



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:30 AM GMT

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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

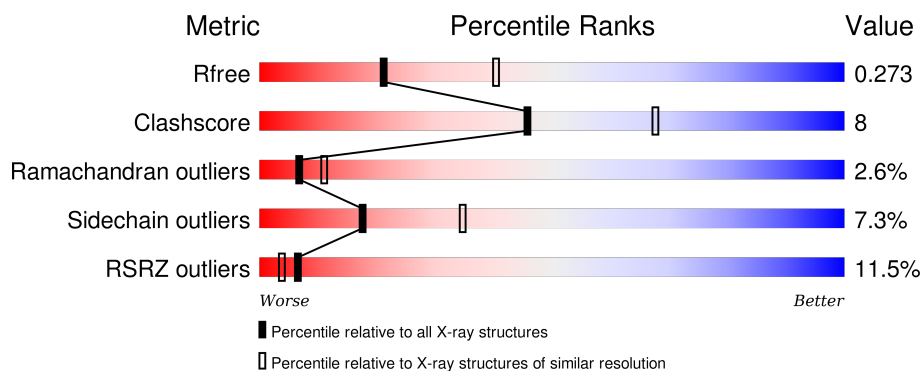
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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. 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	
1	B	456	
1	C	456	
1	D	456	
1	E	456	

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Mol	Chain	Length	Quality of chain
1	F	456	
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.

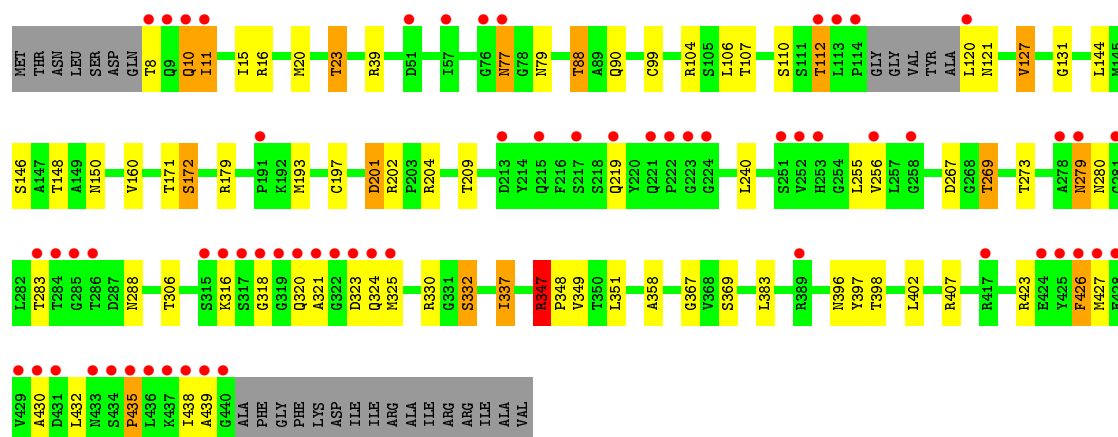
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	4	Total	O	0	0
			4	4		

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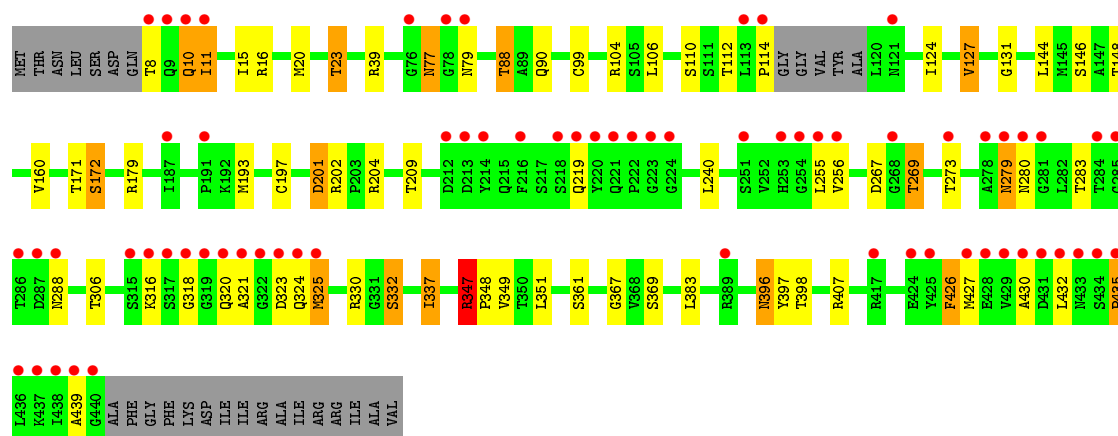
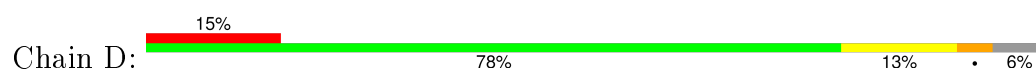
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total 2	O 2	0	0
3	D	2	Total 2	O 2	0	0
3	E	8	Total 8	O 8	0	0
3	F	4	Total 4	O 4	0	0
3	G	6	Total 6	O 6	0	0
3	H	7	Total 7	O 7	0	0
3	I	6	Total 6	O 6	0	0
3	J	1	Total 1	O 1	0	0
3	K	7	Total 7	O 7	0	0
3	L	6	Total 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

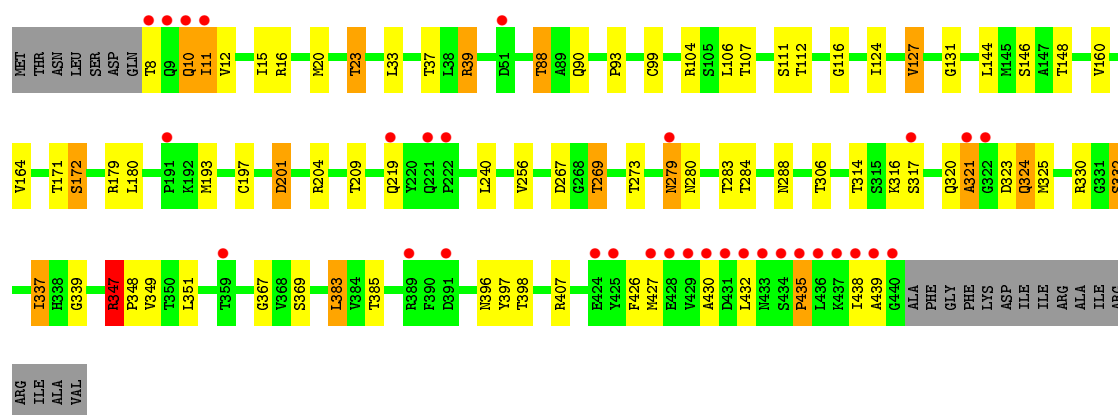
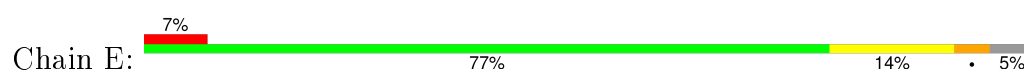




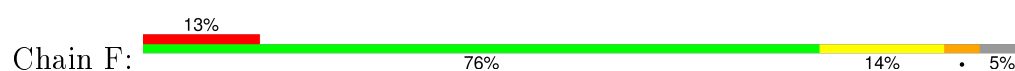
• Molecule 1: polypeptide



• Molecule 1: polypeptide

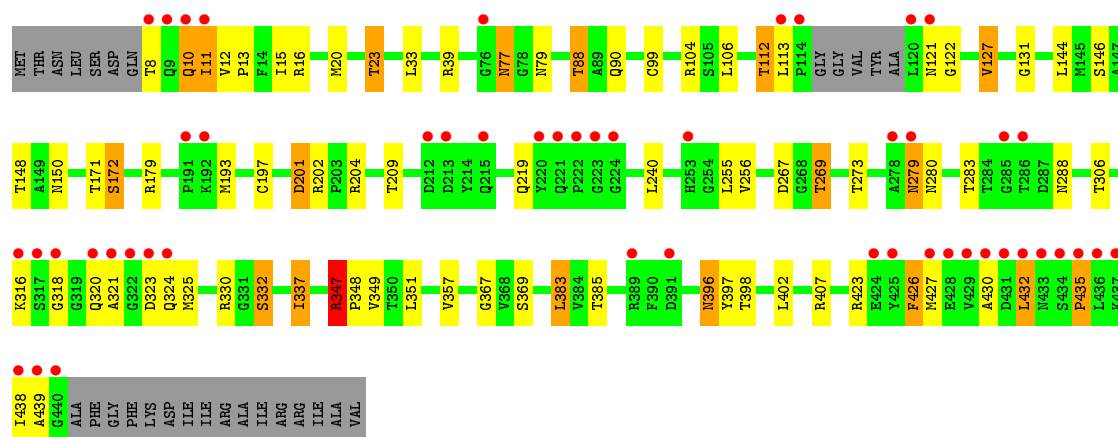


• Molecule 1: polypeptide

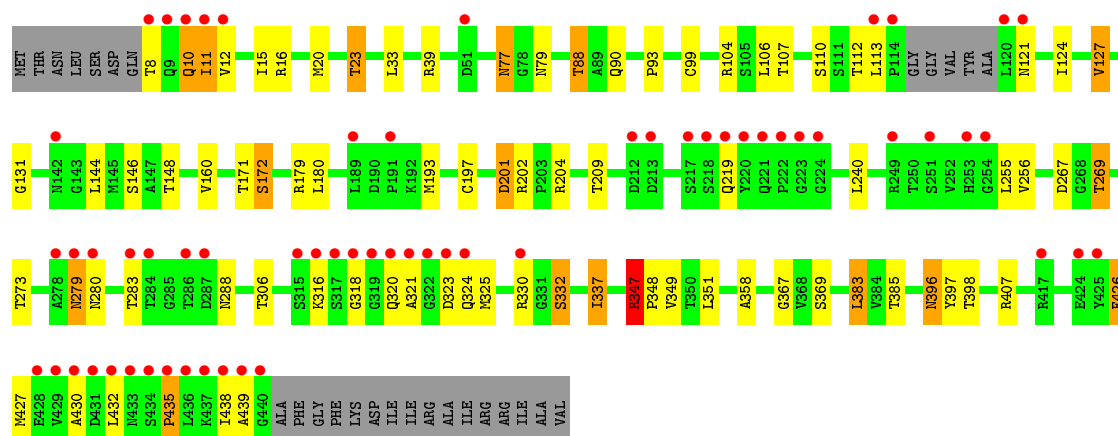
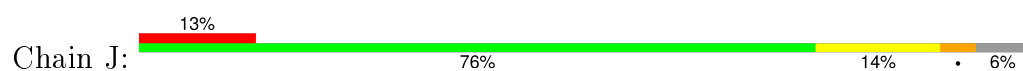




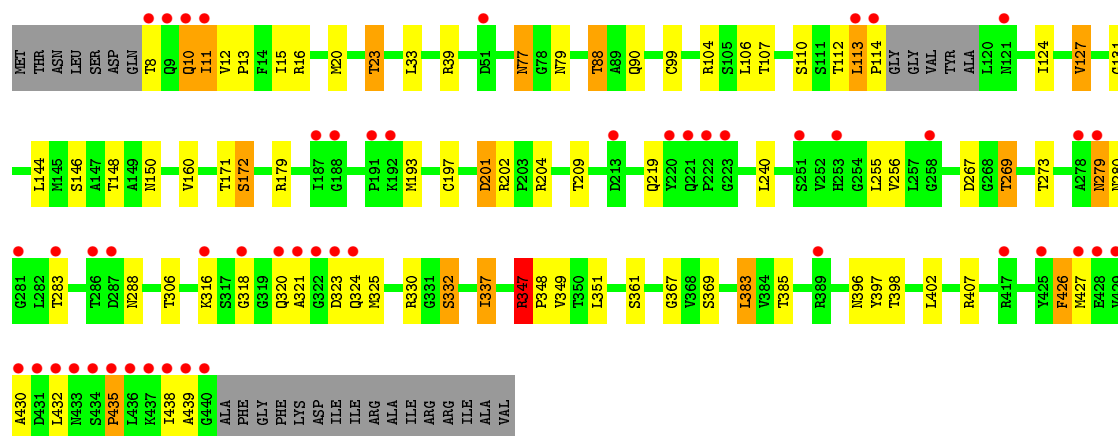
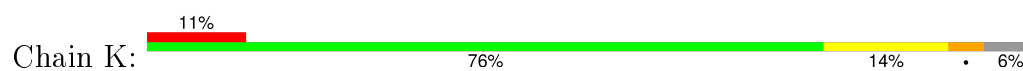




