



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:41 PM UTC

PDB ID : 2GSY / pdb_00002gsy
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

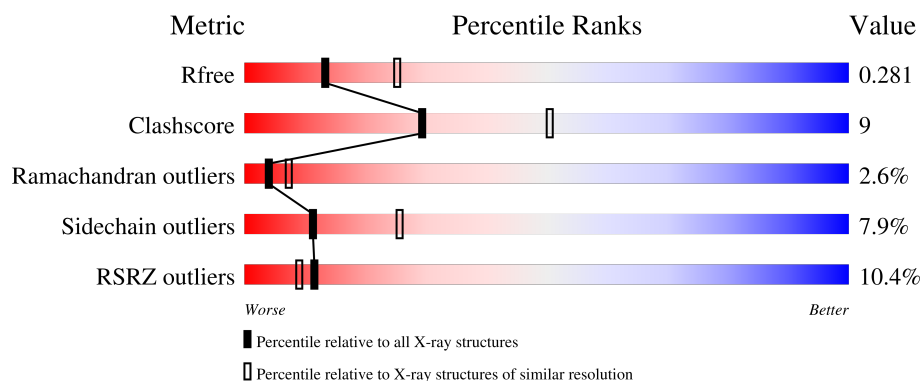
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	456	8% 74% 15% 6%
1	B	456	10% 76% 14% 6%
1	C	456	9% 75% 15% 6%
1	D	456	11% 76% 14% 6%
1	E	456	7% 75% 16% 5%

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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 (CCD ID: CA) (formula: Ca).

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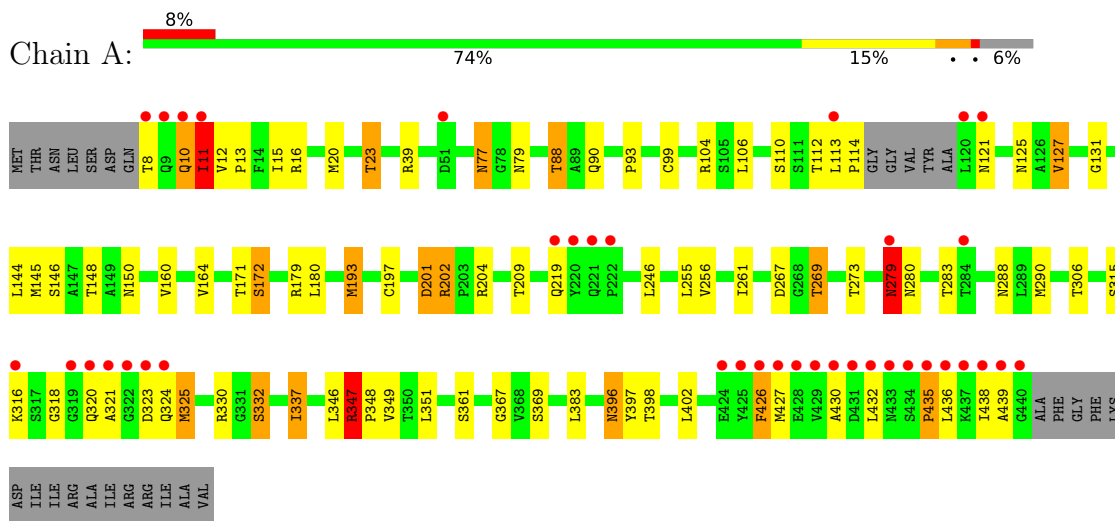
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total O 2 2	0	0
3	D	2	Total O 2 2	0	0
3	E	8	Total O 8 8	0	0
3	F	4	Total O 4 4	0	0
3	G	6	Total O 6 6	0	0
3	H	7	Total O 7 7	0	0
3	I	6	Total O 6 6	0	0
3	J	1	Total O 1 1	0	0
3	K	7	Total O 7 7	0	0
3	L	6	Total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

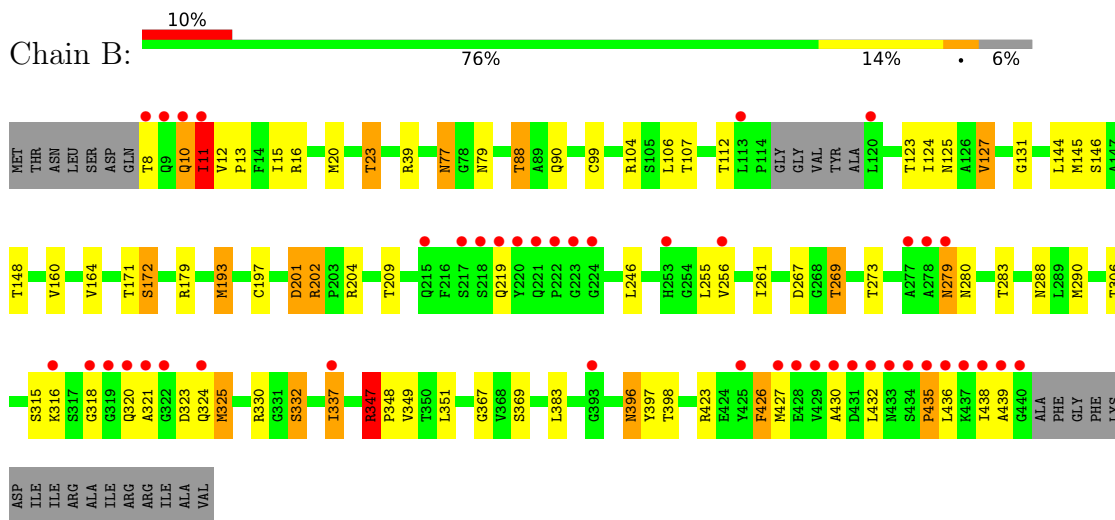
3 Residue-property plots [i](#)

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

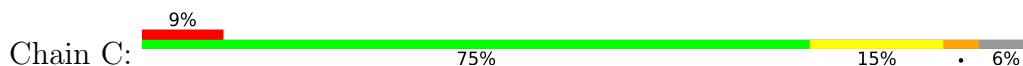
- Molecule 1: polyprotein

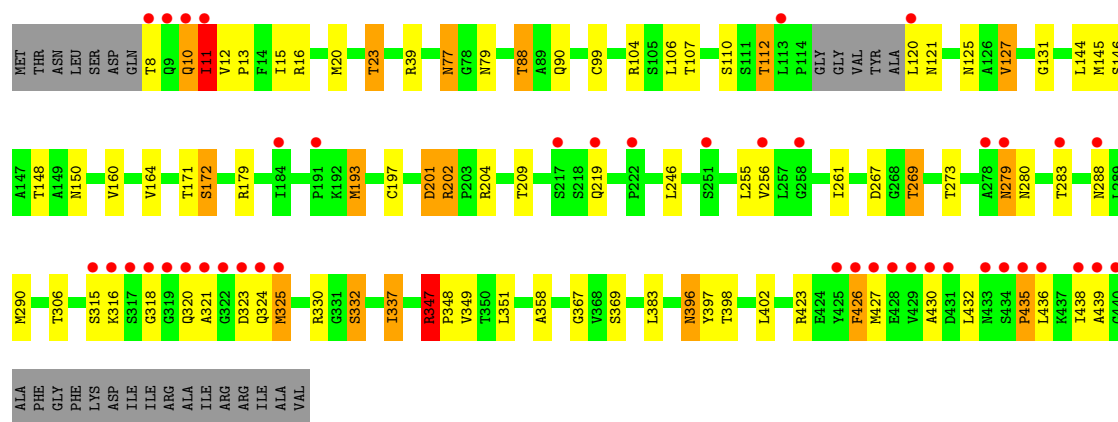


- Molecule 1: polyprotein

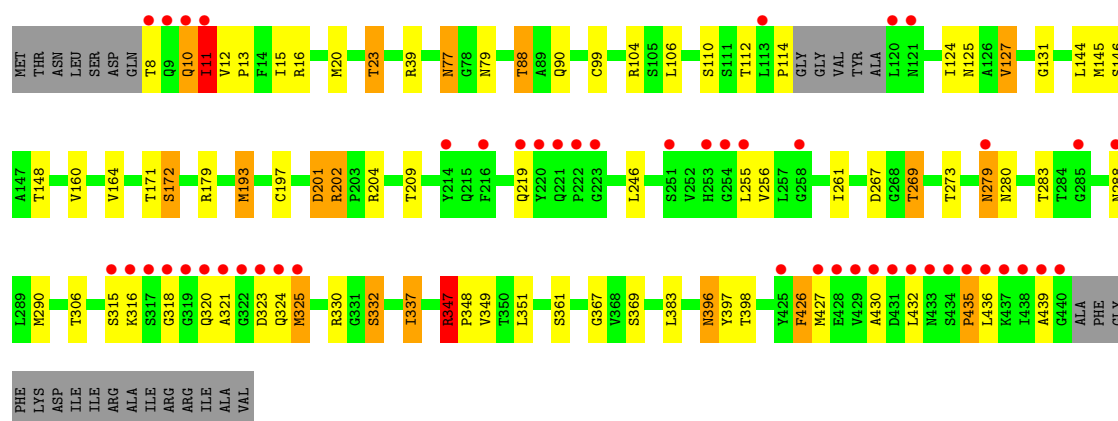
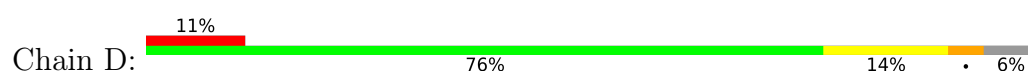


- Molecule 1: polyprotein

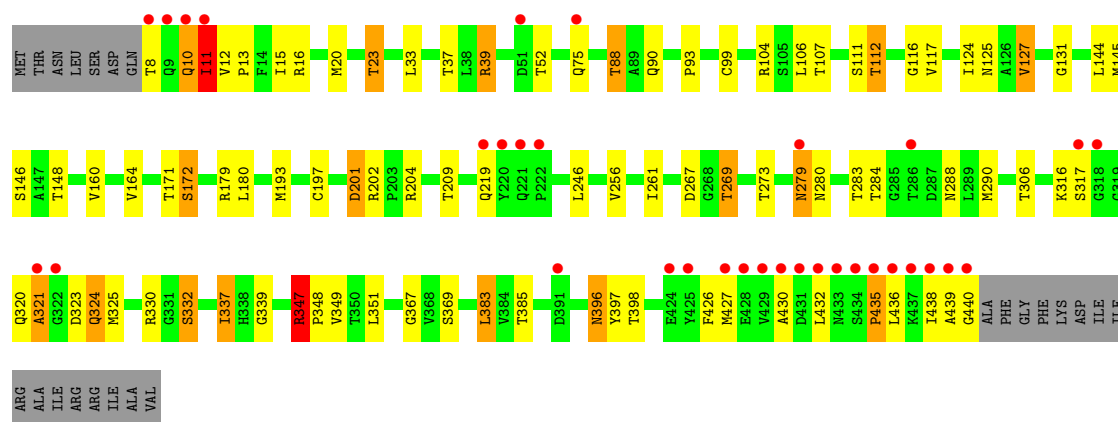
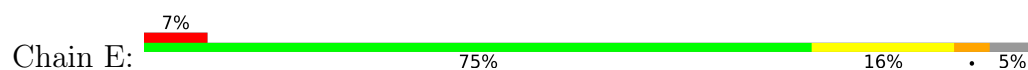




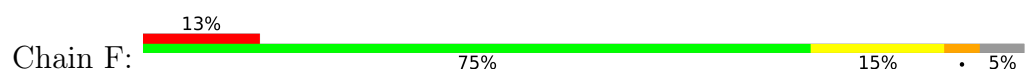
• Molecule 1: polyprotein

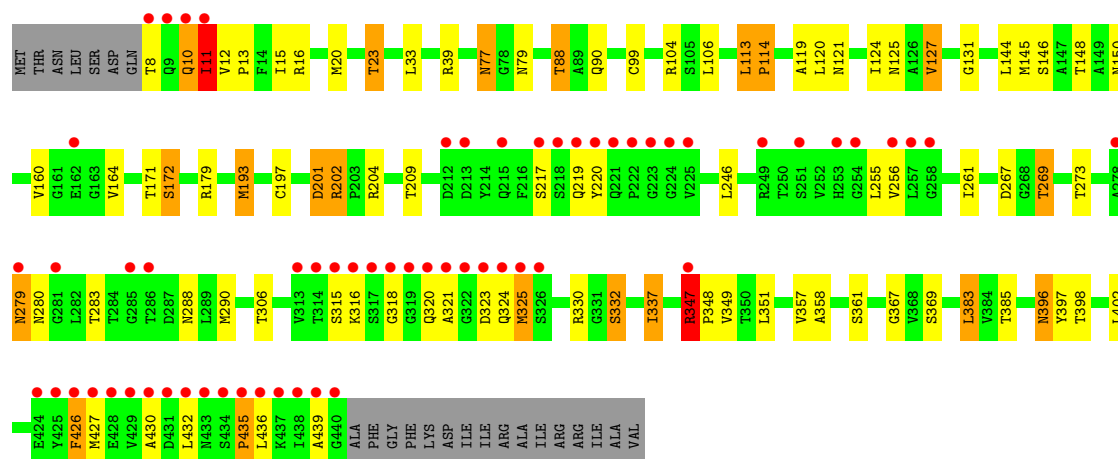


• Molecule 1: polyprotein

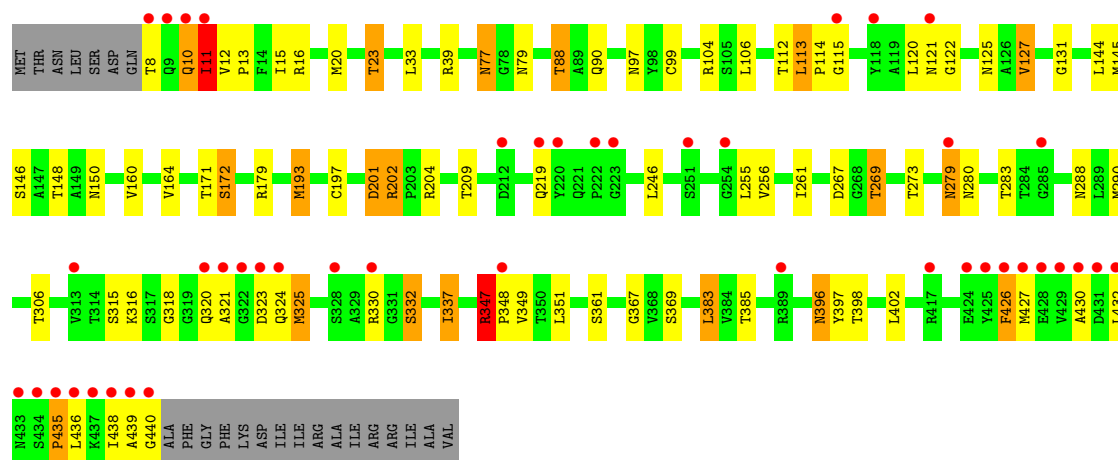
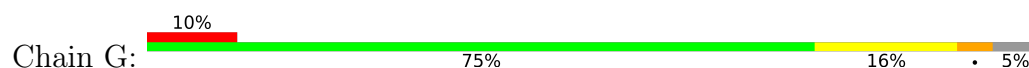


• Molecule 1: polyprotein

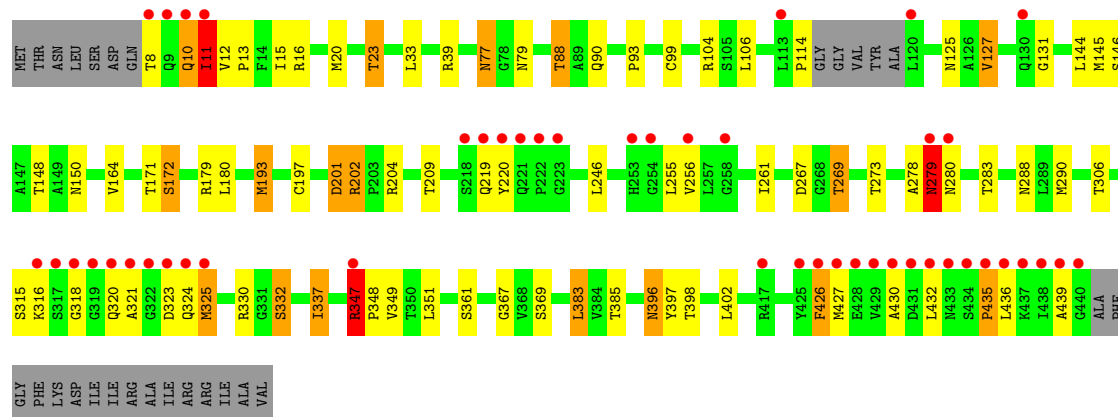
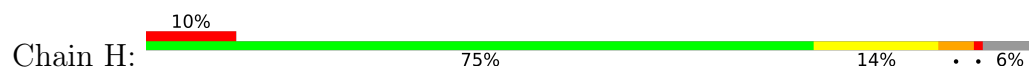




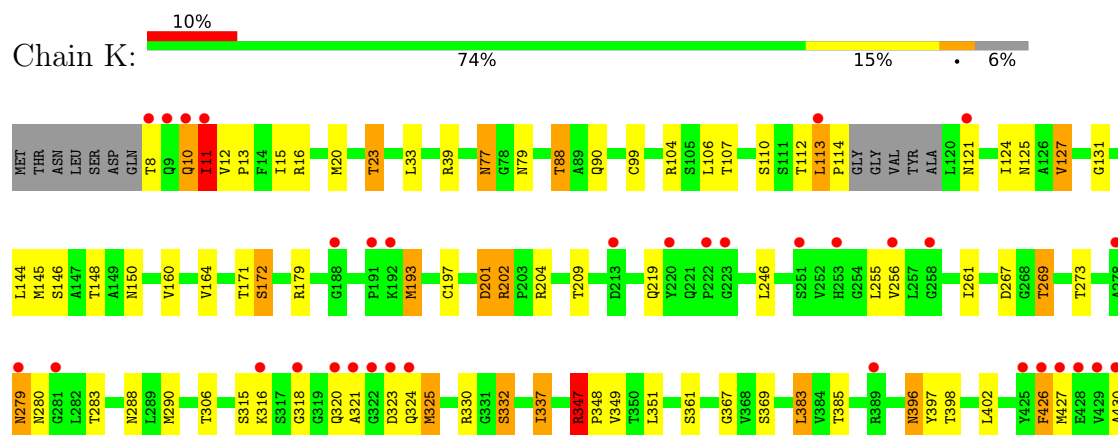
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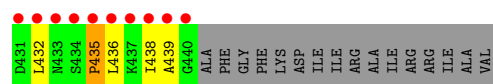


• Molecule 1: polyprotein

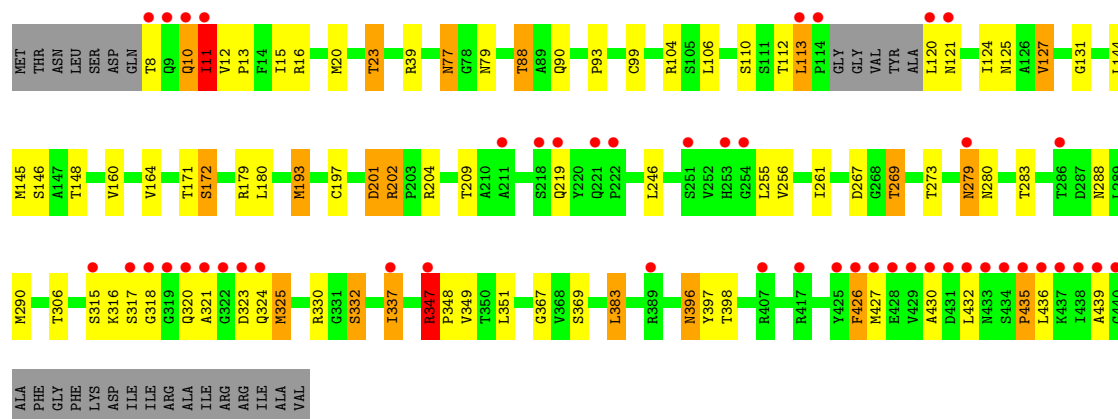
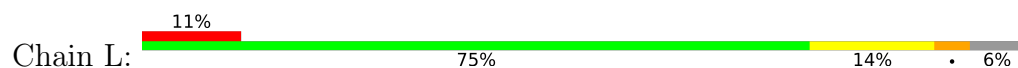


• Molecule 1: polyprotein

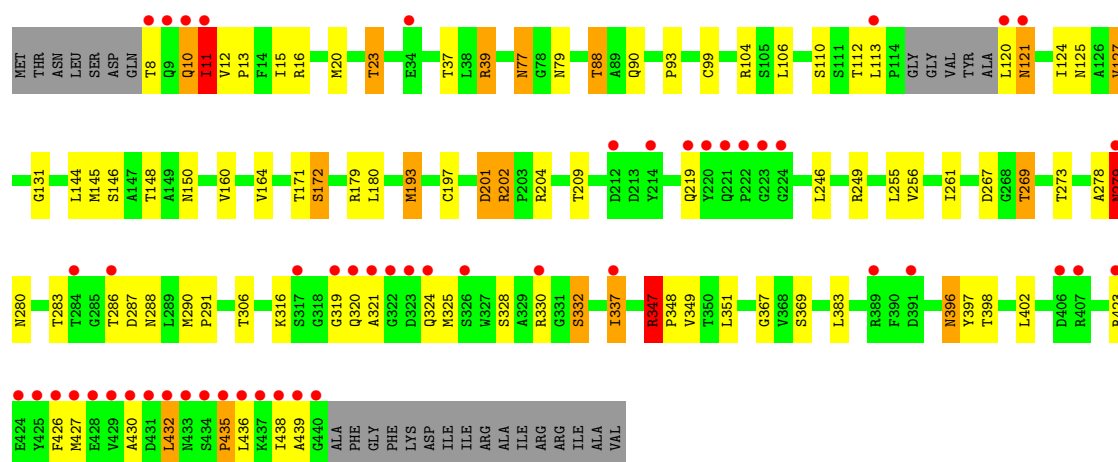
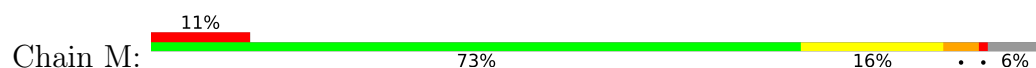




