ILE:HD11	2.01	0.41
1:I:204:ARG:HB3	1:I:337:ILE:HD11	2.00	0.41
1:P:110:SER:HB3	1:P:160:VAL:CG1	2.45	0.41
1:N:201:ASP:O	1:N:202:ARG:HB2	2.19	0.41
1:R:276:VAL:HG22	1:R:294:LEU:HD21	2.02	0.41
1:B:11:ILE:HB	1:B:12:VAL:H	1.64	0.41
1:D:201:ASP:N	1:D:201:ASP:OD1	2.49	0.41
1:I:201:ASP:O	1:I:202:ARG:HB2	2.19	0.41
1:E:283:THR:H	1:E:288:ASN:ND2	2.17	0.41
1:L:93:PRO:HG3	1:L:180:LEU:HB3	2.03	0.41
1:B:171:THR:O	1:B:172:SER:CB	2.67	0.41
1:D:316:LYS:HB2	1:D:325:MET:HE2	2.02	0.41
1:M:110:SER:HB3	1:M:160:VAL:HG12	2.02	0.41
1:M:438:ILE:O	1:M:438:ILE:HG22	2.20	0.41
1:B:337:ILE:HG21	1:B:337:ILE:HD12	1.88	0.41
1:E:320:GLN:O	1:E:321:ALA:C	2.60	0.41
1:F:201:ASP:OD2	1:I:202:ARG:HD2	2.20	0.41
1:H:93:PRO:HG3	1:H:180:LEU:HB3	2.03	0.41
1:J:438:ILE:O	1:J:438:ILE:HG22	2.21	0.41
1:N:20:MET:HG2	1:N:423:ARG:HG2	2.03	0.41
1:O:15:ILE:HG13	1:O:397:TYR:CD2	2.52	0.41
1:R:110:SER:HB3	1:R:160:VAL:HG11	1.97	0.41
1:S:12:VAL:O	1:S:13:PRO:C	2.59	0.41
1:T:283:THR:H	1:T:288:ASN:ND2	2.15	0.41
1:A:12:VAL:O	1:A:13:PRO:C	2.60	0.41
1:E:93:PRO:HG3	1:E:180:LEU:HB3	2.02	0.41
1:A:279:ASN:ND2	1:A:279:ASN:O	2.54	0.41
1:C:20:MET:HG2	1:C:423:ARG:HG2	2.03	0.41
1:K:15:ILE:HD13	1:K:15:ILE:HA	1.86	0.41
1:L:12:VAL:O	1:L:13:PRO:C	2.60	0.41
1:N:438:ILE:HG22	1:N:438:ILE:O	2.21	0.41
1:S:171:THR:O	1:S:172:SER:CB	2.69	0.41
1:A:438:ILE:HG22	1:A:438:ILE:O	2.21	0.40
1:E:124:ILE:HG13	1:E:160:VAL:HG22	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:ASP:O	1:E:339:GLY:HA2	2.21	0.40
1:F:220:TYR:HD2	1:F:320:GLN:O	2.04	0.40
1:N:93:PRO:HG3	1:N:180:LEU:HB3	2.03	0.40
1:Q:93:PRO:HG3	1:Q:180:LEU:HB3	2.03	0.40
1:T:20:MET:HG2	1:T:423:ARG:HG2	2.03	0.40
1:B:20:MET:HG2	1:B:423:ARG:HG2	2.03	0.40
1:E:37:THR:OG1	1:E:39:ARG:NH1	2.55	0.40
1:F:15:ILE:HG13	1:F:397:TYR:CD2	2.52	0.40
1:G:438:ILE:HG22	1:G:438:ILE:O	2.21	0.40
1:J:93:PRO:HG3	1:J:180:LEU:HB3	2.03	0.40
1:K:113:LEU:HA	1:K:114:PRO:HD3	1.93	0.40
1:K:438:ILE:HG22	1:K:438:ILE:O	2.21	0.40
1:L:110:SER:CB	1:L:160:VAL:HG12	2.50	0.40
1:O:438:ILE:HG22	1:O:438:ILE:O	2.22	0.40
1:O:93:PRO:HG3	1:O:180:LEU:HB3	2.03	0.40
1:P:97:ASN:O	1:P:179:ARG:HG3	2.21	0.40
1:Q:20:MET:HG2	1:Q:423:ARG:HG2	2.03	0.40
1:S:20:MET:HG2	1:S:423:ARG:HG2	2.03	0.40
1:S:438:ILE:O	1:S:438:ILE:HG22	2.21	0.40
1:B:283:THR:H	1:B:288:ASN:ND2	2.16	0.40
1:E:438:ILE:HG22	1:E:438:ILE:O	2.22	0.40
1:M:121:ASN:O	1:M:160:VAL:HB	2.22	0.40
1:R:267:ASP:OD1	1:R:269:THR:HB	2.22	0.40
1:S:397:TYR:OH	1:T:432:LEU:HD13	2.22	0.40
1:B:438:ILE:HG22	1:B:438:ILE:O	2.22	0.40
1:D:114:PRO:HD3	1:D:361:SER:HB3	2.03	0.40
1:G:97:ASN:O	1:G:179:ARG:HG3	2.22	0.40
1:H:220:TYR:HD2	1:H:320:GLN:O	2.05	0.40
1:I:12:VAL:O	1:I:13:PRO:C	2.60	0.40
1:K:12:VAL:O	1:K:13:PRO:C	2.60	0.40
1:O:124:ILE:HG13	1:O:160:VAL:HG22	2.02	0.40
1:P:20:MET:HG2	1:P:423:ARG:HG2	2.04	0.40
1:P:93:PRO:HG3	1:P:180:LEU:HB3	2.02	0.40
1:Q:220:TYR:HD2	1:Q:320:GLN:O	2.05	0.40
1:Q:316:LYS:HB2	1:Q:325:MET:HE2	2.03	0.40
1:Q:438:ILE:O	1:Q:438:ILE:HG22	2.22	0.40
1:T:201:ASP:OD1	1:T:201:ASP:N	2.50	0.40
1:G:113:LEU:HA	1:G:114:PRO:HD3	1.88	0.40
1:I:20:MET:HG2	1:I:423:ARG:HG2	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:GLN:OE1	1:F:217:SER:OG[3_545]	1.77	0.43
1:E:284:THR:CG2	1:T:217:SER:CB[11_456]	2.06	0.14
1:L:317:SER:O	1:T:284:THR:CG2[7_564]	2.12	0.08

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	5	9
1	B	424/456 (93%)	394 (93%)	19 (4%)	11 (3%)	5	9
1	C	424/456 (93%)	395 (93%)	18 (4%)	11 (3%)	5	9
1	D	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	5	9
1	E	431/456 (94%)	401 (93%)	20 (5%)	10 (2%)	6	11
1	F	431/456 (94%)	401 (93%)	18 (4%)	12 (3%)	5	7
1	G	431/456 (94%)	403 (94%)	17 (4%)	11 (3%)	5	9
1	H	424/456 (93%)	395 (93%)	18 (4%)	11 (3%)	5	9
1	I	424/456 (93%)	396 (93%)	16 (4%)	12 (3%)	5	7
1	J	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	5	9
1	K	424/456 (93%)	395 (93%)	18 (4%)	11 (3%)	5	9
1	L	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	5	9
1	M	424/456 (93%)	396 (93%)	18 (4%)	10 (2%)	6	10
1	N	424/456 (93%)	395 (93%)	17 (4%)	12 (3%)	5	7
1	O	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	5	9
1	P	426/456 (93%)	397 (93%)	17 (4%)	12 (3%)	5	7
1	Q	425/456 (93%)	396 (93%)	18 (4%)	11 (3%)	5	9
1	R	431/456 (94%)	401 (93%)	23 (5%)	7 (2%)	9	19
1	S	424/456 (93%)	394 (93%)	19 (4%)	11 (3%)	5	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	424/456 (93%)	395 (93%)	18 (4%)	11 (3%)	5	9
All	All	8511/9120 (93%)	7934 (93%)	359 (4%)	218 (3%)	5	9