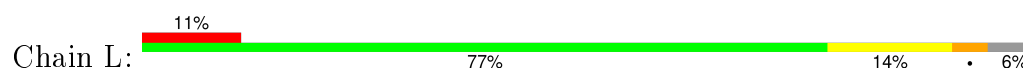
• Molecule 1: polypeptide

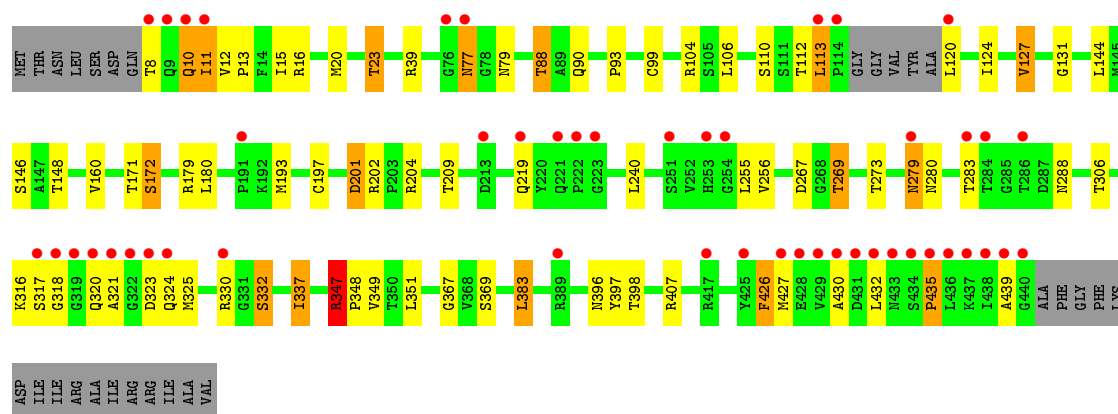


• Molecule 1: polypeptide

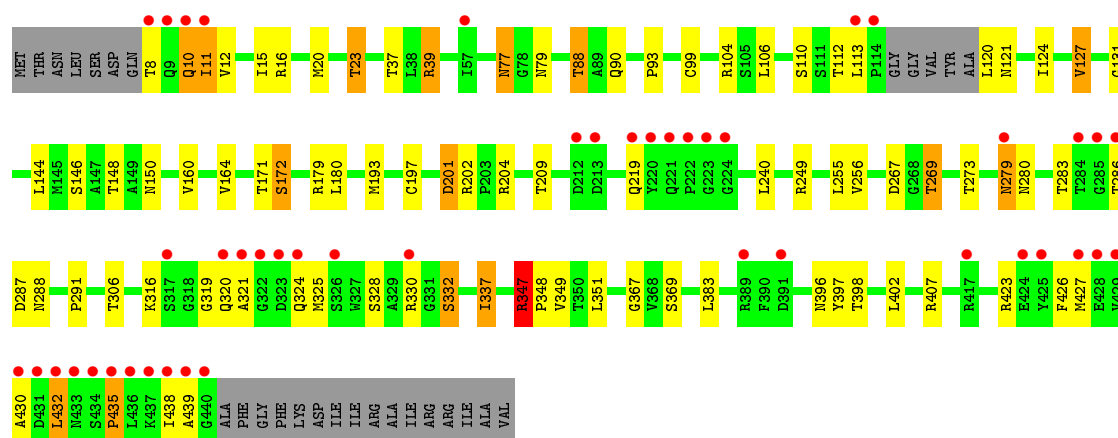
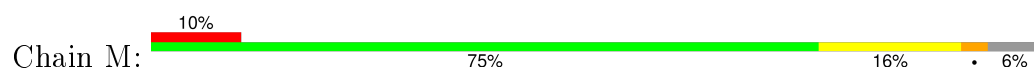


• Molecule 1: polypeptide

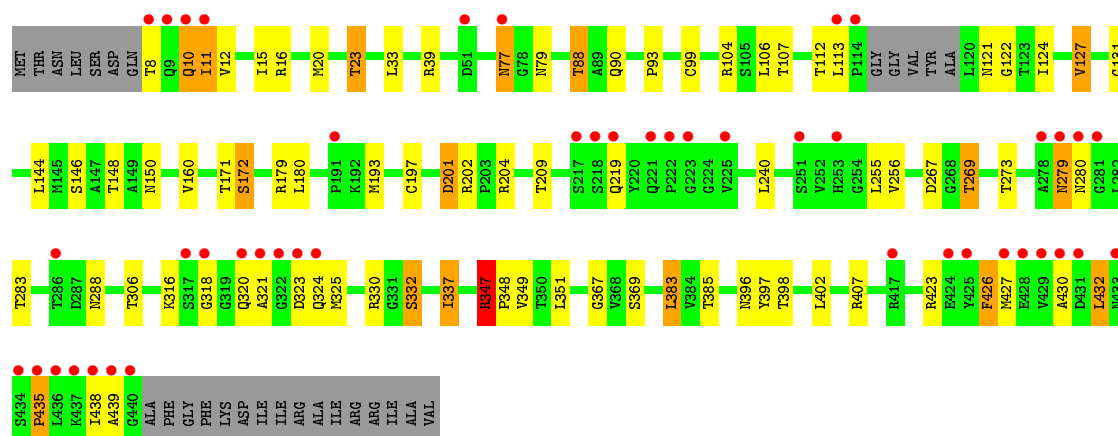
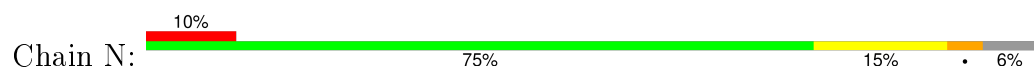




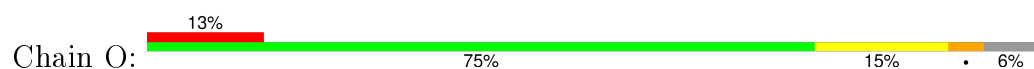
• Molecule 1: polyprotein

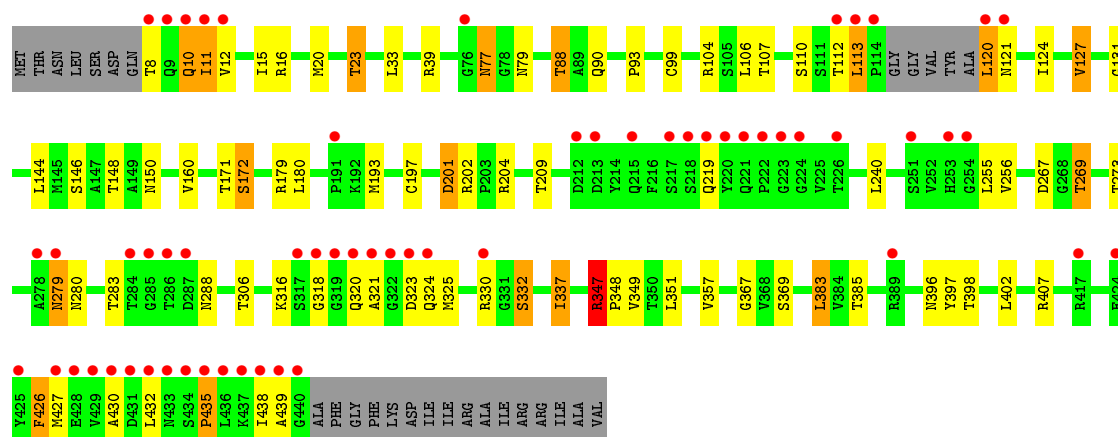


• Molecule 1: polyprotein

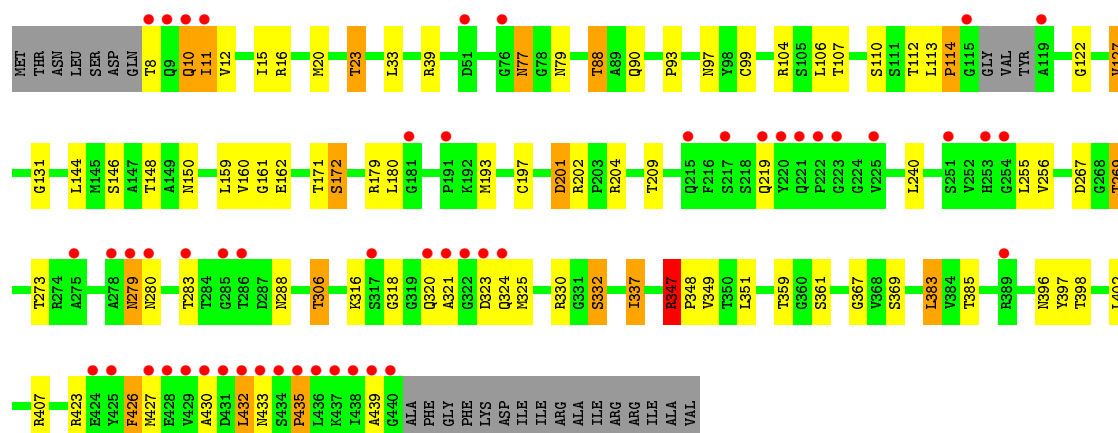
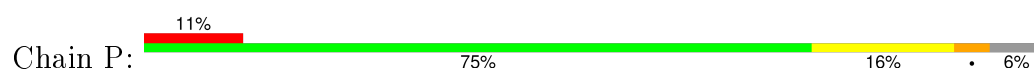


• Molecule 1: polyprotein

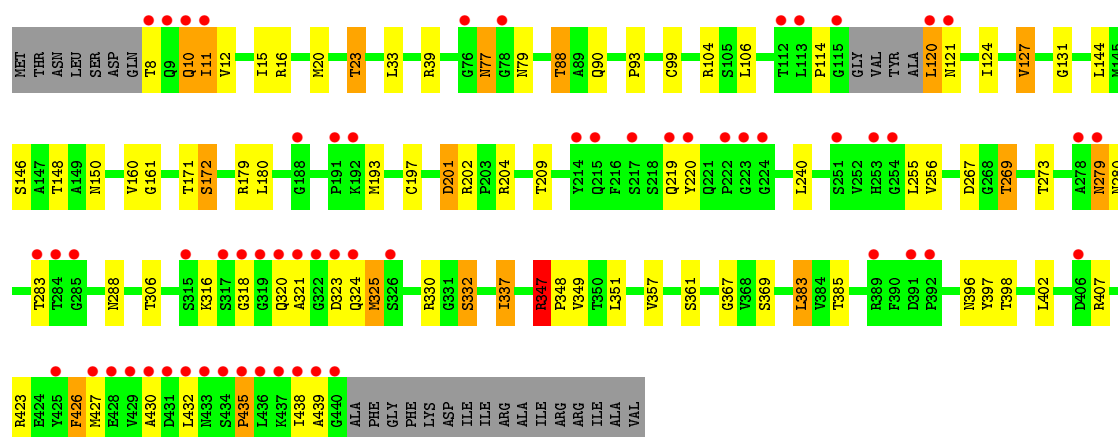
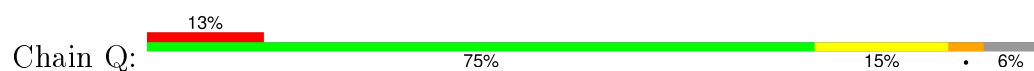




