



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:35 PM UTC

PDB ID : 7TIF / pdb_00007tif
Title : 2.85 Angstrom crystal structure of Arginyltransferase 1 (ATE1) from *Saccharomyces cerevisiae*
Authors : Van, V.; Ejimogu, N.-E.; Smith, A.T.
Deposited on : 2022-01-13
Resolution : 2.85 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
Mogul : 2022.3.0, CSD as543be (2022)
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

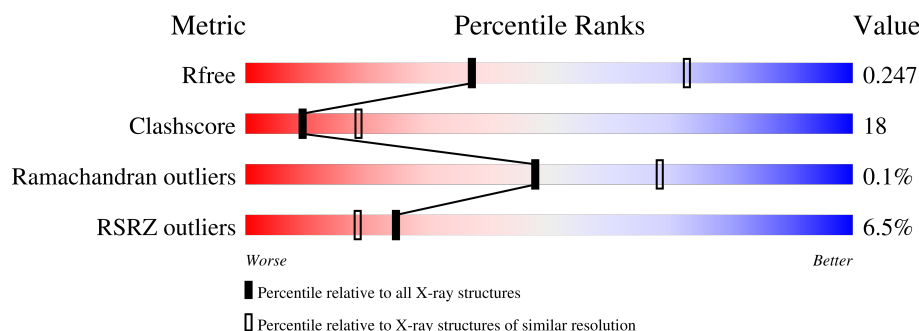
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	518	3% 65%25%10%
1	B	518	4% 65%25%10%
1	C	518	5% 65%25%10%
1	D	518	3% 61%27%12%
1	E	518	4% 67%23%10%
1	F	518	4% 58%31%10%

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Mol	Chain	Length	Quality of chain
1	G	518	
1	H	518	
1	I	518	
1	J	518	
1	K	518	
1	L	518	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	601	-	-	X	-
2	SO4	C	604	-	-	X	-
2	SO4	D	609	-	-	X	-
2	SO4	E	601	-	-	X	-
2	SO4	E	612	-	-	X	-
2	SO4	G	608	-	-	X	-
2	SO4	G	617	-	-	X	-
2	SO4	H	601	-	-	X	-
2	SO4	H	612	-	-	X	-
2	SO4	I	602	-	-	X	-
2	SO4	I	611	-	-	X	-
2	SO4	J	603	-	-	X	-
2	SO4	K	605	-	-	X	-
2	SO4	L	604	-	-	X	-
2	SO4	L	611	-	-	X	-
3	GOL	A	625	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46039 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 Arginyl-tRNA--protein transferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	1	0
			3800	2447	621	706	26			
1	B	464	Total	C	N	O	S	0	0	0
			3775	2430	615	704	26			
1	C	464	Total	C	N	O	S	0	1	0
			3776	2434	618	698	26			
1	D	456	Total	C	N	O	S	0	0	0
			3715	2391	608	691	25			
1	E	465	Total	C	N	O	S	0	0	0
			3783	2437	618	704	24			
1	F	464	Total	C	N	O	S	0	0	0
			3777	2432	617	702	26			
1	G	457	Total	C	N	O	S	0	0	0
			3718	2394	607	692	25			
1	H	456	Total	C	N	O	S	0	0	0
			3721	2397	609	690	25			
1	I	452	Total	C	N	O	S	0	0	0
			3676	2367	602	682	25			
1	J	449	Total	C	N	O	S	0	0	0
			3651	2357	598	671	25			
1	K	459	Total	C	N	O	S	0	0	0
			3733	2405	610	693	25			
1	L	441	Total	C	N	O	S	0	0	0
			3589	2318	588	658	25			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	504	GLU	-	expression tag	UNP P16639
A	505	ASN	-	expression tag	UNP P16639
A	506	LEU	-	expression tag	UNP P16639
A	507	TYR	-	expression tag	UNP P16639
A	508	PHE	-	expression tag	UNP P16639

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Chain	Residue	Modelled	Actual	Comment	Reference
A	509	GLN	-	expression tag	UNP P16639
A	510	SER	-	expression tag	UNP P16639
A	511	LEU	-	expression tag	UNP P16639
A	512	GLU	-	expression tag	UNP P16639
A	513	HIS	-	expression tag	UNP P16639
A	514	HIS	-	expression tag	UNP P16639
A	515	HIS	-	expression tag	UNP P16639
A	516	HIS	-	expression tag	UNP P16639
A	517	HIS	-	expression tag	UNP P16639
A	518	HIS	-	expression tag	UNP P16639
B	504	GLU	-	expression tag	UNP P16639
B	505	ASN	-	expression tag	UNP P16639
B	506	LEU	-	expression tag	UNP P16639
B	507	TYR	-	expression tag	UNP P16639
B	508	PHE	-	expression tag	UNP P16639
B	509	GLN	-	expression tag	UNP P16639
B	510	SER	-	expression tag	UNP P16639
B	511	LEU	-	expression tag	UNP P16639
B	512	GLU	-	expression tag	UNP P16639
B	513	HIS	-	expression tag	UNP P16639
B	514	HIS	-	expression tag	UNP P16639
B	515	HIS	-	expression tag	UNP P16639
B	516	HIS	-	expression tag	UNP P16639
B	517	HIS	-	expression tag	UNP P16639
B	518	HIS	-	expression tag	UNP P16639
C	504	GLU	-	expression tag	UNP P16639
C	505	ASN	-	expression tag	UNP P16639
C	506	LEU	-	expression tag	UNP P16639
C	507	TYR	-	expression tag	UNP P16639
C	508	PHE	-	expression tag	UNP P16639
C	509	GLN	-	expression tag	UNP P16639
C	510	SER	-	expression tag	UNP P16639
C	511	LEU	-	expression tag	UNP P16639
C	512	GLU	-	expression tag	UNP P16639
C	513	HIS	-	expression tag	UNP P16639
C	514	HIS	-	expression tag	UNP P16639
C	515	HIS	-	expression tag	UNP P16639
C	516	HIS	-	expression tag	UNP P16639
C	517	HIS	-	expression tag	UNP P16639
C	518	HIS	-	expression tag	UNP P16639
D	504	GLU	-	expression tag	UNP P16639
D	505	ASN	-	expression tag	UNP P16639

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Chain	Residue	Modelled	Actual	Comment	Reference
D	506	LEU	-	expression tag	UNP P16639
D	507	TYR	-	expression tag	UNP P16639
D	508	PHE	-	expression tag	UNP P16639
D	509	GLN	-	expression tag	UNP P16639
D	510	SER	-	expression tag	UNP P16639
D	511	LEU	-	expression tag	UNP P16639
D	512	GLU	-	expression tag	UNP P16639
D	513	HIS	-	expression tag	UNP P16639
D	514	HIS	-	expression tag	UNP P16639
D	515	HIS	-	expression tag	UNP P16639
D	516	HIS	-	expression tag	UNP P16639
D	517	HIS	-	expression tag	UNP P16639
D	518	HIS	-	expression tag	UNP P16639
E	504	GLU	-	expression tag	UNP P16639
E	505	ASN	-	expression tag	UNP P16639
E	506	LEU	-	expression tag	UNP P16639
E	507	TYR	-	expression tag	UNP P16639
E	508	PHE	-	expression tag	UNP P16639
E	509	GLN	-	expression tag	UNP P16639
E	510	SER	-	expression tag	UNP P16639
E	511	LEU	-	expression tag	UNP P16639
E	512	GLU	-	expression tag	UNP P16639
E	513	HIS	-	expression tag	UNP P16639
E	514	HIS	-	expression tag	UNP P16639
E	515	HIS	-	expression tag	UNP P16639
E	516	HIS	-	expression tag	UNP P16639
E	517	HIS	-	expression tag	UNP P16639
E	518	HIS	-	expression tag	UNP P16639
F	504	GLU	-	expression tag	UNP P16639
F	505	ASN	-	expression tag	UNP P16639
F	506	LEU	-	expression tag	UNP P16639
F	507	TYR	-	expression tag	UNP P16639
F	508	PHE	-	expression tag	UNP P16639
F	509	GLN	-	expression tag	UNP P16639
F	510	SER	-	expression tag	UNP P16639
F	511	LEU	-	expression tag	UNP P16639
F	512	GLU	-	expression tag	UNP P16639
F	513	HIS	-	expression tag	UNP P16639
F	514	HIS	-	expression tag	UNP P16639
F	515	HIS	-	expression tag	UNP P16639
F	516	HIS	-	expression tag	UNP P16639
F	517	HIS	-	expression tag	UNP P16639