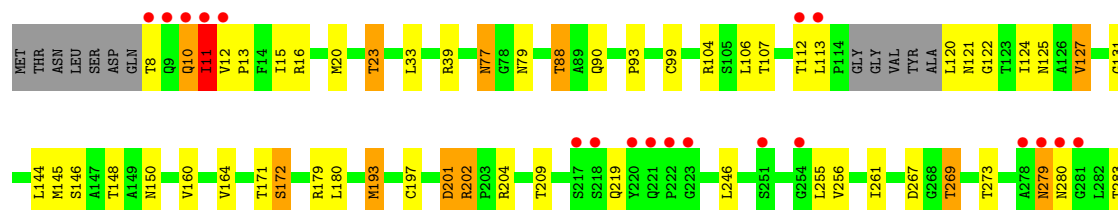
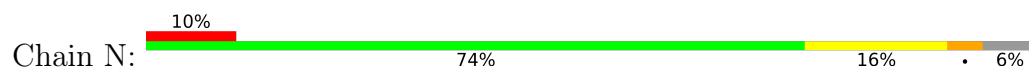
• Molecule 1: polyprotein



• Molecule 1: polyprotein

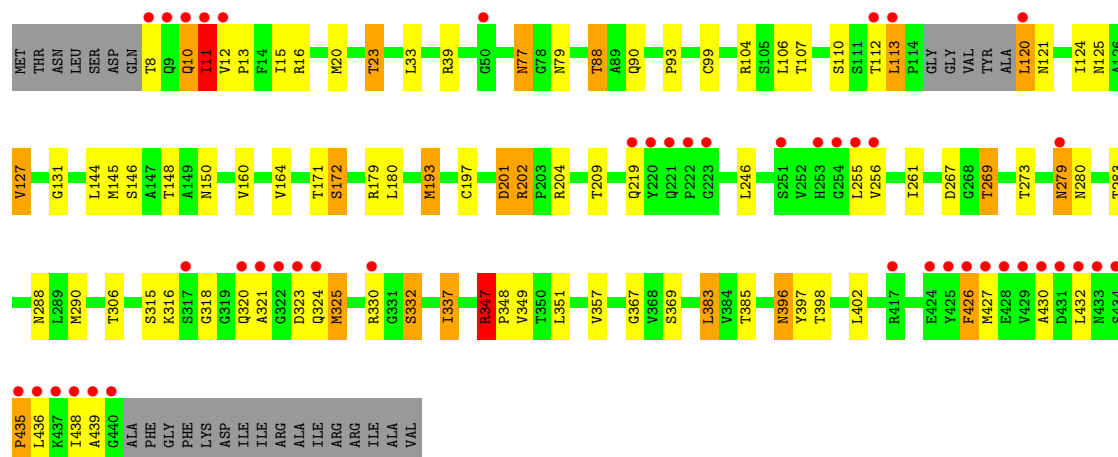
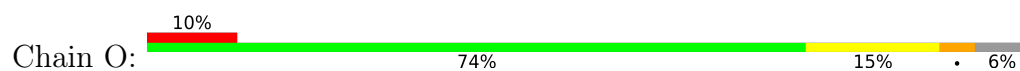


• Molecule 1: polyprotein

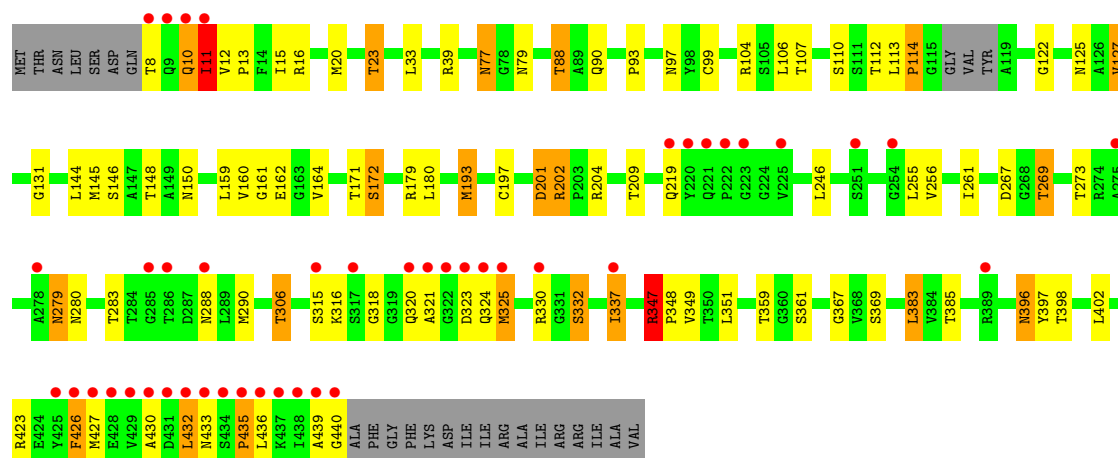
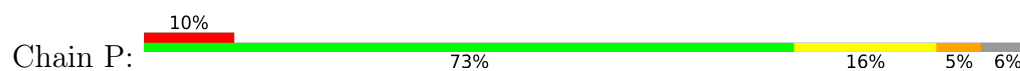




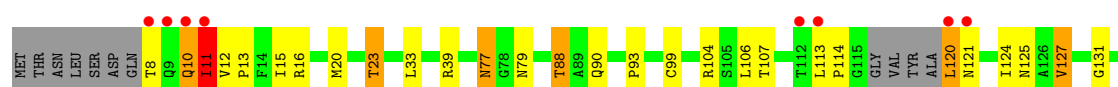
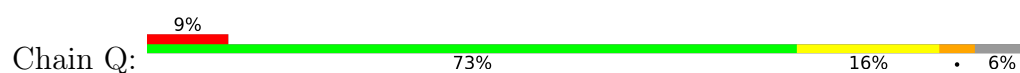
• Molecule 1: polypeptide

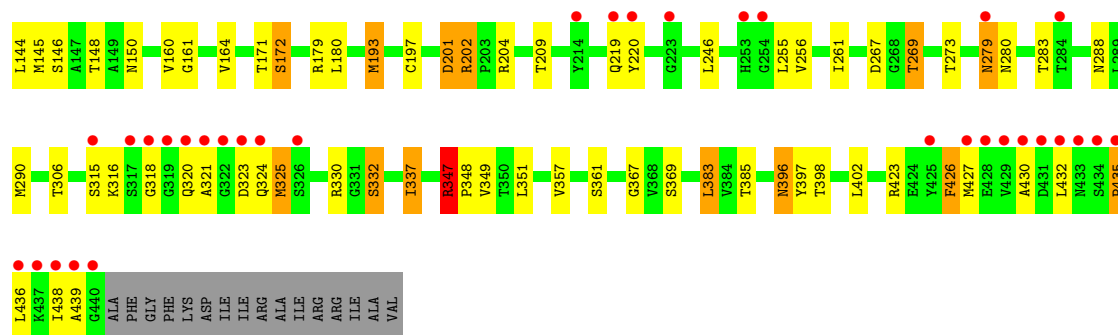


• Molecule 1: polypeptide

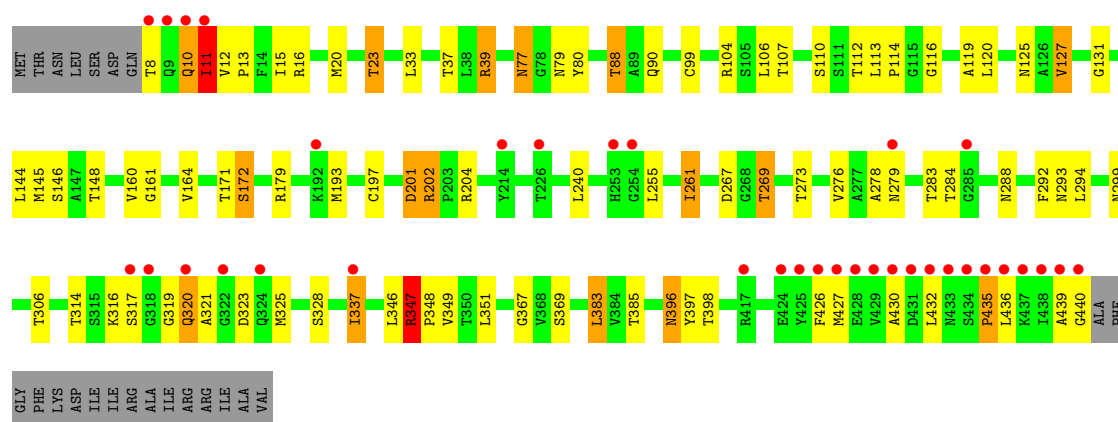
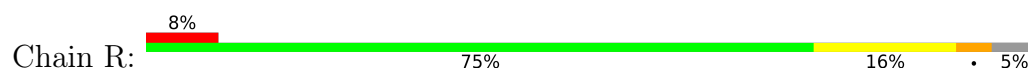


• Molecule 1: polypeptide

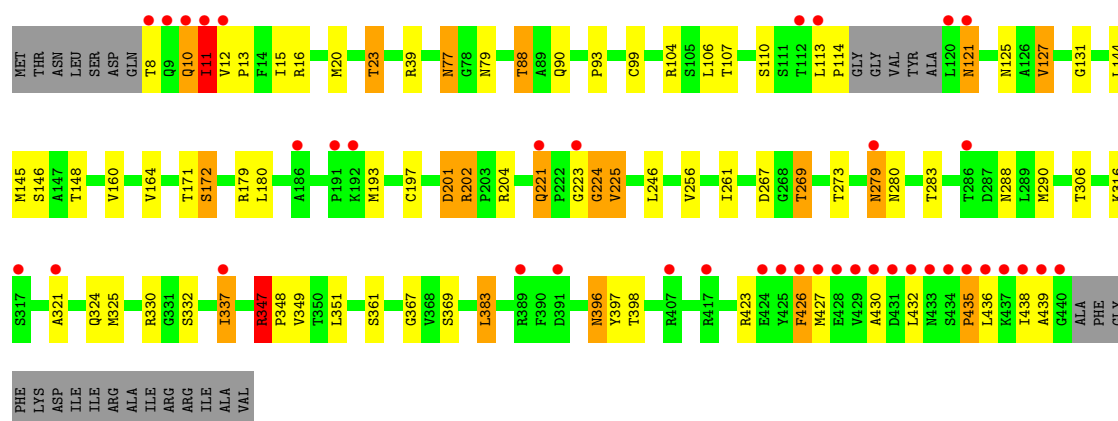
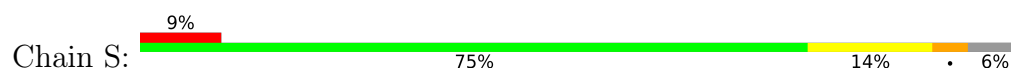




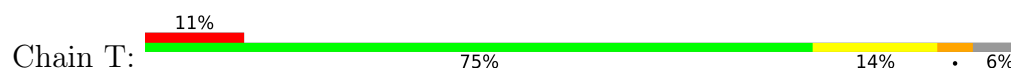
• Molecule 1: polypeptide

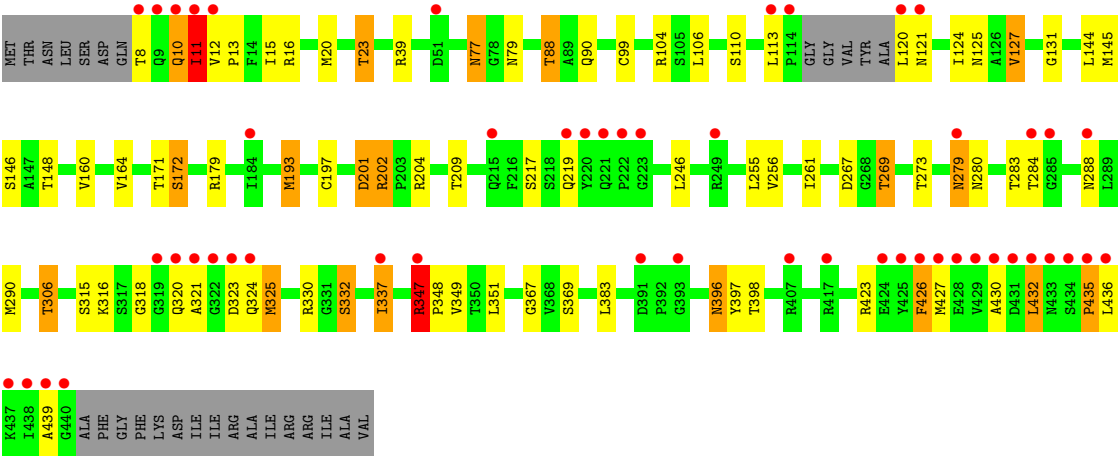


• Molecule 1: polypeptide



• Molecule 1: polypeptide





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	326.30Å 326.30Å 326.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.60 19.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.8 (19.97-2.60) 88.6 (19.97-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.267 0.274 , 0.281	Depositor DCC
R_{free} test set	15643 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 7.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	64447	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.49	0/3272	0.84	4/4471 (0.1%)
1	B	0.48	0/3272	0.84	3/4471 (0.1%)
1	C	0.49	0/3272	0.84	3/4471 (0.1%)
1	D	0.49	0/3272	0.84	3/4471 (0.1%)
1	E	0.48	0/3306	0.83	3/4519 (0.1%)
1	F	0.49	0/3306	0.86	5/4519 (0.1%)
1	G	0.49	0/3306	0.85	4/4519 (0.1%)
1	H	0.49	0/3272	0.84	3/4471 (0.1%)
1	I	0.50	0/3272	0.85	4/4471 (0.1%)
1	J	0.49	0/3272	0.84	3/4471 (0.1%)
1	K	0.49	0/3272	0.84	4/4471 (0.1%)
1	L	0.49	0/3272	0.85	4/4471 (0.1%)
1	M	0.47	0/3272	0.83	4/4471 (0.1%)
1	N	0.49	0/3272	0.84	3/4471 (0.1%)
1	O	0.49	0/3272	0.84	3/4471 (0.1%)
1	P	0.49	0/3281	0.84	3/4483 (0.1%)
1	Q	0.49	0/3276	0.84	3/4476 (0.1%)
1	R	0.48	0/3306	0.83	4/4519 (0.1%)
1	S	0.48	0/3272	0.85	5/4471 (0.1%)
1	T	0.50	0/3272	0.84	3/4471 (0.1%)
All	All	0.49	0/65589	0.84	71/89629 (0.1%)

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 (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	347	ARG	CA-C-N	-9.93	109.83	119.76
1	G	347	ARG	C-N-CA	-9.93	109.83	119.76
1	P	347	ARG	CA-C-N	-9.87	109.89	119.76
1	P	347	ARG	C-N-CA	-9.87	109.89	119.76
1	J	347	ARG	CA-C-N	-9.81	109.95	119.76
1	J	347	ARG	C-N-CA	-9.81	109.95	119.76
1	F	347	ARG	CA-C-N	-9.80	109.96	119.76
1	F	347	ARG	C-N-CA	-9.80	109.96	119.76
1	B	347	ARG	CA-C-N	-9.77	109.99	119.76
1	B	347	ARG	C-N-CA	-9.77	109.99	119.76
1	T	347	ARG	CA-C-N	-9.77	109.99	119.76
1	T	347	ARG	C-N-CA	-9.77	109.99	119.76
1	H	347	ARG	CA-C-N	-9.76	110.00	119.76
1	H	347	ARG	C-N-CA	-9.76	110.00	119.76
1	L	347	ARG	CA-C-N	-9.76	110.00	119.76
1	L	347	ARG	C-N-CA	-9.76	110.00	119.76
1	O	347	ARG	CA-C-N	-9.76	110.00	119.76
1	O	347	ARG	C-N-CA	-9.76	110.00	119.76
1	K	347	ARG	CA-C-N	-9.75	110.01	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	347	ARG	C-N-CA	-9.75	110.01	119.76
1	Q	347	ARG	CA-C-N	-9.75	110.01	119.76
1	Q	347	ARG	C-N-CA	-9.75	110.01	119.76
1	D	347	ARG	CA-C-N	-9.74	110.02	119.76
1	D	347	ARG	C-N-CA	-9.74	110.02	119.76
1	I	347	ARG	CA-C-N	-9.74	110.02	119.76
1	I	347	ARG	C-N-CA	-9.74	110.02	119.76
1	C	347	ARG	CA-C-N	-9.72	110.04	119.76
1	C	347	ARG	C-N-CA	-9.72	110.04	119.76
1	A	347	ARG	CA-C-N	-9.65	110.11	119.76
1	A	347	ARG	C-N-CA	-9.65	110.11	119.76
1	N	347	ARG	CA-C-N	-9.61	110.16	119.76
1	N	347	ARG	C-N-CA	-9.61	110.16	119.76
1	M	347	ARG	CA-C-N	-9.52	110.24	119.76
1	M	347	ARG	C-N-CA	-9.52	110.24	119.76
1	S	347	ARG	CA-C-N	-9.51	110.25	119.76
1	S	347	ARG	C-N-CA	-9.51	110.25	119.76
1	E	347	ARG	CA-C-N	-9.42	110.34	119.76
1	E	347	ARG	C-N-CA	-9.42	110.34	119.76
1	R	347	ARG	CA-C-N	-9.08	110.68	119.76
1	R	347	ARG	C-N-CA	-9.08	110.68	119.76
1	F	113	LEU	CA-C-N	7.80	129.59	119.84
1	F	113	LEU	C-N-CA	7.80	129.59	119.84
1	E	436	LEU	N-CA-C	-7.53	102.43	111.69
1	R	436	LEU	N-CA-C	-7.34	102.66	111.69
1	C	436	LEU	N-CA-C	-7.33	102.67	111.69
1	Q	436	LEU	N-CA-C	-7.29	102.72	111.69
1	F	436	LEU	N-CA-C	-7.26	102.76	111.69
1	K	436	LEU	N-CA-C	-7.25	102.77	111.69
1	S	436	LEU	N-CA-C	-7.24	102.78	111.69
1	M	436	LEU	N-CA-C	-7.24	102.79	111.69
1	O	436	LEU	N-CA-C	-7.23	102.80	111.69
1	G	436	LEU	N-CA-C	-7.20	102.83	111.69
1	T	436	LEU	N-CA-C	-7.20	102.83	111.69
1	D	436	LEU	N-CA-C	-7.19	102.84	111.69
1	K	121	ASN	N-CA-C	7.19	118.67	108.54
1	A	436	LEU	N-CA-C	-7.17	102.87	111.69
1	J	436	LEU	N-CA-C	-7.17	102.87	111.69
1	I	436	LEU	N-CA-C	-7.16	102.88	111.69
1	L	436	LEU	N-CA-C	-7.15	102.90	111.69
1	B	436	LEU	N-CA-C	-7.12	102.94	111.69
1	H	436	LEU	N-CA-C	-7.10	102.96	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	436	LEU	N-CA-C	-7.04	103.03	111.69
1	N	436	LEU	N-CA-C	-7.04	102.81	111.40
1	S	224	GLY	N-CA-C	6.99	124.80	112.64
1	L	121	ASN	N-CA-C	5.69	117.27	110.44
1	G	115	GLY	N-CA-C	5.54	119.35	112.64
1	S	121	ASN	N-CA-C	5.49	117.34	108.34
1	M	121	ASN	N-CA-C	5.42	116.19	108.54
1	R	346	LEU	N-CA-C	-5.06	108.38	114.75
1	I	346	LEU	N-CA-C	-5.03	108.41	114.75
1	A	346	LEU	N-CA-C	-5.03	108.41	114.75

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
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

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Mol	Chain	Res	Type	Group
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
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 ⓘ

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	53	0
1	B	3209	0	3191	52	0
1	C	3209	0	3191	56	0
1	D	3209	0	3191	50	1
1	E	3241	0	3221	61	1
1	F	3241	0	3221	61	1
1	G	3241	0	3221	60	0
1	H	3209	0	3191	56	0
1	I	3209	0	3191	60	0
1	J	3209	0	3191	57	0
1	K	3209	0	3191	60	0
1	L	3209	0	3191	53	1
1	M	3209	0	3191	61	0
1	N	3209	0	3191	62	0
1	O	3209	0	3191	60	0
1	P	3218	0	3199	70	0
1	Q	3213	0	3194	62	0
1	R	3241	0	3221	67	0
1	S	3209	0	3191	51	0
1	T	3209	0	3191	56	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1103	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 9.