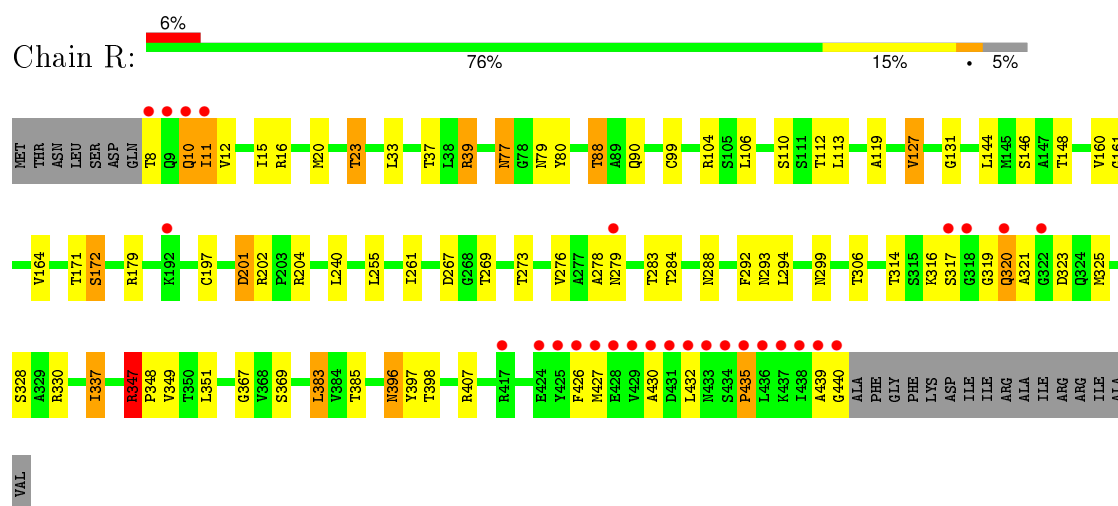
- Molecule 1: polypeptide



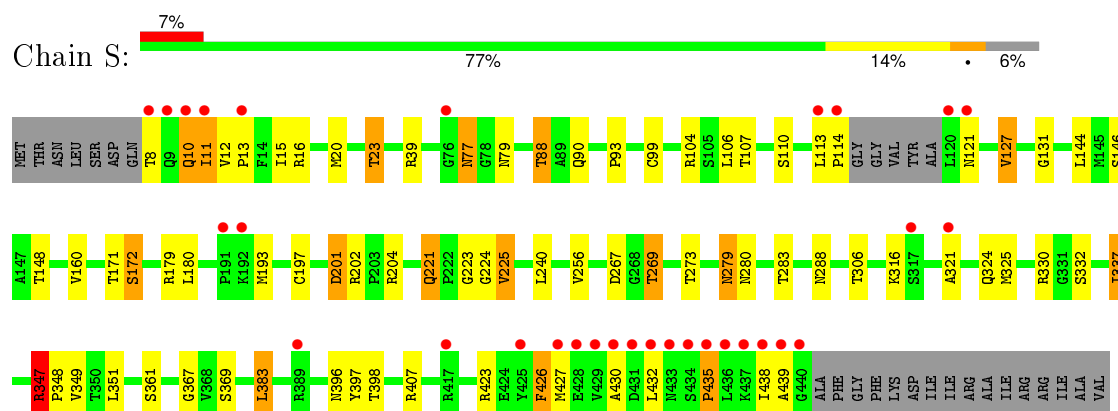
- Molecule 1: polypeptide



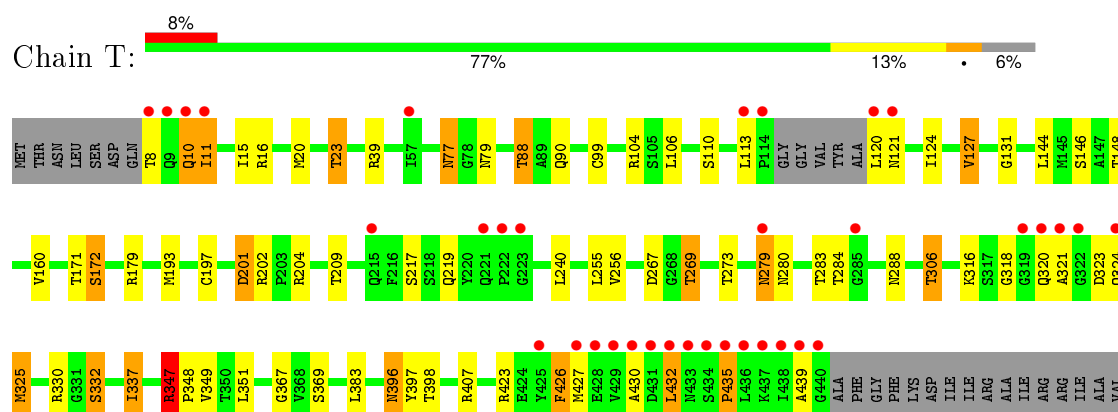
- Molecule 1: polypeptide



- Molecule 1: polyprotein



- Molecule 1: polyprotein



## 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 0.266 , 0.273	Depositor DCC
$R_{free}$ test set	15645 reflections (5.03%)	DCC
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 , 12.3	EDS
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 311078 reflections	Xtriage
$F_o, F_c$ correlation	0.87	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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:R:110:SER:HB3	1:R:160:VAL:CG1	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:204:ARG:HD2	1:L:337:ILE:HD11	1.57	0.87
1:C:204:ARG:HD2	1:C:337:ILE:HD11	1.57	0.86
1:B:204:ARG:HD2	1:B:337:ILE:HD11	1.57	0.86
1:P:204:ARG:HD2	1:P:337:ILE:HD11	1.57	0.86
1:A:204:ARG:HD2	1:A:337:ILE:HD11	1.56	0.86
1:F:204:ARG:HD2	1:F:337:ILE:HD11	1.56	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:R:204:ARG:HB3	1:R:337:ILE:CD1	2.07	0.85
1:O:204:ARG:HD2	1:O:337:ILE:HD11	1.57	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:C:150:ASN:HD21	1:J:385:THR:H	1.29	0.81
1:F:150:ASN:HD21	1:K:385:THR:H	1.26	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:P:306:THR:HG22	3:P:720:HOH:O	1.82	0.78
1:O:385:THR:H	1:Q:150:ASN:HD21	1.28	0.78
1:G:88:THR:HG22	1:G:90:GLN:O	1.83	0.78
1:F:88:THR:HG22	1:F: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:A:88:THR:HG22	1:A: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:K:20:MET:O	1:K:23:THR:HB	1.85	0.77
1:E:20:MET:O	1:E:23:THR:HB	1.84	0.77
1:O:20:MET:O	1:O:23:THR:HB	1.85	0.77
1:L:88:THR:HG22	1:L:90:GLN:O	1.84	0.77
1:S:88:THR:HG22	1:S:90:GLN:O	1.85	0.77
1:J:20:MET:O	1:J:23:THR:HB	1.85	0.77
1:G:20:MET:O	1:G:23:THR:HB	1.85	0.77
1:S:316:LYS:HB2	1:S:325:MET:HE2	1.65	0.77
1:L:20:MET:O	1:L:23:THR:HB	1.85	0.77
1:C:20:MET:O	1:C: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:F:347:ARG:HB3	1:F:348:PRO:HD3	1.69	0.74
1:E:347:ARG:HB3	1:E: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:I:347:ARG:HB3	1:I:348:PRO:HD3	1.69	0.74
1:D:347:ARG:HB3	1:D:348:PRO:HD3	1.68	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:L:16:ARG:HG2	1:L:23:THR:HG21	1.74	0.69
1:F:16:ARG:HG2	1:F:23:THR:HG21	1.74	0.69
1:S:16:ARG:HG2	1:S:23:THR:HG21	1.74	0.69
1:K:11:ILE:HD11	1:K:16:ARG:HD2	1.75	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:16:ARG:HG2	1:K:23:THR:HG21	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:C:11:ILE:HD11	1:C:16:ARG:HD2	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:L:11:ILE:HD11	1:L: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: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: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:M:104:ARG:HD3	1:M:369:SER:OG	1.94	0.68
1:A:16:ARG:HG2	1:A:23:THR:HG21	1.75	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:D:267:ASP:OD1	1:D:269:THR:HB	1.94	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:N:16:ARG:HG2	1:N:23:THR:HG21	1.75	0.68
1:A:267:ASP:OD1	1:A:269:THR:HB	1.94	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:I:11:ILE:HD11	1:I:16:ARG:HD2	1.75	0.67
1:F:11:ILE:HD11	1:F:16:ARG:HD2	1.76	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:Q:11:ILE:HD11	1:Q:16:ARG:HD2	1.75	0.67
1:G:104:ARG:HD3	1:G:369:SER:OG	1.95	0.67
1:T:267:ASP:OD1	1:T:269:THR:HB	1.95	0.67
1:T:131:GLY:O	1:T:347:ARG:O	2.13	0.67
1:M:11:ILE:HD11	1:M:16:ARG:HD2	1.75	0.67
1:H:267:ASP:OD1	1:H:269:THR:HB	1.95	0.67
1:T:16:ARG:HG2	1:T:23:THR:HG21	1.75	0.67
1:N:11:ILE:HD11	1:N:16:ARG:HD2	1.75	0.67
1:J:267:ASP:OD1	1:J:269:THR:HB	1.95	0.67
1:P:104:ARG:HD3	1:P:369:SER:OG	1.95	0.67
1:K:267:ASP:OD1	1:K:269:THR:HB	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:R:11:ILE:HD11	1:R:16:ARG:HD2	1.76	0.66
1:L:267:ASP:OD1	1:L:269:THR:HB	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: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:S:267:ASP:OD1	1:S:269:THR:HB	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:N:131:GLY:O	1:N:347:ARG:O	2.14	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:A:104:ARG:HD3	1:A:369:SER:OG	1.96	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

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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:Q:131:GLY:O	1:Q:347:ARG:O	2.14	0.66
1:O:283:THR:H	1:O:288:ASN:HD21	1.44	0.66
1:G:283:THR:H	1:G:288:ASN:HD21	1.43	0.66
1:C:104:ARG:HD3	1:C:369:SER:OG	1.95	0.66
1:Q:267:ASP:OD1	1:Q:269:THR:HB	1.96	0.66
1:G:131:GLY:O	1:G:347:ARG:O	2.13	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:C:283:THR:H	1:C:288:ASN:HD21	1.44	0.66
1:H:104:ARG:HD3	1:H:369:SER:OG	1.96	0.66
1:D:131:GLY:O	1:D:347:ARG:O	2.14	0.66
1:L:110:SER:HB3	1:L:160:VAL:HG12	1.78	0.66
1:T:110:SER:HB3	1:T:160:VAL:HG12	1.78	0.66
1:F:283:THR:H	1:F:288:ASN:HD21	1.44	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: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:349:VAL:HG12	1:P:351:LEU:HD12	1.78	0.65
1:P:267:ASP:OD1	1:P:269:THR:HB	1.95	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:F:267:ASP:OD1	1:F:269:THR:HB	1.95	0.65
1:C:349:VAL:HG12	1:C:351:LEU:HD12	1.78	0.65
1:P:131:GLY:O	1:P:347:ARG:O	2.13	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: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:L:131:GLY:O	1:L:347:ARG:O	2.14	0.65
1:J:349:VAL:HG12	1:J:351:LEU:HD12	1.79	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: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:349:VAL:HG12	1:E:351:LEU:HD12	1.79	0.64
1:E:267:ASP:OD1	1:E:269:THR:HB	1.97	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: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:D:349:VAL:HG12	1:D:351:LEU:HD12	1.79	0.64
1:J:283:THR:H	1:J:288:ASN:HD21	1.44	0.64
1:E:16:ARG:HG2	1:E:23:THR:HG21	1.77	0.64
1:K:131:GLY:O	1:K:347:ARG:O	2.14	0.64
1:H:349:VAL:HG12	1:H:351:LEU:HD12	1.78	0.64
1:R:316:LYS:HB2	1:R:325:MET:HE3	1.80	0.64
1:M:283:THR:H	1:M:288:ASN:HD21	1.46	0.64
1:A:131:GLY:O	1:A:347:ARG:O	2.15	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:B:283:THR:H	1:B:288:ASN:HD21	1.44	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: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:K:349:VAL:HG12	1:K:351:LEU:HD12	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: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:A:283:THR:H	1:A:288:ASN:HD21	1.44	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:S:121:ASN:O	1:S:160:VAL:HB	1.99	0.62
1:N:179:ARG:HD3	1:N:197:CYS:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:179:ARG:HD3	1:O:197:CYS:HB3	1.82	0.61
1:I:179:ARG:HD3	1:I: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:K:383:LEU:HD22	1:P:383:LEU:HD22	1.82	0.61
1:E:314:THR:HG22	1:E:325:MET:HE1	1.82	0.61
1:Q:179:ARG:HD3	1:Q:197:CYS:HB3	1.82	0.61
1:J:383:LEU:HD22	1:O:383:LEU:HD22	1.82	0.61
1:C:179:ARG:HD3	1:C:197:CYS:HB3	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:L:179:ARG:HD3	1:L:197:CYS:HB3	1.83	0.60
1:H:179:ARG:HD3	1:H:197:CYS:HB3	1.82	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:D:88:THR:CG2	1:D:90:GLN:O	2.51	0.58
1:C:88:THR:CG2	1:C:90:GLN:O	2.52	0.58
1:T:88:THR:CG2	1:T:90:GLN:O	2.52	0.58
1:J:88:THR:CG2	1:J:90:GLN:O	2.52	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:I:255:LEU:HD23	1:I:316:LYS:HG3	1.86	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:K:88:THR:CG2	1:K:90:GLN:O	2.52	0.57
1:L:255:LEU:HD23	1:L:316:LYS:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:255:LEU:HD23	1:K:316:LYS:HG3	1.86	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:M:15:ILE:HG13	1:M:397:TYR:HD2	1.70	0.57
1:C:255:LEU:HD23	1:C:316:LYS:HG3	1.86	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:G:385:THR:N	1:N:150:ASN:HD21	2.00	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: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:Q:88:THR:CG2	1:Q:90:GLN:O	2.52	0.56
1:M:316:LYS:HE2	1:M:319:GLY:H	1.70	0.56
1:Q:114:PRO:HD3	1:Q:361:SER:HB3	1.88	0.56
1:P:15:ILE:HG13	1:P:397:TYR:HD2	1.70	0.56
1:P:88:THR:CG2	1:P:90:GLN:O	2.51	0.56
1:R:88:THR:CG2	1:R:90:GLN:O	2.52	0.56
1:R:319:GLY:C	1:R:320:GLN:HG2	2.26	0.56
1:E:15:ILE:HG13	1:E:397:TYR:HD2	1.70	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:F:383:LEU:HD22	1:S:383:LEU:HD22	1.88	0.56
1:K:15:ILE:HG13	1:K:397:TYR:HD2	1.70	0.56
1:H:88:THR:CG2	1:H:90:GLN:O	2.53	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: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:P:11:ILE:CD1	1:P:16:ARG:HD2	2.36	0.56
1:L:88:THR:CG2	1:L:90:GLN:O	2.52	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: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:N:15:ILE:HG13	1:N:397:TYR:HD2	1.70	0.55
1:B:88:THR:CG2	1:B:90:GLN:O	2.52	0.55
1:A:88:THR:CG2	1:A:90:GLN:O	2.52	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: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:J:11:ILE:CD1	1:J:16:ARG:HD2	2.37	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:R:283:THR:H	1:R:288:ASN:ND2	2.05	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:S:88:THR:CG2	1:S:90:GLN:O	2.54	0.55
1:L:11:ILE:CD1	1:L:16:ARG:HD2	2.36	0.55
1:I:11:ILE:CD1	1:I:16:ARG:HD2	2.36	0.55
1:S:347:ARG:HB3	1:S:348:PRO:CD	2.35	0.55
1:D:15:ILE:HG13	1:D:397:TYR:HD2	1.70	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:Q:11:ILE:CD1	1:Q:16:ARG:HD2	2.37	0.55
1:M:11:ILE:CD1	1:M:16:ARG:HD2	2.36	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:S:11:ILE:CD1	1:S:16:ARG:HD2	2.37	0.54
1:P:114:PRO:HG3	1:P:359:THR:O	2.08	0.54
1:H:426:PHE:CG	1:H:427:MET:N	2.76	0.54
1:R:349:VAL:HG12	1:R:351:LEU:CD1	2.37	0.54
1:O:15:ILE:HG13	1:O:397:TYR:HD2	1.70	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: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: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: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:I:347:ARG:HB3	1:I:348:PRO:CD	2.38	0.53
1:B:426:PHE:CG	1:B:427:MET:N	2.76	0.53
1:K:347:ARG:HB3	1:K:348:PRO:CD	2.38	0.53
1:D:347:ARG:HB3	1:D:348:PRO:CD	2.38	0.53
1:T:426:PHE:CG	1:T:427:MET:N	2.76	0.53
1:Q:426:PHE:CG	1:Q:427:MET:N	2.76	0.53
1:T:11:ILE:CD1	1:T:16:ARG:HD2	2.36	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:I:349:VAL:HG12	1:I:351:LEU:CD1	2.39	0.53
1:A:426:PHE:CG	1:A:427:MET:N	2.76	0.53
1:S:349:VAL:HG12	1:S:351:LEU:CD1	2.38	0.53
1:M:15:ILE:HD11	1:M:398:THR:HA	1.90	0.53
1:G:426:PHE:CG	1:G:427:MET:N	2.76	0.53
1:R:11:ILE:CD1	1:R:16:ARG:HD2	2.37	0.53
1:G:349:VAL:HG12	1:G:351:LEU:CD1	2.39	0.53
1:S:426:PHE:CG	1:S:427:MET:N	2.77	0.53
1:M:426:PHE:CG	1:M:427:MET:N	2.76	0.53
1:L:426:PHE:CG	1:L:427:MET:N	2.76	0.53
1:A:402:LEU:HD12	1:E:33:LEU:HD13	1.88	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: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:L:349:VAL:HG12	1:L:351:LEU:CD1	2.39	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:E:11:ILE:CD1	1:E:16:ARG:HD2	2.39	0.53
1:O:171:THR:HG21	1:O:348:PRO:HG3	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:110:SER:CB	1:R:160:VAL:HG12	2.29	0.53
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:S:179:ARG:CD	1:S:197:CYS:SG	2.96	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:T:347:ARG:HB3	1:T:348:PRO:CD	2.38	0.53
1:N:349:VAL:HG12	1:N:351:LEU:CD1	2.39	0.53
1:E:396:ASN:H	1:E:396:ASN:HD22	1.57	0.53
1:L:171:THR:HG21	1:L:348:PRO:HG3	1.91	0.52
1:D:171:THR:HG21	1:D:348:PRO:HG3	1.91	0.52
1:A:349:VAL:HG12	1:A:351:LEU:CD1	2.39	0.52
1:O:402:LEU:HD12	1:P:33:LEU:HD13	1.91	0.52
1:D:396:ASN:H	1:D:396:ASN:HD22	1.57	0.52
1:G:171:THR:HG21	1:G:348:PRO:HG3	1.91	0.52
1:B:349:VAL:HG12	1:B:351:LEU:CD1	2.39	0.52
1:H:349:VAL:HG12	1:H:351:LEU:CD1	2.39	0.52
1:C:426:PHE:CG	1:C:427:MET:N	2.76	0.52
1:I:396:ASN:HD22	1:I:396:ASN:H	1.57	0.52
1:C:396:ASN:HD22	1:C:396:ASN:H	1.58	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:H:171:THR:HG21	1:H:348:PRO:HG3	1.92	0.52
1:C:349:VAL:HG12	1:C:351:LEU:CD1	2.39	0.52
1:R:171:THR:HG21	1:R:348:PRO:HG3	1.90	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:F:119:ALA:HB3	1:P:113:LEU:HD11	1.92	0.52
1:H:396:ASN:HD22	1:H:396:ASN:H	1.57	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:T:171:THR:HG21	1:T:348:PRO:HG3	1.92	0.52
1:B:171:THR:HG21	1:B:348:PRO:HG3	1.91	0.52
1:M:349:VAL:HG12	1:M:351:LEU:CD1	2.40	0.52