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Chain	Residue	Modelled	Actual	Comment	Reference
F	518	HIS	-	expression tag	UNP P16639
G	504	GLU	-	expression tag	UNP P16639
G	505	ASN	-	expression tag	UNP P16639
G	506	LEU	-	expression tag	UNP P16639
G	507	TYR	-	expression tag	UNP P16639
G	508	PHE	-	expression tag	UNP P16639
G	509	GLN	-	expression tag	UNP P16639
G	510	SER	-	expression tag	UNP P16639
G	511	LEU	-	expression tag	UNP P16639
G	512	GLU	-	expression tag	UNP P16639
G	513	HIS	-	expression tag	UNP P16639
G	514	HIS	-	expression tag	UNP P16639
G	515	HIS	-	expression tag	UNP P16639
G	516	HIS	-	expression tag	UNP P16639
G	517	HIS	-	expression tag	UNP P16639
G	518	HIS	-	expression tag	UNP P16639
H	504	GLU	-	expression tag	UNP P16639
H	505	ASN	-	expression tag	UNP P16639
H	506	LEU	-	expression tag	UNP P16639
H	507	TYR	-	expression tag	UNP P16639
H	508	PHE	-	expression tag	UNP P16639
H	509	GLN	-	expression tag	UNP P16639
H	510	SER	-	expression tag	UNP P16639
H	511	LEU	-	expression tag	UNP P16639
H	512	GLU	-	expression tag	UNP P16639
H	513	HIS	-	expression tag	UNP P16639
H	514	HIS	-	expression tag	UNP P16639
H	515	HIS	-	expression tag	UNP P16639
H	516	HIS	-	expression tag	UNP P16639
H	517	HIS	-	expression tag	UNP P16639
H	518	HIS	-	expression tag	UNP P16639
I	504	GLU	-	expression tag	UNP P16639
I	505	ASN	-	expression tag	UNP P16639
I	506	LEU	-	expression tag	UNP P16639
I	507	TYR	-	expression tag	UNP P16639
I	508	PHE	-	expression tag	UNP P16639
I	509	GLN	-	expression tag	UNP P16639
I	510	SER	-	expression tag	UNP P16639
I	511	LEU	-	expression tag	UNP P16639
I	512	GLU	-	expression tag	UNP P16639
I	513	HIS	-	expression tag	UNP P16639
I	514	HIS	-	expression tag	UNP P16639

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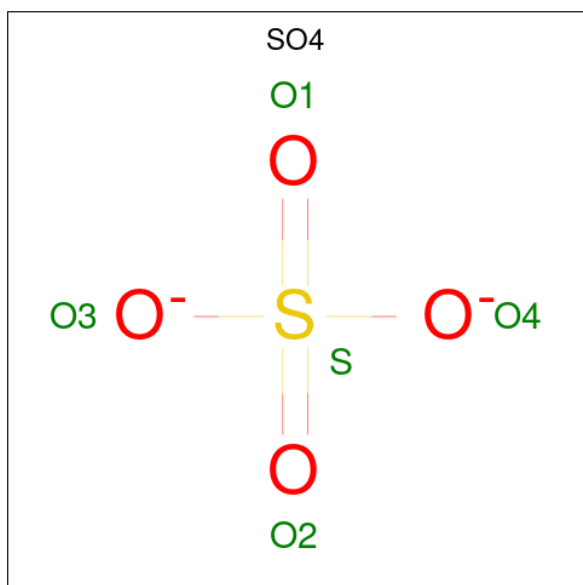
Chain	Residue	Modelled	Actual	Comment	Reference
I	515	HIS	-	expression tag	UNP P16639
I	516	HIS	-	expression tag	UNP P16639
I	517	HIS	-	expression tag	UNP P16639
I	518	HIS	-	expression tag	UNP P16639
J	504	GLU	-	expression tag	UNP P16639
J	505	ASN	-	expression tag	UNP P16639
J	506	LEU	-	expression tag	UNP P16639
J	507	TYR	-	expression tag	UNP P16639
J	508	PHE	-	expression tag	UNP P16639
J	509	GLN	-	expression tag	UNP P16639
J	510	SER	-	expression tag	UNP P16639
J	511	LEU	-	expression tag	UNP P16639
J	512	GLU	-	expression tag	UNP P16639
J	513	HIS	-	expression tag	UNP P16639
J	514	HIS	-	expression tag	UNP P16639
J	515	HIS	-	expression tag	UNP P16639
J	516	HIS	-	expression tag	UNP P16639
J	517	HIS	-	expression tag	UNP P16639
J	518	HIS	-	expression tag	UNP P16639
K	504	GLU	-	expression tag	UNP P16639
K	505	ASN	-	expression tag	UNP P16639
K	506	LEU	-	expression tag	UNP P16639
K	507	TYR	-	expression tag	UNP P16639
K	508	PHE	-	expression tag	UNP P16639
K	509	GLN	-	expression tag	UNP P16639
K	510	SER	-	expression tag	UNP P16639
K	511	LEU	-	expression tag	UNP P16639
K	512	GLU	-	expression tag	UNP P16639
K	513	HIS	-	expression tag	UNP P16639
K	514	HIS	-	expression tag	UNP P16639
K	515	HIS	-	expression tag	UNP P16639
K	516	HIS	-	expression tag	UNP P16639
K	517	HIS	-	expression tag	UNP P16639
K	518	HIS	-	expression tag	UNP P16639
L	504	GLU	-	expression tag	UNP P16639
L	505	ASN	-	expression tag	UNP P16639
L	506	LEU	-	expression tag	UNP P16639
L	507	TYR	-	expression tag	UNP P16639
L	508	PHE	-	expression tag	UNP P16639
L	509	GLN	-	expression tag	UNP P16639
L	510	SER	-	expression tag	UNP P16639
L	511	LEU	-	expression tag	UNP P16639

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Chain	Residue	Modelled	Actual	Comment	Reference
L	512	GLU	-	expression tag	UNP P16639
L	513	HIS	-	expression tag	UNP P16639
L	514	HIS	-	expression tag	UNP P16639
L	515	HIS	-	expression tag	UNP P16639
L	516	HIS	-	expression tag	UNP P16639
L	517	HIS	-	expression tag	UNP P16639
L	518	HIS	-	expression tag	UNP P16639

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

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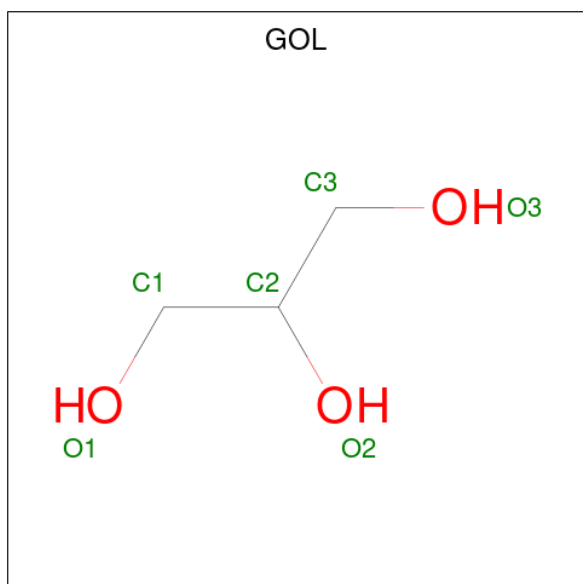
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	12	Total O 12 12	0	0
4	C	5	Total O 5 5	0	0
4	D	7	Total O 7 7	0	0

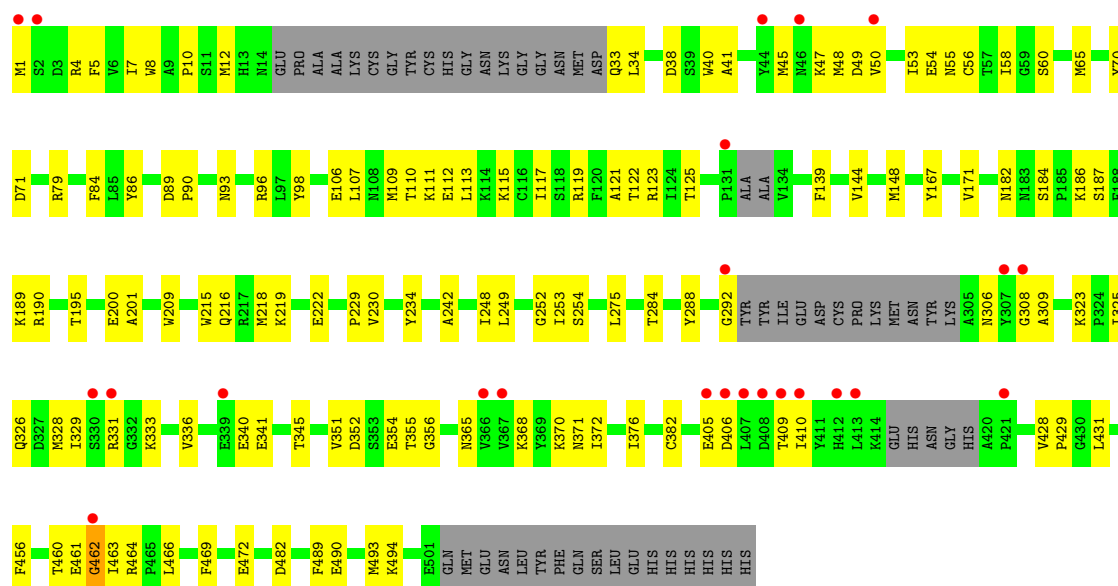
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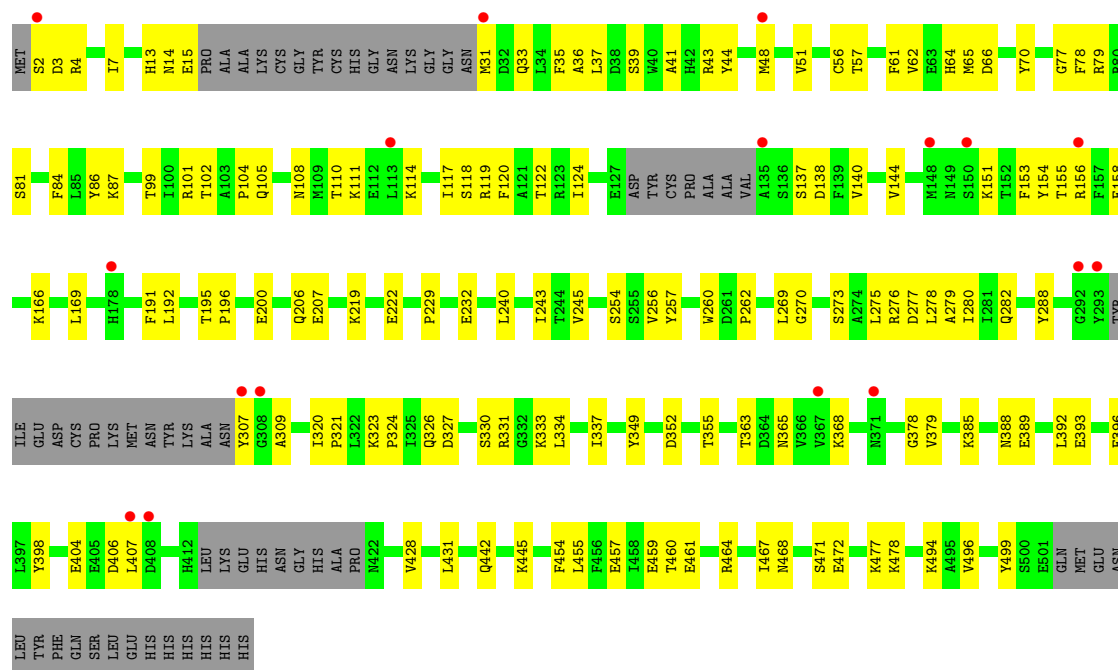
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	9	Total	O	0	0
			9	9		
4	F	5	Total	O	0	0
			5	5		
4	G	7	Total	O	0	0
			7	7		
4	H	3	Total	O	0	0
			3	3		
4	I	2	Total	O	0	0
			2	2		
4	J	2	Total	O	0	0
			2	2		
4	K	5	Total	O	0	0
			5	5		
4	L	2	Total	O	0	0
			2	2		