All (218) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	279	ASN
1	A	435	PRO
1	B	11	ILE
1	B	279	ASN
1	B	435	PRO
1	C	11	ILE
1	C	279	ASN
1	C	435	PRO
1	D	11	ILE
1	D	279	ASN
1	D	435	PRO
1	E	11	ILE
1	E	279	ASN
1	E	321	ALA
1	E	435	PRO
1	F	11	ILE
1	F	279	ASN
1	F	435	PRO
1	G	11	ILE
1	G	279	ASN
1	G	435	PRO
1	H	11	ILE
1	H	279	ASN
1	H	435	PRO
1	I	11	ILE
1	I	279	ASN
1	I	435	PRO
1	J	11	ILE
1	J	279	ASN
1	J	435	PRO
1	K	11	ILE
1	K	279	ASN
1	K	435	PRO
1	L	11	ILE
1	L	279	ASN

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Mol	Chain	Res	Type
1	L	435	PRO
1	M	11	ILE
1	M	279	ASN
1	M	435	PRO
1	N	11	ILE
1	N	279	ASN
1	N	435	PRO
1	O	11	ILE
1	O	279	ASN
1	O	435	PRO
1	P	11	ILE
1	P	279	ASN
1	P	435	PRO
1	Q	11	ILE
1	Q	279	ASN
1	Q	435	PRO
1	R	11	ILE
1	R	317	SER
1	R	435	PRO
1	S	11	ILE
1	S	279	ASN
1	S	324	GLN
1	S	435	PRO
1	T	11	ILE
1	T	279	ASN
1	T	435	PRO
1	A	321	ALA
1	A	324	GLN
1	B	321	ALA
1	B	324	GLN
1	C	321	ALA
1	C	324	GLN
1	D	321	ALA
1	D	324	GLN
1	F	321	ALA
1	F	324	GLN
1	G	321	ALA
1	G	324	GLN
1	H	321	ALA
1	H	324	GLN
1	I	122	GLY
1	I	321	ALA

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Mol	Chain	Res	Type
1	I	324	GLN
1	J	321	ALA
1	J	324	GLN
1	K	321	ALA
1	K	324	GLN
1	L	321	ALA
1	L	324	GLN
1	M	321	ALA
1	N	122	GLY
1	N	321	ALA
1	N	324	GLN
1	O	321	ALA
1	O	324	GLN
1	P	114	PRO
1	P	321	ALA
1	P	324	GLN
1	Q	321	ALA
1	Q	324	GLN
1	S	225	VAL
1	T	321	ALA
1	T	324	GLN
1	A	10	GLN
1	A	439	ALA
1	B	10	GLN
1	B	439	ALA
1	C	10	GLN
1	C	318	GLY
1	C	439	ALA
1	D	10	GLN
1	D	318	GLY
1	D	439	ALA
1	E	10	GLN
1	E	439	ALA
1	F	10	GLN
1	F	439	ALA
1	G	10	GLN
1	G	318	GLY
1	G	439	ALA
1	H	10	GLN
1	H	318	GLY
1	H	439	ALA
1	I	10	GLN

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Mol	Chain	Res	Type
1	I	318	GLY
1	I	439	ALA
1	J	10	GLN
1	J	439	ALA
1	K	10	GLN
1	K	318	GLY
1	K	439	ALA
1	L	10	GLN
1	L	318	GLY
1	L	439	ALA
1	M	10	GLN
1	M	320	GLN
1	M	439	ALA
1	N	10	GLN
1	N	439	ALA
1	O	10	GLN
1	O	439	ALA
1	P	10	GLN
1	P	318	GLY
1	P	439	ALA
1	Q	10	GLN
1	Q	439	ALA
1	R	10	GLN
1	R	439	ALA
1	S	10	GLN
1	S	439	ALA
1	T	10	GLN
1	T	439	ALA
1	A	318	GLY
1	A	426	PHE
1	B	318	GLY
1	B	426	PHE
1	C	426	PHE
1	D	426	PHE
1	E	172	SER
1	F	318	GLY
1	F	426	PHE
1	G	426	PHE
1	H	426	PHE
1	I	426	PHE
1	J	318	GLY
1	J	426	PHE

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Mol	Chain	Res	Type
1	K	426	PHE
1	L	426	PHE
1	M	324	GLN
1	N	318	GLY
1	N	426	PHE
1	O	318	GLY
1	O	426	PHE
1	Q	318	GLY
1	Q	426	PHE
1	S	321	ALA
1	S	426	PHE
1	T	318	GLY
1	T	426	PHE
1	A	172	SER
1	B	172	SER
1	C	172	SER
1	D	172	SER
1	E	324	GLN
1	F	172	SER
1	G	172	SER
1	H	172	SER
1	I	172	SER
1	J	172	SER
1	K	172	SER
1	L	172	SER
1	M	172	SER
1	N	172	SER
1	O	172	SER
1	P	172	SER
1	P	426	PHE
1	Q	172	SER
1	R	172	SER
1	S	172	SER
1	T	172	SER
1	E	111	SER
1	S	347	ARG
1	A	347	ARG
1	B	347	ARG
1	C	347	ARG
1	D	347	ARG
1	E	347	ARG
1	F	347	ARG

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Mol	Chain	Res	Type
1	G	347	ARG
1	H	347	ARG
1	I	347	ARG
1	J	347	ARG
1	K	347	ARG
1	L	347	ARG
1	M	347	ARG
1	N	347	ARG
1	O	347	ARG
1	P	347	ARG
1	Q	347	ARG
1	R	347	ARG
1	T	347	ARG
1	F	114	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	354/380 (93%)	328 (93%)	26 (7%)	14	28
1	B	354/380 (93%)	328 (93%)	26 (7%)	14	28
1	C	354/380 (93%)	328 (93%)	26 (7%)	14	28
1	D	354/380 (93%)	328 (93%)	26 (7%)	14	28
1	E	356/380 (94%)	332 (93%)	24 (7%)	16	33
1	F	356/380 (94%)	329 (92%)	27 (8%)	13	26
1	G	356/380 (94%)	330 (93%)	26 (7%)	14	28
1	H	354/380 (93%)	329 (93%)	25 (7%)	14	29
1	I	354/380 (93%)	328 (93%)	26 (7%)	14	28
1	J	354/380 (93%)	326 (92%)	28 (8%)	12	24
1	K	354/380 (93%)	327 (92%)	27 (8%)	13	26
1	L	354/380 (93%)	329 (93%)	25 (7%)	14	29
1	M	354/380 (93%)	328 (93%)	26 (7%)	14	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	354/380 (93%)	329 (93%)	25 (7%)	14	29
1	O	354/380 (93%)	326 (92%)	28 (8%)	12	24
1	P	354/380 (93%)	329 (93%)	25 (7%)	14	29
1	Q	354/380 (93%)	329 (93%)	25 (7%)	14	29
1	R	356/380 (94%)	332 (93%)	24 (7%)	16	33
1	S	354/380 (93%)	328 (93%)	26 (7%)	14	28
1	T	354/380 (93%)	329 (93%)	25 (7%)	14	29
All	All	7088/7600 (93%)	6572 (93%)	516 (7%)	14	28

All (516) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	39	ARG
1	A	77	ASN
1	A	88	THR
1	A	99	CYS
1	A	112	THR
1	A	113	LEU
1	A	127	VAL
1	A	146	SER
1	A	148	THR
1	A	193	MET
1	A	201	ASP
1	A	219	GLN
1	A	240	LEU
1	A	269	THR
1	A	273	THR
1	A	279	ASN
1	A	306	THR
1	A	325	MET
1	A	330	ARG
1	A	332	SER
1	A	337	ILE
1	A	347	ARG
1	A	383	LEU
1	A	407	ARG
1	A	432	LEU
1	B	23	THR
1	B	39	ARG

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Mol	Chain	Res	Type
1	B	77	ASN
1	B	88	THR
1	B	99	CYS
1	B	107	THR
1	B	112	THR
1	B	127	VAL
1	B	146	SER
1	B	148	THR
1	B	193	MET
1	B	201	ASP
1	B	219	GLN
1	B	240	LEU
1	B	269	THR
1	B	273	THR
1	B	279	ASN
1	B	306	THR
1	B	325	MET
1	B	330	ARG
1	B	332	SER
1	B	337	ILE
1	B	347	ARG
1	B	383	LEU
1	B	407	ARG
1	B	432	LEU
1	C	23	THR
1	C	39	ARG
1	C	77	ASN
1	C	88	THR
1	C	99	CYS
1	C	107	THR
1	C	112	THR
1	C	127	VAL
1	C	146	SER
1	C	148	THR
1	C	193	MET
1	C	201	ASP
1	C	219	GLN
1	C	240	LEU
1	C	269	THR
1	C	273	THR
1	C	279	ASN
1	C	306	THR