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:15:ILE:HD11	1:Q:398:THR:HA	1.93	0.50
1:F:15:ILE:HD11	1:F:398:THR:HA	1.93	0.50
1:B:396:ASN:H	1:B:396:ASN:HD22	1.57	0.50
1:R:171:THR:O	1:R:172:SER:HB3	2.11	0.50
1:Q:171:THR:HG21	1:Q:348:PRO:HG3	1.91	0.50
1:H:15:ILE:HD11	1:H:398:THR:HA	1.93	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:J:15:ILE:HD11	1:J:398:THR:HA	1.93	0.50
1:R:15:ILE:HD11	1:R:398:THR:HA	1.93	0.50
1:A:15:ILE:HD11	1:A:398:THR:HA	1.93	0.50
1:O:15:ILE:HD11	1:O:398:THR:HA	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: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: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:I:179:ARG:CD	1:I:197:CYS:SG	3.00	0.50
1:F:179:ARG:CD	1:F:197:CYS:SG	3.00	0.50
1:B:15:ILE:HD11	1:B:398:THR:HA	1.93	0.50
1:L:15:ILE:HD11	1:L:398:THR:HA	1.93	0.50
1:K:15:ILE:HD11	1:K:398:THR:HA	1.93	0.50
1:F:385:THR:N	1:I:150:ASN:HD21	2.04	0.49
1:G:15:ILE:HD11	1:G:398:THR:HA	1.93	0.49
1:K:171:THR:O	1:K:172:SER:HB3	2.12	0.49
1:T:110:SER:CB	1:T:160:VAL:HG12	2.41	0.49
1:L:179:ARG:CD	1:L:197:CYS:SG	3.00	0.49
1:B:179:ARG:CD	1:B:197:CYS:SG	3.01	0.49
1:F:150:ASN:HD21	1:K:385:THR:N	2.02	0.49
1:C:15:ILE:HD11	1:C:398:THR:HA	1.93	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:R:204:ARG:HB3	1:R:337:ILE:HD11	1.89	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: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: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:I:256:VAL:HG13	1:I:280:ASN:H	1.78	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:R:80:TYR:O	1:R:267:ASP:HB2	2.12	0.49
1:J:256:VAL:HG13	1:J:280:ASN:H	1.78	0.49
1:E:204:ARG:HB3	1:E:337:ILE:CD1	2.43	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:H:179:ARG:CD	1:H:197:CYS:SG	3.01	0.48
1:G:383:LEU:HD22	1:L:383:LEU:HD22	1.94	0.48
1:E:316:LYS:O	1:E:317:SER:HB3	2.12	0.48
1:G:179:ARG:CD	1:G:197:CYS:SG	3.01	0.48
1:T:124:ILE:HG13	1:T:160:VAL:HG22	1.95	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:G:171:THR:O	1:G:172:SER:HB3	2.13	0.48
1:O:110:SER:HB3	1:O:160:VAL:HG12	1.95	0.48
1:H:114:PRO:HD3	1:H:361:SER:HB3	1.94	0.48
1:L:171:THR:O	1:L:172:SER:HB3	2.13	0.48
1:D:171:THR:O	1:D:172:SER:HB3	2.13	0.48
1:N:179:ARG:HD2	1:N:197:CYS:SG	2.53	0.48
1:K:256:VAL:HG13	1:K:280:ASN:H	1.79	0.48
1:G:256:VAL:HG13	1:G:280:ASN:H	1.78	0.48
1:Q:124:ILE:HG13	1:Q:160:VAL:HG22	1.95	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: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: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:P:171:THR:O	1:P:172:SER:HB3	2.13	0.48
1:L:110:SER:HB3	1:L:160:VAL:CG1	2.42	0.48
1:T:121:ASN:O	1:T:160:VAL:HB	2.14	0.48
1:O:121:ASN:HB3	1:O:357:VAL:HG13	1.96	0.48
1:A:256:VAL:HG13	1:A:280:ASN:H	1.78	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:M:204:ARG:HB3	1:M:337:ILE:CD1	2.44	0.48
1:A:110:SER:HB3	1:A:160:VAL:HG12	1.95	0.48
1:T:256:VAL:HG13	1:T:280:ASN:H	1.78	0.48
1:O:171:THR:O	1:O:172:SER:HB3	2.13	0.47
1:F:33:LEU:HD13	1:I:402:LEU:HD12	1.96	0.47
1:H:402:LEU:HD12	1:N:33:LEU:HD13	1.96	0.47
1:C:256:VAL:HG13	1:C:280:ASN:H	1.78	0.47
1:S:171:THR:O	1:S: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:L:124:ILE:HG13	1:L:160:VAL:HG22	1.96	0.47
1:O:204:ARG:HB3	1:O:337:ILE:CD1	2.44	0.47
1:M:179:ARG:HD2	1:M:197:CYS:SG	2.55	0.47
1:I:179:ARG:HD2	1:I:197:CYS:SG	2.55	0.47
1:F:179:ARG:HD2	1:F:197:CYS:SG	2.54	0.47
1:K:110:SER:HB3	1:K:160:VAL:CG1	2.44	0.47
1:H:256:VAL:HG13	1:H:280:ASN:H	1.79	0.47
1:M:8:THR:HG22	1:M:11:ILE:HG22	1.97	0.47
1:E:179:ARG:HD2	1:E:197:CYS:SG	2.54	0.47
1:C:396:ASN:HD22	1:C:396:ASN:N	2.13	0.47
1:E:256:VAL:HG13	1:E:280:ASN:H	1.79	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:G:114:PRO:HD3	1:G:361:SER:HB3	1.96	0.47
1:F:204:ARG:HB3	1:F:337:ILE:CD1	2.44	0.47
1:L:179:ARG:HD2	1:L:197:CYS:SG	2.54	0.47
1:A:179:ARG:HD2	1:A:197:CYS:SG	2.55	0.47
1:J:396:ASN:HD22	1:J:396:ASN:N	2.13	0.47
1:H:396:ASN:N	1:H:396:ASN:HD22	2.12	0.47
1:F:256:VAL:HG13	1:F:280:ASN:H	1.79	0.47
1:S:396:ASN:HD22	1:S:396:ASN:H	1.62	0.47
1:J:204:ARG:HB3	1:J:337:ILE:CD1	2.44	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:K:396:ASN:HD22	1:K:396:ASN:N	2.12	0.47
1:D:396:ASN:HD22	1:D:396:ASN:N	2.12	0.47
1:N:396:ASN:N	1:N:396:ASN:HD22	2.13	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:T:204:ARG:HB3	1:T:337:ILE:CD1	2.45	0.47
1:I:8:THR:HG22	1:I:11:ILE:HG22	1.97	0.47
1:D:8:THR:HG22	1:D:11:ILE:HG22	1.97	0.47
1:K:397:TYR:OH	1:N:432:LEU:HD13	2.14	0.47
1:M:106:LEU:HD23	1:M:367:GLY:HA3	1.97	0.47
1:O:256:VAL:HG13	1:O:280:ASN:H	1.79	0.47
1:N:204:ARG:HB3	1:N:337:ILE:CD1	2.45	0.47
1:K:204:ARG:HB3	1:K:337:ILE:CD1	2.45	0.47
1:T:396:ASN:N	1:T:396:ASN:HD22	2.13	0.47
1:A:396:ASN:HD22	1:A:396:ASN:N	2.13	0.47
1:C:204:ARG:HB3	1:C:337:ILE:CD1	2.45	0.46
1:A:204:ARG:HB3	1:A:337:ILE:CD1	2.45	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:L:256:VAL:HG13	1:L:280:ASN:H	1.78	0.46
1:B:124:ILE:HG13	1:B:160:VAL:HG22	1.96	0.46
1:G:8:THR:HG22	1:G:11:ILE:HG22	1.97	0.46
1:F:8:THR:HG22	1:F:11:ILE:HG22	1.97	0.46
1:B:179:ARG:HD2	1:B:197:CYS:SG	2.55	0.46
1:I:396:ASN:HD22	1:I:396:ASN:N	2.13	0.46
1:F:396:ASN:HD22	1:F:396:ASN:N	2.12	0.46
1:B:396:ASN:N	1:B:396:ASN:HD22	2.13	0.46
1:Q:256:VAL:HG13	1:Q:280:ASN:H	1.79	0.46
1:N:256:VAL:HG13	1:N: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:T:8:THR:HG22	1:T:11:ILE:HG22	1.98	0.46
1:P:122:GLY:C	1:P:160:VAL:HG23	2.36	0.46
1:J:121:ASN:HD21	1:J:358:ALA:H	1.62	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:K:8:THR:HG22	1:K:11:ILE:HG22	1.97	0.46
1:H:8:THR:HG22	1:H:11:ILE:HG22	1.97	0.46
1:T:171:THR:O	1:T:172:SER:HB3	2.14	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:P:8:THR:HG22	1:P:11:ILE:HG22	1.98	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:Q:396:ASN:N	1:Q:396:ASN:HD22	2.13	0.46
1:H:204:ARG:HB3	1:H:337:ILE:CD1	2.45	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:A:8:THR:HG22	1:A:11:ILE:HG22	1.97	0.46
1:N:124:ILE:HG13	1:N:160:VAL:HG22	1.98	0.46
1:M:396:ASN:N	1:M:396:ASN:HD22	2.13	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:R:396:ASN:N	1:R:396:ASN:HD22	2.13	0.46
1:Q:106:LEU:HD23	1:Q:367:GLY:HA3	1.98	0.46
1:N:106:LEU:HD23	1:N:367:GLY:HA3	1.98	0.46
1:L:8:THR:HG22	1:L:11:ILE:HG22	1.98	0.46
1:S:256:VAL:HG13	1:S:280:ASN:H	1.81	0.46
1:E:106:LEU:HD23	1:E:367:GLY:HA3	1.98	0.46
1:R:77:ASN:HD21	1:R:79:ASN:HB2	1.80	0.46
1:O:106:LEU:HD23	1:O:367:GLY:HA3	1.98	0.45
1:I:106:LEU:HD23	1:I:367:GLY:HA3	1.98	0.45
1:N:11:ILE:HB	1:N:12:VAL:H	1.64	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:H:150:ASN:HD21	1:N:385:THR:N	2.07	0.45
1:G:15:ILE:HD13	1:G:15:ILE:HA	1.86	0.45
1:C:120:LEU:HG	1:O:113:LEU:HD21	1.99	0.45
1:O:8:THR:HG22	1:O:11:ILE:HG22	1.97	0.45
1:O:11:ILE:HB	1:O:12:VAL:H	1.64	0.45
1:B:8:THR:HG22	1:B:11:ILE:HG22	1.97	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:B:77:ASN:HD21	1:B:79:ASN:HB2	1.82	0.45
1:S:204:ARG:HB3	1:S:337:ILE:CD1	2.47	0.45
1:R:8:THR:HG22	1:R:11:ILE:HG22	1.98	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:O:77:ASN:HD21	1:O:79:ASN:HB2	1.82	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:J:8:THR:HG22	1:J:11:ILE:HG22	1.97	0.45
1:F:124:ILE:HG13	1:F:160:VAL:HG22	1.99	0.45
1:P:77:ASN:HD21	1:P:79:ASN:HB2	1.82	0.45
1:T:106:LEU:HD23	1:T:367:GLY:HA3	1.99	0.45
1:F:77:ASN:HD21	1:F:79:ASN:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:77:ASN:HD21	1:M:79:ASN:HB2	1.82	0.45
1:S:8:THR:HG22	1:S:11:ILE:HG22	1.99	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:N:77:ASN:HD21	1:N:79:ASN:HB2	1.82	0.45
1:E:204:ARG:HB3	1:E:337:ILE:HD11	1.99	0.44
1:D:15:ILE:HG13	1:D:397:TYR:CD2	2.52	0.44
1:G:120:LEU:HD23	1:R:113:LEU:HD12	1.98	0.44
1:L:106:LEU:HD23	1:L:367:GLY:HA3	1.98	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:M:127:VAL:HG22	1:M:144:LEU:HB3	1.99	0.44
1:I:127:VAL:HG22	1:I:144:LEU:HB3	1.99	0.44
1:I:77:ASN:HD21	1:I:79:ASN:HB2	1.82	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: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: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: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:T:113:LEU:HD22	1:T:120:LEU:HD22	2.00	0.44
1:Q:204:ARG:HB3	1:Q:337:ILE:HD11	1.99	0.44
1:E:15:ILE:HG13	1:E:397:TYR:CD2	2.51	0.44
1:C:15:ILE:HG13	1:C:397:TYR:CD2	2.52	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:K:77:ASN:HD21	1:K:79:ASN:HB2	1.82	0.44
1:E:127:VAL:HG22	1:E:144:LEU:HB3	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:J:124:ILE:HG13	1:J:160:VAL:HG22	2.00	0.44
1:F:11:ILE:HB	1:F:12:VAL:H	1.65	0.44
1:R:261:ILE:HD12	1:R:276:VAL:HG21	1.99	0.44
1:H:15:ILE:HG13	1:H:397:TYR:CD2	2.52	0.44
1:A:77:ASN:HD21	1:A:79:ASN:HB2	1.82	0.44
1:A:209:THR:HA	1:A:332:SER:HB3	1.99	0.44
1:H:127:VAL:HG22	1:H: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:K:127:VAL:HG22	1:K:144:LEU:HB3	2.00	0.44
1:M:112:THR:HG22	1:M:113:LEU:N	2.33	0.44
1:T:204:ARG:HB3	1:T:337:ILE:HD11	2.00	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: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:K:320:GLN:N	1:K:323:ASP:OD2	2.51	0.44
1:C:204:ARG:HB3	1:C:337:ILE:HD11	2.00	0.44
1:I:385:THR:N	1:K:150:ASN:HD21	2.09	0.44
1:T:15:ILE:HG13	1:T:397:TYR:CD2	2.52	0.44
1:I:15:ILE:HG13	1:I:397:TYR:CD2	2.52	0.44
1:B:320:GLN:N	1:B:323:ASP:OD2	2.51	0.44
1:O:209:THR:HA	1:O:332:SER:HB3	2.00	0.44
1:L:77:ASN:HD21	1:L:79:ASN:HB2	1.82	0.44
1:C:112:THR:HA	1:L:120:LEU:O	2.18	0.44