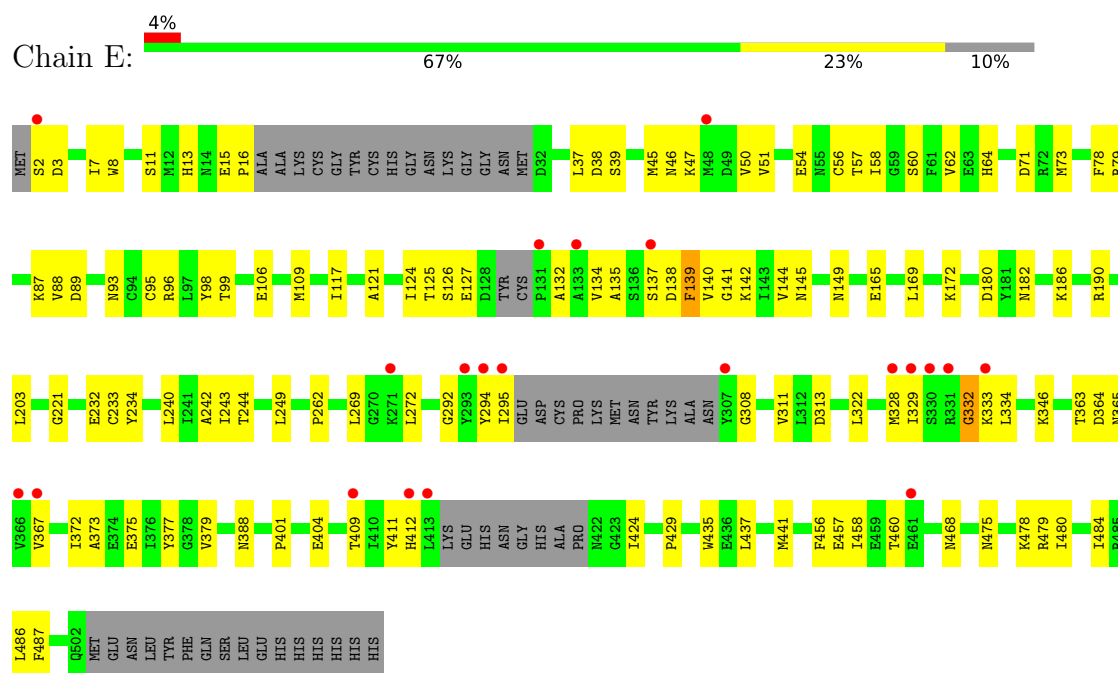
• Molecule 1: Arginyl-tRNA--protein transferase 1



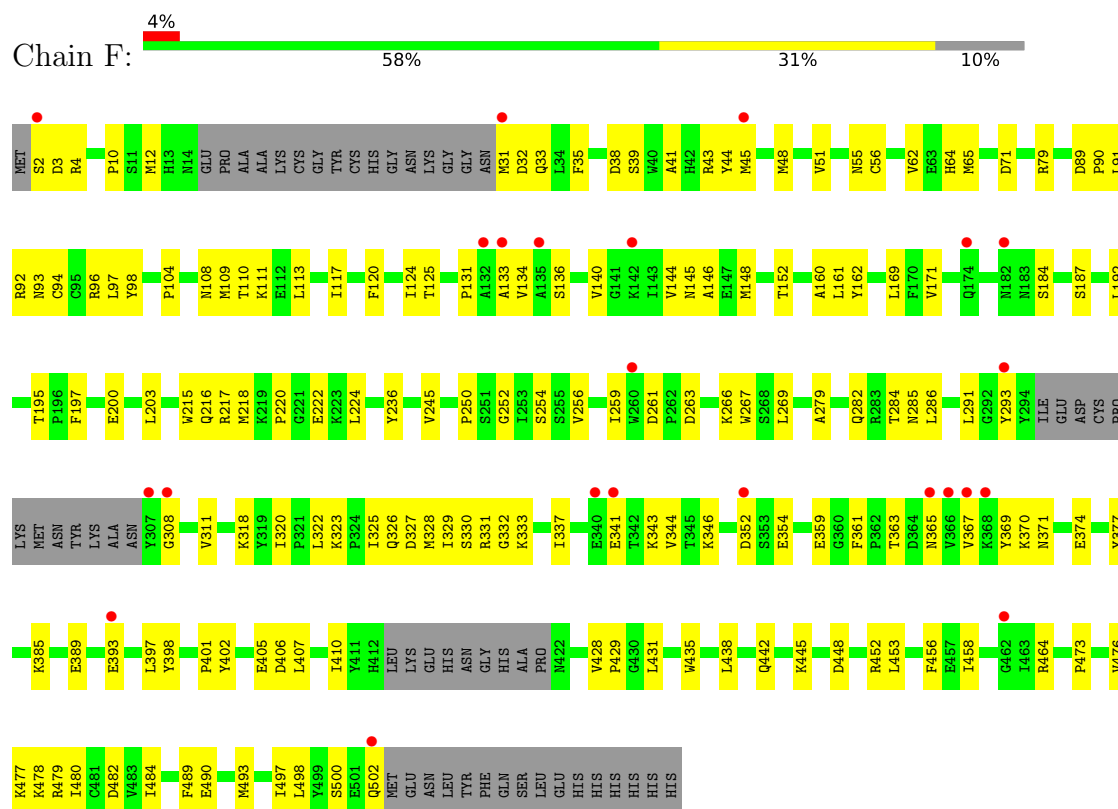
• Molecule 1: Arginyl-tRNA--protein transferase 1