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Mol	Chain	Res	Type
1	C	325	MET
1	C	330	ARG
1	C	332	SER
1	C	337	ILE
1	C	347	ARG
1	C	383	LEU
1	C	407	ARG
1	C	432	LEU
1	D	23	THR
1	D	39	ARG
1	D	77	ASN
1	D	88	THR
1	D	99	CYS
1	D	112	THR
1	D	127	VAL
1	D	146	SER
1	D	148	THR
1	D	193	MET
1	D	201	ASP
1	D	219	GLN
1	D	240	LEU
1	D	269	THR
1	D	273	THR
1	D	279	ASN
1	D	306	THR
1	D	325	MET
1	D	330	ARG
1	D	332	SER
1	D	337	ILE
1	D	347	ARG
1	D	383	LEU
1	D	396	ASN
1	D	407	ARG
1	D	432	LEU
1	E	23	THR
1	E	39	ARG
1	E	88	THR
1	E	99	CYS
1	E	107	THR
1	E	127	VAL
1	E	146	SER
1	E	148	THR

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Mol	Chain	Res	Type
1	E	164	VAL
1	E	193	MET
1	E	201	ASP
1	E	219	GLN
1	E	240	LEU
1	E	269	THR
1	E	273	THR
1	E	279	ASN
1	E	306	THR
1	E	330	ARG
1	E	332	SER
1	E	337	ILE
1	E	347	ARG
1	E	383	LEU
1	E	407	ARG
1	E	432	LEU
1	F	23	THR
1	F	39	ARG
1	F	77	ASN
1	F	88	THR
1	F	99	CYS
1	F	120	LEU
1	F	121	ASN
1	F	127	VAL
1	F	146	SER
1	F	148	THR
1	F	193	MET
1	F	201	ASP
1	F	219	GLN
1	F	240	LEU
1	F	269	THR
1	F	273	THR
1	F	279	ASN
1	F	306	THR
1	F	325	MET
1	F	330	ARG
1	F	332	SER
1	F	337	ILE
1	F	347	ARG
1	F	383	LEU
1	F	396	ASN
1	F	407	ARG

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Mol	Chain	Res	Type
1	F	432	LEU
1	G	23	THR
1	G	39	ARG
1	G	77	ASN
1	G	88	THR
1	G	99	CYS
1	G	113	LEU
1	G	127	VAL
1	G	146	SER
1	G	148	THR
1	G	193	MET
1	G	201	ASP
1	G	219	GLN
1	G	240	LEU
1	G	269	THR
1	G	273	THR
1	G	279	ASN
1	G	306	THR
1	G	325	MET
1	G	330	ARG
1	G	332	SER
1	G	337	ILE
1	G	347	ARG
1	G	383	LEU
1	G	396	ASN
1	G	407	ARG
1	G	432	LEU
1	H	23	THR
1	H	39	ARG
1	H	77	ASN
1	H	88	THR
1	H	99	CYS
1	H	127	VAL
1	H	146	SER
1	H	148	THR
1	H	193	MET
1	H	201	ASP
1	H	219	GLN
1	H	240	LEU
1	H	269	THR
1	H	273	THR
1	H	279	ASN

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Mol	Chain	Res	Type
1	H	306	THR
1	H	325	MET
1	H	330	ARG
1	H	332	SER
1	H	337	ILE
1	H	347	ARG
1	H	383	LEU
1	H	396	ASN
1	H	407	ARG
1	H	432	LEU
1	I	23	THR
1	I	39	ARG
1	I	77	ASN
1	I	88	THR
1	I	99	CYS
1	I	112	THR
1	I	127	VAL
1	I	146	SER
1	I	148	THR
1	I	193	MET
1	I	201	ASP
1	I	219	GLN
1	I	240	LEU
1	I	269	THR
1	I	273	THR
1	I	279	ASN
1	I	306	THR
1	I	325	MET
1	I	330	ARG
1	I	332	SER
1	I	337	ILE
1	I	347	ARG
1	I	383	LEU
1	I	396	ASN
1	I	407	ARG
1	I	432	LEU
1	J	23	THR
1	J	39	ARG
1	J	77	ASN
1	J	88	THR
1	J	99	CYS
1	J	107	THR

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Mol	Chain	Res	Type
1	J	112	THR
1	J	113	LEU
1	J	127	VAL
1	J	146	SER
1	J	148	THR
1	J	193	MET
1	J	201	ASP
1	J	219	GLN
1	J	240	LEU
1	J	269	THR
1	J	273	THR
1	J	279	ASN
1	J	306	THR
1	J	325	MET
1	J	330	ARG
1	J	332	SER
1	J	337	ILE
1	J	347	ARG
1	J	383	LEU
1	J	396	ASN
1	J	407	ARG
1	J	432	LEU
1	K	23	THR
1	K	39	ARG
1	K	77	ASN
1	K	88	THR
1	K	99	CYS
1	K	107	THR
1	K	112	THR
1	K	113	LEU
1	K	127	VAL
1	K	146	SER
1	K	148	THR
1	K	193	MET
1	K	201	ASP
1	K	219	GLN
1	K	240	LEU
1	K	269	THR
1	K	273	THR
1	K	279	ASN
1	K	306	THR
1	K	325	MET

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Mol	Chain	Res	Type
1	K	330	ARG
1	K	332	SER
1	K	337	ILE
1	K	347	ARG
1	K	383	LEU
1	K	407	ARG
1	K	432	LEU
1	L	23	THR
1	L	39	ARG
1	L	77	ASN
1	L	88	THR
1	L	99	CYS
1	L	113	LEU
1	L	127	VAL
1	L	146	SER
1	L	148	THR
1	L	193	MET
1	L	201	ASP
1	L	219	GLN
1	L	240	LEU
1	L	269	THR
1	L	273	THR
1	L	279	ASN
1	L	306	THR
1	L	325	MET
1	L	330	ARG
1	L	332	SER
1	L	337	ILE
1	L	347	ARG
1	L	383	LEU
1	L	407	ARG
1	L	432	LEU
1	M	23	THR
1	M	39	ARG
1	M	77	ASN
1	M	88	THR
1	M	99	CYS
1	M	120	LEU
1	M	127	VAL
1	M	146	SER
1	M	148	THR
1	M	164	VAL

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Mol	Chain	Res	Type
1	M	193	MET
1	M	201	ASP
1	M	219	GLN
1	M	240	LEU
1	M	269	THR
1	M	273	THR
1	M	279	ASN
1	M	306	THR
1	M	325	MET
1	M	330	ARG
1	M	332	SER
1	M	337	ILE
1	M	347	ARG
1	M	383	LEU
1	M	407	ARG
1	M	432	LEU
1	N	23	THR
1	N	39	ARG
1	N	77	ASN
1	N	88	THR
1	N	99	CYS
1	N	107	THR
1	N	127	VAL
1	N	146	SER
1	N	148	THR
1	N	193	MET
1	N	201	ASP
1	N	219	GLN
1	N	240	LEU
1	N	269	THR
1	N	273	THR
1	N	279	ASN
1	N	306	THR
1	N	325	MET
1	N	330	ARG
1	N	332	SER
1	N	337	ILE
1	N	347	ARG
1	N	383	LEU
1	N	407	ARG
1	N	432	LEU
1	O	23	THR

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Mol	Chain	Res	Type
1	O	39	ARG
1	O	77	ASN
1	O	88	THR
1	O	99	CYS
1	O	107	THR
1	O	112	THR
1	O	113	LEU
1	O	120	LEU
1	O	127	VAL
1	O	146	SER
1	O	148	THR
1	O	193	MET
1	O	201	ASP
1	O	219	GLN
1	O	240	LEU
1	O	269	THR
1	O	273	THR
1	O	279	ASN
1	O	306	THR
1	O	325	MET
1	O	330	ARG
1	O	332	SER
1	O	337	ILE
1	O	347	ARG
1	O	383	LEU
1	O	407	ARG
1	O	432	LEU
1	P	23	THR
1	P	39	ARG
1	P	77	ASN
1	P	88	THR
1	P	99	CYS
1	P	107	THR
1	P	127	VAL
1	P	146	SER
1	P	148	THR
1	P	193	MET
1	P	201	ASP
1	P	219	GLN
1	P	240	LEU
1	P	269	THR
1	P	273	THR