1:A:204:ARG:HB3	1:A:337:ILE:HD11	2.00	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: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:E:8:THR:HG22	1:E:11:ILE:HG22	1.98	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:H:209:THR:HA	1:H:332:SER:HB3	2.01	0.43
1:K:204:ARG:HB3	1:K:337:ILE:HD11	2.00	0.43
1:B:15:ILE:HG13	1:B:397:TYR:CD2	2.52	0.43
1:Q:15:ILE:HG13	1:Q:397:TYR:CD2	2.52	0.43
1:F:15:ILE:HD13	1:F:15:ILE:HA	1.86	0.43
1:D:320:GLN:N	1:D:323:ASP:OD2	2.50	0.43
1:S:114:PRO:HD3	1:S:361:SER:HB3	2.00	0.43
1:M:201:ASP:O	1:M:202:ARG:HB2	2.18	0.43
1:I:33:LEU:HD13	1:K:402:LEU:HD12	1.99	0.43
1:B:201:ASP:OD1	1:B:201:ASP:N	2.50	0.43
1:J:171:THR:O	1:J:172:SER:CB	2.66	0.43
1:E:171:THR:O	1:E:172:SER:CB	2.66	0.43
1:K:15:ILE:HG13	1:K:397:TYR:CD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:GLN:N	1:C:323:ASP:OD2	2.51	0.43
1:S:201:ASP:O	1:S:202:ARG:HB2	2.18	0.43
1:G:201:ASP:O	1:G:202:ARG:HB2	2.19	0.43
1:F:204:ARG:HB3	1:F:337:ILE:HD11	2.00	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: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:F:320:GLN:N	1:F:323:ASP:OD2	2.52	0.43
1:D:77:ASN:HD21	1:D:79:ASN:HB2	1.82	0.43
1:I:320:GLN:N	1:I:323:ASP:OD2	2.52	0.43
1:A:114:PRO:HD3	1:A:361:SER:HB3	2.01	0.43
1:O:204:ARG:HB3	1:O:337:ILE:HD11	2.00	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:D:283:THR:H	1:D:288:ASN:ND2	2.15	0.43
1:N:320:GLN:N	1:N:323:ASP:OD2	2.51	0.43
1:C:77:ASN:HD21	1:C:79:ASN:HB2	1.83	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: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:G:127:VAL:HG22	1:G:144:LEU:HB3	2.00	0.43
1:A:127:VAL:HG22	1:A: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:F:209:THR:HA	1:F:332:SER:HB3	2.00	0.43
1:S:93:PRO:HG3	1:S:180:LEU:HB3	2.01	0.43
1:C:106:LEU:HD23	1:C:367:GLY:HA3	1.98	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:F:121:ASN:ND2	1:F:358:ALA:H	2.16	0.43
1:O:113:LEU:HD22	1:O:120:LEU:HD22	2.00	0.43
1:F:201:ASP:O	1:F:202:ARG:HB2	2.19	0.43
1:D:201:ASP:O	1:D:202:ARG:HB2	2.19	0.43
1:F:171:THR:O	1:F:172:SER:CB	2.67	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:T:127:VAL:HG22	1:T:144:LEU:HB3	1.99	0.43
1:N:127:VAL:HG22	1:N:144:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:320:GLN:N	1:O:323:ASP:OD2	2.52	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:S:77:ASN:HD21	1:S:79:ASN:HB2	1.83	0.43
1:L:209:THR:HA	1:L:332:SER:HB3	2.00	0.43
1:G:320:GLN:N	1:G:323:ASP:OD2	2.51	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:A:171:THR:O	1:A:172:SER:CB	2.67	0.43
1:S:110:SER:HB3	1:S:160:VAL:CG1	2.49	0.43
1:B:15:ILE:HA	1:B:15:ILE:HD13	1.86	0.43
1:A:15:ILE:HG13	1:A:397:TYR:CD2	2.52	0.43
1:B:201:ASP:O	1:B:202:ARG:HB2	2.19	0.43
1:I:209:THR:HA	1:I:332:SER:HB3	2.01	0.43
1:D:124:ILE:HG13	1:D:160:VAL:HG22	2.00	0.43
1:M:291:PRO:HB3	1:R:293:ASN:ND2	2.34	0.43
1:R:106:LEU:HD23	1:R:367:GLY:HA3	2.00	0.43
1:P:320:GLN:N	1:P:323:ASP:OD2	2.51	0.43
1:J:320:GLN:N	1:J:323:ASP:OD2	2.52	0.43
1:R:201:ASP:O	1:R:202:ARG:HB2	2.19	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:P:204:ARG:HB3	1:P:337:ILE:HD11	2.01	0.42
1:T:171:THR:O	1:T:172:SER:CB	2.67	0.42
1:S:11:ILE:HB	1:S:12:VAL:H	1.64	0.42
1:K:171:THR:O	1:K:172:SER:CB	2.66	0.42
1:P:201:ASP:O	1:P:202:ARG:HB2	2.19	0.42
1:K:201:ASP:OD1	1:K:201:ASP:N	2.49	0.42
1:Q:127:VAL:HG22	1:Q:144:LEU:HB3	2.00	0.42
1:K:209:THR:HA	1:K:332:SER:HB3	2.00	0.42
1:H:77:ASN:HD21	1:H:79:ASN:HB2	1.83	0.42
1:R:11:ILE:HB	1:R:12:VAL:H	1.64	0.42
1:M:110:SER:CB	1:M:160:VAL:HG12	2.49	0.42
1:J:201:ASP:O	1:J:202:ARG:HB2	2.19	0.42
1:D:127:VAL:HG22	1:D:144:LEU:HB3	2.00	0.42
1:P:209:THR:HA	1:P:332:SER:HB3	2.00	0.42
1:E:116:GLY:HA2	1:P:162:GLU:HA	2.02	0.42
1:A:201:ASP:O	1:A:202:ARG:HB2	2.20	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:M:150:ASN:HD21	1:R:385:THR:N	2.11	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:124:ILE:HG13	1:K:160:VAL:HG22	2.02	0.42
1:J:15:ILE:HG13	1:J:397:TYR:CD2	2.52	0.42
1:M:37:THR:OG1	1:M:39:ARG:NH1	2.53	0.42
1:H:201:ASP:O	1:H:202:ARG:HB2	2.19	0.42
1:G:209:THR:HA	1:G:332:SER:HB3	2.00	0.42
1:J:204:ARG:HB3	1:J:337:ILE:HD11	2.00	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:N:15:ILE:HA	1:N:15:ILE:HD13	1.86	0.42
1:L:201:ASP:N	1:L:201:ASP:OD1	2.49	0.42
1:L:204:ARG:HB3	1:L:337:ILE:HD11	2.00	0.42
1:B:204:ARG:HB3	1:B:337:ILE:HD11	2.01	0.42
1:R:171:THR:O	1:R:172:SER:CB	2.67	0.42
1:M:20:MET:HG2	1:M:423:ARG:HG2	2.02	0.42
1:L:171:THR:O	1:L:172:SER:CB	2.67	0.42
1:F:127:VAL:HG22	1:F:144:LEU:HB3	2.00	0.42
1:M:249:ARG:HB2	1:M:328:SER:HB3	2.01	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:S:110:SER:HB3	1:S:160:VAL:HG12	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:T:320:GLN:N	1:T:323:ASP:OD2	2.52	0.42
1:P:11:ILE:HB	1:P:12:VAL:H	1.65	0.42
1:M:432:LEU:HD13	1:T:397:TYR:OH	2.20	0.42
1:L:201:ASP:O	1:L:202:ARG:HB2	2.20	0.42
1:R:37:THR:OG1	1:R:39:ARG:NH1	2.53	0.42
1:N:209:THR:HA	1:N:332:SER:HB3	2.01	0.42
1:J:127:VAL:HG22	1:J:144:LEU:HB3	2.00	0.42
1:Q:201:ASP:O	1:Q:202:ARG:HB2	2.19	0.42
1:P:432:LEU:HB2	1:P:433:ASN:H	1.67	0.42
1:H:204:ARG:HB3	1:H:337:ILE:HD11	2.00	0.42
1:Q:171:THR:O	1:Q:172:SER:CB	2.67	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:D:110:SER:HB3	1:D:160:VAL:HG12	2.01	0.42
1:C:201:ASP:O	1:C:202:ARG:HB2	2.19	0.42
1:L:112:THR:HG22	1:L:113:LEU:N	2.35	0.42
1:R:127:VAL:HG22	1:R:144:LEU:HB3	2.01	0.42
1:S:204:ARG:HB3	1:S:337:ILE:HD11	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:A:93:PRO:HG3	1:A:180:LEU:HB3	2.02	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:R:15:ILE:HG13	1:R:397:TYR:CD2	2.51	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: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:R:276:VAL:HG22	1:R:294:LEU:HD21	2.02	0.41
1:N:201:ASP:O	1:N:202:ARG:HB2	2.19	0.41
1:B:11:ILE:HB	1:B:12:VAL:H	1.64	0.41
1:I:201:ASP:O	1:I:202:ARG:HB2	2.19	0.41
1:D:201:ASP:N	1:D:201:ASP:OD1	2.49	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:R:110:SER:HB3	1:R:160:VAL:HG11	1.97	0.41
1:B:337:ILE:HG21	1:B:337:ILE:HD12	1.88	0.41
1:N:20:MET:HG2	1:N:423:ARG:HG2	2.03	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:O:15:ILE:HG13	1:O:397:TYR:CD2	2.52	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:E:320:GLN:O	1:E:321:ALA:C	2.60	0.41
1:J:438:ILE:O	1:J:438:ILE:HG22	2.21	0.41
1:E:93:PRO:HG3	1:E:180:LEU:HB3	2.02	0.41
1:A:12:VAL:O	1:A:13:PRO:C	2.60	0.41
1:C:20:MET:HG2	1:C:423:ARG:HG2	2.03	0.41
1:S:171:THR:O	1:S:172:SER:CB	2.69	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:A:279:ASN:ND2	1:A:279:ASN:O	2.54	0.41
1:T:20:MET:HG2	1:T:423:ARG:HG2	2.03	0.40
1:F:220:TYR:HD2	1:F:320:GLN:O	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:93:PRO:HG3	1:N:180:LEU:HB3	2.03	0.40
1:E:201:ASP:O	1:E:339:GLY:HA2	2.21	0.40
1:E:124:ILE:HG13	1:E:160:VAL:HG22	2.01	0.40
1:Q:93:PRO:HG3	1:Q:180:LEU:HB3	2.03	0.40
1:A:438:ILE:HG22	1:A:438:ILE:O	2.21	0.40
1:B:20:MET:HG2	1:B:423:ARG:HG2	2.03	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:L:110:SER:CB	1:L:160:VAL:HG12	2.50	0.40
1:P:97:ASN:O	1:P:179:ARG:HG3	2.21	0.40
1:F:15:ILE:HG13	1:F:397:TYR:CD2	2.52	0.40
1:K:113:LEU:HA	1:K:114:PRO:HD3	1.93	0.40
1:E:37:THR:OG1	1:E:39:ARG:NH1	2.55	0.40
1:O:93:PRO:HG3	1:O:180:LEU:HB3	2.03	0.40
1:J:93:PRO:HG3	1:J:180:LEU:HB3	2.03	0.40
1:K:438:ILE:HG22	1:K:438:ILE:O	2.21	0.40
1:S:438:ILE:O	1:S:438:ILE:HG22	2.21	0.40
1:G:438:ILE:HG22	1:G:438:ILE:O	2.21	0.40
1:O:438:ILE:HG22	1:O:438:ILE:O	2.22	0.40
1:B:283:THR:H	1:B:288:ASN:ND2	2.16	0.40
1:S:397:TYR:OH	1:T:432:LEU:HD13	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:E:438:ILE:HG22	1:E:438:ILE:O	2.22	0.40
1:P:20:MET:HG2	1:P:423:ARG:HG2	2.04	0.40
1:I:12:VAL:O	1:I:13:PRO:C	2.60	0.40
1:G:97:ASN:O	1:G:179:ARG:HG3	2.22	0.40
1:Q:316:LYS:HB2	1:Q:325:MET:HE2	2.03	0.40
1:O:124:ILE:HG13	1:O:160:VAL:HG22	2.02	0.40
1:Q:220:TYR:HD2	1:Q:320:GLN:O	2.05	0.40
1:H:220:TYR:HD2	1:H:320:GLN:O	2.05	0.40
1:T:201:ASP:OD1	1:T:201:ASP:N	2.50	0.40
1:D:114:PRO:HD3	1:D:361:SER:HB3	2.03	0.40
1:P:93:PRO:HG3	1:P:180:LEU:HB3	2.02	0.40
1:K:12:VAL:O	1:K:13:PRO:C	2.60	0.40
1:Q:438:ILE:O	1:Q:438:ILE:HG22	2.22	0.40
1:B:438:ILE:HG22	1:B:438:ILE:O	2.22	0.40
1:I:20:MET:HG2	1:I:423:ARG:HG2	2.03	0.40
1:G:113:LEU:HA	1:G:114:PRO:HD3	1.88	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%)	7	11
1	B	424/456 (93%)	394 (93%)	19 (4%)	11 (3%)	7	11
1	C	424/456 (93%)	395 (93%)	18 (4%)	11 (3%)	7	11
1	D	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	7	11
1	E	431/456 (94%)	401 (93%)	20 (5%)	10 (2%)	8	14
1	F	431/456 (94%)	401 (93%)	18 (4%)	12 (3%)	6	10
1	G	431/456 (94%)	403 (94%)	17 (4%)	11 (3%)	7	11
1	H	424/456 (93%)	395 (93%)	18 (4%)	11 (3%)	7	11
1	I	424/456 (93%)	396 (93%)	16 (4%)	12 (3%)	6	10
1	J	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	7	11
1	K	424/456 (93%)	395 (93%)	18 (4%)	11 (3%)	7	11
1	L	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	7	11
1	M	424/456 (93%)	396 (93%)	18 (4%)	10 (2%)	7	13
1	N	424/456 (93%)	395 (93%)	17 (4%)	12 (3%)	6	10
1	O	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	7	11
1	P	426/456 (93%)	397 (93%)	17 (4%)	12 (3%)	6	10
1	Q	425/456 (93%)	396 (93%)	18 (4%)	11 (3%)	7	11
1	R	431/456 (94%)	401 (93%)	23 (5%)	7 (2%)	12	24
1	S	424/456 (93%)	394 (93%)	19 (4%)	11 (3%)	7	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	424/456 (93%)	395 (93%)	18 (4%)	11 (3%)	7	11
All	All	8511/9120 (93%)	7934 (93%)	359 (4%)	218 (3%)	7	11