All (1103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:110:SER:HB3	1:R:160:VAL:HG12	1.43	0.97
1:M:286:THR:HG21	1:R:279:ASN:HB2	1.44	0.96
1:R:204:ARG:HB3	1:R:337:ILE:HD13	1.56	0.88
1:G:204:ARG:HD2	1:G:337:ILE:HD11	1.56	0.87
1:P:150:ASN:HD21	1:Q:385:THR:H	1.20	0.87
1:H:204:ARG:HD2	1:H:337:ILE:HD11	1.57	0.87
1:D:204:ARG:HD2	1:D:337:ILE:HD11	1.56	0.87
1:L:204:ARG:HD2	1:L:337:ILE:HD11	1.57	0.87
1:R:110:SER:HB3	1:R:160:VAL:CG1	2.04	0.87
1:A:204:ARG:HD2	1:A:337:ILE:HD11	1.56	0.86
1:B:204:ARG:HD2	1:B:337:ILE:HD11	1.57	0.86
1:C:204:ARG:HD2	1:C:337:ILE:HD11	1.57	0.86
1:F:204:ARG:HD2	1:F:337:ILE:HD11	1.56	0.86
1:P:204:ARG:HD2	1:P:337:ILE:HD11	1.57	0.86
1:E:204:ARG:HD2	1:E:337:ILE:HD11	1.54	0.86
1:N:204:ARG:HD2	1:N:337:ILE:HD11	1.57	0.86
1:I:204:ARG:HD2	1:I:337:ILE:HD11	1.57	0.86
1:S:204:ARG:HD2	1:S:337:ILE:HD11	1.57	0.85
1:M:204:ARG:HD2	1:M:337:ILE:HD11	1.56	0.85
1:T:204:ARG:HD2	1:T:337:ILE:HD11	1.57	0.85
1:O:204:ARG:HD2	1:O:337:ILE:HD11	1.57	0.85
1:R:204:ARG:HB3	1:R:337:ILE:CD1	2.07	0.85
1:S:221:GLN:HB3	1:S:224:GLY:HA3	1.57	0.85
1:K:204:ARG:HD2	1:K:337:ILE:HD11	1.56	0.85
1:J:204:ARG:HD2	1:J:337:ILE:HD11	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:385:THR:H	1:Q:150:ASN:HD21	1.28	0.78
1:P:306:THR:HG22	3:P:720:HOH:O	1.82	0.78
1:F:88:THR:HG22	1:F:90:GLN:O	1.83	0.78
1:G:88:THR:HG22	1:G:90:GLN:O	1.83	0.78
1:A:88:THR:HG22	1:A:90:GLN:O	1.83	0.78
1:H:88:THR:HG22	1:H:90:GLN:O	1.84	0.78
1:J:88:THR:HG22	1:J:90:GLN:O	1.83	0.78
1:R:347:ARG:HB3	1:R:348:PRO:HD3	1.66	0.78
1:A:150:ASN:HD21	1:E:385:THR:H	1.30	0.78
1:C:88:THR:HG22	1:C:90:GLN:O	1.83	0.78
1:K:88:THR:HG22	1:K:90:GLN:O	1.83	0.78
1:Q:88:THR:HG22	1:Q:90:GLN:O	1.83	0.78
1:H:150:ASN:HD21	1:N:385:THR:H	1.31	0.77
1:P:20:MET:O	1:P:23:THR:HB	1.85	0.77
1:E:20:MET:O	1:E:23:THR:HB	1.84	0.77
1:K:20:MET:O	1:K:23:THR:HB	1.85	0.77
1:L:88:THR:HG22	1:L:90:GLN:O	1.84	0.77
1:O:20:MET:O	1:O:23:THR:HB	1.85	0.77
1:S:88:THR:HG22	1:S:90:GLN:O	1.85	0.77
1:G:20:MET:O	1:G:23:THR:HB	1.85	0.77
1:J:20:MET:O	1:J:23:THR:HB	1.85	0.77
1:C:20:MET:O	1:C:23:THR:HB	1.85	0.77
1:L:20:MET:O	1:L:23:THR:HB	1.85	0.77
1:A:20:MET:O	1:A:23:THR:HB	1.85	0.77
1:O:88:THR:HG22	1:O:90:GLN:O	1.83	0.77
1:B:20:MET:O	1:B:23:THR:HB	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:MET:O	1:I:23:THR:HB	1.85	0.76
1:F:20:MET:O	1:F:23:THR:HB	1.84	0.76
1:M:88:THR:HG22	1:M:90:GLN:O	1.86	0.76
1:D:20:MET:O	1:D:23:THR:HB	1.85	0.76
1:H:20:MET:O	1:H:23:THR:HB	1.85	0.76
1:I:385:THR:H	1:K:150:ASN:HD21	1.34	0.76
1:Q:20:MET:O	1:Q:23:THR:HB	1.85	0.76
1:T:20:MET:O	1:T:23:THR:HB	1.85	0.76
1:H:347:ARG:HB3	1:H:348:PRO:HD3	1.68	0.76
1:J:347:ARG:HB3	1:J:348:PRO:HD3	1.68	0.76
1:N:347:ARG:HB3	1:N:348:PRO:HD3	1.68	0.75
1:O:347:ARG:HB3	1:O:348:PRO:HD3	1.68	0.75
1:G:347:ARG:HB3	1:G:348:PRO:HD3	1.68	0.75
1:N:20:MET:O	1:N:23:THR:HB	1.85	0.75
1:A:347:ARG:HB3	1:A:348:PRO:HD3	1.68	0.75
1:T:347:ARG:HB3	1:T:348:PRO:HD3	1.69	0.75
1:M:20:MET:O	1:M:23:THR:HB	1.86	0.75
1:S:20:MET:O	1:S:23:THR:HB	1.87	0.75
1:K:347:ARG:HB3	1:K:348:PRO:HD3	1.69	0.75
1:S:347:ARG:HB3	1:S:348:PRO:HD3	1.68	0.74
1:L:347:ARG:HB3	1:L:348:PRO:HD3	1.68	0.74
1:E:112:THR:HG21	1:P:161:GLY:H	1.53	0.74
1:E:347:ARG:HB3	1:E:348:PRO:HD3	1.69	0.74
1:F:347:ARG:HB3	1:F:348:PRO:HD3	1.69	0.74
1:M:347:ARG:HB3	1:M:348:PRO:HD3	1.68	0.74
1:Q:347:ARG:HB3	1:Q:348:PRO:HD3	1.68	0.74
1:C:347:ARG:HB3	1:C:348:PRO:HD3	1.68	0.74
1:B:347:ARG:HB3	1:B:348:PRO:HD3	1.69	0.74
1:D:347:ARG:HB3	1:D:348:PRO:HD3	1.68	0.74
1:I:347:ARG:HB3	1:I:348:PRO:HD3	1.69	0.74
1:R:20:MET:O	1:R:23:THR:HB	1.87	0.73
1:P:347:ARG:HB3	1:P:348:PRO:HD3	1.69	0.73
1:P:110:SER:HB3	1:P:160:VAL:HG12	1.71	0.72
1:M:150:ASN:HD21	1:R:385:THR:H	1.36	0.72
1:M:255:LEU:HD23	1:M:316:LYS:HG3	1.69	0.72
1:E:323:ASP:O	1:E:324:GLN:HB2	1.90	0.71
1:D:16:ARG:HG2	1:D:23:THR:HG21	1.75	0.69
1:F:16:ARG:HG2	1:F:23:THR:HG21	1.74	0.69
1:L:16:ARG:HG2	1:L:23:THR:HG21	1.74	0.69
1:S:16:ARG:HG2	1:S:23:THR:HG21	1.74	0.69
1:H:11:ILE:HD11	1:H:16:ARG:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:ARG:HG2	1:H:23:THR:HG21	1.75	0.69
1:K:11:ILE:HD11	1:K:16:ARG:HD2	1.75	0.69
1:C:11:ILE:HD11	1:C:16:ARG:HD2	1.75	0.69
1:J:11:ILE:HD11	1:J:16:ARG:HD2	1.75	0.69
1:J:16:ARG:HG2	1:J:23:THR:HG21	1.74	0.69
1:K:16:ARG:HG2	1:K:23:THR:HG21	1.75	0.69
1:G:11:ILE:HD11	1:G:16:ARG:HD2	1.75	0.69
1:T:11:ILE:HD11	1:T:16:ARG:HD2	1.75	0.69
1:B:16:ARG:HG2	1:B:23:THR:HG21	1.75	0.69
1:D:11:ILE:HD11	1:D:16:ARG:HD2	1.75	0.69
1:H:383:LEU:HD22	1:R:383:LEU:HD22	1.75	0.69
1:L:11:ILE:HD11	1:L:16:ARG:HD2	1.75	0.69
1:M:16:ARG:HG2	1:M:23:THR:HG21	1.75	0.68
1:B:11:ILE:HD11	1:B:16:ARG:HD2	1.75	0.68
1:E:112:THR:HG23	1:P:159:LEU:HB3	1.74	0.68
1:M:104:ARG:HD3	1:M:369:SER:OG	1.94	0.68
1:P:11:ILE:HD11	1:P:16:ARG:HD2	1.75	0.68
1:P:16:ARG:HG2	1:P:23:THR:HG21	1.75	0.68
1:A:16:ARG:HG2	1:A:23:THR:HG21	1.75	0.68
1:D:267:ASP:OD1	1:D:269:THR:HB	1.94	0.68
1:I:16:ARG:HG2	1:I:23:THR:HG21	1.75	0.68
1:S:11:ILE:HD11	1:S:16:ARG:HD2	1.76	0.68
1:G:16:ARG:HG2	1:G:23:THR:HG21	1.75	0.68
1:A:267:ASP:OD1	1:A:269:THR:HB	1.94	0.68
1:N:16:ARG:HG2	1:N:23:THR:HG21	1.75	0.68
1:O:11:ILE:HD11	1:O:16:ARG:HD2	1.75	0.68
1:Q:16:ARG:HG2	1:Q:23:THR:HG21	1.75	0.68
1:R:16:ARG:HG2	1:R:23:THR:HG21	1.76	0.67
1:O:16:ARG:HG2	1:O:23:THR:HG21	1.75	0.67
1:Q:104:ARG:HD3	1:Q:369:SER:OG	1.95	0.67
1:A:11:ILE:HD11	1:A:16:ARG:HD2	1.75	0.67
1:F:11:ILE:HD11	1:F:16:ARG:HD2	1.76	0.67
1:I:11:ILE:HD11	1:I:16:ARG:HD2	1.75	0.67
1:C:16:ARG:HG2	1:C:23:THR:HG21	1.75	0.67
1:R:104:ARG:HD3	1:R:369:SER:OG	1.95	0.67
1:G:104:ARG:HD3	1:G:369:SER:OG	1.95	0.67
1:Q:11:ILE:HD11	1:Q:16:ARG:HD2	1.75	0.67
1:T:267:ASP:OD1	1:T:269:THR:HB	1.95	0.67
1:H:267:ASP:OD1	1:H:269:THR:HB	1.95	0.67
1:M:11:ILE:HD11	1:M:16:ARG:HD2	1.75	0.67
1:T:131:GLY:O	1:T:347:ARG:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:267:ASP:OD1	1:J:269:THR:HB	1.95	0.67
1:N:11:ILE:HD11	1:N:16:ARG:HD2	1.75	0.67
1:T:16:ARG:HG2	1:T:23:THR:HG21	1.75	0.67
1:K:267:ASP:OD1	1:K:269:THR:HB	1.95	0.67
1:P:104:ARG:HD3	1:P:369:SER:OG	1.95	0.67
1:J:131:GLY:O	1:J:347:ARG:O	2.13	0.67
1:S:131:GLY:O	1:S:347:ARG:O	2.13	0.67
1:N:104:ARG:HD3	1:N:369:SER:OG	1.95	0.66
1:B:267:ASP:OD1	1:B:269:THR:HB	1.95	0.66
1:C:267:ASP:OD1	1:C:269:THR:HB	1.95	0.66
1:L:267:ASP:OD1	1:L:269:THR:HB	1.95	0.66
1:R:11:ILE:HD11	1:R:16:ARG:HD2	1.76	0.66
1:R:349:VAL:HG12	1:R:351:LEU:HD12	1.77	0.66
1:T:104:ARG:HD3	1:T:369:SER:OG	1.95	0.66
1:K:104:ARG:HD3	1:K:369:SER:OG	1.95	0.66
1:N:267:ASP:OD1	1:N:269:THR:HB	1.95	0.66
1:S:267:ASP:OD1	1:S:269:THR:HB	1.95	0.66
1:A:104:ARG:HD3	1:A:369:SER:OG	1.96	0.66
1:F:131:GLY:O	1:F:347:ARG:O	2.14	0.66
1:G:267:ASP:OD1	1:G:269:THR:HB	1.95	0.66
1:H:283:THR:H	1:H:288:ASN:HD21	1.44	0.66
1:J:104:ARG:HD3	1:J:369:SER:OG	1.96	0.66
1:N:131:GLY:O	1:N:347:ARG:O	2.14	0.66
1:Q:283:THR:H	1:Q:288:ASN:HD21	1.44	0.66
1:C:104:ARG:HD3	1:C:369:SER:OG	1.95	0.66
1:G:283:THR:H	1:G:288:ASN:HD21	1.43	0.66
1:O:283:THR:H	1:O:288:ASN:HD21	1.44	0.66
1:Q:131:GLY:O	1:Q:347:ARG:O	2.14	0.66
1:Q:267:ASP:OD1	1:Q:269:THR:HB	1.96	0.66
1:C:283:THR:H	1:C:288:ASN:HD21	1.44	0.66
1:G:131:GLY:O	1:G:347:ARG:O	2.13	0.66
1:H:104:ARG:HD3	1:H:369:SER:OG	1.96	0.66
1:K:283:THR:H	1:K:288:ASN:HD21	1.44	0.66
1:L:104:ARG:HD3	1:L:369:SER:OG	1.96	0.66
1:D:131:GLY:O	1:D:347:ARG:O	2.14	0.66
1:F:283:THR:H	1:F:288:ASN:HD21	1.44	0.66
1:L:110:SER:HB3	1:L:160:VAL:HG12	1.78	0.66
1:N:112:THR:HG22	1:N:113:LEU:H	1.61	0.66
1:O:267:ASP:OD1	1:O:269:THR:HB	1.95	0.66
1:T:110:SER:HB3	1:T:160:VAL:HG12	1.78	0.66
1:B:131:GLY:O	1:B:347:ARG:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:349:VAL:HG12	1:L:351:LEU:HD12	1.78	0.66
1:C:131:GLY:O	1:C:347:ARG:O	2.14	0.65
1:I:131:GLY:O	1:I:347:ARG:O	2.13	0.65
1:P:267:ASP:OD1	1:P:269:THR:HB	1.95	0.65
1:P:349:VAL:HG12	1:P:351:LEU:HD12	1.78	0.65
1:R:316:LYS:HB2	1:R:325:MET:HE3	1.78	0.65
1:I:104:ARG:HD3	1:I:369:SER:OG	1.95	0.65
1:P:283:THR:H	1:P:288:ASN:HD21	1.44	0.65
1:C:349:VAL:HG12	1:C:351:LEU:HD12	1.78	0.65
1:F:267:ASP:OD1	1:F:269:THR:HB	1.95	0.65
1:B:349:VAL:HG12	1:B:351:LEU:HD12	1.78	0.65
1:I:267:ASP:OD1	1:I:269:THR:HB	1.95	0.65
1:P:131:GLY:O	1:P:347:ARG:O	2.13	0.65
1:F:104:ARG:HD3	1:F:369:SER:OG	1.96	0.65
1:E:131:GLY:O	1:E:347:ARG:O	2.15	0.65
1:F:349:VAL:HG12	1:F:351:LEU:HD12	1.79	0.65
1:O:104:ARG:HD3	1:O:369:SER:OG	1.96	0.65
1:O:349:VAL:HG12	1:O:351:LEU:HD12	1.78	0.65
1:D:104:ARG:HD3	1:D:369:SER:OG	1.96	0.65
1:D:283:THR:H	1:D:288:ASN:HD21	1.44	0.65
1:J:349:VAL:HG12	1:J:351:LEU:HD12	1.79	0.65
1:L:131:GLY:O	1:L:347:ARG:O	2.14	0.65
1:I:283:THR:H	1:I:288:ASN:HD21	1.44	0.65
1:M:267:ASP:OD1	1:M:269:THR:HB	1.97	0.65
1:M:349:VAL:HG12	1:M:351:LEU:HD12	1.79	0.65
1:Q:349:VAL:HG12	1:Q:351:LEU:HD12	1.78	0.64
1:B:104:ARG:HD3	1:B:369:SER:OG	1.95	0.64
1:E:267:ASP:OD1	1:E:269:THR:HB	1.97	0.64
1:E:349:VAL:HG12	1:E:351:LEU:HD12	1.79	0.64
1:D:349:VAL:HG12	1:D:351:LEU:HD12	1.79	0.64
1:E:11:ILE:HD11	1:E:16:ARG:HD2	1.78	0.64
1:H:131:GLY:O	1:H:347:ARG:O	2.14	0.64
1:J:283:THR:H	1:J:288:ASN:HD21	1.44	0.64
1:L:283:THR:H	1:L:288:ASN:HD21	1.44	0.64
1:S:283:THR:H	1:S:288:ASN:HD21	1.46	0.64
1:E:16:ARG:HG2	1:E:23:THR:HG21	1.77	0.64
1:H:349:VAL:HG12	1:H:351:LEU:HD12	1.78	0.64
1:K:131:GLY:O	1:K:347:ARG:O	2.14	0.64
1:M:283:THR:H	1:M:288:ASN:HD21	1.46	0.64
1:A:131:GLY:O	1:A:347:ARG:O	2.15	0.64
1:B:283:THR:H	1:B:288:ASN:HD21	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:ARG:HD3	1:E:369:SER:OG	1.98	0.64
1:T:349:VAL:HG12	1:T:351:LEU:HD12	1.79	0.64
1:O:131:GLY:O	1:O:347:ARG:O	2.14	0.64
1:T:283:THR:H	1:T:288:ASN:HD21	1.44	0.64
1:G:349:VAL:HG12	1:G:351:LEU:HD12	1.78	0.64
1:I:349:VAL:HG12	1:I:351:LEU:HD12	1.78	0.64
1:N:349:VAL:HG12	1:N:351:LEU:HD12	1.78	0.64
1: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:M:179:ARG:HD3	1:M:197:CYS:HB3	1.78	0.64
1:N:283:THR:H	1:N:288:ASN:HD21	1.44	0.63
1:A:349:VAL:HG12	1:A:351:LEU:HD12	1.79	0.63
1:A:283:THR:H	1:A:288:ASN:HD21	1.44	0.63
1:E:179:ARG:HD3	1:E:197:CYS:HB3	1.79	0.63
1:R:276:VAL:HG11	1:R:292:PHE:CD2	2.33	0.63
1:S:349:VAL:HG12	1:S:351:LEU:HD12	1.79	0.63
1:S:104:ARG:HD3	1:S:369:SER:OG	1.99	0.63
1:R:179:ARG:HD3	1:R:197:CYS:HB3	1.81	0.62
1:P:150:ASN:HD21	1:Q:385:THR:N	1.94	0.62
1:I:121:ASN:HB3	1:I:357:VAL:HA	1.80	0.62
1:G:179:ARG:HD3	1:G:197:CYS:HB3	1.82	0.62
1:S:125:ASN:HB3	1:S:145:MET:HE3	1.82	0.62
1:N:179:ARG:HD3	1:N:197:CYS:HB3	1.82	0.62
1:S:121:ASN:O	1:S:160:VAL:HB	1.99	0.62
1:I:179:ARG:HD3	1:I:197:CYS:HB3	1.82	0.61
1:O:179:ARG:HD3	1:O:197:CYS:HB3	1.82	0.61
1:R:131:GLY:O	1:R:347:ARG:O	2.18	0.61
1:E:283:THR:H	1:E:288:ASN:HD21	1.45	0.61
1:K:125:ASN:HB3	1:K:145:MET:HE3	1.83	0.61
1:K:383:LEU:HD22	1:P:383:LEU:HD22	1.82	0.61
1:Q:179:ARG:HD3	1:Q:197:CYS:HB3	1.82	0.61
1:C:179:ARG:HD3	1:C:197:CYS:HB3	1.82	0.61
1:J:383:LEU:HD22	1:O:383:LEU:HD22	1.82	0.61
1:L:125:ASN:HB3	1:L:145:MET:HE3	1.83	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:R:319:GLY:C	1:R:320:GLN:HG2	2.26	0.61
1:F:125:ASN:HB3	1:F:145:MET:HE3	1.83	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:179:ARG:HD3	1:H:197:CYS:HB3	1.82	0.60
1:L:179:ARG:HD3	1:L:197:CYS:HB3	1.83	0.60
1:R:125:ASN:HB3	1:R:145:MET:HE3	1.82	0.60
1:B:179:ARG:HD3	1:B:197:CYS:HB3	1.82	0.60
1:P:125:ASN:HB3	1:P:145:MET:HE3	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:C:125:ASN:HB3	1:C:145:MET:HE3	1.83	0.60
1:J:125:ASN:HB3	1:J:145:MET:HE3	1.83	0.60
1:S:316:LYS:HB2	1:S:325:MET:HE2	1.83	0.60
1:B:125:ASN:HB3	1:B:145:MET:HE3	1.83	0.59
1:T:306:THR:HG22	3:T:705:HOH:O	2.01	0.59
1:H:125:ASN:HB3	1:H:145:MET:HE3	1.83	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:D:125:ASN:HB3	1:D:145:MET:HE3	1.84	0.59
1:N:125:ASN:HB3	1:N:145:MET:HE3	1.83	0.59
1:Q:125:ASN:HB3	1:Q:145:MET:HE3	1.83	0.59
1:T:125:ASN:HB3	1:T:145:MET:HE3	1.83	0.59
1:A:125:ASN:HB3	1:A:145:MET:HE3	1.83	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:O:125:ASN:HB3	1:O:145:MET:HE3	1.83	0.59
1:I:125:ASN:HB3	1:I:145:MET:HE3	1.83	0.59
1:R:283:THR:H	1:R:288:ASN:HD21	1.50	0.58
1:G:125:ASN:HB3	1:G:145:MET:HE3	1.84	0.58
1:M:125:ASN:HB3	1:M:145:MET:HE3	1.85	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:E:316:LYS:HB2	1:E:325:MET:HE3	1.85	0.58
1:T:110:SER:HB3	1:T:160:VAL:CG1	2.34	0.58
1:I:88:THR:CG2	1:I:90:GLN:O	2.52	0.58
1:C:88:THR:CG2	1:C:90:GLN:O	2.52	0.58
1:D:88:THR:CG2	1:D:90:GLN:O	2.51	0.58
1:E:125:ASN:HB3	1:E:145:MET:HE3	1.85	0.58
1:J:88:THR:CG2	1:J:90:GLN:O	2.52	0.58
1:T:88:THR:CG2	1:T:90:GLN:O	2.52	0.58
1:A:121:ASN:O	1:A:160:VAL:HB	2.04	0.58
1:A:255:LEU:HD23	1:A:316:LYS:HG3	1.86	0.58
1:G:121:ASN:HB3	1:R:112:THR:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:255:LEU:HD23	1:I:316:LYS:HG3	1.86	0.58
1:N:255:LEU:HD23	1:N:316:LYS:HG3	1.86	0.58
1:K:88:THR:CG2	1:K:90:GLN:O	2.52	0.57
1:K:255:LEU:HD23	1:K:316:LYS:HG3	1.86	0.57
1:L:255:LEU:HD23	1:L:316:LYS:HG3	1.85	0.57
1:B:255:LEU:HD23	1:B:316:LYS:HG3	1.86	0.57
1:P:255:LEU:HD23	1:P:316:LYS:HG3	1.87	0.57
1:F:255:LEU:HD23	1:F:316:LYS:HG3	1.87	0.57
1:C:255:LEU:HD23	1:C:316:LYS:HG3	1.86	0.57
1:M:15:ILE:HG13	1:M:397:TYR:HD2	1.70	0.57
1:T:15:ILE:HG13	1:T:397:TYR:HD2	1.70	0.57
1:B:15:ILE:HG13	1:B:397:TYR:HD2	1.70	0.57
1:D:255:LEU:HD23	1:D:316:LYS:HG3	1.86	0.57
1:S:15:ILE:HG13	1:S:397:TYR:HD2	1.70	0.57
1:S:316:LYS:HB2	1:S:325:MET:CE	2.35	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:G:385:THR:N	1:N:150:ASN:HD21	2.00	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:I:438:ILE:HG23	1:R:440:GLY:C	2.31	0.56
1:L:15:ILE:HG13	1:L:397:TYR:HD2	1.70	0.56
1:G:88:THR:CG2	1:G:90:GLN:O	2.52	0.56
1:M:316:LYS:HE2	1:M:319:GLY:H	1.70	0.56
1:P:15:ILE:HG13	1:P:397:TYR:HD2	1.70	0.56
1:Q:88:THR:CG2	1:Q:90:GLN:O	2.52	0.56
1:Q:114:PRO:HD3	1:Q:361:SER:HB3	1.88	0.56
1:E:15:ILE:HG13	1:E:397:TYR:HD2	1.70	0.56
1:P:88:THR:CG2	1:P:90:GLN:O	2.51	0.56
1:R:88:THR:CG2	1:R:90:GLN:O	2.52	0.56
1:F:15:ILE:HG13	1:F:397:TYR:HD2	1.70	0.56
1:F:383:LEU:HD22	1:S:383:LEU:HD22	1.88	0.56
1:H:15:ILE:HG13	1:H:397:TYR:HD2	1.70	0.56
1:K:15:ILE:HG13	1:K:397:TYR:HD2	1.70	0.56
1:E:112:THR:CG2	1:P:159:LEU:HB3	2.36	0.56
1:G:15:ILE:HG13	1:G:397:TYR:HD2	1.70	0.56
1:H:88:THR:CG2	1:H:90:GLN:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ASN:O	1:C:160:VAL:HB	2.05	0.56
1:Q:255:LEU:HD23	1:Q:316:LYS:HG3	1.86	0.56
1:L:88:THR:CG2	1:L:90:GLN:O	2.52	0.56
1:P:11:ILE:CD1	1:P:16:ARG:HD2	2.36	0.56
1:I:15:ILE:HG13	1:I:397:TYR:HD2	1.70	0.56
1:N:15:ILE:HG13	1:N:397:TYR:HD2	1.70	0.55
1:R:347:ARG:HB3	1:R:348:PRO:CD	2.36	0.55
1:A:88:THR:CG2	1:A:90:GLN:O	2.52	0.55
1:B:88:THR:CG2	1:B:90:GLN:O	2.52	0.55
1:G:11:ILE:CD1	1:G:16:ARG:HD2	2.36	0.55
1:J:255:LEU:HD23	1:J:316:LYS:HG3	1.86	0.55
1:K:11:ILE:CD1	1:K:16:ARG:HD2	2.36	0.55
1:O:11:ILE:CD1	1:O:16:ARG:HD2	2.36	0.55
1:D:11:ILE:CD1	1:D:16:ARG:HD2	2.36	0.55
1:H:11:ILE:CD1	1:H:16:ARG:HD2	2.36	0.55
1:J:11:ILE:CD1	1:J:16:ARG:HD2	2.37	0.55
1:A:15:ILE:HG13	1:A:397:TYR:HD2	1.70	0.55
1:C:15:ILE:HG13	1:C:397:TYR:HD2	1.70	0.55
1:R:283:THR:H	1:R:288:ASN:ND2	2.05	0.55
1:D:15:ILE:HG13	1:D:397:TYR:HD2	1.70	0.55
1:I:11:ILE:CD1	1:I:16:ARG:HD2	2.36	0.55
1:L:11:ILE:CD1	1:L:16:ARG:HD2	2.36	0.55
1:S:88:THR:CG2	1:S:90:GLN:O	2.54	0.55
1:S:347:ARG:HB3	1:S:348:PRO:CD	2.35	0.55
1:I:112:THR:HG22	1:I:113:LEU:H	1.71	0.55
1:H:347:ARG:HB3	1:H:348:PRO:CD	2.37	0.55
1:N:11:ILE:CD1	1:N:16:ARG:HD2	2.37	0.55
1:R:276:VAL:HG11	1:R:292:PHE:CE2	2.41	0.55
1:A:11:ILE:CD1	1:A:16:ARG:HD2	2.36	0.55
1:M:11:ILE:CD1	1:M:16:ARG:HD2	2.36	0.55
1:Q:11:ILE:CD1	1:Q:16:ARG:HD2	2.37	0.55
1:Q:347:ARG:HB3	1:Q:348:PRO:CD	2.37	0.55
1:J:347:ARG:HB3	1:J:348:PRO:CD	2.37	0.55
1:N:347:ARG:HB3	1:N:348:PRO:CD	2.37	0.55
1:M:88:THR:CG2	1:M:90:GLN:O	2.55	0.55
1:P:402:LEU:HD12	1:Q:33:LEU:HD13	1.90	0.54
1:E:88:THR:CG2	1:E:90:GLN:O	2.52	0.54
1:F:11:ILE:CD1	1:F:16:ARG:HD2	2.37	0.54
1:P:114:PRO:HG3	1:P:359:THR:O	2.08	0.54
1:S:11:ILE:CD1	1:S:16:ARG:HD2	2.37	0.54
1:H:426:PHE:CG	1:H:427:MET:N	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:15:ILE:HG13	1:O:397:TYR:HD2	1.70	0.54
1:R:349:VAL:HG12	1:R:351:LEU:CD1	2.37	0.54
1:C:11:ILE:CD1	1:C:16:ARG:HD2	2.37	0.54
1:M:347:ARG:HB3	1:M:348:PRO:CD	2.37	0.54
1:R:426:PHE:CG	1:R:427:MET:N	2.76	0.54
1:B:11:ILE:CD1	1:B:16:ARG:HD2	2.37	0.54
1:I:426:PHE:CG	1:I:427:MET:N	2.76	0.54
1:J:426:PHE:CG	1:J:427:MET:N	2.76	0.54
1:N:426:PHE:CG	1:N:427:MET:N	2.76	0.54
1:C:347:ARG:HB3	1:C:348:PRO:CD	2.37	0.54
1:D:426:PHE:CG	1:D:427:MET:N	2.76	0.54
1:B:426:PHE:CG	1:B:427:MET:N	2.76	0.53
1:I:347:ARG:HB3	1:I:348:PRO:CD	2.38	0.53
1:D:347:ARG:HB3	1:D:348:PRO:CD	2.38	0.53
1:K:347:ARG:HB3	1:K:348:PRO:CD	2.38	0.53
1:Q:426:PHE:CG	1:Q:427:MET:N	2.76	0.53
1:T:426:PHE:CG	1:T:427:MET:N	2.76	0.53
1:E:171:THR:HG21	1:E:348:PRO:HG3	1.89	0.53
1:N:121:ASN:O	1:N:160:VAL:HB	2.08	0.53
1:T:11:ILE:CD1	1:T:16:ARG:HD2	2.36	0.53
1:A:426:PHE:CG	1:A:427:MET:N	2.76	0.53
1:I:349:VAL:HG12	1:I:351:LEU:CD1	2.39	0.53
1:G:426:PHE:CG	1:G:427:MET:N	2.76	0.53
1:M:15:ILE:HD11	1:M:398:THR:HA	1.90	0.53
1:S:349:VAL:HG12	1:S:351:LEU:CD1	2.38	0.53
1:A:402:LEU:HD12	1:E:33:LEU:HD13	1.88	0.53
1:G:349:VAL:HG12	1:G:351:LEU:CD1	2.39	0.53
1:L:426:PHE:CG	1:L:427:MET:N	2.76	0.53
1:M:426:PHE:CG	1:M:427:MET:N	2.76	0.53
1:R:11:ILE:CD1	1:R:16:ARG:HD2	2.37	0.53
1:S:426:PHE:CG	1:S:427:MET:N	2.77	0.53
1:D:349:VAL:HG12	1:D:351:LEU:CD1	2.39	0.53
1:F:426:PHE:CG	1:F:427:MET:N	2.76	0.53
1:G:347:ARG:HB3	1:G:348:PRO:CD	2.37	0.53
1:L:347:ARG:HB3	1:L:348:PRO:CD	2.38	0.53
1:L:349:VAL:HG12	1:L:351:LEU:CD1	2.39	0.53
1:M:171:THR:HG21	1:M:348:PRO:HG3	1.89	0.53
1:P:347:ARG:HB3	1:P:348:PRO:CD	2.37	0.53
1:E:11:ILE:CD1	1:E:16:ARG:HD2	2.39	0.53
1:E:179:ARG:CD	1:E:197:CYS:SG	2.97	0.53
1:K:396:ASN:HD22	1:K:396:ASN:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:396:ASN:H	1:L:396:ASN:HD22	1.57	0.53
1:O:171:THR:HG21	1:O:348:PRO:HG3	1.91	0.53
1:F:171:THR:HG21	1:F:348:PRO:HG3	1.91	0.53
1:K:349:VAL:HG12	1:K:351:LEU:CD1	2.39	0.53
1:K:426:PHE:CG	1:K:427:MET:N	2.77	0.53
1:M:396:ASN:H	1:M:396:ASN:HD22	1.57	0.53
1:R:110:SER:CB	1:R:160:VAL:HG12	2.29	0.53
1:S:179:ARG:CD	1:S:197:CYS:SG	2.96	0.53
1:E:396:ASN:H	1:E:396:ASN:HD22	1.57	0.53
1:N:349:VAL:HG12	1:N:351:LEU:CD1	2.39	0.53
1:T:347:ARG:HB3	1:T:348:PRO:CD	2.38	0.53
1:A:349:VAL:HG12	1:A:351:LEU:CD1	2.39	0.52
1:D:171:THR:HG21	1:D:348:PRO:HG3	1.91	0.52
1:D:396:ASN:HD22	1:D:396:ASN:H	1.57	0.52
1:L:171:THR:HG21	1:L:348:PRO:HG3	1.91	0.52
1:O:402:LEU:HD12	1:P:33:LEU:HD13	1.91	0.52
1:B:349:VAL:HG12	1:B:351:LEU:CD1	2.39	0.52
1:C:396:ASN:H	1:C:396:ASN:HD22	1.58	0.52
1:C:426:PHE:CG	1:C:427:MET:N	2.76	0.52
1:G:171:THR:HG21	1:G:348:PRO:HG3	1.91	0.52
1:H:349:VAL:HG12	1:H:351:LEU:CD1	2.39	0.52
1:I:396:ASN:HD22	1:I:396:ASN:H	1.57	0.52
1:P:396:ASN:HD22	1:P:396:ASN:H	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:H	1:J:396:ASN:HD22	1.58	0.52
1:C:171:THR:HG21	1:C:348:PRO:HG3	1.91	0.52
1:E:15:ILE:HD11	1:E:398:THR:HA	1.91	0.52
1:P:426:PHE:CG	1:P:427:MET:N	2.76	0.52
1:C:349:VAL:HG12	1:C:351:LEU:CD1	2.39	0.52
1:H:171:THR:HG21	1:H:348:PRO:HG3	1.92	0.52
1:F:119:ALA:HB3	1:P:113:LEU:HD11	1.92	0.52
1:F:347:ARG:HB3	1:F:348:PRO:CD	2.38	0.52
1:F:349:VAL:HG12	1:F:351:LEU:CD1	2.39	0.52
1:H:396:ASN:H	1:H:396:ASN:HD22	1.57	0.52
1:O:426:PHE:CG	1:O:427:MET:N	2.76	0.52
1:R:171:THR:HG21	1:R:348:PRO:HG3	1.90	0.52
1:G:396:ASN:H	1:G:396:ASN:HD22	1.57	0.52
1:R:314:THR:HG22	1:R:325:MET:HE2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:THR:HG21	1:A:348:PRO:HG3	1.91	0.52
1:A:396:ASN:HD22	1:A:396:ASN:H	1.58	0.52
1:B:171:THR:HG21	1:B:348:PRO:HG3	1.91	0.52
1:C:402:LEU:HD12	1:J:33:LEU:HD13	1.92	0.52
1:M:349:VAL:HG12	1:M:351:LEU:CD1	2.40	0.52
1:T:171:THR:HG21	1:T:348:PRO:HG3	1.92	0.52
1:J:349:VAL:HG12	1:J:351:LEU:CD1	2.39	0.52
1:K:171:THR:HG21	1:K:348:PRO:HG3	1.91	0.52
1:P:349:VAL:HG12	1:P:351:LEU:CD1	2.39	0.52
1:R:396:ASN:HD22	1:R:396:ASN:H	1.58	0.52
1:S:15:ILE:HD11	1:S:398:THR:HA	1.92	0.52
1:S:171:THR:HG21	1:S:348:PRO:HG3	1.92	0.52
1:T:179:ARG:CD	1:T:197:CYS:SG	2.98	0.52
1:A:150:ASN:HD21	1:E:385:THR:N	2.03	0.51
1:F:396:ASN:HD22	1:F:396:ASN:H	1.57	0.51
1:N:112:THR:HG22	1:N:113:LEU:N	2.24	0.51
1:P:171:THR:HG21	1:P:348:PRO:HG3	1.91	0.51
1:B:347:ARG:HB3	1:B:348:PRO:CD	2.38	0.51
1:E:426:PHE:CG	1:E:427:MET:N	2.78	0.51
1:O:349:VAL:HG12	1:O:351:LEU:CD1	2.39	0.51
1:O:396:ASN:H	1:O:396:ASN:HD22	1.57	0.51
1:P:122:GLY:C	1:P:160:VAL:HG23	2.36	0.51
1:E:349:VAL:HG12	1:E:351:LEU:CD1	2.41	0.51
1:M:287:ASP:HB2	1:R:278:ALA:HB3	1.92	0.51
1:P:15:ILE:HD11	1:P:398:THR:HA	1.93	0.51
1:Q:349:VAL:HG12	1:Q:351:LEU:CD1	2.39	0.51
1:Q:396:ASN:H	1:Q:396:ASN:HD22	1.57	0.51
1:F:121:ASN:HD22	1:F:357:VAL:HA	1.76	0.51
1:J:171:THR:HG21	1:J:348:PRO:HG3	1.91	0.51
1:M:124:ILE:HG13	1:M:160:VAL:HG22	1.92	0.51
1:M:179:ARG:CD	1:M:197:CYS:SG	2.99	0.51
1:N:171:THR:HG21	1:N:348:PRO:HG3	1.91	0.51
1:T:255:LEU:HD23	1:T:316:LYS:HG3	1.93	0.51
1:R:179:ARG:CD	1:R:197:CYS:SG	2.99	0.51
1:D:15:ILE:HD11	1:D:398:THR:HA	1.93	0.51
1:G:33:LEU:HD13	1:N:402:LEU:HD12	1.93	0.51
1:G:402:LEU:HD12	1:H:33:LEU:HD13	1.92	0.51
1:N:15:ILE:HD11	1:N:398:THR:HA	1.93	0.51
1:O:385:THR:N	1:Q:150:ASN:HD21	2.04	0.51
1:S:179:ARG:HD2	1:S:197:CYS:SG	2.51	0.51
1:E:171:THR:O	1:E:172:SER:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:179:ARG:CD	1:N:197:CYS:SG	2.99	0.51
1:O:179:ARG:CD	1:O:197:CYS:SG	2.99	0.51
1:T:15:ILE:HD11	1:T:398:THR:HA	1.93	0.51
1:B:396:ASN:HD22	1:B:396:ASN:H	1.57	0.50
1:F:15:ILE:HD11	1:F:398:THR:HA	1.93	0.50
1:Q:15:ILE:HD11	1:Q:398:THR:HA	1.93	0.50
1:Q:179:ARG:CD	1:Q:197:CYS:SG	2.99	0.50
1:H:15:ILE:HD11	1:H:398:THR:HA	1.93	0.50
1:Q:171:THR:HG21	1:Q:348:PRO:HG3	1.91	0.50
1:R:171:THR:O	1:R:172:SER:HB3	2.11	0.50
1:D:179:ARG:CD	1:D:197:CYS:SG	2.99	0.50
1:N:396:ASN:HD22	1:N:396:ASN:H	1.58	0.50
1:M:402:LEU:HD12	1:R:33:LEU:HD13	1.94	0.50
1:O:33:LEU:HD13	1:Q:402:LEU:HD12	1.93	0.50
1:A:15:ILE:HD11	1:A:398:THR:HA	1.93	0.50
1:J:15:ILE:HD11	1:J:398:THR:HA	1.93	0.50
1:O:15:ILE:HD11	1:O:398:THR:HA	1.93	0.50
1:R:15:ILE:HD11	1:R:398:THR:HA	1.93	0.50
1:F:114:PRO:HD3	1:F:361:SER:HB3	1.93	0.50
1:F:402:LEU:HD12	1:K:33:LEU:HD13	1.93	0.50
1:K:114:PRO:HD3	1:K:361:SER:HB3	1.93	0.50
1:K:179:ARG:CD	1:K:197:CYS:SG	3.00	0.50
1:C:150:ASN:HD21	1:J:385:THR:N	2.04	0.50
1:O:347:ARG:HB3	1:O:348:PRO:CD	2.38	0.50
1:H:397:TYR:OH	1:I:432:LEU:HD13	2.11	0.50
1:B:15:ILE:HD11	1:B:398:THR:HA	1.93	0.50
1:F:179:ARG:CD	1:F:197:CYS:SG	3.00	0.50
1:I:179:ARG:CD	1:I:197:CYS:SG	3.00	0.50
1:K:15:ILE:HD11	1:K:398:THR:HA	1.93	0.50
1:L:15:ILE:HD11	1:L:398:THR:HA	1.93	0.50
1: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:B:179:ARG:CD	1:B:197:CYS:SG	3.01	0.49
1:K:171:THR:O	1:K:172:SER:HB3	2.12	0.49
1:L:179:ARG:CD	1:L:197:CYS:SG	3.00	0.49
1:T:110:SER:CB	1:T:160:VAL:HG12	2.41	0.49
1:C:15:ILE:HD11	1:C:398:THR:HA	1.93	0.49
1:F:150:ASN:HD21	1:K:385:THR:N	2.02	0.49
1:I:15:ILE:HD11	1:I:398:THR:HA	1.93	0.49
1:C:179:ARG:CD	1:C:197:CYS:SG	3.01	0.49
1:A:179:ARG:CD	1:A:197:CYS:SG	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:121:ASN:O	1:O:160:VAL:HB	2.12	0.49