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Mol	Chain	Res	Type
1	P	279	ASN
1	P	306	THR
1	P	325	MET
1	P	330	ARG
1	P	332	SER
1	P	337	ILE
1	P	347	ARG
1	P	383	LEU
1	P	407	ARG
1	P	432	LEU
1	Q	23	THR
1	Q	39	ARG
1	Q	77	ASN
1	Q	88	THR
1	Q	99	CYS
1	Q	120	LEU
1	Q	127	VAL
1	Q	146	SER
1	Q	148	THR
1	Q	193	MET
1	Q	201	ASP
1	Q	219	GLN
1	Q	240	LEU
1	Q	269	THR
1	Q	273	THR
1	Q	279	ASN
1	Q	306	THR
1	Q	325	MET
1	Q	330	ARG
1	Q	332	SER
1	Q	337	ILE
1	Q	347	ARG
1	Q	383	LEU
1	Q	407	ARG
1	Q	432	LEU
1	R	23	THR
1	R	39	ARG
1	R	77	ASN
1	R	88	THR
1	R	99	CYS
1	R	127	VAL
1	R	146	SER

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Mol	Chain	Res	Type
1	R	148	THR
1	R	164	VAL
1	R	201	ASP
1	R	240	LEU
1	R	273	THR
1	R	284	THR
1	R	299	ASN
1	R	306	THR
1	R	320	GLN
1	R	328	SER
1	R	330	ARG
1	R	337	ILE
1	R	347	ARG
1	R	383	LEU
1	R	396	ASN
1	R	407	ARG
1	R	432	LEU
1	S	23	THR
1	S	39	ARG
1	S	77	ASN
1	S	88	THR
1	S	99	CYS
1	S	107	THR
1	S	113	LEU
1	S	127	VAL
1	S	146	SER
1	S	148	THR
1	S	193	MET
1	S	201	ASP
1	S	221	GLN
1	S	225	VAL
1	S	240	LEU
1	S	269	THR
1	S	273	THR
1	S	279	ASN
1	S	306	THR
1	S	330	ARG
1	S	332	SER
1	S	337	ILE
1	S	347	ARG
1	S	383	LEU
1	S	407	ARG

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Mol	Chain	Res	Type
1	S	432	LEU
1	T	23	THR
1	T	39	ARG
1	T	77	ASN
1	T	88	THR
1	T	99	CYS
1	T	127	VAL
1	T	146	SER
1	T	148	THR
1	T	193	MET
1	T	201	ASP
1	T	219	GLN
1	T	240	LEU
1	T	269	THR
1	T	273	THR
1	T	279	ASN
1	T	306	THR
1	T	325	MET
1	T	330	ARG
1	T	332	SER
1	T	337	ILE
1	T	347	ARG
1	T	383	LEU
1	T	396	ASN
1	T	407	ARG
1	T	432	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (161) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	77	ASN
1	A	90	GLN
1	A	121	ASN
1	A	130	GLN
1	A	150	ASN
1	A	219	GLN
1	A	288	ASN
1	A	396	ASN
1	B	75	GLN
1	B	77	ASN
1	B	90	GLN

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Mol	Chain	Res	Type
1	B	150	ASN
1	B	219	GLN
1	B	288	ASN
1	B	396	ASN
1	C	75	GLN
1	C	77	ASN
1	C	90	GLN
1	C	130	GLN
1	C	150	ASN
1	C	219	GLN
1	C	288	ASN
1	C	396	ASN
1	D	75	GLN
1	D	77	ASN
1	D	90	GLN
1	D	150	ASN
1	D	219	GLN
1	D	288	ASN
1	D	396	ASN
1	E	75	GLN
1	E	90	GLN
1	E	150	ASN
1	E	219	GLN
1	E	288	ASN
1	E	324	GLN
1	E	396	ASN
1	F	75	GLN
1	F	77	ASN
1	F	90	GLN
1	F	121	ASN
1	F	130	GLN
1	F	150	ASN
1	F	219	GLN
1	F	288	ASN
1	F	293	ASN
1	F	396	ASN
1	G	75	GLN
1	G	77	ASN
1	G	130	GLN
1	G	150	ASN
1	G	219	GLN
1	G	288	ASN

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Mol	Chain	Res	Type
1	G	293	ASN
1	G	396	ASN
1	H	75	GLN
1	H	77	ASN
1	H	90	GLN
1	H	130	GLN
1	H	150	ASN
1	H	219	GLN
1	H	288	ASN
1	H	396	ASN
1	I	75	GLN
1	I	77	ASN
1	I	90	GLN
1	I	130	GLN
1	I	150	ASN
1	I	219	GLN
1	I	288	ASN
1	I	396	ASN
1	J	75	GLN
1	J	77	ASN
1	J	90	GLN
1	J	121	ASN
1	J	150	ASN
1	J	219	GLN
1	J	288	ASN
1	J	396	ASN
1	K	75	GLN
1	K	77	ASN
1	K	90	GLN
1	K	130	GLN
1	K	150	ASN
1	K	219	GLN
1	K	288	ASN
1	K	396	ASN
1	L	75	GLN
1	L	77	ASN
1	L	90	GLN
1	L	150	ASN
1	L	219	GLN
1	L	288	ASN
1	L	396	ASN
1	M	75	GLN

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Mol	Chain	Res	Type
1	M	77	ASN
1	M	90	GLN
1	M	130	GLN
1	M	150	ASN
1	M	219	GLN
1	M	288	ASN
1	M	396	ASN
1	N	75	GLN
1	N	77	ASN
1	N	90	GLN
1	N	130	GLN
1	N	150	ASN
1	N	219	GLN
1	N	288	ASN
1	N	396	ASN
1	O	75	GLN
1	O	77	ASN
1	O	90	GLN
1	O	130	GLN
1	O	150	ASN
1	O	219	GLN
1	O	288	ASN
1	O	396	ASN
1	P	75	GLN
1	P	77	ASN
1	P	90	GLN
1	P	121	ASN
1	P	130	GLN
1	P	150	ASN
1	P	219	GLN
1	P	288	ASN
1	P	396	ASN
1	Q	75	GLN
1	Q	77	ASN
1	Q	90	GLN
1	Q	130	GLN
1	Q	150	ASN
1	Q	219	GLN
1	Q	288	ASN
1	Q	293	ASN
1	Q	396	ASN
1	R	75	GLN

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Mol	Chain	Res	Type
1	R	77	ASN
1	R	90	GLN
1	R	150	ASN
1	R	215	GLN
1	R	219	GLN
1	R	288	ASN
1	R	293	ASN
1	R	299	ASN
1	R	396	ASN
1	S	75	GLN
1	S	77	ASN
1	S	90	GLN
1	S	150	ASN
1	S	219	GLN
1	S	288	ASN
1	S	396	ASN
1	T	75	GLN
1	T	77	ASN
1	T	90	GLN
1	T	150	ASN
1	T	219	GLN
1	T	288	ASN
1	T	396	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	428/456 (93%)	0.56	52 (12%) 4 2	8, 12, 17, 24	0
1	B	428/456 (93%)	0.74	53 (12%) 4 2	8, 12, 17, 24	0
1	C	428/456 (93%)	0.70	60 (14%) 2 1	8, 12, 18, 24	0
1	D	428/456 (93%)	0.73	66 (15%) 2 1	8, 12, 16, 24	0
1	E	433/456 (94%)	0.46	31 (7%) 15 11	5, 11, 16, 24	0
1	F	433/456 (94%)	0.76	57 (13%) 3 2	8, 12, 17, 24	0
1	G	433/456 (94%)	0.60	40 (9%) 9 6	6, 12, 17, 24	0
1	H	428/456 (93%)	0.65	43 (10%) 7 4	8, 12, 18, 24	0
1	I	428/456 (93%)	0.68	50 (11%) 4 3	8, 12, 18, 24	0
1	J	428/456 (93%)	0.68	60 (14%) 2 1	8, 12, 17, 24	0
1	K	428/456 (93%)	0.63	48 (11%) 5 3	8, 12, 18, 24	0
1	L	428/456 (93%)	0.56	44 (10%) 6 4	8, 12, 18, 24	0
1	M	428/456 (93%)	0.66	42 (9%) 7 5	8, 12, 18, 24	0
1	N	428/456 (93%)	0.63	46 (10%) 6 3	8, 12, 18, 24	0
1	O	428/456 (93%)	0.66	60 (14%) 2 1	8, 12, 18, 24	0
1	P	430/456 (94%)	0.63	48 (11%) 5 3	8, 12, 17, 24	0
1	Q	429/456 (94%)	0.66	55 (12%) 3 2	8, 12, 18, 24	0
1	R	433/456 (94%)	0.54	27 (6%) 20 15	2, 11, 17, 24	0
1	S	428/456 (93%)	0.61	30 (7%) 16 12	4, 11, 18, 24	0
1	T	428/456 (93%)	0.69	33 (7%) 13 10	8, 12, 18, 24	0
All	All	8583/9120 (94%)	0.64	945 (11%) 5 3	2, 12, 18, 24	0