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 ⓘ

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%)	17	35
1	B	354/380 (93%)	328 (93%)	26 (7%)	17	35
1	C	354/380 (93%)	328 (93%)	26 (7%)	17	35
1	D	354/380 (93%)	328 (93%)	26 (7%)	17	35
1	E	356/380 (94%)	332 (93%)	24 (7%)	20	40
1	F	356/380 (94%)	329 (92%)	27 (8%)	16	32
1	G	356/380 (94%)	330 (93%)	26 (7%)	17	35
1	H	354/380 (93%)	329 (93%)	25 (7%)	18	36
1	I	354/380 (93%)	328 (93%)	26 (7%)	17	35
1	J	354/380 (93%)	326 (92%)	28 (8%)	15	30
1	K	354/380 (93%)	327 (92%)	27 (8%)	16	32
1	L	354/380 (93%)	329 (93%)	25 (7%)	18	36
1	M	354/380 (93%)	328 (93%)	26 (7%)	17	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	354/380 (93%)	329 (93%)	25 (7%)	18	36
1	O	354/380 (93%)	326 (92%)	28 (8%)	15	30
1	P	354/380 (93%)	329 (93%)	25 (7%)	18	36
1	Q	354/380 (93%)	329 (93%)	25 (7%)	18	36
1	R	356/380 (94%)	332 (93%)	24 (7%)	20	40
1	S	354/380 (93%)	328 (93%)	26 (7%)	17	35
1	T	354/380 (93%)	329 (93%)	25 (7%)	18	36
All	All	7088/7600 (93%)	6572 (93%)	516 (7%)	17	35

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

*Continued on next page...*

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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

*Continued on next page...*

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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%)	0.60	52 (12%) 6 3	8, 12, 17, 24	0
1	B	428/456 (93%)	0.78	59 (13%) 4 2	8, 12, 17, 24	0
1	C	428/456 (93%)	0.74	62 (14%) 3 2	8, 12, 18, 24	0
1	D	428/456 (93%)	0.78	68 (15%) 3 1	8, 12, 16, 24	0
1	E	433/456 (94%)	0.50	32 (7%) 17 12	5, 11, 16, 24	0
1	F	433/456 (94%)	0.80	58 (13%) 4 2	8, 12, 17, 24	0
1	G	433/456 (94%)	0.64	42 (9%) 10 6	6, 12, 17, 24	0
1	H	428/456 (93%)	0.69	45 (10%) 8 5	8, 12, 18, 24	0
1	I	428/456 (93%)	0.72	50 (11%) 6 4	8, 12, 18, 24	0
1	J	428/456 (93%)	0.72	61 (14%) 4 2	8, 12, 17, 24	0
1	K	428/456 (93%)	0.67	50 (11%) 6 4	8, 12, 18, 24	0
1	L	428/456 (93%)	0.60	48 (11%) 7 4	8, 12, 18, 24	0
1	M	428/456 (93%)	0.70	46 (10%) 8 4	8, 12, 18, 24	0
1	N	428/456 (93%)	0.67	46 (10%) 8 4	8, 12, 18, 24	0
1	O	428/456 (93%)	0.70	60 (14%) 4 2	8, 12, 18, 24	0
1	P	430/456 (94%)	0.67	51 (11%) 6 4	8, 12, 17, 24	0
1	Q	429/456 (94%)	0.70	59 (13%) 4 2	8, 12, 18, 24	0
1	R	433/456 (94%)	0.58	28 (6%) 22 16	2, 11, 17, 24	0
1	S	428/456 (93%)	0.65	31 (7%) 18 13	4, 11, 18, 24	0
1	T	428/456 (93%)	0.73	35 (8%) 14 10	8, 12, 18, 24	0
All	All	8583/9120 (94%)	0.68	983 (11%) 6 4	2, 12, 18, 24	0

All (983) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	440	GLY	14.3
1	Q	439	ALA	13.1
1	R	439	ALA	12.9
1	N	439	ALA	11.5
1	K	439	ALA	11.5
1	B	439	ALA	11.4
1	E	440	GLY	11.3
1	I	440	GLY	11.2
1	J	439	ALA	10.9
1	A	439	ALA	10.9
1	O	436	LEU	10.8
1	P	439	ALA	10.8
1	H	434	SER	10.4
1	G	439	ALA	10.3
1	Q	436	LEU	10.2
1	I	322	GLY	10.2
1	A	435	PRO	10.1
1	L	440	GLY	10.1
1	C	439	ALA	10.1
1	B	440	GLY	10.0
1	J	434	SER	9.9
1	F	322	GLY	9.7
1	C	9	GLN	9.7
1	R	430	ALA	9.7
1	L	439	ALA	9.5
1	J	440	GLY	9.5
1	I	439	ALA	9.5
1	R	435	PRO	9.5
1	H	440	GLY	9.4
1	F	439	ALA	9.4
1	D	429	VAL	9.3
1	O	430	ALA	9.3
1	Q	438	ILE	9.2
1	E	439	ALA	9.2
1	H	439	ALA	9.2
1	N	434	SER	9.1
1	R	434	SER	9.1
1	H	438	ILE	9.1
1	N	438	ILE	9.1
1	B	435	PRO	9.1
1	B	430	ALA	9.1
1	S	435	PRO	9.0
1	P	434	SER	9.0

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Mol	Chain	Res	Type	RSRZ
1	Q	434	SER	8.9
1	I	438	ILE	8.9
1	M	439	ALA	8.9
1	A	433	ASN	8.9
1	B	433	ASN	8.8
1	T	436	LEU	8.8
1	A	440	GLY	8.8
1	L	435	PRO	8.8
1	K	436	LEU	8.7
1	J	435	PRO	8.7
1	G	321	ALA	8.6
1	S	433	ASN	8.6
1	M	433	ASN	8.6
1	L	436	LEU	8.6
1	R	438	ILE	8.6
1	I	435	PRO	8.5
1	Q	433	ASN	8.5
1	B	434	SER	8.5
1	S	439	ALA	8.4
1	M	434	SER	8.4
1	L	438	ILE	8.4
1	F	434	SER	8.4
1	H	433	ASN	8.4
1	D	440	GLY	8.3
1	A	436	LEU	8.3
1	O	435	PRO	8.3
1	O	434	SER	8.3
1	F	433	ASN	8.2
1	F	321	ALA	8.2
1	C	434	SER	8.2
1	N	436	LEU	8.2
1	I	430	ALA	8.1
1	J	433	ASN	8.1
1	O	429	VAL	8.1
1	O	437	LYS	8.1
1	O	439	ALA	8.0
1	J	438	ILE	8.0
1	S	438	ILE	8.0
1	E	10	GLN	8.0
1	M	10	GLN	8.0
1	B	429	VAL	8.0
1	S	10	GLN	7.9

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Mol	Chain	Res	Type	RSRZ
1	G	8	THR	7.9
1	O	440	GLY	7.9
1	H	435	PRO	7.9
1	H	10	GLN	7.9
1	H	436	LEU	7.9
1	F	440	GLY	7.9
1	N	8	THR	7.8
1	O	433	ASN	7.7
1	Q	8	THR	7.7
1	N	430	ALA	7.7
1	M	440	GLY	7.7
1	T	439	ALA	7.7
1	F	430	ALA	7.7
1	P	429	VAL	7.7
1	Q	435	PRO	7.7
1	D	435	PRO	7.6
1	O	322	GLY	7.6
1	D	433	ASN	7.6
1	R	9	GLN	7.6
1	I	434	SER	7.5
1	G	434	SER	7.5
1	C	430	ALA	7.5
1	E	433	ASN	7.5
1	D	434	SER	7.4
1	D	439	ALA	7.4
1	M	436	LEU	7.4
1	N	435	PRO	7.4
1	M	9	GLN	7.4
1	P	430	ALA	7.4
1	G	11	ILE	7.4
1	G	440	GLY	7.4
1	R	429	VAL	7.4
1	K	435	PRO	7.4
1	K	440	GLY	7.4
1	M	429	VAL	7.3
1	S	434	SER	7.3
1	D	320	GLN	7.3
1	S	9	GLN	7.2
1	K	433	ASN	7.2
1	A	434	SER	7.2
1	F	10	GLN	7.2
1	A	430	ALA	7.2