• Molecule 1: Arginyl-tRNA--protein transferase 1

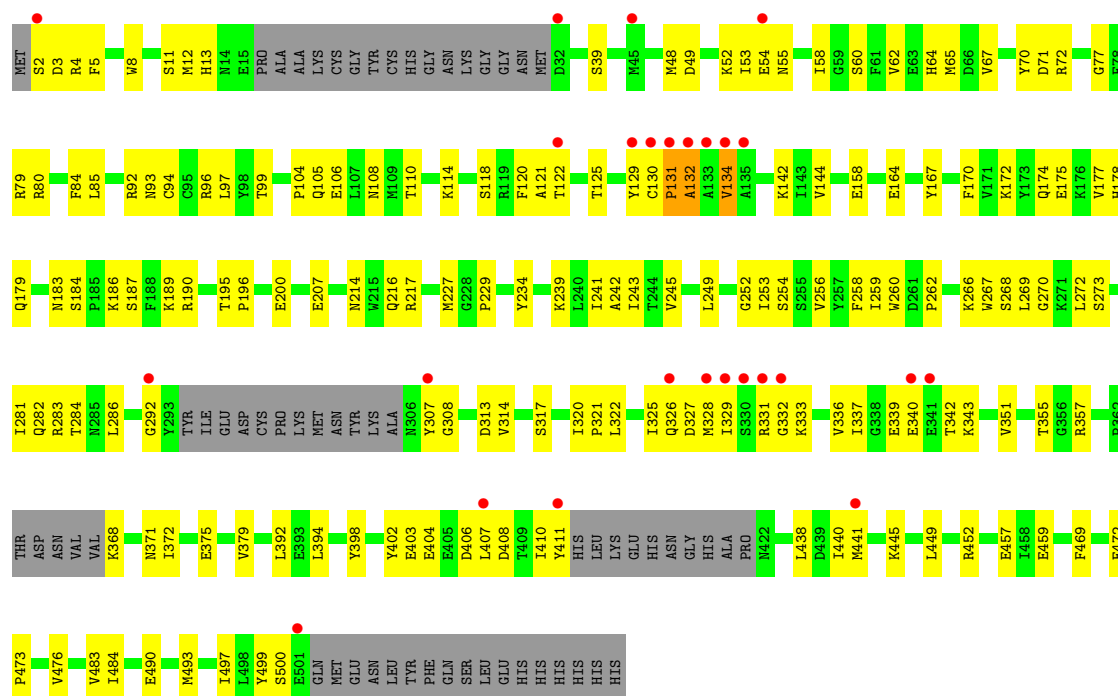


- Molecule 1: Arginyl-tRNA--protein transferase 1

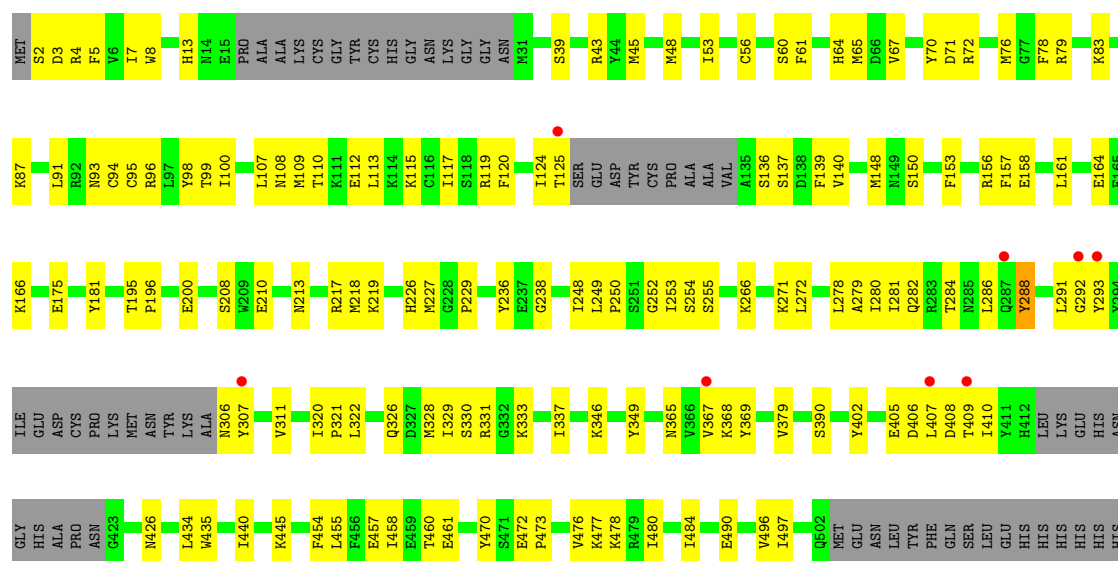


- Molecule 1: Arginyl-tRNA--protein transferase 1

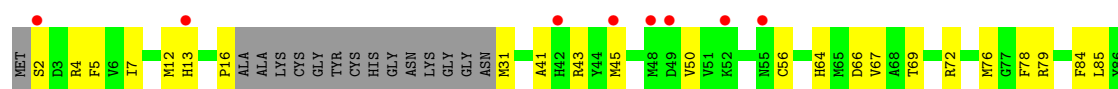


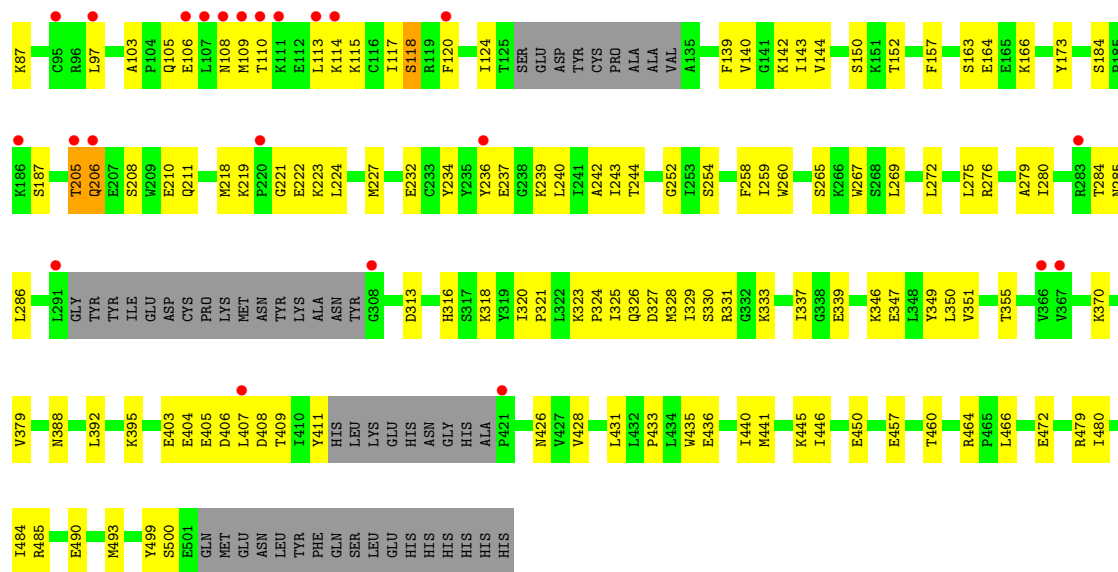


• Molecule 1: Arginyl-tRNA--protein transferase 1

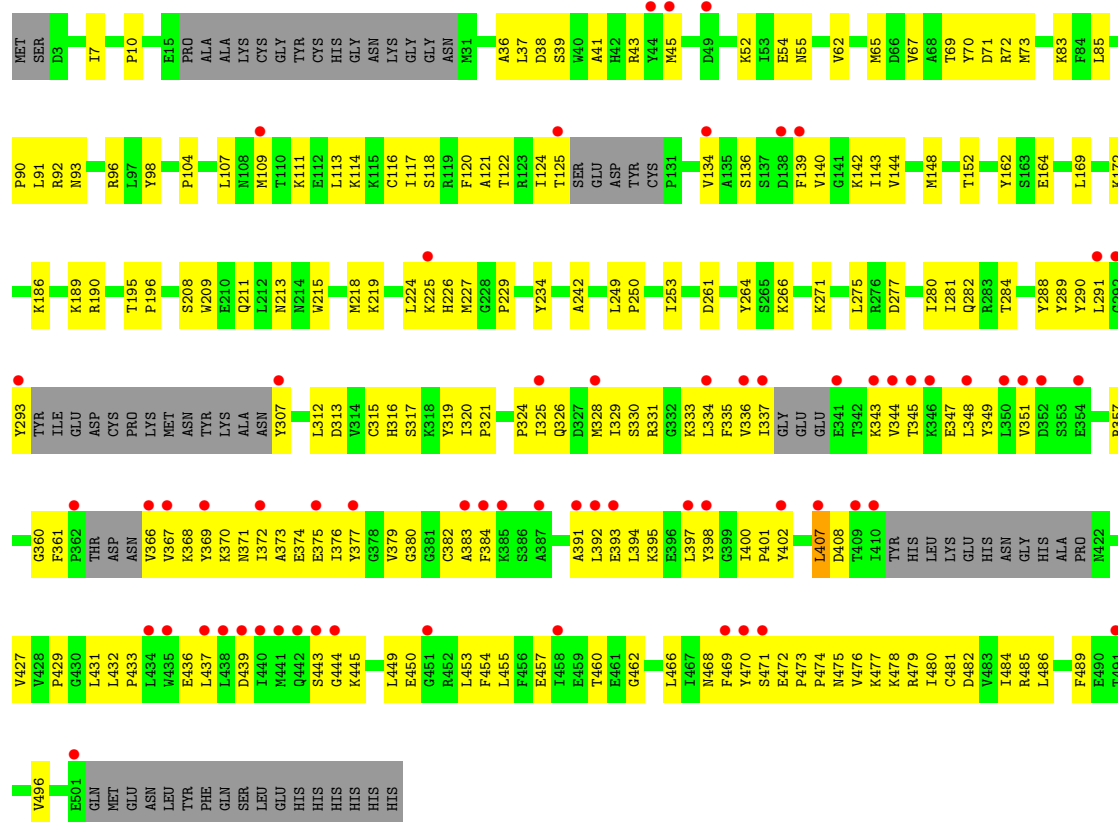


• Molecule 1: Arginyl-tRNA--protein transferase 1



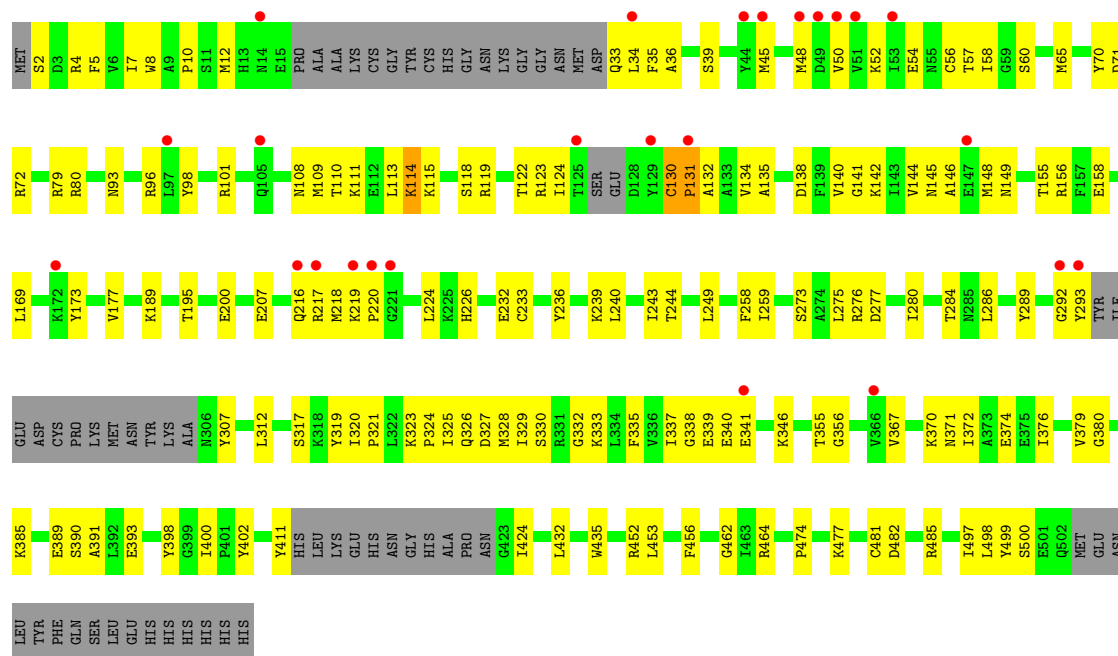


• Molecule 1: Arginyl-tRNA--protein transferase 1



• Molecule 1: Arginyl-tRNA--protein transferase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	235.27Å 235.27Å 171.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.25 – 2.85 65.25 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.25-2.85) 99.8 (65.25-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.200 , 0.257 (Not available) , 0.247	Depositor DCC
R_{free} test set	10893 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 82.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	46039	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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: SO4, GOL

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	0.46	0/3898	0.74	1/5269 (0.0%)
1	B	0.48	0/3867	0.76	2/5226 (0.0%)
1	C	0.51	0/3871	0.79	5/5229 (0.1%)
1	D	0.44	0/3804	0.69	1/5136 (0.0%)
1	E	0.46	0/3875	0.73	2/5236 (0.0%)
1	F	0.47	0/3870	0.70	1/5230 (0.0%)
1	G	0.44	0/3808	0.70	2/5143 (0.0%)
1	H	0.42	0/3811	0.68	1/5146 (0.0%)
1	I	0.44	0/3764	0.77	6/5083 (0.1%)
1	J	0.44	0/3737	0.75	2/5043 (0.0%)
1	K	0.45	0/3823	0.79	5/5165 (0.1%)
1	L	0.47	0/3675	0.84	9/4956 (0.2%)
All	All	0.46	0/45803	0.75	37/61862 (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	L	0	1

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	220	PRO	N-CA-C	11.61	129.57	111.11
1	K	220	PRO	CB-CA-C	-10.74	97.65	111.39
1	C	462	GLY	CA-C-N	8.21	131.81	120.49
1	C	462	GLY	C-N-CA	8.21	131.81	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	205	THR	CA-C-N	8.05	135.53	121.52
1	I	205	THR	C-N-CA	8.05	135.53	121.52
1	I	118	SER	CA-C-N	7.76	131.32	120.29
1	I	118	SER	C-N-CA	7.76	131.32	120.29