1:R:204:ARG:HB3	1:R:337:ILE:HD11	1.89	0.49
1:C:438:ILE:HG23	1:G:440:GLY:C	2.37	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
1:P:179:ARG:CD	1:P:197:CYS:SG	3.01	0.49
1:H:171:THR:O	1:H:172:SER:HB3	2.13	0.49
1:I:256:VAL:HG13	1:I:280:ASN:H	1.78	0.49
1:J:171:THR:O	1:J:172:SER:HB3	2.13	0.49
1:N:171:THR:O	1:N:172:SER:HB3	2.13	0.49
1:A:171:THR:O	1:A:172:SER:HB3	2.13	0.49
1:E:347:ARG:HB3	1:E:348:PRO:CD	2.39	0.49
1:I:171:THR:O	1:I:172:SER:HB3	2.13	0.49
1:J:256:VAL:HG13	1:J:280:ASN:H	1.78	0.49
1:R:80:TYR:O	1:R:267:ASP:HB2	2.12	0.49
1:E:204:ARG:HB3	1:E:337:ILE:CD1	2.43	0.48
1:E:316:LYS:O	1:E:317:SER:HB3	2.12	0.48
1:G:383:LEU:HD22	1:L:383:LEU:HD22	1.94	0.48
1:H:179:ARG:CD	1:H:197:CYS:SG	3.01	0.48
1:Q:171:THR:O	1:Q:172:SER:HB3	2.13	0.48
1:Q:179:ARG:HD2	1:Q:197:CYS:SG	2.53	0.48
1:G:179:ARG:CD	1:G:197:CYS:SG	3.01	0.48
1:D:179:ARG:HD2	1:D:197:CYS:SG	2.53	0.48
1:Q:120:LEU:HD21	1:Q:161:GLY:H	1.78	0.48
1:T:124:ILE:HG13	1:T:160:VAL:HG22	1.95	0.48
1:G:171:THR:O	1:G:172:SER:HB3	2.13	0.48
1:H:114:PRO:HD3	1:H:361:SER:HB3	1.94	0.48
1:O:110:SER:HB3	1:O:160:VAL:HG12	1.95	0.48
1:D:171:THR:O	1:D:172:SER:HB3	2.13	0.48
1:G:256:VAL:HG13	1:G:280:ASN:H	1.78	0.48
1:K:256:VAL:HG13	1:K:280:ASN:H	1.79	0.48
1:L:171:THR:O	1:L:172:SER:HB3	2.13	0.48
1:N:179:ARG:HD2	1:N:197:CYS:SG	2.53	0.48
1:Q:124:ILE:HG13	1:Q:160:VAL:HG22	1.95	0.48
1:B:256:VAL:HG13	1:B:280:ASN:H	1.79	0.48
1:D:256:VAL:HG13	1:D:280:ASN:H	1.78	0.48
1:G:150:ASN:HD21	1:H:385:THR:N	2.04	0.48
1:T:179:ARG:HD2	1:T:197:CYS:SG	2.53	0.48
1:C:171:THR:O	1:C:172:SER:HB3	2.13	0.48
1:O:179:ARG:HD2	1:O:197:CYS:SG	2.54	0.48
1:A:256:VAL:HG13	1:A:280:ASN:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:110:SER:HB3	1:L:160:VAL:CG1	2.42	0.48
1:O:121:ASN:HB3	1:O:357:VAL:HG13	1.96	0.48
1:P:171:THR:O	1:P:172:SER:HB3	2.13	0.48
1:T:121:ASN:O	1:T:160:VAL:HB	2.14	0.48
1:B:171:THR:O	1:B:172:SER:HB3	2.13	0.48
1:K:179:ARG:HD2	1:K:197:CYS:SG	2.54	0.48
1:P:256:VAL:HG13	1:P:280:ASN:H	1.79	0.48
1:A:110:SER:HB3	1:A:160:VAL:HG12	1.95	0.48
1:M:204:ARG:HB3	1:M:337:ILE:CD1	2.44	0.48
1:T:256:VAL:HG13	1:T:280:ASN:H	1.78	0.48
1:C:256:VAL:HG13	1:C:280:ASN:H	1.78	0.47
1: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:O:171:THR:O	1:O:172:SER:HB3	2.13	0.47
1:L:396:ASN:HD22	1:L:396:ASN:N	2.12	0.47
1:O:396:ASN:HD22	1:O:396:ASN:N	2.13	0.47
1:S:171:THR:O	1:S:172:SER:HB3	2.13	0.47
1:L:124:ILE:HG13	1:L:160:VAL:HG22	1.96	0.47
1:F:179:ARG:HD2	1:F:197:CYS:SG	2.54	0.47
1:H:256:VAL:HG13	1:H:280:ASN:H	1.79	0.47
1:I:179:ARG:HD2	1:I:197:CYS:SG	2.55	0.47
1:K:110:SER:HB3	1:K:160:VAL:CG1	2.44	0.47
1:M:179:ARG:HD2	1:M:197:CYS:SG	2.55	0.47
1:O:204:ARG:HB3	1:O:337:ILE:CD1	2.44	0.47
1:C:396:ASN:HD22	1:C:396:ASN:N	2.13	0.47
1:E:179:ARG:HD2	1:E:197:CYS:SG	2.54	0.47
1:E:256:VAL:HG13	1:E:280:ASN:H	1.79	0.47
1:M:8:THR:HG22	1:M:11:ILE:HG22	1.97	0.47
1:G:114:PRO:HD3	1:G:361:SER:HB3	1.96	0.47
1:L:204:ARG:HB3	1:L:337:ILE:CD1	2.45	0.47
1:P:204:ARG:HB3	1:P:337:ILE:CD1	2.45	0.47
1:R:255:LEU:HD22	1:R:325:MET:HE2	1.97	0.47
1:A:179:ARG:HD2	1:A:197:CYS:SG	2.55	0.47
1:F:204:ARG:HB3	1:F:337:ILE:CD1	2.44	0.47
1:F:256:VAL:HG13	1:F:280:ASN:H	1.79	0.47
1:H:396:ASN:HD22	1:H:396:ASN:N	2.12	0.47
1:J:396:ASN:HD22	1:J:396:ASN:N	2.13	0.47
1:L:179:ARG:HD2	1:L:197:CYS:SG	2.54	0.47
1:S:396:ASN:HD22	1:S:396:ASN:H	1.62	0.47
1:D:396:ASN:HD22	1:D:396:ASN:N	2.12	0.47
1:J:204:ARG:HB3	1:J:337:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:396:ASN:HD22	1:K:396:ASN:N	2.12	0.47
1:N:396:ASN:HD22	1:N:396:ASN:N	2.13	0.47
1:Q:8:THR:HG22	1:Q:11:ILE:HG22	1.97	0.47
1:Q:204:ARG:HB3	1:Q:337:ILE:CD1	2.44	0.47
1:R:179:ARG:HD2	1:R:197:CYS:SG	2.54	0.47
1:B:204:ARG:HB3	1:B:337:ILE:CD1	2.45	0.47
1:D:8:THR:HG22	1:D:11:ILE:HG22	1.97	0.47
1:I:8:THR:HG22	1:I:11:ILE:HG22	1.97	0.47
1: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:T:204:ARG:HB3	1:T:337:ILE:CD1	2.45	0.47
1:A:396:ASN:HD22	1:A:396:ASN:N	2.13	0.47
1:K:204:ARG:HB3	1:K:337:ILE:CD1	2.45	0.47
1:N:204:ARG:HB3	1:N:337:ILE:CD1	2.45	0.47
1:T:396:ASN:HD22	1:T:396:ASN:N	2.13	0.47
1:A:204:ARG:HB3	1:A:337:ILE:CD1	2.45	0.46
1:B:124:ILE:HG13	1:B:160:VAL:HG22	1.96	0.46
1:C:204:ARG:HB3	1:C:337:ILE:CD1	2.45	0.46
1:L:256:VAL:HG13	1:L:280:ASN:H	1.78	0.46
1:M:171:THR:O	1:M:172:SER:HB3	2.15	0.46
1:P:179:ARG:HD2	1:P:197:CYS:SG	2.55	0.46
1:B:179:ARG:HD2	1:B:197:CYS:SG	2.55	0.46
1:B:396:ASN:HD22	1:B:396:ASN:N	2.13	0.46
1:F:8:THR:HG22	1:F:11:ILE:HG22	1.97	0.46
1:F:396:ASN:HD22	1:F:396:ASN:N	2.12	0.46
1:G:8:THR:HG22	1:G:11:ILE:HG22	1.97	0.46
1:H:315:SER:HA	1:H:325:MET:HE1	1.97	0.46
1:I:396:ASN:HD22	1:I:396:ASN:N	2.13	0.46
1:N:256:VAL:HG13	1:N:280:ASN:H	1.79	0.46
1:Q:256:VAL:HG13	1:Q:280:ASN:H	1.79	0.46
1:G:204:ARG:HB3	1:G:337:ILE:CD1	2.45	0.46
1:I:204:ARG:HB3	1:I:337:ILE:CD1	2.45	0.46
1:J:121:ASN:HD21	1:J:358:ALA:H	1.62	0.46
1:R:321:ALA:C	1:R:323:ASP:H	2.22	0.46
1:T:8:THR:HG22	1:T:11:ILE:HG22	1.98	0.46
1:J:179:ARG:HD2	1:J:197:CYS:SG	2.55	0.46
1:O:315:SER:HA	1:O:325:MET:HE1	1.97	0.46
1:B:315:SER:HA	1:B:325:MET:HE1	1.97	0.46
1:D:204:ARG:HB3	1:D:337:ILE:CD1	2.45	0.46
1:G:179:ARG:HD2	1:G:197:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:396:ASN:HD22	1:G:396:ASN:N	2.13	0.46
1:H:8:THR:HG22	1:H:11:ILE:HG22	1.97	0.46
1:K:8:THR:HG22	1:K:11:ILE:HG22	1.97	0.46
1:T:171:THR:O	1:T:172:SER:HB3	2.14	0.46
1:F:315:SER:HA	1:F:325:MET:HE1	1.97	0.46
1:I:315:SER:HA	1:I:325:MET:HE1	1.96	0.46
1:N:8:THR:HG22	1:N:11:ILE:HG22	1.97	0.46
1:P:8:THR:HG22	1:P:11:ILE:HG22	1.98	0.46
1:P:396:ASN:HD22	1:P:396:ASN:N	2.13	0.46
1:Q:315:SER:HA	1:Q:325:MET:HE1	1.98	0.46
1:Q:396:ASN:HD22	1:Q:396:ASN:N	2.13	0.46
1:A:8:THR:HG22	1:A:11:ILE:HG22	1.97	0.46
1:A:315:SER:HA	1:A:325:MET:HE1	1.97	0.46
1:C:8:THR:HG22	1:C:11:ILE:HG22	1.97	0.46
1:G:315:SER:HA	1:G:325:MET:HE1	1.98	0.46
1:H:204:ARG:HB3	1:H:337:ILE:CD1	2.45	0.46
1:M:396:ASN:HD22	1:M:396:ASN:N	2.13	0.46
1:N:124:ILE:HG13	1:N:160:VAL:HG22	1.98	0.46
1:C:179:ARG:HD2	1:C:197:CYS:SG	2.55	0.46
1:J:315:SER:HA	1:J:325:MET:HE1	1.97	0.46
1:Q:121:ASN:HB3	1:Q:357:VAL:HG13	1.98	0.46
1:D:315:SER:HA	1:D:325:MET:HE1	1.98	0.46
1:E:396:ASN:HD22	1:E:396:ASN:N	2.14	0.46
1:N:106:LEU:HD23	1:N:367:GLY:HA3	1.98	0.46
1:P:315:SER:HA	1:P:325:MET:HE1	1.98	0.46
1:Q:106:LEU:HD23	1:Q:367:GLY:HA3	1.98	0.46
1:R:396:ASN:HD22	1:R:396:ASN:N	2.13	0.46
1:E:106:LEU:HD23	1:E:367:GLY:HA3	1.98	0.46
1:L:8:THR:HG22	1:L:11:ILE:HG22	1.98	0.46
1:R:77:ASN:HD21	1:R:79:ASN:HB2	1.80	0.46
1:S:256:VAL:HG13	1:S:280:ASN:H	1.81	0.46
1:E:320:GLN:O	1:E:321:ALA:C	2.60	0.45
1:I:106:LEU:HD23	1:I:367:GLY:HA3	1.98	0.45
1:O:106:LEU:HD23	1:O:367:GLY:HA3	1.98	0.45
1:A:12:VAL:O	1:A:13:PRO:C	2.60	0.45
1:H:179:ARG:HD2	1:H:197:CYS:SG	2.56	0.45
1:K:106:LEU:HD23	1:K:367:GLY:HA3	1.97	0.45
1:N:11:ILE:HB	1:N:12:VAL:H	1.64	0.45
1:N:315:SER:HA	1:N:325:MET:HE1	1.97	0.45
1:T:315:SER:HA	1:T:325:MET:HE1	1.98	0.45
1:L:12:VAL:O	1:L:13:PRO:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LEU:HG	1:O:113:LEU:HD21	1.99	0.45
1:C:315:SER:HA	1:C:325:MET:HE1	1.97	0.45
1:G:15:ILE:HD13	1:G:15:ILE:HA	1.86	0.45
1:H:150:ASN:HD21	1:N:385:THR:N	2.07	0.45
1:K:315:SER:HA	1:K:325:MET:HE1	1.98	0.45
1:S:12:VAL:O	1:S:13:PRO:C	2.59	0.45
1:A:246:LEU:HD12	1:A:290:MET:HE2	1.99	0.45
1:B:8:THR:HG22	1:B:11:ILE:HG22	1.97	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:77:ASN:HD21	1:B:79:ASN:HB2	1.82	0.45
1:I:15:ILE:HD13	1:I:15:ILE:HA	1.86	0.45
1:M:209:THR:HA	1:M:332:SER:HB3	1.99	0.45
1:M:256:VAL:HG13	1:M:280:ASN:H	1.80	0.45
1:T:246:LEU:HD12	1:T:290:MET:HE2	1.99	0.45
1:I:12:VAL:O	1:I:13:PRO:C	2.60	0.45
1:K:12:VAL:O	1:K:13:PRO:C	2.60	0.45
1:R:8:THR:HG22	1:R:11:ILE:HG22	1.98	0.45
1:S:204:ARG:HB3	1:S:337:ILE:CD1	2.47	0.45
1:A:106:LEU:HD23	1:A:367:GLY:HA3	1.98	0.45
1:D:106:LEU:HD23	1:D:367:GLY:HA3	1.98	0.45
1:O:77:ASN:HD21	1:O:79:ASN:HB2	1.82	0.45
1:S:15:ILE:HG13	1:S:397:TYR:CD2	2.51	0.45
1:F:77:ASN:HD21	1:F:79:ASN:HB2	1.82	0.45
1:F:124:ILE:HG13	1:F:160:VAL:HG22	1.99	0.45
1:J:8:THR:HG22	1:J:11:ILE:HG22	1.97	0.45
1:M:77:ASN:HD21	1:M:79:ASN:HB2	1.82	0.45
1:P:77:ASN:HD21	1:P:79:ASN:HB2	1.82	0.45
1:T:106:LEU:HD23	1:T:367:GLY:HA3	1.99	0.45
1:C:12:VAL:O	1:C:13:PRO:C	2.60	0.45
1:F:12:VAL:O	1:F:13:PRO:C	2.60	0.45
1:L:315:SER:HA	1:L:325:MET:HE1	1.97	0.45
1:N:77:ASN:HD21	1:N:79:ASN:HB2	1.82	0.45
1:P:246:LEU:HD12	1:P:290:MET:HE2	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:8:THR:HG22	1:S:11:ILE:HG22	1.99	0.45
1:S:106:LEU:HD23	1:S:367:GLY:HA3	1.99	0.45
1:C:246:LEU:HD12	1:C:290:MET:HE2	1.99	0.44
1:D:15:ILE:HG13	1:D:397:TYR:CD2	2.52	0.44
1:E:204:ARG:HB3	1:E:337:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:120:LEU:HD23	1:R:113:LEU:HD12	1.98	0.44
1:G:246:LEU:HD12	1:G:290:MET:HE2	1.99	0.44
1:L:106:LEU:HD23	1:L:367:GLY:HA3	1.98	0.44
1:M:127:VAL:HG22	1:M:144:LEU:HB3	1.99	0.44
1:D:246:LEU:HD12	1:D:290:MET:HE2	2.00	0.44
1:I:127:VAL:HG22	1:I:144:LEU:HB3	1.99	0.44
1:B:106:LEU:HD23	1:B:367:GLY:HA3	1.98	0.44
1:I:77:ASN:HD21	1:I:79:ASN:HB2	1.82	0.44
1:M:12:VAL:O	1:M:13:PRO:C	2.60	0.44
1:B:12:VAL:O	1:B:13:PRO:C	2.60	0.44
1:C:110:SER:HB3	1:C:160:VAL:CG1	2.46	0.44
1:C:121:ASN:HD21	1:C:358:ALA:HB3	1.82	0.44
1:C:209:THR:HA	1:C:332:SER:HB3	2.00	0.44
1:G:12:VAL:O	1:G:13:PRO:C	2.60	0.44
1:G:193:MET:HE2	1:G:193:MET:C	2.43	0.44
1:I:201:ASP:OD1	1:I:201:ASP:N	2.49	0.44
1:N:246:LEU:HD12	1:N:290:MET:HE2	1.99	0.44
1:P:15:ILE:HD13	1:P:15:ILE:HA	1.86	0.44
1:P:106:LEU:HD23	1:P:367:GLY:HA3	1.99	0.44
1:R:114:PRO:C	1:R:116:GLY:H	2.26	0.44
1:T:113:LEU:HD22	1:T:120:LEU:HD22	2.00	0.44
1:B:127:VAL:HG22	1:B:144:LEU:HB3	2.00	0.44
1:B:209:THR:HA	1:B:332:SER:HB3	2.00	0.44
1:C:15:ILE:HG13	1:C:397:TYR:CD2	2.52	0.44
1:E:15:ILE:HG13	1:E:397:TYR:CD2	2.51	0.44
1:E:127:VAL:HG22	1:E:144:LEU:HB3	2.00	0.44
1:I:246:LEU:HD12	1:I:290:MET:HE2	1.99	0.44
1:K:77:ASN:HD21	1:K:79:ASN:HB2	1.82	0.44
1:Q:204:ARG:HB3	1:Q:337:ILE:HD11	1.99	0.44
1:D:12:VAL:O	1:D:13:PRO:C	2.60	0.44
1:G:122:GLY:C	1:G:160:VAL:HG23	2.43	0.44
1:J:12:VAL:O	1:J:13:PRO:C	2.60	0.44
1:J:77:ASN:HD21	1:J:79:ASN:HB2	1.82	0.44
1:J:124:ILE:HG13	1:J:160:VAL:HG22	2.00	0.44
1:J:201:ASP:OD1	1:J:201:ASP:N	2.49	0.44
1:O:12:VAL:O	1:O:13:PRO:C	2.60	0.44
1:P:127:VAL:HG22	1:P:144:LEU:HB3	2.00	0.44
1:R:12:VAL:O	1:R:13:PRO:C	2.61	0.44
1:A:77:ASN:HD21	1:A:79:ASN:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:THR:HA	1:A:332:SER:HB3	1.99	0.44
1:F:11:ILE:HB	1:F:12:VAL:H	1.65	0.44
1:F:193:MET:C	1:F:193:MET:HE2	2.43	0.44
1:H:15:ILE:HG13	1:H:397:TYR:CD2	2.52	0.44
1:H:127:VAL:HG22	1:H:144:LEU:HB3	2.00	0.44
1:K:127:VAL:HG22	1:K:144:LEU:HB3	2.00	0.44
1:K:193:MET:C	1:K:193:MET:HE2	2.43	0.44
1:L:127:VAL:HG22	1:L:144:LEU:HB3	2.00	0.44
1:M:112:THR:HG22	1:M:113:LEU:N	2.33	0.44
1:R:261:ILE:HD12	1:R:276:VAL:HG21	1.99	0.44
1:A:320:GLN:N	1:A:323:ASP:OD2	2.51	0.44
1:E:52:THR:HG21	1:E:75:GLN:C	2.43	0.44
1:J:106:LEU:HD23	1:J:367:GLY:HA3	1.99	0.44
1:K:320:GLN:N	1:K:323:ASP:OD2	2.51	0.44
1:O:127:VAL:HG22	1:O:144:LEU:HB3	2.00	0.44
1:O:193:MET:C	1:O:193:MET:HE2	2.43	0.44
1:Q:320:GLN:N	1:Q:323:ASP:OD2	2.51	0.44
1:T:204:ARG:HB3	1:T:337:ILE:HD11	2.00	0.44
1:B:320:GLN:N	1:B:323:ASP:OD2	2.51	0.44
1:C:112:THR:HA	1:L:120:LEU:O	2.18	0.44
1:C:204:ARG:HB3	1:C:337:ILE:HD11	2.00	0.44
1:I:15:ILE:HG13	1:I:397:TYR:CD2	2.52	0.44
1:I:385:THR:N	1:K:150:ASN:HD21	2.09	0.44
1:L:77:ASN:HD21	1:L:79:ASN:HB2	1.82	0.44
1:O:209:THR:HA	1:O:332:SER:HB3	2.00	0.44
1:Q:12:VAL:O	1:Q:13:PRO:C	2.59	0.44
1:T:12:VAL:O	1:T:13:PRO:C	2.59	0.44
1:T:15:ILE:HG13	1:T:397:TYR:CD2	2.52	0.44
1:A:204:ARG:HB3	1:A:337:ILE:HD11	2.00	0.43
1:D:193:MET:C	1:D:193:MET:HE2	2.43	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:I:193:MET:HE2	1:I:193:MET:C	2.42	0.43
1:J:193:MET:C	1:J:193:MET:HE2	2.43	0.43
1:M:193:MET:C	1:M:193:MET:HE2	2.43	0.43
1:M:204:ARG:HB3	1:M:337:ILE:HD11	2.00	0.43
1:P:12:VAL:O	1:P:13:PRO:C	2.59	0.43
1:P:193:MET:C	1:P:193:MET:HE2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:HD12	1:B:290:MET:HE2	1.99	0.43
1:E:8:THR:HG22	1:E:11:ILE:HG22	1.98	0.43
1:H:209:THR:HA	1:H:332:SER:HB3	2.01	0.43
1:L:320:GLN:N	1:L:323:ASP:OD2	2.51	0.43
1:N:193:MET:HE2	1:N:193:MET:C	2.43	0.43
1:P:112:THR:O	1:P:361:SER:HB2	2.17	0.43
1:T:209:THR:HA	1:T:332:SER:HB3	2.00	0.43
1:B:15:ILE:HG13	1:B:397:TYR:CD2	2.52	0.43
1:B:201:ASP:OD1	1:B:201:ASP:N	2.50	0.43
1:C:193:MET:C	1:C:193:MET:HE2	2.43	0.43
1:D:320:GLN:N	1:D:323:ASP:OD2	2.50	0.43
1:F:15:ILE:HD13	1:F:15:ILE:HA	1.86	0.43
1:H:12:VAL:O	1:H:13:PRO:C	2.60	0.43
1:I:33:LEU:HD13	1:K:402:LEU:HD12	1.99	0.43
1:K:204:ARG:HB3	1:K:337:ILE:HD11	2.00	0.43
1:M:201:ASP:O	1:M:202:ARG:HB2	2.18	0.43
1:Q:15:ILE:HG13	1:Q:397:TYR:CD2	2.52	0.43
1:Q:246:LEU:HD12	1:Q:290:MET:HE2	1.99	0.43
1:S:114:PRO:HD3	1:S:361:SER:HB3	2.00	0.43
1:C:320:GLN:N	1:C:323:ASP:OD2	2.51	0.43
1:E:171:THR:O	1:E:172:SER:CB	2.66	0.43
1:H:246:LEU:HD12	1:H:290:MET:HE2	2.00	0.43
1:J:171:THR:O	1:J:172:SER:CB	2.66	0.43
1:K:15:ILE:HG13	1:K:397:TYR:CD2	2.51	0.43
1:N:12:VAL:O	1:N:13:PRO:C	2.60	0.43
1:S:201:ASP:O	1:S:202:ARG:HB2	2.18	0.43
1:A:114:PRO:HD3	1:A:361:SER:HB3	2.01	0.43
1:D:77:ASN:HD21	1:D:79:ASN:HB2	1.82	0.43
1:E:12:VAL:O	1:E:13:PRO:C	2.62	0.43
1:E:246:LEU:HD12	1:E:290:MET:HE2	2.00	0.43
1:F:204:ARG:HB3	1:F:337:ILE:HD11	2.00	0.43
1:F:320:GLN:N	1:F:323:ASP:OD2	2.52	0.43
1:G:201:ASP:OD1	1:G:201:ASP:N	2.49	0.43
1:H:320:GLN:N	1:H:323:ASP:OD2	2.51	0.43
1:I:320:GLN:N	1:I:323:ASP:OD2	2.52	0.43
1:L:246:LEU:HD12	1:L:290:MET:HE2	1.99	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:O:246:LEU:HD12	1:O:290:MET:HE2	2.00	0.43
1:Q:121:ASN:O	1:Q:160:VAL:HB	2.18	0.43
1:C:77:ASN:HD21	1:C:79:ASN:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:THR:H	1:D:288:ASN:ND2	2.15	0.43
1:G:171:THR:O	1:G:172:SER:CB	2.66	0.43
1:L:193:MET:HE2	1:L:193:MET:C	2.43	0.43
1:M:11:ILE:HB	1:M:12:VAL:H	1.65	0.43
1:N:320:GLN:N	1:N:323:ASP:OD2	2.51	0.43
1:O:204:ARG:HB3	1:O:337:ILE:HD11	2.00	0.43
1:T:77:ASN:HD21	1:T:79:ASN:HB2	1.82	0.43
1:T:201:ASP:O	1:T:202:ARG:HB2	2.18	0.43
1:A:127:VAL:HG22	1:A:144:LEU:HB3	2.00	0.43
1:C:106:LEU:HD23	1:C:367:GLY:HA3	1.98	0.43
1:F:209:THR:HA	1:F:332:SER:HB3	2.00	0.43
1:G:127:VAL:HG22	1:G:144:LEU:HB3	2.00	0.43
1:J:209:THR:HA	1:J:332:SER:HB3	2.00	0.43
1:J:246:LEU:HD12	1:J:290:MET:HE2	1.99	0.43
1:K:246:LEU:HD12	1:K:290:MET:HE2	2.00	0.43
1:M:93:PRO:HG3	1:M:180:LEU:HB3	2.00	0.43
1:N:171:THR:O	1:N:172:SER:CB	2.67	0.43
1:P:171:THR:O	1:P:172:SER:CB	2.66	0.43
1:Q:193:MET:HE2	1:Q:193:MET:C	2.43	0.43
1:S:93:PRO:HG3	1:S:180:LEU:HB3	2.01	0.43
1:D:201:ASP:O	1:D:202:ARG:HB2	2.19	0.43
1:F:121:ASN:ND2	1:F:358:ALA:H	2.16	0.43
1:F:201:ASP:O	1:F:202:ARG:HB2	2.19	0.43
1:H:171:THR:O	1:H:172:SER:CB	2.66	0.43
1:N:15:ILE:HG13	1:N:397:TYR:CD2	2.51	0.43
1:O:113:LEU:HD22	1:O:120:LEU:HD22	2.00	0.43
1:R:145:MET:HA	1:R:145:MET:HE2	2.01	0.43
1:A:193:MET:C	1:A:193:MET:HE2	2.43	0.43
1:B:193:MET:HE2	1:B:193:MET:C	2.43	0.43
1:C:127:VAL:HG22	1:C:144:LEU:HB3	2.00	0.43
1:E:209:THR:HA	1:E:332:SER:HB3	1.99	0.43
1:F:171:THR:O	1:F:172:SER:CB	2.67	0.43
1:G:320:GLN:N	1:G:323:ASP:OD2	2.51	0.43
1:L:209:THR:HA	1:L:332:SER:HB3	2.00	0.43
1:N:127:VAL:HG22	1:N:144:LEU:HB3	2.01	0.43
1:O:320:GLN:N	1:O:323:ASP:OD2	2.52	0.43
1:Q:121:ASN:HB3	1:Q:357:VAL:HA	2.01	0.43
1:S:77:ASN:HD21	1:S:79:ASN:HB2	1.83	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:A:15:ILE:HG13	1:A:397:TYR:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:THR:O	1:A:172:SER:CB	2.67	0.43
1:B:15:ILE:HD13	1:B:15:ILE:HA	1.86	0.43
1:B:201:ASP:O	1:B:202:ARG:HB2	2.19	0.43
1:D:124:ILE:HG13	1:D:160:VAL:HG22	2.00	0.43
1:E:11:ILE:HB	1:E:12:VAL:H	1.65	0.43
1:H:193:MET:C	1:H:193:MET:HE2	2.44	0.43
1:I:11:ILE:HB	1:I:12:VAL:H	1.65	0.43
1:I:209:THR:HA	1:I:332:SER:HB3	2.01	0.43
1:J:320:GLN:N	1:J:323:ASP:OD2	2.52	0.43
1:M:145:MET:HA	1:M:145:MET:HE2	2.00	0.43
1:M:291:PRO:HB3	1:R:293:ASN:ND2	2.34	0.43
1:P:320:GLN:N	1:P:323:ASP:OD2	2.51	0.43
1:R:106:LEU:HD23	1:R:367:GLY:HA3	2.00	0.43
1:R:201:ASP:O	1:R:202:ARG:HB2	2.19	0.43
1:S:110:SER:HB3	1:S:160:VAL:CG1	2.49	0.43
1:F:246:LEU:HD12	1:F:290:MET:HE2	1.99	0.42
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:T:193:MET:C	1:T:193:MET:HE2	2.44	0.42
1:H:77:ASN:HD21	1:H:79:ASN:HB2	1.83	0.42
1:K:171:THR:O	1:K:172:SER:CB	2.66	0.42
1:K:201:ASP:OD1	1:K:201:ASP:N	2.49	0.42
1:K:209:THR:HA	1:K:332:SER:HB3	2.00	0.42
1:P:201:ASP:O	1:P:202:ARG:HB2	2.19	0.42
1:P:204:ARG:HB3	1:P:337:ILE:HD11	2.01	0.42
1:Q:127:VAL:HG22	1:Q:144:LEU:HB3	2.00	0.42
1:S:11:ILE:HB	1:S:12:VAL:H	1.64	0.42
1:T:171:THR:O	1:T:172:SER:CB	2.67	0.42
1:A:201:ASP:O	1:A:202:ARG:HB2	2.20	0.42
1:D:127:VAL:HG22	1:D:144:LEU:HB3	2.00	0.42
1:E:116:GLY:HA2	1:P:162:GLU:HA	2.02	0.42
1:J:201:ASP:O	1:J:202:ARG:HB2	2.19	0.42
1:M:110:SER:CB	1:M:160:VAL:HG12	2.49	0.42
1:P:209:THR:HA	1:P:332:SER:HB3	2.00	0.42
1:R:11:ILE:HB	1:R:12:VAL:H	1.64	0.42
1:C:171:THR:O	1:C:172:SER:CB	2.67	0.42
1:D:171:THR:O	1:D:172:SER:CB	2.67	0.42
1:G:209:THR:HA	1:G:332:SER:HB3	2.00	0.42
1:H:201:ASP:O	1:H:202:ARG:HB2	2.19	0.42
1:J:15:ILE:HG13	1:J:397:TYR:CD2	2.52	0.42
1:K:124:ILE:HG13	1:K:160:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:145:MET:HE2	1:L:145:MET:HA	2.02	0.42
1:M:37:THR:OG1	1:M:39:ARG:NH1	2.53	0.42
1:M:150:ASN:HD21	1:R:385:THR:N	2.11	0.42
1:F:145:MET:HE2	1:F:145:MET:HA	2.02	0.42
1:J:204:ARG:HB3	1:J:337:ILE:HD11	2.00	0.42
1:L:201:ASP:OD1	1:L:201:ASP:N	2.49	0.42
1:N:15:ILE:HD13	1:N:15:ILE:HA	1.86	0.42
1:O:171:THR:O	1:O:172:SER:CB	2.67	0.42
1:P:15:ILE:HG13	1:P:397:TYR:CD2	2.52	0.42
1:B:204:ARG:HB3	1:B:337:ILE:HD11	2.01	0.42
1:D:145:MET:HE2	1:D:145:MET:HA	2.02	0.42
1:F:127:VAL:HG22	1:F:144:LEU:HB3	2.00	0.42
1:L:171:THR:O	1:L:172:SER:CB	2.67	0.42
1:L:204:ARG:HB3	1:L:337:ILE:HD11	2.00	0.42
1:M:20:MET:HG2	1:M:423:ARG:HG2	2.02	0.42
1:M:249:ARG:HB2	1:M:328:SER:HB3	2.01	0.42
1:R:171:THR:O	1:R:172:SER:CB	2.67	0.42
1:T:145:MET:HA	1:T:145:MET:HE2	2.02	0.42
1:P:145:MET:HE2	1:P:145:MET:HA	2.02	0.42
1:R:347:ARG:HG2	1:R:347:ARG:HH11	1.85	0.42
1:A:145:MET:HE2	1:A:145:MET:HA	2.02	0.42
1:C:110:SER:CB	1:C:160:VAL:HG12	2.47	0.42
1:E:145:MET:HA	1:E:145:MET:HE2	2.00	0.42
1:E:440:GLY:C	1:J:438:ILE:HG23	2.44	0.42
1:F:113:LEU:HA	1:F:114:PRO:HD3	1.83	0.42
1:J:145:MET:HA	1:J:145:MET:HE2	2.01	0.42
1:M:246:LEU:HD12	1:M:290:MET:HE2	2.01	0.42
1:S:110:SER:HB3	1:S:160:VAL:HG12	2.01	0.42
1:S:246:LEU:HD12	1:S:290:MET:HE2	2.01	0.42
1:T:320:GLN:N	1:T:323:ASP:OD2	2.52	0.42
1:J:127:VAL:HG22	1:J:144:LEU:HB3	2.00	0.42
1:M:432:LEU:HD13	1:T:397:TYR:OH	2.20	0.42
1:N:209:THR:HA	1:N:332:SER:HB3	2.01	0.42
1:P:11:ILE:HB	1:P:12:VAL:H	1.65	0.42
1:P:432:LEU:HB2	1:P:433:ASN:H	1.67	0.42
1:Q:201:ASP:O	1:Q:202:ARG:HB2	2.19	0.42
1:R:37:THR:OG1	1:R:39:ARG:NH1	2.53	0.42
1:C:201:ASP:O	1:C:202:ARG:HB2	2.19	0.42
1:D:110:SER:HB3	1:D:160:VAL:HG12	2.01	0.42
1:H:204:ARG:HB3	1:H:337:ILE:HD11	2.00	0.42
1:I:171:THR:O	1:I:172:SER:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:110:SER:HB3	1:J:160:VAL:HG12	2.01	0.42
1:L:112:THR:HG22	1:L:113:LEU:N	2.35	0.42
1:Q:145:MET:HE2	1:Q:145:MET:HA	2.01	0.42
1:Q:171:THR:O	1:Q:172:SER:CB	2.67	0.42
1:R:127:VAL:HG22	1:R:144:LEU:HB3	2.01	0.42
1:A:93:PRO:HG3	1:A:180:LEU:HB3	2.02	0.41
1:J:11:ILE:HB	1:J:12:VAL:H	1.65	0.41
1:K:145:MET:HE2	1:K:145:MET:HA	2.02	0.41
1:K:201:ASP:O	1:K:202:ARG:HB2	2.20	0.41
1:N:438:ILE:HG23	1:P:440:GLY:C	2.45	0.41
1:S:127:VAL:HG22	1:S:144:LEU:HB3	2.01	0.41
1:S:204:ARG:HB3	1:S:337:ILE:HD11	2.02	0.41
1:B:145:MET:HE2	1:B:145:MET:HA	2.01	0.41
1:L:15:ILE:HG13	1:L:397:TYR:CD2	2.52	0.41
1:O:201:ASP:O	1:O:202:ARG:HB2	2.20	0.41
1:R:15:ILE:HG13	1:R:397:TYR:CD2	2.51	0.41
1:D:204:ARG:HB3	1:D:337:ILE:HD11	2.01	0.41
1:I:204:ARG:HB3	1:I:337:ILE:HD11	2.00	0.41
1:N:145:MET:HE2	1:N:145:MET:HA	2.02	0.41
1:P:110:SER:HB3	1:P:160:VAL:CG1	2.45	0.41
1:C:145:MET:HA	1:C:145:MET:HE2	2.01	0.41
1:G:145:MET:HE2	1:G:145:MET:HA	2.02	0.41
1:I:145:MET:HE2	1:I:145:MET:HA	2.02	0.41
1:N:201:ASP:O	1:N:202:ARG:HB2	2.19	0.41
1:R:276:VAL:HG22	1:R:294:LEU:HD21	2.02	0.41
1:B:11:ILE:HB	1:B:12:VAL:H	1.64	0.41
1:D:201:ASP:OD1	1:D:201:ASP:N	2.49	0.41
1:G:201:ASP:O	1:G:202:ARG:HB2	2.19	0.41
1:I:201:ASP:O	1:I:202:ARG:HB2	2.19	0.41
1:L:201:ASP:O	1:L:202:ARG:HB2	2.20	0.41
1:E:283:THR:H	1:E:288:ASN:ND2	2.17	0.41
1:H:145:MET:HA	1:H:145:MET:HE2	2.02	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:E:52:THR:CG2	1:E:75:GLN:C	2.94	0.41
1:M:110:SER:HB3	1:M:160:VAL:HG12	2.02	0.41
1:M:438:ILE:O	1:M:438:ILE:HG22	2.20	0.41
1:B:337:ILE:HG21	1:B:337:ILE:HD12	1.88	0.41
1:E:93:PRO:HG3	1:E:180:LEU:HB3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:438:ILE:O	1:J:438:ILE:HG22	2.21	0.41
1:M:278:ALA:O	1:M:279:ASN:C	2.64	0.41
1:N:20:MET:HG2	1:N:423:ARG:HG2	2.03	0.41
1:O:15:ILE:HG13	1:O:397:TYR:CD2	2.52	0.41
1:O:145:MET:HA	1:O:145:MET:HE2	2.01	0.41
1:R:110:SER:HB3	1:R:160:VAL:HG11	1.97	0.41
1:T:283:THR:H	1:T:288:ASN:ND2	2.15	0.41
1:A:279:ASN:O	1:A:279:ASN:ND2	2.54	0.41
1:C:20:MET:HG2	1:C:423:ARG:HG2	2.03	0.41
1:K:15:ILE:HD13	1:K:15:ILE:HA	1.86	0.41
1:N:438:ILE:HG22	1:N:438:ILE:O	2.21	0.41
1:S:171:THR:O	1:S:172:SER:CB	2.69	0.41
1:A:438:ILE:HG22	1:A:438:ILE:O	2.21	0.40
1:E:124:ILE:HG13	1:E:160:VAL:HG22	2.01	0.40
1:E:201:ASP:O	1:E:339:GLY:HA2	2.21	0.40
1:F:220:TYR:HD2	1:F:320:GLN:O	2.04	0.40
1:N:93:PRO:HG3	1:N:180:LEU:HB3	2.03	0.40
1:Q:93:PRO:HG3	1:Q:180:LEU:HB3	2.03	0.40
1:T:20:MET:HG2	1:T:423:ARG:HG2	2.03	0.40
1:B:20:MET:HG2	1:B:423:ARG:HG2	2.03	0.40
1:E:37:THR:OG1	1:E:39:ARG:NH1	2.55	0.40
1:F:15:ILE:HG13	1:F:397:TYR:CD2	2.52	0.40
1:G:438:ILE:HG22	1:G:438:ILE:O	2.21	0.40
1:H:278:ALA:O	1:H:279:ASN:C	2.64	0.40
1:J:93:PRO:HG3	1:J:180:LEU:HB3	2.03	0.40
1:K:113:LEU:HA	1:K:114:PRO:HD3	1.93	0.40
1:K:438:ILE:O	1:K:438:ILE:HG22	2.21	0.40
1:L:110:SER:CB	1:L:160:VAL:HG12	2.50	0.40
1:O:93:PRO:HG3	1:O:180:LEU:HB3	2.03	0.40
1:O:438:ILE:HG22	1:O:438:ILE:O	2.22	0.40
1:P:97:ASN:O	1:P:179:ARG:HG3	2.21	0.40
1:Q:20:MET:HG2	1:Q:423:ARG:HG2	2.03	0.40
1:S:20:MET:HG2	1:S:423:ARG:HG2	2.03	0.40
1:S:438:ILE:HG22	1:S:438:ILE:O	2.21	0.40
1:B:283:THR:H	1:B:288:ASN:ND2	2.16	0.40
1:E:438:ILE:O	1:E:438:ILE:HG22	2.22	0.40
1:J:316:LYS:HB2	1:J:325:MET:HE3	2.03	0.40
1:M:121:ASN:O	1:M:160:VAL:HB	2.22	0.40
1:R:267:ASP:OD1	1:R:269:THR:HB	2.22	0.40
1:S:397:TYR:OH	1:T:432:LEU:HD13	2.22	0.40
1:B:438:ILE:HG22	1:B:438:ILE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:PRO:HD3	1:D:361:SER:HB3	2.03	0.40
1:D:316:LYS:HB2	1:D:325:MET:HE3	2.04	0.40
1:G:97:ASN:O	1:G:179:ARG:HG3	2.22	0.40
1:H:220:TYR:HD2	1:H:320:GLN:O	2.05	0.40
1:O:124:ILE:HG13	1:O:160:VAL:HG22	2.02	0.40
1:P:20:MET:HG2	1:P:423:ARG:HG2	2.04	0.40
1:P:93:PRO:HG3	1:P:180:LEU:HB3	2.02	0.40
1:Q:220:TYR:HD2	1:Q:320:GLN:O	2.05	0.40
1:Q:438:ILE:HG22	1:Q:438:ILE:O	2.22	0.40
1:T:201:ASP:OD1	1:T:201:ASP:N	2.50	0.40
1:G:113:LEU:HA	1:G:114:PRO:HD3	1.88	0.40
1:I:20:MET:HG2	1:I:423:ARG:HG2	2.03	0.40