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Mol	Chain	Res	Type	RSRZ
1	T	440	GLY	7.2
1	D	425	TYR	7.1
1	J	322	GLY	7.1
1	G	430	ALA	7.1
1	P	436	LEU	7.1
1	S	436	LEU	7.1
1	S	8	THR	7.1
1	O	10	GLN	7.0
1	H	8	THR	7.0
1	M	8	THR	7.0
1	S	440	GLY	7.0
1	H	9	GLN	7.0
1	F	435	PRO	7.0
1	P	433	ASN	7.0
1	E	429	VAL	7.0
1	T	434	SER	7.0
1	E	435	PRO	7.0
1	L	9	GLN	6.9
1	M	430	ALA	6.9
1	Q	10	GLN	6.9
1	N	440	GLY	6.9
1	C	322	GLY	6.9
1	N	425	TYR	6.9
1	I	429	VAL	6.8
1	D	431	ASP	6.8
1	B	437	LYS	6.8
1	G	435	PRO	6.8
1	I	433	ASN	6.8
1	K	429	VAL	6.8
1	A	10	GLN	6.8
1	R	440	GLY	6.8
1	D	10	GLN	6.8
1	I	436	LEU	6.8
1	R	436	LEU	6.8
1	M	435	PRO	6.8
1	H	430	ALA	6.8
1	E	430	ALA	6.7
1	Q	440	GLY	6.7
1	D	8	THR	6.7
1	K	8	THR	6.7
1	C	10	GLN	6.7
1	F	425	TYR	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	435	PRO	6.7
1	K	321	ALA	6.7
1	N	433	ASN	6.6
1	J	436	LEU	6.6
1	B	438	ILE	6.6
1	A	321	ALA	6.6
1	G	436	LEU	6.6
1	P	435	PRO	6.6
1	P	440	GLY	6.6
1	A	438	ILE	6.6
1	C	11	ILE	6.6
1	C	431	ASP	6.6
1	L	8	THR	6.5
1	R	11	ILE	6.5
1	R	8	THR	6.5
1	B	436	LEU	6.5
1	M	438	ILE	6.4
1	F	220	TYR	6.4
1	J	9	GLN	6.4
1	L	430	ALA	6.4
1	I	9	GLN	6.4
1	K	430	ALA	6.3
1	B	322	GLY	6.3
1	I	8	THR	6.3
1	L	434	SER	6.3
1	C	429	VAL	6.3
1	F	428	GLU	6.3
1	O	9	GLN	6.3
1	T	425	TYR	6.3
1	J	8	THR	6.3
1	F	9	GLN	6.3
1	C	438	ILE	6.3
1	B	8	THR	6.3
1	K	113	LEU	6.3
1	R	433	ASN	6.3
1	K	10	GLN	6.2
1	F	224	GLY	6.2
1	M	428	GLU	6.2
1	A	437	LYS	6.2
1	N	321	ALA	6.2
1	S	429	VAL	6.2
1	P	8	THR	6.2

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Mol	Chain	Res	Type	RSRZ
1	R	437	LYS	6.2
1	I	431	ASP	6.2
1	O	321	ALA	6.2
1	G	428	GLU	6.2
1	H	429	VAL	6.2
1	B	321	ALA	6.1
1	O	438	ILE	6.1
1	D	438	ILE	6.1
1	Q	321	ALA	6.1
1	K	322	GLY	6.1
1	P	321	ALA	6.1
1	C	113	LEU	6.1
1	L	429	VAL	6.1
1	D	11	ILE	6.1
1	P	11	ILE	6.1
1	J	429	VAL	6.1
1	J	10	GLN	6.0
1	K	434	SER	6.0
1	Q	9	GLN	6.0
1	B	9	GLN	6.0
1	R	431	ASP	6.0
1	L	431	ASP	5.9
1	E	9	GLN	5.9
1	F	320	GLN	5.9
1	Q	11	ILE	5.9
1	F	324	GLN	5.9
1	F	429	VAL	5.9
1	Q	429	VAL	5.9
1	N	428	GLU	5.9
1	J	430	ALA	5.9
1	O	11	ILE	5.9
1	K	437	LYS	5.9
1	A	8	THR	5.9
1	B	10	GLN	5.8
1	Q	430	ALA	5.8
1	J	113	LEU	5.8
1	I	10	GLN	5.8
1	F	8	THR	5.8
1	S	428	GLU	5.8
1	I	321	ALA	5.8
1	G	433	ASN	5.8
1	A	322	GLY	5.8