1	I	206	GLN	N-CA-C	-7.71	105.04	114.75
1	G	132	ALA	N-CA-C	7.48	126.73	110.80
1	L	221	GLY	CA-C-N	7.33	131.79	121.24
1	L	221	GLY	C-N-CA	7.33	131.79	121.24
1	E	137	SER	N-CA-C	-6.95	95.99	110.80
1	L	467	ILE	CB-CA-C	-6.58	103.46	111.88
1	K	114	LYS	O-C-N	6.44	128.94	122.12
1	A	2	SER	N-CA-C	6.43	121.74	113.18
1	L	467	ILE	O-C-N	6.40	128.34	121.94
1	C	284	THR	N-CA-C	-6.36	102.31	110.19
1	C	284	THR	CA-C-N	-6.25	109.61	121.54
1	C	284	THR	C-N-CA	-6.25	109.61	121.54
1	L	481	CYS	CB-CA-C	-6.19	99.35	110.37
1	D	406	ASP	N-CA-C	6.17	118.13	110.91
1	I	407	LEU	N-CA-C	-6.17	97.66	110.80
1	E	332	GLY	N-CA-C	6.08	123.52	114.95
1	F	405	GLU	N-CA-C	5.86	118.55	110.35
1	J	407	LEU	CA-C-N	-5.76	113.49	122.42
1	J	407	LEU	C-N-CA	-5.76	113.49	122.42
1	L	484	ILE	N-CA-C	-5.70	104.79	111.00
1	L	119	ARG	N-CA-C	-5.63	105.14	111.28
1	K	219	LYS	CA-C-N	5.57	125.57	119.89
1	K	219	LYS	C-N-CA	5.57	125.57	119.89
1	H	288	TYR	CB-CA-C	-5.46	98.06	110.07
1	L	467	ILE	N-CA-C	5.44	116.07	110.36
1	L	321	PRO	O-C-N	-5.43	115.30	122.64
1	B	409	THR	CA-C-N	5.43	127.98	121.84
1	B	409	THR	C-N-CA	5.43	127.98	121.84
1	G	130	CYS	N-CA-C	-5.28	98.15	109.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	104	PRO	Mainchain

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	3800	0	3733	107	2
1	B	3775	0	3707	105	0
1	C	3776	0	3727	125	0
1	D	3715	0	3654	114	0
1	E	3783	0	3722	127	0
1	F	3777	0	3710	137	0
1	G	3718	0	3653	164	0
1	H	3721	0	3660	132	0
1	I	3676	0	3629	138	2
1	J	3651	0	3615	187	0
1	K	3733	0	3675	147	0
1	L	3589	0	3546	210	3
2	A	115	0	0	2	1
2	B	125	0	0	3	0
2	C	115	0	0	6	0
2	D	110	0	0	2	0
2	E	125	0	0	6	0
2	F	65	0	0	1	0
2	G	85	0	0	7	0
2	H	65	0	0	6	0
2	I	65	0	0	5	0
2	J	40	0	0	2	0
2	K	50	0	0	5	0
2	L	55	0	0	9	0
3	A	48	0	64	9	0
3	B	30	0	39	2	0
3	C	18	0	24	0	0
3	D	24	0	32	3	0
3	E	18	0	24	3	0
3	F	12	0	16	2	0
3	G	36	0	48	5	0
3	H	24	0	32	4	0
3	I	6	0	8	0	0
3	J	6	0	8	0	0
3	K	18	0	24	1	0
3	L	6	0	8	0	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	12	0	0	1	0
4	C	5	0	0	0	0
4	D	7	0	0	0	0
4	E	9	0	0	3	0
4	F	5	0	0	0	0
4	G	7	0	0	0	0
4	H	3	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	5	0	0	0	0
4	L	2	0	0	0	0
All	All	46039	0	44358	1623	4

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 18.