All (945) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	440	GLY	14.1
1	Q	439	ALA	12.9
1	R	439	ALA	12.5
1	N	439	ALA	11.4
1	K	439	ALA	11.3
1	B	439	ALA	11.2
1	I	440	GLY	11.0
1	O	436	LEU	11.0
1	E	440	GLY	10.8
1	J	439	ALA	10.7
1	P	439	ALA	10.7
1	A	439	ALA	10.6
1	H	434	SER	10.3
1	Q	436	LEU	10.3
1	I	322	GLY	10.2
1	G	439	ALA	10.1
1	A	435	PRO	9.9
1	C	439	ALA	9.9
1	B	440	GLY	9.9
1	L	440	GLY	9.8
1	J	434	SER	9.8
1	C	9	GLN	9.6
1	F	322	GLY	9.6
1	R	430	ALA	9.5
1	J	440	GLY	9.4
1	I	439	ALA	9.3
1	R	435	PRO	9.3
1	L	439	ALA	9.3
1	O	430	ALA	9.2
1	H	440	GLY	9.2
1	F	439	ALA	9.2
1	Q	438	ILE	9.2
1	B	430	ALA	9.2
1	D	429	VAL	9.1
1	E	439	ALA	9.1
1	H	439	ALA	9.0
1	H	438	ILE	9.0
1	R	434	SER	9.0
1	B	435	PRO	9.0
1	N	434	SER	8.9
1	T	436	LEU	8.9
1	N	438	ILE	8.9
1	M	439	ALA	8.9

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Mol	Chain	Res	Type	RSRZ
1	I	438	ILE	8.8
1	P	434	SER	8.8
1	S	435	PRO	8.8
1	Q	434	SER	8.8
1	B	433	ASN	8.7
1	A	433	ASN	8.7
1	A	440	GLY	8.7
1	L	435	PRO	8.6
1	S	433	ASN	8.6
1	K	436	LEU	8.6
1	L	436	LEU	8.6
1	J	435	PRO	8.6
1	R	438	ILE	8.5
1	M	433	ASN	8.5
1	G	321	ALA	8.4
1	Q	433	ASN	8.4
1	I	435	PRO	8.4
1	S	439	ALA	8.4
1	F	434	SER	8.4
1	L	438	ILE	8.4
1	B	434	SER	8.3
1	M	434	SER	8.3
1	O	435	PRO	8.3
1	H	433	ASN	8.3
1	D	440	GLY	8.2
1	O	434	SER	8.2
1	I	430	ALA	8.2
1	N	436	LEU	8.2
1	A	436	LEU	8.1
1	F	433	ASN	8.1
1	F	321	ALA	8.1
1	O	429	VAL	8.1
1	S	438	ILE	8.0
1	O	437	LYS	8.0
1	J	433	ASN	7.9
1	O	439	ALA	7.9
1	C	434	SER	7.9
1	B	429	VAL	7.9
1	J	438	ILE	7.9
1	G	8	THR	7.9
1	H	10	GLN	7.8
1	T	439	ALA	7.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	10	GLN	7.8
1	O	440	GLY	7.8
1	N	8	THR	7.8
1	H	436	LEU	7.8
1	S	10	GLN	7.7
1	Q	8	THR	7.7
1	E	10	GLN	7.7
1	H	435	PRO	7.7
1	P	429	VAL	7.7
1	O	433	ASN	7.6
1	M	440	GLY	7.6
1	F	440	GLY	7.6
1	Q	435	PRO	7.6
1	O	322	GLY	7.5
1	F	430	ALA	7.5
1	N	430	ALA	7.5
1	R	9	GLN	7.5
1	D	433	ASN	7.4
1	G	434	SER	7.4
1	C	430	ALA	7.4
1	P	430	ALA	7.4
1	M	429	VAL	7.4
1	N	435	PRO	7.4
1	M	436	LEU	7.4
1	D	435	PRO	7.3
1	I	434	SER	7.3
1	E	433	ASN	7.3
1	G	11	ILE	7.3
1	D	434	SER	7.3
1	M	9	GLN	7.3
1	G	440	GLY	7.2
1	R	429	VAL	7.2
1	D	439	ALA	7.2
1	K	440	GLY	7.2
1	K	435	PRO	7.2
1	K	433	ASN	7.2
1	D	320	GLN	7.2
1	P	436	LEU	7.1
1	S	434	SER	7.1
1	S	436	LEU	7.1
1	F	10	GLN	7.1
1	J	322	GLY	7.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	T	440	GLY	7.1
1	A	434	SER	7.1
1	S	9	GLN	7.0
1	M	8	THR	7.0
1	S	440	GLY	7.0
1	H	8	THR	7.0
1	A	430	ALA	7.0
1	S	8	THR	7.0
1	O	10	GLN	7.0
1	E	429	VAL	6.9
1	F	435	PRO	6.9
1	H	9	GLN	6.9
1	E	435	PRO	6.9
1	P	433	ASN	6.9
1	T	434	SER	6.9
1	D	10	GLN	6.9
1	D	425	TYR	6.9
1	N	440	GLY	6.9
1	G	430	ALA	6.8
1	I	436	LEU	6.8
1	Q	10	GLN	6.8
1	I	429	VAL	6.8
1	M	430	ALA	6.8
1	L	9	GLN	6.8
1	M	435	PRO	6.8
1	R	436	LEU	6.8
1	C	322	GLY	6.8
1	N	425	TYR	6.8
1	D	8	THR	6.7
1	I	433	ASN	6.7
1	K	429	VAL	6.7
1	A	10	GLN	6.7
1	G	435	PRO	6.6
1	E	430	ALA	6.6
1	K	8	THR	6.6
1	D	431	ASP	6.6
1	K	321	ALA	6.6
1	B	437	LYS	6.6
1	Q	440	GLY	6.6
1	R	440	GLY	6.6
1	C	10	GLN	6.6
1	C	435	PRO	6.5