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	4	7
1	B	424/456 (93%)	394 (93%)	19 (4%)	11 (3%)	4	7
1	C	424/456 (93%)	395 (93%)	18 (4%)	11 (3%)	4	7
1	D	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	4	7
1	E	431/456 (94%)	401 (93%)	20 (5%)	10 (2%)	5	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	431/456 (94%)	401 (93%)	18 (4%)	12 (3%)	4	6
1	G	431/456 (94%)	403 (94%)	17 (4%)	11 (3%)	4	7
1	H	424/456 (93%)	395 (93%)	18 (4%)	11 (3%)	4	7
1	I	424/456 (93%)	396 (93%)	16 (4%)	12 (3%)	4	6
1	J	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	4	7
1	K	424/456 (93%)	395 (93%)	18 (4%)	11 (3%)	4	7
1	L	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	4	7
1	M	424/456 (93%)	396 (93%)	18 (4%)	10 (2%)	4	9
1	N	424/456 (93%)	395 (93%)	17 (4%)	12 (3%)	4	6
1	O	424/456 (93%)	396 (93%)	17 (4%)	11 (3%)	4	7
1	P	426/456 (93%)	397 (93%)	17 (4%)	12 (3%)	4	6
1	Q	425/456 (93%)	396 (93%)	18 (4%)	11 (3%)	4	7
1	R	431/456 (94%)	401 (93%)	23 (5%)	7 (2%)	7	16
1	S	424/456 (93%)	394 (93%)	19 (4%)	11 (3%)	4	7
1	T	424/456 (93%)	395 (93%)	18 (4%)	11 (3%)	4	7
All	All	8511/9120 (93%)	7934 (93%)	359 (4%)	218 (3%)	4	7