All (1623) 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:L:79:ARG:NH1	1:L:292:GLY:HA3	1.21	1.45
1:H:266:LYS:HD2	2:H:601:SO4:O1	1.25	1.35
1:C:189:LYS:NZ	2:C:601:SO4:O1	1.56	1.34
1:L:79:ARG:NH1	1:L:292:GLY:CA	1.93	1.30
1:D:282:GLN:NE2	2:D:609:SO4:O2	1.65	1.29
1:L:432:LEU:HD11	2:L:604:SO4:O2	1.15	1.25
1:K:424:ILE:N	2:K:605:SO4:O1	1.69	1.24
1:L:432:LEU:CD1	2:L:604:SO4:O2	1.86	1.24
1:C:47:LYS:O	1:C:50:VAL:HG12	1.35	1.24
1:D:138:ASP:OD1	2:D:609:SO4:O1	1.57	1.20
1:C:38:ASP:OD2	1:C:331:ARG:NH2	1.72	1.19
1:A:43:ARG:NH2	1:A:409:THR:CG2	2.06	1.19
1:I:103:ALA:HB3	1:I:106:GLU:CG	1.74	1.17
1:I:103:ALA:HB3	1:I:106:GLU:HG2	1.17	1.16
1:E:96:ARG:NE	1:E:332:GLY:O	1.78	1.15
1:A:43:ARG:NH2	1:A:409:THR:HG22	1.66	1.10
1:K:130:CYS:HB3	1:K:131:PRO:HD3	1.23	1.10
1:A:43:ARG:HH21	1:A:409:THR:CG2	1.61	1.10
1:E:15:GLU:HB3	1:E:16:PRO:HD3	1.18	1.10
1:K:130:CYS:HB3	1:K:131:PRO:CD	1.82	1.09
1:H:266:LYS:CD	2:H:601:SO4:O1	2.00	1.09
1:G:129:TYR:CE2	1:G:131:PRO:HD3	1.88	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:156:ARG:NH2	1:K:158:GLU:OE2	1.89	1.05
1:L:79:ARG:HH11	1:L:292:GLY:CA	1.58	1.05
1:G:129:TYR:OH	1:G:131:PRO:HB3	1.57	1.04
1:B:135:ALA:HB2	1:G:132:ALA:HB2	1.40	1.03
1:J:208:SER:HB3	1:J:225:LYS:HD3	1.39	1.03
1:G:266:LYS:HB3	2:G:610:SO4:O3	1.61	1.01
1:C:38:ASP:CG	1:C:331:ARG:NH2	2.19	1.01
1:J:104:PRO:HG2	1:J:282:GLN:HB2	1.44	1.00
1:L:69:THR:HG22	1:L:73:MET:HE1	1.43	1.00
1:G:329:ILE:HD11	1:G:371:ASN:ND2	1.77	0.99
1:J:445:LYS:HB2	1:L:349:TYR:CG	1.98	0.98
1:D:396:GLU:OE1	3:D:625:GOL:H11	1.65	0.97
1:K:130:CYS:CB	1:K:131:PRO:CD	2.42	0.97
1:A:43:ARG:HH21	1:A:409:THR:HG21	1.27	0.96
1:F:393:GLU:HB2	1:F:397:LEU:HD13	1.45	0.96
1:I:43:ARG:NH1	2:I:610:SO4:O2	1.99	0.96
1:J:380:GLY:HA2	1:J:407:LEU:HD21	1.44	0.96
1:G:129:TYR:CE2	1:G:131:PRO:HG3	2.02	0.95
1:F:352:ASP:OD2	1:F:490:GLU:HG3	1.67	0.94
1:L:322:LEU:HA	1:L:325:ILE:CG1	1.97	0.94
1:I:113:LEU:CD2	1:I:275:LEU:HD21	1.97	0.94
1:H:284:THR:HG23	1:H:286:LEU:HG	1.47	0.93
1:L:478:LYS:C	1:L:481:CYS:SG	2.51	0.93
1:C:47:LYS:O	1:C:50:VAL:CG1	2.17	0.92
1:L:478:LYS:HA	1:L:481:CYS:SG	2.09	0.92
1:A:32:ASP:N	1:A:45:MET:HE1	1.84	0.92
1:L:325:ILE:HG23	1:L:328:MET:HE1	1.52	0.91
1:E:47:LYS:NZ	2:E:601:SO4:O3	2.03	0.91
1:B:119:ARG:HH12	1:B:123:ARG:HB2	1.35	0.91
1:E:15:GLU:CB	1:E:16:PRO:HD3	1.97	0.91
1:G:342:THR:O	1:G:343:LYS:HG3	1.71	0.91
1:F:31:MET:N	1:F:48:MET:HE1	1.84	0.91
1:L:478:LYS:O	1:L:481:CYS:SG	2.30	0.90
1:F:96:ARG:HD2	1:F:332:GLY:O	1.72	0.90
1:G:129:TYR:CE2	1:G:131:PRO:CD	2.56	0.89
1:I:325:ILE:HG13	1:I:328:MET:CE	2.01	0.89
1:G:172:LYS:NZ	2:G:608:SO4:O1	2.04	0.89
1:H:148:MET:HE1	1:H:217:ARG:HD3	1.53	0.89
1:G:322:LEU:O	1:G:326:GLN:CB	2.21	0.88
1:I:392:LEU:HD11	1:I:404:GLU:HG3	1.52	0.88
1:J:444:GLY:O	1:L:349:TYR:CE1	2.26	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:TYR:OH	1:G:142:LYS:NZ	2.07	0.88
1:L:104:PRO:HA	1:L:278:LEU:HD22	1.56	0.88
1:F:352:ASP:CG	1:F:490:GLU:HG3	1.99	0.87
1:L:326:GLN:O	1:L:330:SER:OG	1.93	0.87
1:K:317:SER:OG	1:K:355:THR:O	1.92	0.87
1:E:47:LYS:NZ	2:E:601:SO4:S	2.47	0.87
1:I:409:THR:HG23	1:I:411:TYR:H	1.39	0.87
1:J:481:CYS:HA	1:J:484:ILE:HG12	1.54	0.87
1:E:334:LEU:CD2	1:E:373:ALA:HB1	2.05	0.86
1:E:365:ASN:O	1:E:365:ASN:ND2	2.08	0.86
1:K:200:GLU:HG3	1:L:3:ASP:HB3	1.56	0.86
1:B:119:ARG:NH1	1:B:123:ARG:HB2	1.90	0.86
1:E:87:LYS:NZ	4:E:701:HOH:O	2.07	0.86
1:G:129:TYR:CE2	1:G:131:PRO:CG	2.59	0.86
1:J:407:LEU:O	1:J:407:LEU:HG	1.76	0.86
1:K:218:MET:CE	1:K:284:THR:HA	2.05	0.85
1:G:283:ARG:NH2	2:G:617:SO4:O4	2.08	0.85
1:J:343:LYS:HE2	1:J:345:THR:HG22	1.57	0.85
1:I:113:LEU:HD22	1:I:114:LYS:HD2	1.57	0.85
1:K:72:ARG:HG2	1:K:356:GLY:HA3	1.56	0.85
1:A:39:SER:OG	1:A:374:GLU:OE1	1.94	0.84
1:E:73:MET:HE2	1:E:487:PHE:HD1	1.41	0.84
1:D:39:SER:HB3	1:D:379:VAL:HG23	1.58	0.84
1:K:482:ASP:OD2	2:K:605:SO4:O3	1.94	0.84
1:L:394:LEU:HG	1:L:438:LEU:HD13	1.60	0.84
1:K:145:ASN:HA	1:K:148:MET:HB2	1.58	0.83
1:H:67:VAL:HG23	2:H:612:SO4:O3	1.77	0.83
1:H:326:GLN:HG3	1:H:329:ILE:HD11	1.59	0.83
1:G:322:LEU:HG	1:G:326:GLN:HG3	1.60	0.83
1:H:79:ARG:NH2	1:H:254:SER:OG	2.12	0.83
1:B:311:VAL:HG11	1:B:325:ILE:HD11	1.59	0.82
1:E:15:GLU:HB3	1:E:16:PRO:CD	2.08	0.82
1:L:322:LEU:HA	1:L:325:ILE:HG12	1.59	0.82
1:G:129:TYR:HE2	1:G:131:PRO:HG3	1.40	0.82
1:I:113:LEU:HD21	1:I:275:LEU:HD21	1.62	0.82
1:E:47:LYS:NZ	2:E:601:SO4:O2	2.13	0.81
1:A:90:PRO:HG3	3:A:625:GOL:H11	1.62	0.81
1:I:323:LYS:HA	1:I:326:GLN:HB2	1.60	0.81
1:C:119:ARG:HA	1:C:122:THR:HG23	1.62	0.81
1:L:79:ARG:NH1	1:L:292:GLY:N	2.27	0.81
1:B:135:ALA:CB	1:G:132:ALA:HB2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:232:GLU:OE2	1:I:276:ARG:NH1	2.14	0.81
1:H:266:LYS:CE	2:H:601:SO4:O1	2.29	0.80
1:K:232:GLU:OE1	1:K:276:ARG:NH2	2.14	0.80
1:J:328:MET:SD	1:J:371:ASN:ND2	2.54	0.80
1:G:129:TYR:CD2	1:G:131:PRO:HD3	2.15	0.80
1:C:38:ASP:OD1	1:C:331:ARG:NH2	2.14	0.80
1:I:113:LEU:HD11	1:I:275:LEU:HD11	1.62	0.80
1:A:314:VAL:HG11	3:A:625:GOL:H12	1.63	0.80
1:L:393:GLU:HG3	1:L:397:LEU:HD12	1.61	0.80
1:G:402:TYR:O	1:G:403:GLU:HG3	1.82	0.80
1:B:133:ALA:O	1:F:134:VAL:HG21	1.83	0.79
1:E:38:ASP:OD1	1:E:333:LYS:NZ	2.15	0.79