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	N	113	LEU	5.3
1	T	10	GLN	5.3
1	B	425	TYR	5.2
1	I	428	GLU	5.2
1	Q	428	GLU	5.2
1	E	436	LEU	5.2
1	D	317	SER	5.2
1	C	321	ALA	5.2
1	D	428	GLU	5.2
1	O	428	GLU	5.2
1	D	321	ALA	5.2
1	N	11	ILE	5.2
1	T	430	ALA	5.1
1	R	428	GLU	5.1
1	M	431	ASP	5.1
1	D	436	LEU	5.1
1	H	113	LEU	5.1
1	L	10	GLN	5.1
1	E	434	SER	5.1
1	A	429	VAL	5.1
1	G	322	GLY	5.1
1	C	436	LEU	5.1
1	K	431	ASP	5.1
1	B	223	GLY	5.0
1	K	425	TYR	5.0
1	B	217	SER	5.0
1	H	321	ALA	5.0
1	C	222	PRO	5.0
1	T	428	GLU	5.0
1	M	425	TYR	5.0
1	B	320	GLN	5.0
1	Q	437	LYS	5.0
1	E	8	THR	5.0
1	L	321	ALA	5.0
1	J	428	GLU	5.0
1	K	438	ILE	5.0
1	F	11	ILE	5.0
1	E	431	ASP	5.0
1	B	222	PRO	4.9
1	P	437	LYS	4.9
1	C	433	ASN	4.9
1	N	437	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	Q	113	LEU	4.9
1	P	10	GLN	4.9
1	Q	425	TYR	4.9
1	B	11	ILE	4.8
1	M	321	ALA	4.8
1	D	113	LEU	4.8
1	G	431	ASP	4.8
1	O	223	GLY	4.8
1	T	429	VAL	4.8
1	G	425	TYR	4.8
1	E	321	ALA	4.8
1	T	11	ILE	4.8
1	G	10	GLN	4.7
1	O	431	ASP	4.7
1	A	425	TYR	4.7
1	J	317	SER	4.7
1	E	221	GLN	4.7
1	F	437	LYS	4.7
1	P	9	GLN	4.7
1	G	437	LYS	4.7
1	H	428	GLU	4.6
1	I	220	TYR	4.6
1	D	286	THR	4.6
1	C	425	TYR	4.6
1	N	431	ASP	4.6
1	O	425	TYR	4.6
1	G	9	GLN	4.6
1	L	322	GLY	4.6
1	G	219	GLN	4.6
1	M	427	MET	4.5
1	F	323	ASP	4.5
1	H	425	TYR	4.5
1	O	254	GLY	4.5
1	N	222	PRO	4.5
1	C	428	GLU	4.5
1	P	278	ALA	4.5
1	J	223	GLY	4.5
1	F	222	PRO	4.5
1	K	324	GLN	4.5
1	B	113	LEU	4.5
1	D	222	PRO	4.5
1	J	431	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	I	437	LYS	4.4
1	K	222	PRO	4.4
1	S	430	ALA	4.4
1	A	11	ILE	4.4
1	G	220	TYR	4.4
1	H	320	GLN	4.4
1	C	76	GLY	4.4
1	I	222	PRO	4.4
1	T	113	LEU	4.4
1	T	433	ASN	4.4
1	H	223	GLY	4.4
1	P	322	GLY	4.4
1	P	324	GLN	4.4
1	S	431	ASP	4.4
1	T	437	LYS	4.3
1	N	323	ASP	4.3
1	H	222	PRO	4.3
1	I	279	ASN	4.3
1	Q	220	TYR	4.3
1	P	286	THR	4.3
1	A	431	ASP	4.3
1	E	425	TYR	4.3
1	I	425	TYR	4.3
1	P	222	PRO	4.3
1	J	251	SER	4.2
1	A	428	GLU	4.2
1	M	113	LEU	4.2
1	T	432	LEU	4.2
1	D	9	GLN	4.2
1	P	428	GLU	4.2
1	D	319	GLY	4.2
1	B	428	GLU	4.2
1	J	11	ILE	4.2
1	K	223	GLY	4.2
1	D	323	ASP	4.2
1	F	217	SER	4.1
1	H	322	GLY	4.1
1	M	320	GLN	4.1
1	O	324	GLN	4.1
1	S	317	SER	4.1
1	R	417	ARG	4.1
1	A	222	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	113	LEU	4.1
1	J	432	LEU	4.1
1	K	318	GLY	4.1
1	K	320	GLN	4.0
1	L	427	MET	4.0
1	O	317	SER	4.0
1	M	223	GLY	4.0
1	N	251	SER	4.0
1	K	278	ALA	4.0
1	D	254	GLY	4.0
1	C	256	VAL	4.0
1	Q	320	GLN	4.0
1	F	223	GLY	4.0
1	H	317	SER	3.9
1	O	251	SER	3.9
1	R	425	TYR	3.9
1	A	76	GLY	3.9
1	F	319	GLY	3.9
1	I	427	MET	3.9
1	K	428	GLU	3.9
1	D	253	HIS	3.9
1	H	431	ASP	3.9
1	F	279	ASN	3.9
1	G	223	GLY	3.9
1	N	223	GLY	3.9
1	D	219	GLN	3.9
1	A	432	LEU	3.8
1	H	220	TYR	3.8
1	P	191	PRO	3.8
1	B	317	SER	3.8
1	F	278	ALA	3.8
1	E	428	GLU	3.8
1	T	427	MET	3.8
1	C	317	SER	3.8
1	E	437	LYS	3.8
1	J	425	TYR	3.8
1	L	320	GLN	3.8
1	I	323	ASP	3.8
1	P	317	SER	3.8
1	N	320	GLN	3.8
1	I	120	LEU	3.7
1	I	320	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	J	219	GLN	3.7
1	J	220	TYR	3.7
1	O	323	ASP	3.7
1	B	224	GLY	3.7
1	D	322	GLY	3.7
1	Q	324	GLN	3.7
1	C	320	GLN	3.7
1	C	278	ALA	3.7
1	B	120	LEU	3.7
1	K	427	MET	3.7
1	R	427	MET	3.7
1	C	217	SER	3.7
1	C	324	GLN	3.7
1	P	219	GLN	3.7
1	Q	431	ASP	3.7
1	C	427	MET	3.7
1	D	251	SER	3.7
1	J	315	SER	3.7
1	D	324	GLN	3.7
1	D	79	ASN	3.7
1	S	425	TYR	3.7
1	H	432	LEU	3.6
1	L	114	PRO	3.6
1	B	253	HIS	3.6
1	C	286	THR	3.6
1	G	222	PRO	3.6
1	A	320	GLN	3.6
1	Q	323	ASP	3.6
1	I	114	PRO	3.6
1	L	319	GLY	3.6
1	T	322	GLY	3.6
1	D	437	LYS	3.6
1	J	284	THR	3.6
1	G	279	ASN	3.6
1	H	120	LEU	3.6
1	K	432	LEU	3.6
1	H	324	GLN	3.6
1	N	217	SER	3.6
1	P	285	GLY	3.6
1	H	427	MET	3.6
1	T	222	PRO	3.5
1	Q	317	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	285	GLY	3.5
1	S	192	LYS	3.5
1	D	315	SER	3.5
1	S	437	LYS	3.5
1	O	191	PRO	3.5
1	T	279	ASN	3.5
1	F	256	VAL	3.5
1	A	223	GLY	3.5
1	D	318	GLY	3.5
1	P	220	TYR	3.5
1	C	323	ASP	3.5
1	T	8	THR	3.5
1	B	278	ALA	3.5
1	F	221	GLN	3.5
1	H	219	GLN	3.5
1	T	320	GLN	3.5
1	L	432	LEU	3.5
1	G	324	GLN	3.5
1	H	221	GLN	3.5
1	H	437	LYS	3.5
1	I	223	GLY	3.4
1	D	221	GLN	3.4
1	J	320	GLN	3.4
1	A	417	ARG	3.4
1	P	389	ARG	3.4
1	H	319	GLY	3.4
1	I	432	LEU	3.4
1	B	219	GLN	3.4
1	P	223	GLY	3.4
1	S	114	PRO	3.4
1	B	279	ASN	3.4
1	N	221	GLN	3.4
1	G	389	ARG	3.4
1	Q	284	THR	3.4
1	I	221	GLN	3.4
1	K	251	SER	3.4
1	I	389	ARG	3.4
1	L	425	TYR	3.3
1	Q	432	LEU	3.3
1	C	219	GLN	3.3
1	F	285	GLY	3.3
1	D	427	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	Q	319	GLY	3.3
1	P	251	SER	3.3
1	O	320	GLN	3.3
1	I	113	LEU	3.3
1	C	318	GLY	3.3
1	K	279	ASN	3.3
1	L	389	ARG	3.3
1	Q	253	HIS	3.3
1	A	219	GLN	3.3
1	O	76	GLY	3.3
1	D	284	THR	3.3
1	C	251	SER	3.3
1	F	325	MET	3.3
1	H	256	VAL	3.3
1	N	427	MET	3.3
1	C	114	PRO	3.3
1	H	318	GLY	3.3
1	I	286	THR	3.3
1	P	320	GLN	3.3
1	L	120	LEU	3.3
1	P	432	LEU	3.3
1	F	215	GLN	3.3
1	T	221	GLN	3.3
1	T	324	GLN	3.3
1	L	251	SER	3.3
1	E	322	GLY	3.2
1	F	212	ASP	3.2
1	N	324	GLN	3.2
1	Q	318	GLY	3.2
1	G	427	MET	3.2
1	S	120	LEU	3.2
1	C	285	GLY	3.2
1	F	318	GLY	3.2
1	N	281	GLY	3.2
1	O	279	ASN	3.2
1	H	11	ILE	3.2
1	S	191	PRO	3.2
1	J	279	ASN	3.2
1	C	223	GLY	3.2
1	F	251	SER	3.2
1	A	51	ASP	3.2
1	D	279	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	N	317	SER	3.2
1	I	253	HIS	3.2
1	M	286	THR	3.2
1	R	192	LYS	3.2
1	D	114	PRO	3.2
1	J	319	GLY	3.2
1	B	318	GLY	3.1
1	C	253	HIS	3.1
1	E	432	LEU	3.1
1	A	324	GLN	3.1
1	D	121	ASN	3.1
1	M	221	GLN	3.1
1	Q	219	GLN	3.1
1	I	424	GLU	3.1
1	Q	279	ASN	3.1
1	D	76	GLY	3.1
1	K	192	LYS	3.1
1	P	221	GLN	3.1
1	J	316	LYS	3.1
1	L	437	LYS	3.1
1	D	278	ALA	3.1
1	M	424	GLU	3.1
1	D	287	ASP	3.1
1	J	286	THR	3.1
1	I	278	ALA	3.0
1	C	279	ASN	3.0
1	L	279	ASN	3.0
1	K	187	ILE	3.0
1	O	424	GLU	3.0
1	C	283	THR	3.0
1	K	281	GLY	3.0
1	O	319	GLY	3.0
1	H	323	ASP	3.0
1	L	286	THR	3.0
1	N	280	ASN	3.0
1	Q	251	SER	3.0
1	G	320	GLN	3.0
1	E	424	GLU	3.0
1	K	253	HIS	3.0
1	O	222	PRO	3.0
1	F	431	ASP	3.0
1	O	318	GLY	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	432	LEU	3.0
1	I	324	GLN	3.0
1	F	315	SER	3.0
1	B	191	PRO	3.0
1	L	318	GLY	3.0
1	B	221	GLN	3.0
1	G	432	LEU	3.0
1	Q	427	MET	3.0
1	S	427	MET	3.0
1	B	256	VAL	3.0
1	Q	223	GLY	3.0
1	S	432	LEU	2.9
1	M	317	SER	2.9
1	S	321	ALA	2.9
1	P	254	GLY	2.9
1	A	316	LYS	2.9
1	N	279	ASN	2.9
1	K	286	THR	2.9
1	C	191	PRO	2.9
1	K	188	GLY	2.9
1	K	121	ASN	2.9
1	B	251	SER	2.9
1	M	279	ASN	2.9
1	L	113	LEU	2.9
1	L	317	SER	2.9
1	O	221	GLN	2.9
1	N	114	PRO	2.9
1	B	427	MET	2.9
1	A	253	HIS	2.9
1	O	287	ASP	2.9
1	L	284	THR	2.9
1	F	191	PRO	2.9
1	O	114	PRO	2.9
1	M	324	GLN	2.9
1	J	114	PRO	2.9
1	Q	222	PRO	2.9
1	H	253	HIS	2.8
1	M	322	GLY	2.8
1	B	277	ALA	2.8
1	J	222	PRO	2.8
1	C	215	GLN	2.8
1	G	212	ASP	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	J	120	LEU	2.8
1	A	279	ASN	2.8
1	G	424	GLU	2.8
1	J	249	ARG	2.8
1	E	427	MET	2.8
1	A	120	LEU	2.8
1	F	213	ASP	2.8
1	O	212	ASP	2.8
1	B	114	PRO	2.8
1	D	288	ASN	2.8
1	J	217	SER	2.8
1	O	218	SER	2.8
1	P	323	ASP	2.8
1	B	319	GLY	2.8
1	C	77	ASN	2.8
1	J	287	ASP	2.8
1	E	222	PRO	2.8
1	K	191	PRO	2.8
1	C	315	SER	2.8
1	M	220	TYR	2.8
1	R	317	SER	2.8
1	O	12	VAL	2.8
1	D	389	ARG	2.8
1	O	417	ARG	2.8
1	I	121	ASN	2.8
1	L	222	PRO	2.8
1	E	317	SER	2.8
1	O	215	GLN	2.8
1	J	280	ASN	2.8
1	A	323	ASP	2.8
1	D	281	GLY	2.8
1	J	253	HIS	2.7
1	R	432	LEU	2.7
1	C	258	GLY	2.7
1	K	258	GLY	2.7
1	Q	115	GLY	2.7
1	L	11	ILE	2.7
1	A	427	MET	2.7
1	A	221	GLN	2.7
1	C	221	GLN	2.7
1	P	279	ASN	2.7
1	R	279	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	284	THR	2.7
1	L	254	GLY	2.7
1	Q	112	THR	2.7
1	Q	285	GLY	2.7
1	Q	315	SER	2.7
1	D	316	LYS	2.7
1	N	424	GLU	2.7
1	A	217	SER	2.7
1	P	225	VAL	2.7
1	H	417	ARG	2.7
1	K	389	ARG	2.7
1	Q	392	PRO	2.7
1	A	319	GLY	2.7
1	C	316	LYS	2.7
1	H	192	LYS	2.7
1	D	220	TYR	2.7
1	C	120	LEU	2.6
1	B	77	ASN	2.6
1	M	212	ASP	2.6
1	D	191	PRO	2.6
1	L	221	GLN	2.6
1	M	114	PRO	2.6
1	O	427	MET	2.6
1	Q	254	GLY	2.6
1	D	424	GLU	2.6
1	O	217	SER	2.6
1	L	324	GLN	2.6
1	B	280	ASN	2.6
1	H	285	GLY	2.6
1	O	224	GLY	2.6
1	L	323	ASP	2.6
1	A	317	SER	2.6
1	F	218	SER	2.6
1	F	219	GLN	2.6
1	J	330	ARG	2.6
1	P	275	ALA	2.6
1	C	319	GLY	2.6
1	F	76	GLY	2.6
1	J	318	GLY	2.6
1	F	316	LYS	2.6
1	J	212	ASP	2.6
1	K	323	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	Q	76	GLY	2.6
1	K	51	ASP	2.6
1	Q	391	ASP	2.6
1	L	417	ARG	2.6
1	J	191	PRO	2.6
1	T	114	PRO	2.6
1	B	289	LEU	2.6
1	D	325	MET	2.6
1	F	314	THR	2.6
1	O	226	THR	2.6
1	P	253	HIS	2.6
1	J	417	ARG	2.6
1	Q	389	ARG	2.6
1	J	221	GLN	2.6
1	I	192	LYS	2.6
1	I	318	GLY	2.5
1	J	12	VAL	2.5
1	A	226	THR	2.5
1	F	283	THR	2.5
1	F	424	GLU	2.5
1	I	316	LYS	2.5
1	L	283	THR	2.5
1	O	286	THR	2.5
1	A	114	PRO	2.5
1	M	222	PRO	2.5
1	G	353	ALA	2.5
1	I	212	ASP	2.5
1	F	253	HIS	2.5
1	I	76	GLY	2.5
1	J	224	GLY	2.5
1	A	77	ASN	2.5
1	A	424	GLU	2.5
1	J	142	ASN	2.5
1	B	220	TYR	2.5
1	O	220	TYR	2.5
1	L	223	GLY	2.5
1	E	219	GLN	2.5
1	J	424	GLU	2.5
1	M	323	ASP	2.5
1	Q	278	ALA	2.5
1	C	284	THR	2.5
1	F	249	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	427	MET	2.5
1	N	219	GLN	2.5
1	L	253	HIS	2.5
1	O	285	GLY	2.5
1	Q	326	SER	2.5
1	R	322	GLY	2.5
1	J	283	THR	2.4
1	H	281	GLY	2.4
1	D	212	ASP	2.4
1	H	114	PRO	2.4
1	B	215	GLN	2.4
1	B	76	GLY	2.4
1	D	78	GLY	2.4
1	D	268	GLY	2.4
1	L	76	GLY	2.4
1	A	286	THR	2.4
1	I	317	SER	2.4
1	S	76	GLY	2.4
1	D	417	ARG	2.4
1	P	115	GLY	2.4
1	O	330	ARG	2.4
1	D	214	TYR	2.4
1	N	191	PRO	2.4
1	T	285	GLY	2.4
1	F	317	SER	2.4
1	D	213	ASP	2.4
1	G	323	ASP	2.4
1	B	390	PHE	2.4
1	G	215	GLN	2.4
1	B	218	SER	2.4
1	C	213	ASP	2.4
1	J	51	ASP	2.4
1	C	325	MET	2.4
1	O	278	ALA	2.4
1	F	389	ARG	2.4
1	N	51	ASP	2.4
1	N	417	ARG	2.4
1	Q	121	ASN	2.4
1	B	417	ARG	2.3
1	F	225	VAL	2.3
1	I	391	ASP	2.3
1	D	224	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	192	LYS	2.3
1	Q	217	SER	2.3
1	D	256	VAL	2.3
1	F	187	ILE	2.3
1	J	323	ASP	2.3
1	E	191	PRO	2.3
1	T	319	GLY	2.3
1	P	427	MET	2.3
1	G	278	ALA	2.3
1	A	284	THR	2.3
1	A	215	GLN	2.3
1	A	218	SER	2.3
1	G	317	SER	2.3
1	K	287	ASP	2.3
1	Q	214	TYR	2.3
1	D	187	ILE	2.3
1	J	121	ASN	2.3
1	E	51	ASP	2.3
1	B	316	LYS	2.3
1	O	253	HIS	2.3
1	A	121	ASN	2.3
1	A	220	TYR	2.3
1	G	57	ILE	2.3
1	N	286	THR	2.3
1	O	219	GLN	2.3
1	E	391	ASP	2.3
1	A	278	ALA	2.3
1	C	57	ILE	2.3
1	M	330	ARG	2.3
1	G	251	SER	2.3
1	K	417	ARG	2.3
1	N	77	ASN	2.3
1	O	284	THR	2.3
1	I	191	PRO	2.2
1	N	225	VAL	2.2
1	L	219	GLN	2.2
1	R	320	GLN	2.2
1	K	220	TYR	2.2
1	T	57	ILE	2.2
1	K	316	LYS	2.2
1	N	253	HIS	2.2
1	M	224	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	284	THR	2.2
1	K	114	PRO	2.2
1	B	121	ASN	2.2
1	M	285	GLY	2.2
1	N	318	GLY	2.2
1	P	424	GLU	2.2
1	O	112	THR	2.2
1	C	51	ASP	2.2
1	H	51	ASP	2.2
1	I	213	ASP	2.2
1	Q	120	LEU	2.2
1	A	426	PHE	2.2
1	G	191	PRO	2.2
1	C	424	GLU	2.2
1	I	215	GLN	2.2
1	S	121	ASN	2.2
1	H	286	THR	2.2
1	J	218	SER	2.2
1	P	217	SER	2.2
1	K	221	GLN	2.2
1	P	280	ASN	2.2
1	C	252	VAL	2.2
1	D	273	THR	2.2
1	J	189	LEU	2.2
1	Q	406	ASP	2.2
1	R	426	PHE	2.2
1	C	224	GLY	2.2
1	C	437	LYS	2.2
1	C	417	ARG	2.2
1	E	389	ARG	2.2
1	M	389	ARG	2.2
1	S	389	ARG	2.2
1	I	224	GLY	2.2
1	C	389	ARG	2.2
1	J	278	ALA	2.2
1	Q	283	THR	2.2
1	N	218	SER	2.1
1	I	285	GLY	2.1
1	Q	188	GLY	2.1
1	E	359	THR	2.1
1	D	218	SER	2.1
1	C	281	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	121	ASN	2.1
1	Q	191	PRO	2.1
1	P	283	THR	2.1
1	F	281	GLY	2.1
1	R	424	GLU	2.1
1	F	391	ASP	2.1
1	C	112	THR	2.1
1	J	254	GLY	2.1
1	O	389	ARG	2.1
1	O	213	ASP	2.1
1	N	278	ALA	2.1
1	D	255	LEU	2.1
1	H	279	ASN	2.1
1	K	213	ASP	2.1
1	B	424	GLU	2.1
1	G	218	SER	2.1
1	M	326	SER	2.1
1	M	432	LEU	2.1
1	O	432	LEU	2.1
1	P	76	GLY	2.1
1	B	286	THR	2.1
1	B	323	ASP	2.1
1	J	213	ASP	2.1
1	B	254	GLY	2.1
1	D	432	LEU	2.1
1	T	120	LEU	2.1
1	T	121	ASN	2.1
1	M	219	GLN	2.1
1	P	215	GLN	2.1
1	M	57	ILE	2.1
1	B	212	ASP	2.1
1	L	330	ARG	2.1
1	P	51	ASP	2.1
1	G	254	GLY	2.1
1	P	181	GLY	2.1
1	D	216	PHE	2.0
1	S	417	ARG	2.0
1	Q	78	GLY	2.0
1	Q	224	GLY	2.0
1	R	318	GLY	2.0
1	Q	215	GLN	2.0
1	G	253	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	T	215	GLN	2.0
1	E	279	ASN	2.0
1	Q	192	LYS	2.0
1	H	213	ASP	2.0
1	S	13	PRO	2.0
1	B	281	GLY	2.0
1	D	280	ASN	2.0
1	L	77	ASN	2.0
1	P	119	ALA	2.0
1	M	417	ARG	2.0
1	K	283	THR	2.0
1	C	426	PHE	2.0
1	L	191	PRO	2.0
1	L	213	ASP	2.0
1	M	213	ASP	2.0
1	M	391	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	B	502	1/1	0.98	0.19	0.73	12,12,12,12	1
2	CA	O	509	1/1	0.95	0.19	0.24	2,2,2,2	0
2	CA	C	503	1/1	0.99	0.17	-0.19	2,2,2,2	1
2	CA	G	506	1/1	0.98	0.12	-1.49	2,2,2,2	0
2	CA	A	501	1/1	0.95	0.12	-1.77	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	L	507	1/1	0.95	0.12	-1.77	2,2,2,2	1
2	CA	F	505	1/1	0.99	0.11	-2.00	2,2,2,2	0
2	CA	S	510	1/1	0.97	0.09	-8.04	5,5,5,5	1
2	CA	M	508	1/1	0.97	0.09	-8.04	2,2,2,2	1
2	CA	T	511	1/1	0.99	0.12	-	4,4,4,4	1
2	CA	D	504	1/1	0.97	0.17	-	2,2,2,2	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.