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	326 (92%)	28 (8%)	11	26
1	B	354/380 (93%)	325 (92%)	29 (8%)	10	24
1	C	354/380 (93%)	326 (92%)	28 (8%)	11	26
1	D	354/380 (93%)	327 (92%)	27 (8%)	12	27
1	E	356/380 (94%)	329 (92%)	27 (8%)	12	27
1	F	356/380 (94%)	329 (92%)	27 (8%)	12	27
1	G	356/380 (94%)	328 (92%)	28 (8%)	11	26
1	H	354/380 (93%)	328 (93%)	26 (7%)	13	29
1	I	354/380 (93%)	326 (92%)	28 (8%)	11	26
1	J	354/380 (93%)	324 (92%)	30 (8%)	10	22
1	K	354/380 (93%)	325 (92%)	29 (8%)	10	24
1	L	354/380 (93%)	327 (92%)	27 (8%)	12	27
1	M	354/380 (93%)	327 (92%)	27 (8%)	12	27
1	N	354/380 (93%)	326 (92%)	28 (8%)	11	26
1	O	354/380 (93%)	324 (92%)	30 (8%)	10	22
1	P	354/380 (93%)	327 (92%)	27 (8%)	12	27
1	Q	354/380 (93%)	325 (92%)	29 (8%)	10	24
1	R	356/380 (94%)	328 (92%)	28 (8%)	11	26
1	S	354/380 (93%)	326 (92%)	28 (8%)	11	26
1	T	354/380 (93%)	328 (93%)	26 (7%)	13	29
All	All	7088/7600 (93%)	6531 (92%)	557 (8%)	11	26