1:D:206:GLN:OE1	1:G:452:ARG:NH2	2.15	0.79
1:E:51:VAL:HG13	1:E:412:HIS:O	1.82	0.79
1:E:96:ARG:CD	1:E:332:GLY:O	2.30	0.79
1:H:108:ASN:HB2	1:H:307:TYR:HD2	1.47	0.79
1:E:311:VAL:HG11	1:E:329:ILE:HD11	1.62	0.79
1:K:156:ARG:HH12	1:K:158:GLU:HG3	1.46	0.79
1:J:65:MET:HE1	1:J:85:LEU:HD22	1.65	0.78
1:F:341:GLU:O	1:F:341:GLU:CD	2.26	0.78
1:H:320:ILE:HD12	1:H:321:PRO:HD2	1.64	0.78
1:I:110:THR:H	1:I:114:LYS:NZ	1.82	0.78
1:J:445:LYS:HD2	1:L:349:TYR:CD2	2.19	0.78
1:C:123:ARG:NH2	2:C:604:SO4:O3	2.17	0.77
1:F:184:SER:H	1:F:187:SER:HB3	1.47	0.77
1:J:439:ASP:O	1:J:443:SER:HB3	1.83	0.77
1:L:322:LEU:HA	1:L:325:ILE:HG13	1.66	0.77
1:L:277:ASP:HA	1:L:280:ILE:HD12	1.65	0.77
1:D:388:ASN:HB3	1:D:404:GLU:HG2	1.65	0.77
1:B:331:ARG:HH11	1:B:333:LYS:HE3	1.48	0.77
1:D:320:ILE:HG13	1:D:321:PRO:HD2	1.66	0.77
1:G:322:LEU:CG	1:G:326:GLN:HG3	2.14	0.77
1:L:478:LYS:CA	1:L:481:CYS:SG	2.72	0.77
1:D:65:MET:HE3	1:D:70:TYR:HB2	1.67	0.77
1:K:45:MET:HG2	1:K:48:MET:SD	2.24	0.77
1:I:113:LEU:HD22	1:I:114:LYS:CD	2.14	0.77
1:G:12:MET:HE3	1:G:58:ILE:HG12	1.67	0.77
1:G:129:TYR:OH	1:G:131:PRO:CB	2.32	0.77
1:G:325:ILE:HG23	1:G:329:ILE:HG21	1.67	0.77
1:E:109:MET:HE2	1:E:139:PHE:HB3	1.66	0.76
1:K:115:LYS:HG3	1:K:118:SER:HB3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ARG:HH21	1:C:333:LYS:CD	1.99	0.76
1:L:481:CYS:O	1:L:485:ARG:HG3	1.86	0.76
1:J:71:ASP:HA	1:J:249:LEU:HD13	1.68	0.76
1:J:380:GLY:CA	1:J:407:LEU:HD21	2.15	0.76
1:K:340:GLU:HA	1:K:370:LYS:HE2	1.67	0.76
1:H:108:ASN:HB2	1:H:307:TYR:CD2	2.21	0.76
1:J:384:PHE:CD2	1:J:407:LEU:HD13	2.21	0.76
1:I:103:ALA:HB3	1:I:106:GLU:HG3	1.64	0.75
1:J:344:VAL:HG13	1:L:442:GLN:OE1	1.86	0.75
1:K:115:LYS:HG2	1:K:118:SER:OG	1.87	0.75
1:I:110:THR:H	1:I:114:LYS:HZ3	1.32	0.75
1:L:383:ALA:HB1	1:L:427:VAL:HG11	1.67	0.75
1:I:103:ALA:CB	1:I:106:GLU:HG2	2.09	0.75
1:F:195:THR:HG22	1:F:197:PHE:H	1.51	0.75
1:L:124:ILE:O	1:L:150:SER:OG	2.03	0.74
1:L:79:ARG:HH12	1:L:292:GLY:H	1.33	0.74
1:G:129:TYR:CZ	1:G:131:PRO:HB3	2.21	0.74
1:G:322:LEU:HD12	1:G:326:GLN:HB2	1.69	0.74
1:G:490:GLU:HA	1:G:493:MET:HE2	1.70	0.74
1:J:343:LYS:HG2	1:J:344:VAL:N	2.02	0.74
1:D:13:HIS:O	1:D:56:CYS:HB2	1.87	0.74
1:E:334:LEU:C	1:E:334:LEU:HD23	2.13	0.74
1:F:43:ARG:HE	1:F:44:TYR:HE1	1.32	0.74
1:G:243:ILE:HD12	1:G:259:ILE:HD11	1.70	0.74
1:G:322:LEU:CD1	1:G:326:GLN:HB2	2.18	0.74
1:G:329:ILE:HD11	1:G:371:ASN:HD22	1.50	0.73
1:L:113:LEU:N	1:L:113:LEU:HD23	2.02	0.73
1:A:226:HIS:HA	3:A:631:GOL:O2	1.88	0.73
1:A:311:VAL:HG11	1:A:325:ILE:HD11	1.69	0.73
1:J:208:SER:HB3	1:J:225:LYS:CD	2.18	0.73
1:L:403:GLU:HG2	1:L:404:GLU:H	1.53	0.73
1:E:486:LEU:HD23	1:E:487:PHE:CE2	2.23	0.73
1:K:115:LYS:CG	1:K:118:SER:HB3	2.19	0.73
1:D:43:ARG:NH2	1:D:44:TYR:OH	2.21	0.73
1:G:322:LEU:O	1:G:326:GLN:HB2	1.89	0.73
1:I:450:GLU:HG2	1:I:466:LEU:CD1	2.19	0.73
1:K:277:ASP:HA	1:K:280:ILE:HD12	1.70	0.73
1:G:322:LEU:O	1:G:326:GLN:HB3	1.88	0.73
1:L:79:ARG:HH11	1:L:292:GLY:HA3	0.66	0.73
1:D:77:GLY:HA2	1:D:99:THR:HG21	1.69	0.72
1:D:327:ASP:HA	1:D:330:SER:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:156:ARG:NH1	1:K:158:GLU:HG3	2.04	0.72
1:G:325:ILE:HG23	1:G:329:ILE:CG2	2.19	0.72
1:K:144:VAL:HG13	1:K:216:GLN:HG2	1.69	0.72
1:D:108:ASN:HB2	1:D:307:TYR:HB3	1.71	0.72
1:I:325:ILE:HG13	1:I:328:MET:HE1	1.69	0.72
1:C:109:MET:HE3	1:C:113:LEU:C	2.14	0.72
1:H:248:ILE:HG12	1:H:253:ILE:HD13	1.70	0.72
1:I:379:VAL:O	2:I:611:SO4:O4	2.07	0.72
1:J:375:GLU:O	1:J:382:CYS:N	2.22	0.72
1:L:102:THR:HG23	1:L:309:ALA:HB2	1.71	0.72
1:J:393:GLU:O	1:J:397:LEU:HB2	1.90	0.71
1:L:245:VAL:HG23	1:L:256:VAL:HB	1.69	0.71
1:E:51:VAL:CG1	1:E:412:HIS:O	2.37	0.71
1:H:408:ASP:OD1	1:H:409:THR:N	2.21	0.71
1:A:39:SER:HB3	1:A:379:VAL:HG23	1.71	0.71
1:A:204:GLY:HA2	3:A:631:GOL:H32	1.73	0.71
1:K:140:VAL:O	1:K:144:VAL:HG23	1.89	0.71
1:C:41:ALA:O	1:C:45:MET:HB2	1.90	0.71
1:B:148:MET:HE3	1:B:217:ARG:HH11	1.54	0.71
1:I:113:LEU:HD23	1:I:275:LEU:HD21	1.71	0.71
1:K:113:LEU:HD22	1:K:275:LEU:HD11	1.73	0.71
1:G:322:LEU:HG	1:G:326:GLN:CG	2.19	0.71
1:C:490:GLU:HA	1:C:493:MET:HE3	1.72	0.71
1:H:140:VAL:HG11	1:H:282:GLN:OE1	1.91	0.71
1:B:366:VAL:HG21	1:D:467:ILE:HG21	1.71	0.70
1:J:92:ARG:NH2	1:J:427:VAL:HG23	2.06	0.70
1:J:266:LYS:HB3	2:J:603:SO4:O2	1.91	0.70
1:L:79:ARG:HH12	1:L:292:GLY:N	1.88	0.70
1:B:346:LYS:HD3	2:B:610:SO4:O2	1.91	0.70
1:E:78:PHE:CE2	1:E:486:LEU:HD11	2.26	0.70
1:H:284:THR:CG2	1:H:286:LEU:HG	2.21	0.70
1:J:93:ASN:O	1:J:96:ARG:NH1	2.22	0.70
1:L:79:ARG:CZ	1:L:292:GLY:HA3	2.17	0.70
1:E:8:TRP:HH2	1:E:458:ILE:HD13	1.57	0.70
1:F:134:VAL:HG12	1:F:136:SER:OG	1.91	0.70
1:L:479:ARG:NH1	2:L:602:SO4:O2	2.25	0.70
1:C:463:ILE:HD12	1:C:463:ILE:H	1.56	0.70
1:D:320:ILE:HD13	1:D:337:ILE:HD12	1.74	0.70
1:F:55:ASN:ND2	1:F:94:CYS:SG	2.61	0.70
1:K:115:LYS:HG2	1:K:115:LYS:O	1.92	0.70
1:G:77:GLY:HA2	1:G:99:THR:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:LEU:HD21	1:D:334:LEU:HD23	1.73	0.69
1:J:140:VAL:O	1:J:144:VAL:HG23	1.92	0.69
1:K:33:GLN:HG3	1:K:34:LEU:H	1.55	0.69
1:A:111:LYS:O	1:A:115:LYS:HG3	1.92	0.69
1:J:67:VAL:HG21	1:J:227:MET:HB3	1.75	0.69
1:J:124:ILE:HD12	1:J:125:THR:N	2.08	0.69