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Mol	Chain	Res	Type	RSRZ
1	P	435	PRO	6.5
1	N	433	ASN	6.5
1	G	436	LEU	6.5
1	J	436	LEU	6.5
1	H	430	ALA	6.5
1	B	438	ILE	6.5
1	A	438	ILE	6.5
1	C	11	ILE	6.5
1	L	8	THR	6.5
1	R	11	ILE	6.4
1	F	425	TYR	6.4
1	B	436	LEU	6.4
1	P	440	GLY	6.4
1	C	431	ASP	6.4
1	A	321	ALA	6.4
1	R	8	THR	6.3
1	F	220	TYR	6.3
1	K	113	LEU	6.3
1	C	438	ILE	6.3
1	M	438	ILE	6.3
1	B	322	GLY	6.2
1	K	430	ALA	6.2
1	J	9	GLN	6.2
1	D	11	ILE	6.2
1	F	428	GLU	6.2
1	B	321	ALA	6.2
1	C	429	VAL	6.2
1	B	8	THR	6.2
1	J	8	THR	6.2
1	P	8	THR	6.2
1	K	10	GLN	6.2
1	T	425	TYR	6.2
1	N	321	ALA	6.2
1	F	9	GLN	6.1
1	R	433	ASN	6.1
1	I	9	GLN	6.1
1	O	9	GLN	6.1
1	O	438	ILE	6.1
1	M	428	GLU	6.1
1	K	322	GLY	6.1
1	A	437	LYS	6.1
1	L	430	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
1	L	434	SER	6.1
1	I	8	THR	6.1
1	H	429	VAL	6.0
1	F	224	GLY	6.0
1	Q	321	ALA	6.0
1	O	321	ALA	6.0
1	P	321	ALA	6.0
1	D	438	ILE	6.0
1	R	437	LYS	6.0
1	P	11	ILE	6.0
1	I	431	ASP	6.0
1	J	429	VAL	6.0
1	G	428	GLU	6.0
1	O	11	ILE	5.9
1	S	429	VAL	5.9
1	C	113	LEU	5.9
1	L	429	VAL	5.9
1	K	434	SER	5.9
1	Q	9	GLN	5.8
1	F	429	VAL	5.8
1	F	320	GLN	5.8
1	Q	430	ALA	5.8
1	Q	429	VAL	5.8
1	Q	11	ILE	5.8
1	B	9	GLN	5.8
1	J	10	GLN	5.8
1	A	8	THR	5.8
1	J	430	ALA	5.8
1	F	324	GLN	5.8
1	F	8	THR	5.8
1	R	431	ASP	5.8
1	N	428	GLU	5.8
1	E	9	GLN	5.7
1	I	321	ALA	5.7
1	I	10	GLN	5.7
1	L	431	ASP	5.7
1	G	433	ASN	5.7
1	K	437	LYS	5.7
1	P	438	ILE	5.7
1	J	113	LEU	5.7
1	K	11	ILE	5.7
1	M	11	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	10	GLN	5.7
1	S	11	ILE	5.6
1	T	438	ILE	5.6
1	A	322	GLY	5.6
1	K	9	GLN	5.6
1	D	223	GLY	5.6
1	T	435	PRO	5.6
1	S	428	GLU	5.6
1	I	11	ILE	5.5
1	F	436	LEU	5.5
1	C	8	THR	5.5
1	A	9	GLN	5.5
1	G	438	ILE	5.5
1	B	324	GLN	5.5
1	N	429	VAL	5.5
1	F	438	ILE	5.5
1	N	322	GLY	5.5
1	R	10	GLN	5.4
1	E	438	ILE	5.4
1	O	120	LEU	5.4
1	D	430	ALA	5.4
1	L	428	GLU	5.4
1	G	429	VAL	5.4
1	Q	322	GLY	5.4
1	J	321	ALA	5.4
1	L	433	ASN	5.4
1	M	437	LYS	5.4
1	E	11	ILE	5.3
1	T	321	ALA	5.3
1	T	223	GLY	5.3
1	P	431	ASP	5.3
1	S	113	LEU	5.3
1	J	324	GLN	5.2
1	O	113	LEU	5.2
1	N	10	GLN	5.2
1	T	9	GLN	5.2
1	J	437	LYS	5.2
1	B	431	ASP	5.2
1	E	436	LEU	5.2
1	N	113	LEU	5.2
1	N	9	GLN	5.2
1	P	425	TYR	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	321	ALA	5.2
1	T	431	ASP	5.2
1	I	428	GLU	5.2
1	O	8	THR	5.1
1	H	113	LEU	5.1
1	T	430	ALA	5.1
1	D	317	SER	5.1
1	B	425	TYR	5.1
1	C	436	LEU	5.1
1	N	11	ILE	5.1
1	M	431	ASP	5.1
1	T	10	GLN	5.1
1	C	321	ALA	5.1
1	O	428	GLU	5.1
1	E	434	SER	5.1
1	Q	428	GLU	5.1
1	D	436	LEU	5.1
1	A	429	VAL	5.0
1	F	11	ILE	5.0
1	G	322	GLY	5.0
1	D	428	GLU	5.0
1	L	10	GLN	5.0
1	C	222	PRO	5.0
1	R	428	GLU	5.0
1	B	320	GLN	5.0
1	H	321	ALA	5.0
1	L	321	ALA	5.0
1	B	223	GLY	5.0
1	B	217	SER	4.9
1	B	222	PRO	4.9
1	P	437	LYS	4.9
1	K	438	ILE	4.9
1	E	8	THR	4.9
1	Q	425	TYR	4.9
1	Q	437	LYS	4.9
1	T	428	GLU	4.9
1	K	425	TYR	4.8
1	Q	113	LEU	4.8
1	M	425	TYR	4.8
1	J	428	GLU	4.8
1	C	433	ASN	4.8
1	E	431	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	K	431	ASP	4.8
1	T	11	ILE	4.8
1	N	437	LYS	4.7
1	O	223	GLY	4.7
1	P	10	GLN	4.7
1	B	11	ILE	4.7
1	D	113	LEU	4.7
1	T	429	VAL	4.7
1	G	425	TYR	4.7
1	G	10	GLN	4.6
1	E	321	ALA	4.6
1	M	321	ALA	4.6
1	A	425	TYR	4.6
1	G	431	ASP	4.6
1	E	221	GLN	4.6
1	G	437	LYS	4.6
1	O	254	GLY	4.5
1	P	278	ALA	4.5
1	C	425	TYR	4.5
1	P	9	GLN	4.5
1	O	431	ASP	4.5
1	H	428	GLU	4.5
1	J	317	SER	4.5
1	L	322	GLY	4.5
1	F	437	LYS	4.5
1	G	219	GLN	4.5
1	G	9	GLN	4.5
1	A	11	ILE	4.4
1	J	223	GLY	4.4
1	I	220	TYR	4.4
1	F	222	PRO	4.4
1	N	222	PRO	4.4
1	F	323	ASP	4.4
1	D	286	THR	4.4
1	N	431	ASP	4.4
1	H	425	TYR	4.4
1	D	222	PRO	4.4
1	I	437	LYS	4.4
1	M	427	MET	4.4
1	K	222	PRO	4.4
1	O	425	TYR	4.4
1	B	113	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	H	320	GLN	4.4
1	C	428	GLU	4.4
1	K	324	GLN	4.3
1	J	431	ASP	4.3
1	T	113	LEU	4.3
1	H	222	PRO	4.3
1	I	222	PRO	4.3
1	P	322	GLY	4.3
1	G	220	TYR	4.3
1	S	430	ALA	4.3
1	C	76	GLY	4.3
1	P	324	GLN	4.3
1	I	279	ASN	4.3
1	T	437	LYS	4.2
1	P	286	THR	4.2
1	H	223	GLY	4.2
1	N	323	ASP	4.2
1	J	251	SER	4.2
1	Q	220	TYR	4.2
1	P	222	PRO	4.2
1	T	433	ASN	4.2
1	J	11	ILE	4.2
1	I	425	TYR	4.2
1	A	431	ASP	4.1
1	S	431	ASP	4.1
1	T	432	LEU	4.1
1	E	425	TYR	4.1
1	F	217	SER	4.1
1	M	113	LEU	4.1
1	A	222	PRO	4.1
1	D	9	GLN	4.1
1	D	323	ASP	4.1
1	P	428	GLU	4.1
1	K	223	GLY	4.1
1	B	428	GLU	4.0
1	S	317	SER	4.0
1	A	428	GLU	4.0
1	M	320	GLN	4.0
1	O	324	GLN	4.0
1	D	319	GLY	4.0
1	H	322	GLY	4.0
1	M	223	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	J	432	LEU	4.0
1	N	251	SER	4.0
1	R	417	ARG	4.0
1	K	318	GLY	3.9
1	A	113	LEU	3.9
1	K	320	GLN	3.9
1	H	317	SER	3.9
1	D	254	GLY	3.9
1	C	256	VAL	3.9
1	F	319	GLY	3.9
1	L	427	MET	3.9
1	Q	320	GLN	3.9
1	F	223	GLY	3.9
1	K	278	ALA	3.8
1	D	253	HIS	3.8
1	O	317	SER	3.8
1	F	279	ASN	3.8