All (557) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
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

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Mol	Chain	Res	Type
1	A	164	VAL
1	A	193	MET
1	A	201	ASP
1	A	202	ARG
1	A	219	GLN
1	A	261	ILE
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	383	LEU
1	A	396	ASN
1	A	432	LEU
1	B	11	ILE
1	B	23	THR
1	B	39	ARG
1	B	77	ASN
1	B	88	THR
1	B	99	CYS
1	B	107	THR
1	B	112	THR
1	B	123	THR
1	B	127	VAL
1	B	146	SER
1	B	148	THR
1	B	164	VAL
1	B	193	MET
1	B	201	ASP
1	B	202	ARG
1	B	219	GLN
1	B	261	ILE
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

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Mol	Chain	Res	Type
1	B	337	ILE
1	B	383	LEU
1	B	396	ASN
1	B	432	LEU
1	C	11	ILE
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	164	VAL
1	C	193	MET
1	C	201	ASP
1	C	202	ARG
1	C	219	GLN
1	C	261	ILE
1	C	269	THR
1	C	273	THR
1	C	279	ASN
1	C	306	THR
1	C	325	MET
1	C	330	ARG
1	C	332	SER
1	C	337	ILE
1	C	383	LEU
1	C	396	ASN
1	C	432	LEU
1	D	11	ILE
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

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Mol	Chain	Res	Type
1	D	164	VAL
1	D	193	MET
1	D	201	ASP
1	D	202	ARG
1	D	219	GLN
1	D	261	ILE
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	383	LEU
1	D	396	ASN
1	D	432	LEU
1	E	11	ILE
1	E	23	THR
1	E	39	ARG
1	E	88	THR
1	E	99	CYS
1	E	107	THR
1	E	112	THR
1	E	117	VAL
1	E	127	VAL
1	E	146	SER
1	E	148	THR
1	E	164	VAL
1	E	193	MET
1	E	201	ASP
1	E	202	ARG
1	E	219	GLN
1	E	261	ILE
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	383	LEU

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Mol	Chain	Res	Type
1	E	396	ASN
1	E	432	LEU
1	F	11	ILE
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	127	VAL
1	F	146	SER
1	F	148	THR
1	F	164	VAL
1	F	193	MET
1	F	201	ASP
1	F	202	ARG
1	F	219	GLN
1	F	261	ILE
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	383	LEU
1	F	396	ASN
1	F	432	LEU
1	G	11	ILE
1	G	23	THR
1	G	39	ARG
1	G	77	ASN
1	G	88	THR
1	G	99	CYS
1	G	112	THR
1	G	113	LEU
1	G	127	VAL
1	G	146	SER
1	G	148	THR
1	G	164	VAL
1	G	193	MET

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Mol	Chain	Res	Type
1	G	201	ASP
1	G	202	ARG
1	G	219	GLN
1	G	261	ILE
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	383	LEU
1	G	396	ASN
1	G	432	LEU
1	H	11	ILE
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	164	VAL
1	H	193	MET
1	H	201	ASP
1	H	202	ARG
1	H	219	GLN
1	H	261	ILE
1	H	269	THR
1	H	273	THR
1	H	279	ASN
1	H	306	THR
1	H	325	MET
1	H	330	ARG
1	H	332	SER
1	H	337	ILE
1	H	383	LEU
1	H	396	ASN
1	H	432	LEU
1	I	11	ILE

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Mol	Chain	Res	Type
1	I	23	THR
1	I	39	ARG
1	I	77	ASN
1	I	88	THR
1	I	99	CYS
1	I	107	THR
1	I	112	THR
1	I	127	VAL
1	I	146	SER
1	I	148	THR
1	I	164	VAL
1	I	193	MET
1	I	201	ASP
1	I	202	ARG
1	I	219	GLN
1	I	261	ILE
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	383	LEU
1	I	396	ASN
1	I	432	LEU
1	J	11	ILE
1	J	23	THR
1	J	39	ARG
1	J	77	ASN
1	J	88	THR
1	J	99	CYS
1	J	107	THR
1	J	112	THR
1	J	113	LEU
1	J	120	LEU
1	J	127	VAL
1	J	146	SER
1	J	148	THR
1	J	164	VAL
1	J	193	MET

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Mol	Chain	Res	Type
1	J	201	ASP
1	J	202	ARG
1	J	219	GLN
1	J	261	ILE
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	383	LEU
1	J	396	ASN
1	J	432	LEU
1	K	11	ILE
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	164	VAL
1	K	193	MET
1	K	201	ASP
1	K	202	ARG
1	K	219	GLN
1	K	261	ILE
1	K	269	THR
1	K	273	THR
1	K	279	ASN
1	K	306	THR
1	K	325	MET
1	K	330	ARG
1	K	332	SER
1	K	337	ILE
1	K	383	LEU

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Mol	Chain	Res	Type
1	K	396	ASN
1	K	432	LEU
1	L	11	ILE
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	164	VAL
1	L	193	MET
1	L	201	ASP
1	L	202	ARG
1	L	219	GLN
1	L	261	ILE
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	383	LEU
1	L	396	ASN
1	L	432	LEU
1	M	11	ILE
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
1	M	193	MET
1	M	201	ASP

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Mol	Chain	Res	Type
1	M	202	ARG
1	M	219	GLN
1	M	261	ILE
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	383	LEU
1	M	396	ASN
1	M	432	LEU
1	N	11	ILE
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	120	LEU
1	N	127	VAL
1	N	146	SER
1	N	148	THR
1	N	164	VAL
1	N	193	MET
1	N	201	ASP
1	N	202	ARG
1	N	219	GLN
1	N	261	ILE
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	383	LEU
1	N	396	ASN
1	N	432	LEU

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Mol	Chain	Res	Type
1	O	11	ILE
1	O	23	THR
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	164	VAL
1	O	193	MET
1	O	201	ASP
1	O	202	ARG
1	O	219	GLN
1	O	261	ILE
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	383	LEU
1	O	396	ASN
1	O	432	LEU
1	P	11	ILE
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	164	VAL
1	P	193	MET

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Mol	Chain	Res	Type
1	P	201	ASP
1	P	202	ARG
1	P	219	GLN
1	P	261	ILE
1	P	269	THR
1	P	273	THR
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	383	LEU
1	P	396	ASN
1	P	432	LEU
1	Q	11	ILE
1	Q	23	THR
1	Q	39	ARG
1	Q	77	ASN
1	Q	88	THR
1	Q	99	CYS
1	Q	107	THR
1	Q	113	LEU
1	Q	120	LEU
1	Q	127	VAL
1	Q	146	SER
1	Q	148	THR
1	Q	164	VAL
1	Q	193	MET
1	Q	201	ASP
1	Q	202	ARG
1	Q	219	GLN
1	Q	261	ILE
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	383	LEU

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Mol	Chain	Res	Type
1	Q	396	ASN
1	Q	432	LEU
1	R	11	ILE
1	R	23	THR
1	R	39	ARG
1	R	77	ASN
1	R	88	THR
1	R	99	CYS
1	R	107	THR
1	R	120	LEU
1	R	127	VAL
1	R	146	SER
1	R	148	THR
1	R	164	VAL
1	R	193	MET
1	R	201	ASP
1	R	202	ARG
1	R	240	LEU
1	R	261	ILE
1	R	269	THR
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	337	ILE
1	R	383	LEU
1	R	396	ASN
1	R	432	LEU
1	S	11	ILE
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	164	VAL

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Mol	Chain	Res	Type
1	S	193	MET
1	S	201	ASP
1	S	202	ARG
1	S	221	GLN
1	S	225	VAL
1	S	261	ILE
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	383	LEU
1	S	396	ASN
1	S	432	LEU
1	T	11	ILE
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	164	VAL
1	T	193	MET
1	T	201	ASP
1	T	202	ARG
1	T	219	GLN
1	T	261	ILE
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	383	LEU
1	T	396	ASN
1	T	432	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (222) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	77	ASN
1	A	90	GLN
1	A	97	ASN
1	A	130	GLN
1	A	150	ASN
1	A	219	GLN
1	A	221	GLN
1	A	288	ASN
1	A	293	ASN
1	A	299	ASN
1	A	303	GLN
1	A	396	ASN
1	B	75	GLN
1	B	77	ASN
1	B	90	GLN
1	B	97	ASN
1	B	150	ASN
1	B	219	GLN
1	B	221	GLN
1	B	288	ASN
1	B	299	ASN
1	B	303	GLN
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	221	GLN
1	C	288	ASN
1	C	293	ASN
1	C	303	GLN
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	221	GLN

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Mol	Chain	Res	Type
1	D	288	ASN
1	D	299	ASN
1	D	303	GLN
1	D	396	ASN
1	E	75	GLN
1	E	90	GLN
1	E	97	ASN
1	E	150	ASN
1	E	219	GLN
1	E	221	GLN
1	E	288	ASN
1	E	299	ASN
1	E	303	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	221	GLN
1	F	288	ASN
1	F	293	ASN
1	F	299	ASN
1	F	303	GLN
1	F	396	ASN
1	G	75	GLN
1	G	77	ASN
1	G	97	ASN
1	G	130	GLN
1	G	150	ASN
1	G	219	GLN
1	G	221	GLN
1	G	288	ASN
1	G	293	ASN
1	G	299	ASN
1	G	303	GLN
1	G	396	ASN
1	H	75	GLN
1	H	77	ASN
1	H	90	GLN

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Mol	Chain	Res	Type
1	H	97	ASN
1	H	130	GLN
1	H	150	ASN
1	H	219	GLN
1	H	221	GLN
1	H	288	ASN
1	H	303	GLN
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	221	GLN
1	I	288	ASN
1	I	299	ASN
1	I	303	GLN
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	221	GLN
1	J	288	ASN
1	J	303	GLN
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	221	GLN
1	K	288	ASN
1	K	293	ASN
1	K	299	ASN
1	K	396	ASN
1	L	75	GLN
1	L	77	ASN

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Mol	Chain	Res	Type
1	L	97	ASN
1	L	150	ASN
1	L	219	GLN
1	L	221	GLN
1	L	288	ASN
1	L	299	ASN
1	L	303	GLN
1	L	396	ASN
1	M	75	GLN
1	M	77	ASN
1	M	90	GLN
1	M	130	GLN
1	M	150	ASN
1	M	219	GLN
1	M	221	GLN
1	M	288	ASN
1	M	303	GLN
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	221	GLN
1	N	288	ASN
1	N	299	ASN
1	N	303	GLN
1	N	396	ASN
1	O	75	GLN
1	O	77	ASN
1	O	90	GLN
1	O	97	ASN
1	O	130	GLN
1	O	150	ASN
1	O	219	GLN
1	O	221	GLN
1	O	288	ASN
1	O	303	GLN
1	O	396	ASN
1	P	75	GLN
1	P	77	ASN

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Mol	Chain	Res	Type
1	P	90	GLN
1	P	97	ASN
1	P	121	ASN
1	P	130	GLN
1	P	150	ASN
1	P	219	GLN
1	P	221	GLN
1	P	288	ASN
1	P	299	ASN
1	P	303	GLN
1	P	396	ASN
1	Q	46	ASN
1	Q	75	GLN
1	Q	77	ASN
1	Q	90	GLN
1	Q	97	ASN
1	Q	130	GLN
1	Q	150	ASN
1	Q	219	GLN
1	Q	221	GLN
1	Q	288	ASN
1	Q	293	ASN
1	Q	303	GLN
1	Q	396	ASN
1	R	75	GLN
1	R	77	ASN
1	R	90	GLN
1	R	97	ASN
1	R	150	ASN
1	R	219	GLN
1	R	288	ASN
1	R	293	ASN
1	R	338	HIS
1	R	396	ASN
1	S	75	GLN
1	S	77	ASN
1	S	90	GLN
1	S	97	ASN
1	S	150	ASN
1	S	219	GLN
1	S	288	ASN
1	S	299	ASN

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Mol	Chain	Res	Type
1	S	303	GLN
1	S	396	ASN
1	T	75	GLN
1	T	77	ASN
1	T	90	GLN
1	T	97	ASN
1	T	150	ASN
1	T	219	GLN
1	T	221	GLN
1	T	288	ASN
1	T	299	ASN
1	T	303	GLN
1	T	396	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	428/456 (93%)	0.60	38 (8%) 15 12	8, 12, 17, 24	0
1	B	428/456 (93%)	0.68	44 (10%) 12 9	8, 12, 17, 24	0
1	C	428/456 (93%)	0.65	43 (10%) 12 9	8, 12, 18, 24	0
1	D	428/456 (93%)	0.65	48 (11%) 10 8	8, 12, 16, 24	0
1	E	433/456 (94%)	0.66	33 (7%) 20 16	5, 11, 16, 24	0
1	F	433/456 (94%)	0.93	61 (14%) 6 5	8, 12, 16, 24	0
1	G	433/456 (94%)	0.72	44 (10%) 12 9	6, 12, 16, 24	0
1	H	428/456 (93%)	0.73	47 (10%) 10 8	8, 12, 18, 24	0
1	I	428/456 (93%)	0.79	51 (11%) 9 7	8, 12, 18, 24	0
1	J	428/456 (93%)	0.63	40 (9%) 14 11	8, 12, 17, 24	0
1	K	428/456 (93%)	0.71	44 (10%) 12 9	8, 12, 18, 24	0
1	L	428/456 (93%)	0.63	48 (11%) 10 8	8, 12, 18, 24	0
1	M	428/456 (93%)	0.85	51 (11%) 9 7	8, 12, 18, 24	0
1	N	428/456 (93%)	0.69	44 (10%) 12 9	8, 12, 18, 24	0
1	O	428/456 (93%)	0.66	45 (10%) 11 9	8, 12, 18, 24	0
1	P	430/456 (94%)	0.67	44 (10%) 12 9	8, 12, 16, 24	0
1	Q	429/456 (94%)	0.63	41 (9%) 13 10	8, 12, 18, 24	0
1	R	433/456 (94%)	0.73	35 (8%) 18 14	2, 11, 17, 24	0
1	S	428/456 (93%)	0.78	40 (9%) 14 11	4, 11, 18, 24	0
1	T	428/456 (93%)	1.00	51 (11%) 9 7	8, 12, 18, 24	0
All	All	8583/9120 (94%)	0.72	892 (10%) 11 9	2, 12, 18, 24	0

All (892) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	439	ALA	15.6
1	K	439	ALA	12.4
1	M	434	SER	11.9
1	E	439	ALA	11.8
1	N	434	SER	11.6
1	M	433	ASN	11.5
1	H	434	SER	11.2
1	H	433	ASN	11.1
1	I	440	GLY	10.9
1	T	436	LEU	10.8
1	S	433	ASN	10.6
1	T	434	SER	10.4
1	S	435	PRO	10.3
1	E	440	GLY	10.3
1	Q	439	ALA	10.1
1	R	430	ALA	10.1
1	A	439	ALA	10.1
1	H	9	GLN	10.0
1	M	10	GLN	10.0
1	F	433	ASN	10.0
1	R	9	GLN	9.9
1	N	439	ALA	9.7
1	T	440	GLY	9.5
1	I	322	GLY	9.5
1	R	435	PRO	9.5
1	C	9	GLN	9.4
1	R	434	SER	9.4
1	S	438	ILE	9.3
1	S	10	GLN	9.3
1	A	435	PRO	9.3
1	A	433	ASN	9.2
1	F	439	ALA	9.2
1	B	439	ALA	9.1
1	K	433	ASN	9.1
1	F	434	SER	9.1
1	M	430	ALA	9.1
1	P	439	ALA	9.1
1	M	429	VAL	8.9
1	N	438	ILE	8.9
1	E	10	GLN	8.9
1	H	10	GLN	8.8
1	N	436	LEU	8.8
1	I	433	ASN	8.7

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Mol	Chain	Res	Type	RSRZ
1	G	439	ALA	8.7
1	S	439	ALA	8.7
1	R	438	ILE	8.7
1	O	436	LEU	8.6
1	C	440	GLY	8.5
1	I	434	SER	8.5
1	M	436	LEU	8.5
1	O	433	ASN	8.5
1	I	430	ALA	8.5
1	J	433	ASN	8.4
1	I	435	PRO	8.4
1	B	433	ASN	8.4
1	G	434	SER	8.4
1	I	439	ALA	8.3
1	F	322	GLY	8.3
1	P	434	SER	8.2
1	T	10	GLN	8.2
1	O	434	SER	8.2
1	G	11	ILE	8.2
1	Q	436	LEU	8.2
1	R	436	LEU	8.2
1	J	434	SER	8.2
1	S	9	GLN	8.1
1	T	439	ALA	8.1
1	K	436	LEU	8.1
1	L	439	ALA	8.1
1	P	433	ASN	8.1
1	R	10	GLN	8.1
1	S	436	LEU	8.0
1	T	428	GLU	8.0
1	Q	434	SER	8.0
1	F	430	ALA	8.0
1	F	324	GLN	8.0
1	A	434	SER	7.9
1	O	322	GLY	7.9
1	N	430	ALA	7.9
1	H	436	LEU	7.9
1	M	439	ALA	7.8
1	A	10	GLN	7.8
1	S	8	THR	7.8
1	E	433	ASN	7.8
1	O	430	ALA	7.8

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Mol	Chain	Res	Type	RSRZ
1	R	437	LYS	7.8
1	G	321	ALA	7.7
1	T	425	TYR	7.5
1	Q	433	ASN	7.5
1	S	428	GLU	7.5
1	S	440	GLY	7.5
1	F	321	ALA	7.5
1	T	9	GLN	7.4
1	T	435	PRO	7.4
1	C	439	ALA	7.4
1	A	436	LEU	7.3
1	M	9	GLN	7.3
1	O	439	ALA	7.3
1	K	437	LYS	7.3
1	S	434	SER	7.3
1	J	439	ALA	7.3
1	L	438	ILE	7.2
1	O	437	LYS	7.2
1	G	8	THR	7.2
1	L	440	GLY	7.2
1	R	429	VAL	7.1
1	C	434	SER	7.1
1	D	320	GLN	7.1
1	I	9	GLN	7.1
1	N	425	TYR	7.1
1	D	433	ASN	7.0
1	H	438	ILE	7.0
1	F	10	GLN	7.0
1	I	436	LEU	7.0
1	S	317	SER	7.0
1	G	435	PRO	7.0
1	Q	435	PRO	7.0
1	R	11	ILE	7.0
1	L	436	LEU	7.0
1	M	428	GLU	7.0
1	L	435	PRO	6.9
1	E	430	ALA	6.9
1	G	10	GLN	6.9
1	L	9	GLN	6.9
1	G	433	ASN	6.8
1	N	433	ASN	6.8
1	H	439	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
1	S	430	ALA	6.8
1	L	434	SER	6.8
1	B	440	GLY	6.8
1	G	430	ALA	6.8
1	K	10	GLN	6.8
1	M	8	THR	6.8
1	P	11	ILE	6.8
1	T	430	ALA	6.8
1	O	9	GLN	6.7
1	T	431	ASP	6.7
1	H	435	PRO	6.7
1	R	433	ASN	6.7
1	O	435	PRO	6.6
1	T	321	ALA	6.6
1	D	434	SER	6.6
1	Q	10	GLN	6.6
1	M	11	ILE	6.6
1	T	438	ILE	6.6
1	R	440	GLY	6.5
1	I	321	ALA	6.5
1	K	435	PRO	6.5
1	F	425	TYR	6.5
1	H	440	GLY	6.4
1	J	440	GLY	6.4
1	B	434	SER	6.4
1	I	10	GLN	6.4
1	B	430	ALA	6.4
1	E	435	PRO	6.4
1	M	435	PRO	6.4
1	I	438	ILE	6.4
1	T	433	ASN	6.4
1	O	10	GLN	6.4
1	F	323	ASP	6.4
1	C	430	ALA	6.4
1	C	435	PRO	6.3
1	Q	438	ILE	6.3
1	N	435	PRO	6.3
1	C	10	GLN	6.3
1	L	433	ASN	6.3
1	R	431	ASP	6.3
1	B	435	PRO	6.3
1	G	437	LYS	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	321	ALA	6.2
1	F	429	VAL	6.2
1	R	8	THR	6.2
1	K	9	GLN	6.2
1	L	430	ALA	6.2
1	P	430	ALA	6.2
1	F	435	PRO	6.1
1	M	437	LYS	6.1
1	A	430	ALA	6.1
1	F	224	GLY	6.1
1	F	428	GLU	6.1
1	K	322	GLY	6.1
1	M	440	GLY	6.1
1	K	434	SER	6.1
1	E	221	GLN	6.0
1	C	433	ASN	6.0
1	B	437	LYS	6.0
1	D	429	VAL	6.0
1	K	429	VAL	6.0
1	T	432	LEU	6.0
1	N	10	GLN	6.0
1	Q	430	ALA	6.0
1	E	429	VAL	6.0
1	T	322	GLY	5.9
1	B	429	VAL	5.9
1	F	220	TYR	5.9
1	S	429	VAL	5.9
1	E	434	SER	5.9
1	A	437	LYS	5.8
1	Q	8	THR	5.8
1	F	9	GLN	5.8
1	P	435	PRO	5.8
1	E	9	GLN	5.8
1	J	9	GLN	5.8
1	A	322	GLY	5.8
1	E	438	ILE	5.8
1	T	113	LEU	5.8
1	J	435	PRO	5.8
1	S	11	ILE	5.7
1	K	430	ALA	5.7
1	P	425	TYR	5.7
1	O	11	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	J	10	GLN	5.7
1	M	425	TYR	5.7
1	B	322	GLY	5.7
1	N	9	GLN	5.7
1	C	322	GLY	5.6
1	E	431	ASP	5.6
1	E	437	LYS	5.6
1	G	428	GLU	5.6
1	H	430	ALA	5.6
1	F	320	GLN	5.6
1	M	438	ILE	5.6
1	D	10	GLN	5.5
1	P	9	GLN	5.5
1	O	429	VAL	5.5
1	P	437	LYS	5.5
1	N	429	VAL	5.5
1	G	425	TYR	5.5
1	S	113	LEU	5.5
1	R	428	GLU	5.5
1	S	427	MET	5.4
1	N	322	GLY	5.4
1	T	11	ILE	5.4
1	T	427	MET	5.4
1	K	8	THR	5.4
1	N	8	THR	5.4
1	C	431	ASP	5.4
1	T	221	GLN	5.4
1	I	431	ASP	5.4
1	I	429	VAL	5.4
1	S	425	TYR	5.4
1	N	321	ALA	5.3
1	G	9	GLN	5.3
1	E	11	ILE	5.3
1	G	220	TYR	5.3
1	H	222	PRO	5.3
1	J	438	ILE	5.3
1	K	438	ILE	5.3
1	P	438	ILE	5.3
1	B	10	GLN	5.3
1	L	431	ASP	5.3
1	O	438	ILE	5.3
1	J	430	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	S	437	LYS	5.2
1	K	11	ILE	5.2
1	Q	11	ILE	5.2
1	F	222	PRO	5.2
1	J	324	GLN	5.2
1	P	436	LEU	5.2
1	I	279	ASN	5.2
1	B	436	LEU	5.2
1	M	431	ASP	5.1
1	P	431	ASP	5.1
1	L	429	VAL	5.1
1	T	429	VAL	5.1
1	L	8	THR	5.1
1	J	436	LEU	5.1
1	P	432	LEU	5.1
1	C	436	LEU	5.1
1	I	8	THR	5.0
1	F	436	LEU	5.0
1	A	438	ILE	5.0
1	D	440	GLY	5.0
1	T	223	GLY	5.0
1	H	8	THR	5.0
1	H	113	LEU	5.0
1	G	322	GLY	5.0
1	T	437	LYS	5.0
1	D	431	ASP	5.0
1	N	323	ASP	5.0
1	T	324	GLN	5.0
1	A	440	GLY	5.0
1	T	279	ASN	5.0
1	O	440	GLY	5.0
1	S	432	LEU	4.9
1	B	438	ILE	4.9
1	I	11	ILE	4.9
1	Q	9	GLN	4.9
1	P	222	PRO	4.9
1	K	113	LEU	4.9
1	L	10	GLN	4.9
1	D	430	ALA	4.9
1	C	11	ILE	4.9
1	F	438	ILE	4.9
1	I	427	MET	4.9