1	A	432	LEU	3.8
1	G	223	GLY	3.8
1	N	223	GLY	3.8
1	A	76	GLY	3.8
1	I	427	MET	3.8
1	K	428	GLU	3.8
1	O	251	SER	3.8
1	H	220	TYR	3.8
1	R	425	TYR	3.8
1	C	317	SER	3.8
1	F	278	ALA	3.8
1	H	431	ASP	3.8
1	N	320	GLN	3.8
1	P	191	PRO	3.7
1	E	437	LYS	3.7
1	D	219	GLN	3.7
1	L	320	GLN	3.7
1	J	220	TYR	3.7
1	I	120	LEU	3.7
1	E	428	GLU	3.7
1	B	317	SER	3.7
1	I	323	ASP	3.7
1	C	217	SER	3.7
1	P	219	GLN	3.7
1	C	278	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	T	427	MET	3.7
1	C	320	GLN	3.6
1	P	317	SER	3.6
1	Q	324	GLN	3.6
1	R	427	MET	3.6
1	D	322	GLY	3.6
1	C	324	GLN	3.6
1	L	114	PRO	3.6
1	H	432	LEU	3.6
1	O	323	ASP	3.6
1	B	224	GLY	3.6
1	I	320	GLN	3.6
1	J	425	TYR	3.6
1	B	253	HIS	3.6
1	Q	323	ASP	3.6
1	C	286	THR	3.6
1	B	120	LEU	3.6
1	J	219	GLN	3.6
1	D	251	SER	3.6
1	J	315	SER	3.6
1	C	427	MET	3.6
1	Q	431	ASP	3.5
1	G	222	PRO	3.5
1	Q	317	SER	3.5
1	H	120	LEU	3.5
1	D	324	GLN	3.5
1	D	315	SER	3.5
1	N	217	SER	3.5
1	S	425	TYR	3.5
1	I	114	PRO	3.5
1	T	222	PRO	3.5
1	G	279	ASN	3.5
1	J	284	THR	3.5
1	K	432	LEU	3.5
1	H	324	GLN	3.5
1	K	427	MET	3.5
1	P	285	GLY	3.5
1	D	79	ASN	3.5
1	A	320	GLN	3.5
1	A	223	GLY	3.5
1	D	437	LYS	3.5
1	L	319	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	T	322	GLY	3.5
1	O	191	PRO	3.4
1	S	192	LYS	3.4
1	T	279	ASN	3.4
1	T	8	THR	3.4
1	I	223	GLY	3.4
1	B	278	ALA	3.4
1	G	324	GLN	3.4
1	H	427	MET	3.4
1	S	437	LYS	3.4
1	P	220	TYR	3.4
1	F	256	VAL	3.4
1	L	432	LEU	3.4
1	D	285	GLY	3.4
1	P	389	ARG	3.4
1	D	318	GLY	3.4
1	H	319	GLY	3.4
1	J	320	GLN	3.4
1	C	323	ASP	3.4
1	H	437	LYS	3.4
1	S	114	PRO	3.4
1	F	221	GLN	3.4
1	H	221	GLN	3.3
1	I	432	LEU	3.3
1	Q	432	LEU	3.3
1	H	219	GLN	3.3
1	H	318	GLY	3.3
1	Q	319	GLY	3.3
1	T	320	GLN	3.3
1	K	251	SER	3.3
1	P	251	SER	3.3
1	D	221	GLN	3.3
1	B	219	GLN	3.3
1	N	221	GLN	3.3
1	P	223	GLY	3.3
1	G	389	ARG	3.3
1	I	221	GLN	3.3
1	A	417	ARG	3.3
1	B	279	ASN	3.3
1	C	251	SER	3.3
1	I	286	THR	3.3
1	O	76	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	389	ARG	3.3
1	Q	284	THR	3.2
1	F	285	GLY	3.2
1	C	219	GLN	3.2
1	Q	253	HIS	3.2
1	H	11	ILE	3.2
1	A	219	GLN	3.2
1	D	284	THR	3.2
1	Q	318	GLY	3.2
1	L	425	TYR	3.2
1	L	389	ARG	3.2
1	O	320	GLN	3.2
1	P	320	GLN	3.2
1	D	427	MET	3.2
1	F	325	MET	3.2
1	F	318	GLY	3.2
1	S	120	LEU	3.2
1	K	279	ASN	3.2
1	C	318	GLY	3.2
1	H	256	VAL	3.2
1	C	114	PRO	3.2
1	T	221	GLN	3.2
1	P	432	LEU	3.2
1	F	215	GLN	3.2
1	C	223	GLY	3.2
1	C	285	GLY	3.2
1	J	279	ASN	3.2
1	L	120	LEU	3.2
1	L	251	SER	3.2
1	N	281	GLY	3.2
1	N	317	SER	3.2
1	T	324	GLN	3.2
1	G	427	MET	3.1
1	N	427	MET	3.1
1	E	322	GLY	3.1
1	I	113	LEU	3.1
1	F	212	ASP	3.1
1	N	324	GLN	3.1
1	E	432	LEU	3.1
1	S	191	PRO	3.1
1	J	319	GLY	3.1
1	F	251	SER	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	253	HIS	3.1
1	O	279	ASN	3.1
1	A	324	GLN	3.1
1	D	121	ASN	3.1
1	M	286	THR	3.1
1	A	51	ASP	3.1
1	K	192	LYS	3.1
1	R	192	LYS	3.1
1	C	253	HIS	3.0
1	J	286	THR	3.0
1	I	278	ALA	3.0
1	M	221	GLN	3.0
1	M	424	GLU	3.0
1	D	279	ASN	3.0
1	K	187	ILE	3.0
1	B	318	GLY	3.0
1	I	424	GLU	3.0
1	L	279	ASN	3.0
1	Q	219	GLN	3.0
1	D	114	PRO	3.0
1	J	316	LYS	3.0
1	Q	279	ASN	3.0
1	P	221	GLN	3.0
1	K	253	HIS	3.0
1	L	437	LYS	3.0
1	S	432	LEU	3.0
1	M	317	SER	3.0
1	O	424	GLU	3.0
1	A	316	LYS	2.9
1	C	279	ASN	2.9
1	N	280	ASN	2.9
1	Q	251	SER	2.9
1	K	281	GLY	2.9
1	C	283	THR	2.9
1	L	286	THR	2.9
1	B	191	PRO	2.9
1	O	222	PRO	2.9
1	D	287	ASP	2.9
1	H	323	ASP	2.9
1	B	221	GLN	2.9
1	B	432	LEU	2.9
1	G	320	GLN	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	256	VAL	2.9
1	F	431	ASP	2.9
1	D	76	GLY	2.9
1	G	432	LEU	2.9
1	D	278	ALA	2.9
1	S	321	ALA	2.9
1	I	324	GLN	2.9
1	O	319	GLY	2.9
1	F	315	SER	2.9
1	Q	223	GLY	2.9
1	K	286	THR	2.9
1	L	113	LEU	2.9
1	O	318	GLY	2.9
1	C	191	PRO	2.9
1	J	114	PRO	2.9
1	K	121	ASN	2.9
1	N	279	ASN	2.9
1	K	188	GLY	2.8
1	L	318	GLY	2.8
1	E	424	GLU	2.8
1	S	427	MET	2.8
1	J	222	PRO	2.8
1	P	254	GLY	2.8
1	A	253	HIS	2.8
1	B	277	ALA	2.8
1	O	114	PRO	2.8
1	Q	427	MET	2.8
1	L	317	SER	2.8
1	A	120	LEU	2.8
1	A	279	ASN	2.8
1	G	424	GLU	2.8
1	L	284	THR	2.8
1	M	279	ASN	2.8
1	B	427	MET	2.8
1	B	251	SER	2.8
1	O	218	SER	2.8
1	J	249	ARG	2.8
1	O	221	GLN	2.8
1	Q	222	PRO	2.8
1	M	324	GLN	2.8
1	O	287	ASP	2.8
1	R	432	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	191	PRO	2.8
1	N	114	PRO	2.8
1	B	319	GLY	2.8
1	D	389	ARG	2.8
1	B	114	PRO	2.7
1	E	427	MET	2.7
1	H	253	HIS	2.7
1	P	323	ASP	2.7
1	D	288	ASN	2.7
1	O	417	ARG	2.7
1	L	11	ILE	2.7
1	C	215	GLN	2.7
1	C	315	SER	2.7
1	E	317	SER	2.7
1	K	191	PRO	2.7
1	C	77	ASN	2.7
1	J	287	ASP	2.7
1	D	281	GLY	2.7
1	J	280	ASN	2.7
1	L	222	PRO	2.7
1	O	12	VAL	2.7
1	J	253	HIS	2.7
1	M	322	GLY	2.7
1	E	222	PRO	2.7
1	J	217	SER	2.7
1	Q	392	PRO	2.7
1	R	317	SER	2.7
1	A	221	GLN	2.7
1	K	258	GLY	2.7
1	J	120	LEU	2.7
1	M	220	TYR	2.7
1	O	212	ASP	2.7
1	O	215	GLN	2.7
1	A	427	MET	2.7
1	A	323	ASP	2.7
1	A	217	SER	2.7
1	C	316	LYS	2.7
1	C	221	GLN	2.6
1	D	191	PRO	2.6
1	P	225	VAL	2.6
1	I	121	ASN	2.6
1	Q	112	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	Q	285	GLY	2.6
1	P	279	ASN	2.6
1	K	389	ARG	2.6
1	G	212	ASP	2.6
1	C	258	GLY	2.6
1	N	424	GLU	2.6
1	C	120	LEU	2.6
1	H	417	ARG	2.6
1	A	319	GLY	2.6
1	O	217	SER	2.6
1	D	316	LYS	2.6
1	F	284	THR	2.6
1	F	213	ASP	2.6
1	F	316	LYS	2.6
1	B	77	ASN	2.6
1	R	279	ASN	2.6
1	Q	115	GLY	2.6
1	Q	315	SER	2.6
1	P	275	ALA	2.6
1	L	254	GLY	2.6
1	O	224	GLY	2.6
1	J	191	PRO	2.6
1	D	220	TYR	2.6
1	B	289	LEU	2.6
1	F	218	SER	2.6
1	H	114	PRO	2.5
1	H	192	LYS	2.5
1	L	221	GLN	2.5
1	D	424	GLU	2.5
1	J	318	GLY	2.5
1	Q	254	GLY	2.5
1	O	427	MET	2.5
1	T	114	PRO	2.5
1	Q	76	GLY	2.5
1	A	317	SER	2.5
1	J	221	GLN	2.5
1	F	424	GLU	2.5
1	B	280	ASN	2.5
1	K	323	ASP	2.5
1	L	323	ASP	2.5
1	Q	391	ASP	2.5
1	C	319	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	76	GLY	2.5
1	J	330	ARG	2.5
1	L	324	GLN	2.5
1	K	51	ASP	2.5
1	O	226	THR	2.5
1	Q	389	ARG	2.5
1	H	285	GLY	2.5
1	J	12	VAL	2.5
1	D	325	MET	2.5
1	A	77	ASN	2.5
1	F	314	THR	2.5
1	G	353	ALA	2.5
1	O	286	THR	2.5
1	F	219	GLN	2.5
1	J	212	ASP	2.5
1	J	417	ARG	2.5
1	L	417	ARG	2.5
1	J	224	GLY	2.5
1	M	114	PRO	2.5
1	P	253	HIS	2.5
1	I	316	LYS	2.5
1	M	212	ASP	2.5
1	A	114	PRO	2.4
1	M	222	PRO	2.4
1	F	253	HIS	2.4
1	I	192	LYS	2.4
1	Q	278	ALA	2.4
1	Q	326	SER	2.4
1	I	318	GLY	2.4
1	J	142	ASN	2.4
1	D	268	GLY	2.4
1	E	219	GLN	2.4
1	H	281	GLY	2.4
1	L	223	GLY	2.4
1	R	322	GLY	2.4
1	A	286	THR	2.4
1	L	283	THR	2.4
1	A	226	THR	2.4
1	C	284	THR	2.4
1	F	249	ARG	2.4
1	L	253	HIS	2.4
1	J	283	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	424	GLU	2.4
1	I	212	ASP	2.4
1	B	220	TYR	2.4
1	I	76	GLY	2.4
1	O	220	TYR	2.4
1	F	283	THR	2.4
1	N	219	GLN	2.4
1	S	76	GLY	2.4
1	J	424	GLU	2.4
1	F	427	MET	2.4
1	M	323	ASP	2.4
1	D	78	GLY	2.4
1	T	285	GLY	2.4
1	E	191	PRO	2.3
1	G	215	GLN	2.3
1	N	191	PRO	2.3
1	O	285	GLY	2.3
1	P	115	GLY	2.3
1	Q	121	ASN	2.3
1	B	390	PHE	2.3
1	B	215	GLN	2.3
1	D	212	ASP	2.3
1	B	218	SER	2.3
1	I	317	SER	2.3
1	L	76	GLY	2.3
1	O	278	ALA	2.3
1	J	323	ASP	2.3
1	B	76	GLY	2.3
1	D	417	ARG	2.3
1	F	317	SER	2.3
1	N	417	ARG	2.3
1	D	213	ASP	2.3
1	J	51	ASP	2.3
1	O	330	ARG	2.3
1	C	325	MET	2.3
1	Q	217	SER	2.3
1	A	192	LYS	2.3
1	G	57	ILE	2.3
1	B	417	ARG	2.3
1	D	224	GLY	2.3
1	A	218	SER	2.3
1	G	317	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	253	HIS	2.3
1	N	286	THR	2.3
1	F	187	ILE	2.3
1	N	225	VAL	2.3
1	A	284	THR	2.3
1	D	214	TYR	2.3
1	Q	214	TYR	2.3
1	D	187	ILE	2.3
1	D	256	VAL	2.3
1	F	225	VAL	2.3
1	N	51	ASP	2.3
1	A	278	ALA	2.2
1	G	323	ASP	2.2
1	T	319	GLY	2.2
1	A	215	GLN	2.2
1	A	121	ASN	2.2
1	N	77	ASN	2.2
1	B	316	LYS	2.2
1	G	278	ALA	2.2
1	P	427	MET	2.2
1	E	391	ASP	2.2
1	R	320	GLN	2.2
1	J	189	LEU	2.2
1	F	389	ARG	2.2
1	M	330	ARG	2.2
1	A	426	PHE	2.2
1	O	219	GLN	2.2
1	C	57	ILE	2.2
1	T	57	ILE	2.2
1	G	251	SER	2.2
1	J	121	ASN	2.2
1	N	253	HIS	2.2
1	K	220	TYR	2.2
1	C	213	ASP	2.2
1	I	391	ASP	2.2
1	K	287	ASP	2.2
1	M	284	THR	2.2
1	A	220	TYR	2.2
1	R	426	PHE	2.2
1	G	191	PRO	2.2
1	K	114	PRO	2.2
1	K	316	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	224	GLY	2.2
1	K	417	ARG	2.2
1	I	215	GLN	2.2
1	M	285	GLY	2.2
1	D	273	THR	2.2
1	O	284	THR	2.2
1	J	218	SER	2.1
1	L	219	GLN	2.1
1	I	191	PRO	2.1
1	C	224	GLY	2.1
1	E	51	ASP	2.1
1	I	285	GLY	2.1
1	Q	283	THR	2.1
1	C	252	VAL	2.1
1	C	51	ASP	2.1
1	E	389	ARG	2.1
1	H	286	THR	2.1
1	O	112	THR	2.1
1	P	424	GLU	2.1
1	B	121	ASN	2.1
1	P	217	SER	2.1
1	I	213	ASP	2.1
1	Q	191	PRO	2.1
1	C	437	LYS	2.1
1	S	121	ASN	2.1
1	C	389	ARG	2.1
1	C	417	ARG	2.1
1	N	318	GLY	2.1
1	Q	120	LEU	2.1
1	Q	188	GLY	2.1
1	S	389	ARG	2.1
1	C	424	GLU	2.1
1	P	280	ASN	2.1
1	N	218	SER	2.1
1	D	255	LEU	2.1
1	I	224	GLY	2.1
1	Q	406	ASP	2.1
1	K	221	GLN	2.1
1	O	121	ASN	2.1
1	M	389	ARG	2.1
1	M	432	LEU	2.1
1	E	359	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	218	SER	2.1
1	F	281	GLY	2.1
1	H	51	ASP	2.1
1	J	254	GLY	2.1
1	O	432	LEU	2.0
1	M	57	ILE	2.0
1	J	278	ALA	2.0
1	R	424	GLU	2.0
1	O	213	ASP	2.0
1	P	181	GLY	2.0
1	D	432	LEU	2.0
1	O	389	ARG	2.0
1	N	278	ALA	2.0
1	M	326	SER	2.0
1	C	426	PHE	2.0
1	T	120	LEU	2.0
1	D	218	SER	2.0
1	P	51	ASP	2.0
1	P	76	GLY	2.0
1	S	13	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	L	507	1/1	0.95	0.12	2,2,2,2	1
2	CA	O	509	1/1	0.95	0.19	2,2,2,2	0
2	CA	A	501	1/1	0.95	0.12	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	D	504	1/1	0.97	0.17	2,2,2,2	1
2	CA	M	508	1/1	0.97	0.09	2,2,2,2	1
2	CA	S	510	1/1	0.97	0.09	5,5,5,5	1
2	CA	B	502	1/1	0.98	0.19	12,12,12,12	1
2	CA	G	506	1/1	0.98	0.12	2,2,2,2	0
2	CA	F	505	1/1	0.99	0.11	2,2,2,2	0
2	CA	T	511	1/1	0.99	0.13	4,4,4,4	1
2	CA	C	503	1/1	0.99	0.17	2,2,2,2	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.