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Mol	Chain	Res	Type	RSRZ
1	P	321	ALA	4.9
1	D	438	ILE	4.9
1	M	321	ALA	4.8
1	I	220	TYR	4.8
1	N	113	LEU	4.8
1	Q	113	LEU	4.8
1	D	425	TYR	4.8
1	F	8	THR	4.8
1	E	427	MET	4.8
1	N	428	GLU	4.8
1	G	440	GLY	4.8
1	I	437	LYS	4.8
1	M	427	MET	4.8
1	D	435	PRO	4.8
1	K	321	ALA	4.8
1	K	440	GLY	4.8
1	Q	322	GLY	4.7
1	E	425	TYR	4.7
1	H	429	VAL	4.7
1	A	9	GLN	4.7
1	N	437	LYS	4.7
1	F	315	SER	4.7
1	J	8	THR	4.7
1	D	317	SER	4.7
1	R	425	TYR	4.7
1	I	222	PRO	4.6
1	S	121	ASN	4.6
1	B	425	TYR	4.6
1	J	429	VAL	4.6
1	H	428	GLU	4.6
1	R	432	LEU	4.6
1	T	222	PRO	4.6
1	B	9	GLN	4.6
1	D	254	GLY	4.6
1	G	436	LEU	4.6
1	A	429	VAL	4.6
1	Q	429	VAL	4.6
1	N	427	MET	4.6
1	O	321	ALA	4.5
1	F	437	LYS	4.5
1	P	429	VAL	4.5
1	N	11	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	L	322	GLY	4.5
1	Q	425	TYR	4.5
1	O	254	GLY	4.5
1	B	8	THR	4.5
1	G	431	ASP	4.5
1	L	428	GLU	4.5
1	B	431	ASP	4.4
1	B	222	PRO	4.4
1	A	425	TYR	4.4
1	P	440	GLY	4.4
1	D	319	GLY	4.4
1	G	223	GLY	4.4
1	H	320	GLN	4.4
1	K	425	TYR	4.4
1	P	219	GLN	4.4
1	P	8	THR	4.4
1	I	428	GLU	4.4
1	G	427	MET	4.3
1	G	432	LEU	4.3
1	R	427	MET	4.3
1	Q	437	LYS	4.3
1	H	425	TYR	4.3
1	E	432	LEU	4.3
1	S	431	ASP	4.3
1	L	427	MET	4.3
1	F	440	GLY	4.2
1	P	324	GLN	4.2
1	J	322	GLY	4.2
1	K	427	MET	4.2
1	C	8	THR	4.2
1	H	432	LEU	4.2
1	B	324	GLN	4.2
1	C	219	GLN	4.2
1	K	320	GLN	4.2
1	R	317	SER	4.2
1	A	8	THR	4.2
1	M	320	GLN	4.2
1	O	324	GLN	4.2
1	C	258	GLY	4.2
1	H	319	GLY	4.1
1	I	425	TYR	4.1
1	K	428	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	N	431	ASP	4.1
1	Q	428	GLU	4.1
1	S	191	PRO	4.1
1	K	431	ASP	4.1
1	D	8	THR	4.1
1	S	321	ALA	4.1
1	B	11	ILE	4.1
1	K	121	ASN	4.1
1	L	432	LEU	4.1
1	M	317	SER	4.1
1	C	438	ILE	4.0
1	G	438	ILE	4.0
1	R	426	PHE	4.0
1	D	9	GLN	4.0
1	H	219	GLN	4.0
1	B	321	ALA	4.0
1	A	431	ASP	4.0
1	A	11	ILE	4.0
1	J	432	LEU	4.0
1	L	317	SER	4.0
1	M	326	SER	4.0
1	G	219	GLN	4.0
1	L	254	GLY	4.0
1	K	324	GLN	3.9
1	M	424	GLU	3.9
1	D	285	GLY	3.9
1	C	425	TYR	3.9
1	I	286	THR	3.9
1	T	8	THR	3.9
1	I	320	GLN	3.9
1	T	320	GLN	3.9
1	H	427	MET	3.9
1	F	279	ASN	3.9
1	C	256	VAL	3.9
1	P	220	TYR	3.9
1	C	222	PRO	3.9
1	P	10	GLN	3.9
1	S	192	LYS	3.9
1	F	314	THR	3.8
1	J	437	LYS	3.8
1	L	321	ALA	3.8
1	F	256	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	324	GLN	3.8
1	N	320	GLN	3.8
1	E	436	LEU	3.8
1	O	251	SER	3.8
1	D	439	ALA	3.8
1	F	278	ALA	3.8
1	F	258	GLY	3.8
1	K	258	GLY	3.8
1	D	323	ASP	3.8
1	H	437	LYS	3.8
1	C	428	GLU	3.8
1	E	8	THR	3.8
1	I	432	LEU	3.8
1	J	113	LEU	3.8
1	G	429	VAL	3.8
1	I	316	LYS	3.8
1	M	212	ASP	3.8
1	M	279	ASN	3.8
1	C	113	LEU	3.8
1	Q	317	SER	3.8
1	I	324	GLN	3.7
1	B	113	LEU	3.7
1	M	324	GLN	3.7
1	O	428	GLU	3.7
1	T	424	GLU	3.7
1	F	325	MET	3.7
1	H	220	TYR	3.7
1	O	425	TYR	3.7
1	Q	321	ALA	3.7
1	H	256	VAL	3.7
1	B	320	GLN	3.7
1	A	427	MET	3.7
1	P	254	GLY	3.7
1	G	279	ASN	3.7
1	Q	220	TYR	3.7
1	T	407	ARG	3.7
1	S	426	PHE	3.7
1	M	113	LEU	3.6
1	O	431	ASP	3.6
1	F	217	SER	3.6
1	N	251	SER	3.6
1	D	11	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	11	ILE	3.6
1	D	121	ASN	3.6
1	E	51	ASP	3.6
1	H	321	ALA	3.6
1	N	222	PRO	3.6
1	H	221	GLN	3.6
1	L	437	LYS	3.6
1	C	429	VAL	3.6
1	B	224	GLY	3.6
1	F	319	GLY	3.6
1	O	223	GLY	3.6
1	A	316	LYS	3.6
1	L	323	ASP	3.5
1	L	425	TYR	3.5
1	T	219	GLN	3.5
1	S	120	LEU	3.5
1	H	317	SER	3.5
1	C	321	ALA	3.5
1	D	321	ALA	3.5
1	F	318	GLY	3.5
1	H	258	GLY	3.5
1	D	222	PRO	3.5
1	F	212	ASP	3.5
1	G	212	ASP	3.5
1	J	321	ALA	3.5
1	B	428	GLU	3.5
1	D	436	LEU	3.5
1	Q	324	GLN	3.5
1	M	220	TYR	3.5
1	T	184	ILE	3.5
1	F	316	LYS	3.5
1	A	432	LEU	3.5
1	C	251	SER	3.4
1	T	121	ASN	3.4
1	J	222	PRO	3.4
1	H	323	ASP	3.4
1	J	431	ASP	3.4
1	F	221	GLN	3.4
1	Q	432	LEU	3.4
1	B	217	SER	3.4
1	C	315	SER	3.4
1	J	220	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	223	GLY	3.4
1	H	322	GLY	3.4
1	C	324	GLN	3.4
1	E	391	ASP	3.4
1	F	223	GLY	3.4
1	K	278	ALA	3.4
1	L	279	ASN	3.4
1	T	426	PHE	3.4
1	F	251	SER	3.3
1	J	251	SER	3.3
1	N	217	SER	3.3
1	D	255	LEU	3.3
1	E	322	GLY	3.3
1	R	322	GLY	3.3
1	I	121	ASN	3.3
1	H	426	PHE	3.3
1	I	315	SER	3.3
1	P	286	THR	3.3
1	T	120	LEU	3.3
1	Q	440	GLY	3.3
1	E	279	ASN	3.3
1	K	279	ASN	3.3
1	C	323	ASP	3.3
1	F	225	VAL	3.3
1	I	323	ASP	3.3
1	O	323	ASP	3.3
1	G	251	SER	3.3
1	A	219	GLN	3.3
1	N	280	ASN	3.3
1	H	431	ASP	3.3
1	N	324	GLN	3.3
1	D	318	GLY	3.3
1	E	321	ALA	3.3
1	D	288	ASN	3.3
1	I	256	VAL	3.3
1	F	431	ASP	3.3
1	B	120	LEU	3.2
1	G	222	PRO	3.2
1	B	223	GLY	3.2
1	M	322	GLY	3.2
1	A	222	PRO	3.2
1	Q	320	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	O	220	TYR	3.2
1	O	426	PHE	3.2
1	D	113	LEU	3.2
1	D	428	GLU	3.2
1	O	221	GLN	3.2
1	P	322	GLY	3.2
1	J	425	TYR	3.2
1	S	279	ASN	3.2
1	I	424	GLU	3.2
1	L	120	LEU	3.2
1	E	222	PRO	3.2
1	F	219	GLN	3.2
1	J	317	SER	3.2
1	F	257	LEU	3.1
1	L	319	GLY	3.1
1	T	285	GLY	3.1
1	B	278	ALA	3.1
1	C	317	SER	3.1
1	F	427	MET	3.1
1	F	162	GLU	3.1
1	P	278	ALA	3.1
1	J	315	SER	3.1
1	H	120	LEU	3.1
1	T	323	ASP	3.1
1	A	428	GLU	3.1
1	K	222	PRO	3.1
1	A	320	GLN	3.1
1	E	286	THR	3.1
1	M	224	GLY	3.1
1	H	11	ILE	3.1
1	K	251	SER	3.1
1	Q	427	MET	3.1
1	B	432	LEU	3.1
1	D	324	GLN	3.0
1	M	221	GLN	3.0
1	O	8	THR	3.0
1	O	427	MET	3.0
1	K	426	PHE	3.0
1	O	12	VAL	3.0
1	C	217	SER	3.0
1	O	120	LEU	3.0
1	N	279	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	R	320	GLN	3.0
1	T	391	ASP	3.0
1	O	113	LEU	3.0
1	M	330	ARG	3.0
1	R	417	ARG	3.0
1	D	223	GLY	3.0
1	I	278	ALA	3.0
1	A	113	LEU	3.0
1	D	315	SER	3.0
1	J	428	GLU	3.0
1	C	320	GLN	3.0
1	Q	431	ASP	3.0
1	N	440	GLY	3.0
1	E	424	GLU	2.9
1	H	324	GLN	2.9
1	H	318	GLY	2.9
1	R	318	GLY	2.9
1	K	432	LEU	2.9
1	L	121	ASN	2.9
1	I	223	GLY	2.9
1	R	424	GLU	2.9
1	I	221	GLN	2.9
1	J	320	GLN	2.9
1	L	337	ILE	2.9
1	L	318	GLY	2.9
1	Q	254	GLY	2.9
1	I	211	ALA	2.9
1	E	317	SER	2.9
1	H	280	ASN	2.9
1	S	223	GLY	2.9
1	B	277	ALA	2.9
1	A	221	GLN	2.8
1	E	219	GLN	2.8
1	H	417	ARG	2.8
1	P	320	GLN	2.8
1	T	215	GLN	2.8
1	J	280	ASN	2.8
1	C	318	GLY	2.8
1	K	323	ASP	2.8
1	L	286	THR	2.8
1	O	432	LEU	2.8
1	Q	112	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	427	MET	2.8
1	A	426	PHE	2.8
1	H	325	MET	2.8
1	L	417	ARG	2.8
1	B	221	GLN	2.8
1	J	279	ASN	2.8
1	M	214	TYR	2.8
1	M	219	GLN	2.8
1	E	428	GLU	2.8
1	M	286	THR	2.8
1	P	428	GLU	2.8
1	T	337	ILE	2.7
1	L	251	SER	2.7
1	N	432	LEU	2.7
1	O	424	GLU	2.7
1	Q	219	GLN	2.7
1	I	253	HIS	2.7
1	J	223	GLY	2.7
1	I	212	ASP	2.7
1	T	249	ARG	2.7
1	F	281	GLY	2.7
1	H	253	HIS	2.7
1	A	279	ASN	2.7
1	G	389	ARG	2.7
1	I	347	ARG	2.7
1	P	315	SER	2.7
1	Q	319	GLY	2.7
1	T	319	GLY	2.7
1	G	424	GLU	2.7
1	F	286	THR	2.7
1	N	221	GLN	2.6
1	A	120	LEU	2.6
1	N	347	ARG	2.6
1	C	319	GLY	2.6
1	D	437	LYS	2.6
1	P	221	GLN	2.6
1	B	427	MET	2.6
1	L	389	ARG	2.6
1	N	223	GLY	2.6
1	A	121	ASN	2.6
1	B	279	ASN	2.6
1	L	222	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	N	218	SER	2.6
1	R	324	GLN	2.6
1	A	51	ASP	2.6
1	F	213	ASP	2.6
1	J	212	ASP	2.6
1	M	391	ASP	2.6
1	M	389	ARG	2.6
1	P	223	GLY	2.6
1	O	279	ASN	2.6
1	P	225	VAL	2.6
1	L	320	GLN	2.6
1	K	220	TYR	2.6
1	L	347	ARG	2.6
1	R	254	GLY	2.6
1	O	222	PRO	2.6
1	F	426	PHE	2.6
1	J	217	SER	2.5
1	S	391	ASP	2.5
1	E	220	TYR	2.5
1	M	223	GLY	2.5
1	C	278	ALA	2.5
1	F	249	ARG	2.5
1	H	316	LYS	2.5
1	G	121	ASN	2.5
1	B	220	TYR	2.5
1	K	318	GLY	2.5
1	P	285	GLY	2.5
1	C	427	MET	2.5
1	J	427	MET	2.5
1	D	251	SER	2.5
1	G	328	SER	2.5
1	M	432	LEU	2.5
1	T	417	ARG	2.5
1	T	393	GLY	2.5
1	G	320	GLN	2.5
1	S	12	VAL	2.5
1	F	347	ARG	2.4
1	L	113	LEU	2.4
1	A	323	ASP	2.4
1	B	253	HIS	2.4
1	K	213	ASP	2.4
1	K	253	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	254	GLY	2.4
1	A	220	TYR	2.4
1	D	219	GLN	2.4
1	M	407	ARG	2.4
1	N	112	THR	2.4
1	L	253	HIS	2.4
1	N	317	SER	2.4
1	O	317	SER	2.4
1	Q	323	ASP	2.4
1	C	325	MET	2.4
1	T	114	PRO	2.4
1	C	316	LYS	2.4
1	L	324	GLN	2.4
1	G	118	TYR	2.4
1	I	120	LEU	2.4
1	J	11	ILE	2.4
1	H	279	ASN	2.4
1	I	317	SER	2.4
1	P	317	SER	2.4
1	G	313	VAL	2.4
1	I	389	ARG	2.4
1	Q	121	ASN	2.4
1	T	51	ASP	2.4
1	P	325	MET	2.4
1	B	318	GLY	2.4
1	K	223	GLY	2.4
1	B	219	GLN	2.4
1	H	130	GLN	2.4
1	J	219	GLN	2.4
1	O	320	GLN	2.4
1	F	313	VAL	2.4
1	K	389	ARG	2.4
1	T	347	ARG	2.4
1	C	426	PHE	2.4
1	P	426	PHE	2.4
1	B	337	ILE	2.3
1	T	284	THR	2.3
1	Q	253	HIS	2.3
1	D	279	ASN	2.3
1	P	323	ASP	2.3
1	B	215	GLN	2.3
1	G	115	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	254	GLY	2.3
1	H	254	GLY	2.3
1	N	281	GLY	2.3
1	T	12	VAL	2.3
1	Q	120	LEU	2.3
1	C	184	ILE	2.3
1	R	226	THR	2.3
1	T	288	ASN	2.3
1	F	218	SER	2.3
1	J	287	ASP	2.3
1	L	407	ARG	2.3
1	S	186	ALA	2.3
1	I	391	ASP	2.3
1	P	251	SER	2.3
1	Q	326	SER	2.3
1	P	389	ARG	2.3
1	I	319	GLY	2.3
1	L	221	GLN	2.3
1	G	426	PHE	2.3
1	M	426	PHE	2.3
1	O	255	LEU	2.3
1	P	337	ILE	2.3
1	R	253	HIS	2.3
1	B	316	LYS	2.3
1	N	316	LYS	2.3
1	F	424	GLU	2.3
1	B	218	SER	2.3
1	L	114	PRO	2.3
1	L	219	GLN	2.3
1	C	120	LEU	2.3
1	S	337	ILE	2.2
1	K	192	LYS	2.2
1	K	316	LYS	2.2
1	A	424	GLU	2.2
1	C	288	ASN	2.2
1	M	121	ASN	2.2
1	L	218	SER	2.2
1	I	113	LEU	2.2
1	D	216	PHE	2.2
1	R	279	ASN	2.2
1	S	389	ARG	2.2
1	I	258	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	254	GLY	2.2
1	B	256	VAL	2.2
1	L	426	PHE	2.2
1	I	275	ALA	2.2
1	M	34	GLU	2.2
1	C	279	ASN	2.2
1	D	214	TYR	2.2
1	T	220	TYR	2.2
1	G	348	PRO	2.2
1	K	191	PRO	2.2
1	E	75	GLN	2.2
1	B	319	GLY	2.2
1	D	316	LYS	2.2
1	D	322	GLY	2.2
1	F	254	GLY	2.2
1	M	319	GLY	2.2
1	M	406	ASP	2.2
1	K	256	VAL	2.2
1	A	284	THR	2.2
1	M	284	THR	2.2
1	I	219	GLN	2.2
1	O	219	GLN	2.2
1	F	432	LEU	2.2
1	K	188	GLY	2.2
1	G	323	ASP	2.2
1	M	323	ASP	2.2
1	P	427	MET	2.2
1	L	315	SER	2.2
1	L	11	ILE	2.2
1	N	278	ALA	2.1
1	J	245	GLU	2.1
1	Q	284	THR	2.1
1	M	222	PRO	2.1
1	A	324	GLN	2.1
1	D	221	GLN	2.1
1	D	432	LEU	2.1
1	Q	223	GLY	2.1
1	H	218	SER	2.1
1	N	426	PHE	2.1
1	S	424	GLU	2.1
1	H	347	ARG	2.1
1	P	330	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	191	PRO	2.1
1	I	348	PRO	2.1
1	D	120	LEU	2.1
1	D	325	MET	2.1
1	M	120	LEU	2.1
1	Q	279	ASN	2.1
1	N	220	TYR	2.1
1	I	318	GLY	2.1
1	J	258	GLY	2.1
1	F	253	HIS	2.1
1	L	211	ALA	2.1
1	F	285	GLY	2.1
1	G	285	GLY	2.1
1	R	337	ILE	2.1
1	F	326	SER	2.1
1	N	417	ARG	2.1
1	O	112	THR	2.1
1	F	215	GLN	2.1
1	P	288	ASN	2.1
1	E	318	GLY	2.1
1	D	220	TYR	2.1
1	Q	214	TYR	2.1
1	G	330	ARG	2.0
1	S	407	ARG	2.0
1	F	317	SER	2.0
1	Q	315	SER	2.0
1	R	192	LYS	2.0
1	C	283	THR	2.0
1	S	286	THR	2.0
1	D	253	HIS	2.0
1	J	121	ASN	2.0
1	A	319	GLY	2.0
1	D	258	GLY	2.0
1	O	50	GLY	2.0
1	Q	318	GLY	2.0
1	G	417	ARG	2.0
1	M	423	ARG	2.0
1	O	417	ARG	2.0
1	P	275	ALA	2.0
1	S	112	THR	2.0
1	S	221	GLN	2.0
1	O	253	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	393	GLY	2.0
1	K	281	GLY	2.0
1	M	337	ILE	2.0
1	R	285	GLY	2.0
1	N	12	VAL	2.0
1	O	256	VAL	2.0
1	O	330	ARG	2.0
1	S	417	ARG	2.0
1	R	214	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	D	504	1/1	0.96	0.12	2,2,2,2	1
2	CA	L	507	1/1	0.96	0.10	2,2,2,2	1
2	CA	A	501	1/1	0.97	0.09	10,10,10,10	1
2	CA	S	510	1/1	0.97	0.06	5,5,5,5	1
2	CA	O	509	1/1	0.98	0.15	2,2,2,2	0
2	CA	M	508	1/1	0.98	0.05	2,2,2,2	1
2	CA	T	511	1/1	0.98	0.03	4,4,4,4	1
2	CA	B	502	1/1	0.99	0.12	12,12,12,12	1
2	CA	F	505	1/1	0.99	0.07	2,2,2,2	0
2	CA	G	506	1/1	0.99	0.09	2,2,2,2	0
2	CA	C	503	1/1	0.99	0.12	2,2,2,2	1

6.5 Other polymers [i](#)

There are no such residues in this entry.