1:G:322:LEU:HG	1:G:326:GLN:CB	2.21	0.69
1:I:184:SER:OG	1:I:187:SER:N	2.22	0.69
1:A:51:VAL:HG21	1:A:411:TYR:HB3	1.75	0.69
1:A:388:ASN:HB3	1:A:404:GLU:HG2	1.75	0.69
1:D:277:ASP:HA	1:D:280:ILE:HD12	1.74	0.69
1:L:325:ILE:HG23	1:L:328:MET:CE	2.22	0.69
1:B:45:MET:HA	1:B:48:MET:HE2	1.75	0.68
1:J:432:LEU:HB2	1:J:485:ARG:HA	1.75	0.68
1:B:316:HIS:O	3:B:628:GOL:O2	2.11	0.68
1:C:308:GLY:HA2	1:C:323:LYS:HE2	1.76	0.68
1:I:240:LEU:HD21	1:I:243:ILE:HD11	1.76	0.68
1:F:96:ARG:CD	1:F:332:GLY:O	2.40	0.68
1:J:234:TYR:HB2	1:J:242:ALA:HB3	1.75	0.68
1:C:90:PRO:HG2	1:C:429:PRO:HG2	1.74	0.68
1:G:270:GLY:H	3:G:621:GOL:H2	1.58	0.68
1:J:134:VAL:HG21	1:J:142:LYS:HE2	1.76	0.68
1:C:8:TRP:O	1:C:60:SER:OG	2.11	0.68
1:K:218:MET:HE2	1:K:284:THR:HA	1.75	0.68
1:A:109:MET:HE2	1:A:139:PHE:HB3	1.76	0.68
1:H:164:GLU:HG2	3:H:617:GOL:H31	1.76	0.68
1:G:329:ILE:CD1	1:G:371:ASN:HD22	2.07	0.67
1:G:52:LYS:HE2	1:G:54:GLU:HG2	1.76	0.67
1:C:308:GLY:CA	1:C:323:LYS:HE2	2.24	0.67
1:F:320:ILE:HG23	1:F:361:PHE:CD1	2.30	0.67
1:G:184:SER:HB3	1:G:187:SER:H	1.58	0.67
1:J:343:LYS:HG2	1:J:344:VAL:H	1.60	0.67
1:A:339:GLU:HB2	3:A:629:GOL:H31	1.75	0.66
1:D:14:ASN:N	1:D:14:ASN:HD22	1.93	0.66
1:H:3:ASP:OD2	1:H:64:HIS:NE2	2.28	0.66
1:D:110:THR:HG22	1:D:111:LYS:N	2.11	0.66
1:C:112:GLU:HA	1:C:115:LYS:HD3	1.76	0.66
1:G:342:THR:O	1:G:343:LYS:CG	2.42	0.66
1:L:58:ILE:HG22	1:L:486:LEU:HD21	1.77	0.66
1:C:331:ARG:O	1:C:331:ARG:HG2	1.95	0.66
1:C:406:ASP:O	1:C:409:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:GLU:HB3	3:E:627:GOL:H32	1.78	0.66
1:L:36:ALA:O	1:L:334:LEU:N	2.24	0.66
1:D:119:ARG:O	1:D:122:THR:OG1	2.11	0.66
1:H:140:VAL:HG12	1:H:279:ALA:HA	1.77	0.66
1:J:347:GLU:HG3	1:J:383:ALA:HB1	1.78	0.66
1:J:445:LYS:HA	1:L:349:TYR:CZ	2.31	0.66
1:E:132:ALA:O	1:E:134:VAL:HG13	1.96	0.66
1:J:124:ILE:O	1:J:152:THR:OG1	2.13	0.66
1:K:244:THR:HG22	1:K:258:PHE:CD1	2.31	0.66
1:A:8:TRP:O	1:A:60:SER:OG	2.14	0.66
1:L:309:ALA:O	1:L:322:LEU:HG	1.95	0.66
1:I:218:MET:HE2	1:I:284:THR:HA	1.78	0.65
1:L:457:GLU:HB3	1:L:460:THR:HG23	1.77	0.65
1:A:342:THR:HB	2:A:608:SO4:O3	1.96	0.65
1:C:331:ARG:HH21	1:C:333:LYS:HD3	1.60	0.65
1:J:320:ILE:HG21	1:J:337:ILE:HD11	1.77	0.65
1:J:349:TYR:CE1	1:J:436:GLU:HG2	2.32	0.65
1:F:320:ILE:HD13	1:F:337:ILE:HD11	1.79	0.65
1:K:130:CYS:CB	1:K:131:PRO:HD2	2.24	0.65
1:J:266:LYS:CB	2:J:603:SO4:O2	2.44	0.65
1:L:172:LYS:NZ	2:L:611:SO4:O4	2.30	0.65
1:G:96:ARG:NE	1:G:332:GLY:O	2.29	0.65
1:D:15:GLU:HB3	1:D:57:THR:HG23	1.79	0.65
1:G:329:ILE:CD1	1:G:371:ASN:ND2	2.58	0.65
1:I:244:THR:HG22	1:I:258:PHE:CD1	2.31	0.65
1:J:39:SER:OG	1:J:379:VAL:HG23	1.96	0.65
1:L:350:LEU:HD12	1:L:433:PRO:HD3	1.77	0.65
1:B:370:LYS:HD3	1:B:371:ASN:H	1.61	0.65
1:L:398:TYR:OH	1:L:442:GLN:HB3	1.96	0.65
1:L:432:LEU:HD12	2:L:604:SO4:O2	1.93	0.65
1:L:39:SER:OG	1:L:374:GLU:HG3	1.97	0.65
1:G:65:MET:SD	1:G:70:TYR:HB2	2.37	0.65
1:J:208:SER:CB	1:J:225:LYS:HD3	2.22	0.65
1:E:87:LYS:CE	4:E:701:HOH:O	2.44	0.64
1:E:96:ARG:HD2	1:E:332:GLY:O	1.97	0.64
1:F:38:ASP:OD1	1:F:331:ARG:NH2	2.30	0.64
1:L:93:ASN:C	1:L:96:ARG:HH12	2.04	0.64
1:E:11:SER:OG	1:E:13:HIS:NE2	2.30	0.64
1:G:65:MET:HE1	1:G:85:LEU:HD22	1.79	0.64
1:E:78:PHE:HZ	1:E:486:LEU:CD1	2.11	0.64
1:K:39:SER:HB3	1:K:379:VAL:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:106:GLU:O	1:L:106:GLU:HG2	1.96	0.64
1:B:78:PHE:CE2	1:B:87:LYS:HD2	2.33	0.64
1:J:444:GLY:O	1:L:349:TYR:HE1	1.80	0.64
1:I:223:LYS:HD2	1:I:285:ASN:HB2	1.79	0.64
1:L:403:GLU:HG2	1:L:404:GLU:N	2.11	0.64
1:E:221:GLY:C	2:E:612:SO4:O3	2.41	0.64
1:J:401:PRO:HD2	1:J:478:LYS:HB2	1.79	0.64
1:D:352:ASP:OD2	1:D:445:LYS:NZ	2.32	0.63
1:J:367:VAL:HG22	1:L:468:ASN:HD21	1.63	0.63
1:J:445:LYS:HB2	1:L:349:TYR:CD2	2.33	0.63
1:J:344:VAL:HG11	1:J:348:LEU:CD2	2.28	0.63
1:J:139:PHE:O	1:J:143:ILE:HG13	1.97	0.63
1:E:132:ALA:O	1:E:134:VAL:CG1	2.46	0.63
1:I:244:THR:HG22	1:I:258:PHE:HD1	1.64	0.63
1:K:217:ARG:HG2	1:K:217:ARG:O	1.98	0.63
1:L:205:THR:HG23	1:L:208:SER:H	1.63	0.63
1:I:237:GLU:O	1:I:239:LYS:HG2	1.99	0.63
1:K:79:ARG:HD2	1:K:292:GLY:HA3	1.80	0.63
1:C:336:VAL:HG23	1:C:372:ILE:HG13	1.80	0.63
1:D:110:THR:HG22	1:D:111:LYS:H	1.64	0.63
1:E:180:ASP:OD1	1:E:182:ASN:HB2	1.98	0.63
1:D:3:ASP:HB2	1:G:200:GLU:CD	2.22	0.63
1:G:457:GLU:HG3	1:G:499:TYR:CE1	2.33	0.63
1:H:65:MET:HE3	1:H:70:TYR:HB2	1.81	0.63
1:H:406:ASP:HB3	1:H:408:ASP:OD1	1.99	0.63
1:K:156:ARG:HH22	1:K:158:GLU:CD	2.01	0.63
1:K:239:LYS:HE2	3:K:611:GOL:H12	1.81	0.63
1:C:323:LYS:O	1:C:326:GLN:HB3	1.99	0.63
1:J:349:TYR:HE1	1:J:436:GLU:HG2	1.64	0.63
1:C:98:TYR:OH	1:C:333:LYS:O	2.17	0.63
1:E:334:LEU:HD21	1:E:373:ALA:HB1	1.78	0.63
1:D:118:SER:O	1:D:122:THR:HG23	1.99	0.62
1:E:363:THR:OG1	1:H:210:GLU:OE1	2.12	0.62
1:F:140:VAL:HG22	1:F:279:ALA:HA	1.80	0.62
1:J:384:PHE:CG	1:J:407:LEU:HD13	2.34	0.62
1:B:449:LEU:HD23	1:B:493:MET:HG3	1.81	0.62
1:C:184:SER:H	1:C:187:SER:HB3	1.63	0.62
1:H:100:ILE:HD13	1:H:311:VAL:HG22	1.80	0.62
1:H:108:ASN:HB3	1:H:306:ASN:HB3	1.79	0.62
1:J:172:LYS:NZ	1:J:261:ASP:OD1	2.33	0.62
1:K:464:ARG:NH2	1:K:499:TYR:OH	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:THR:HG22	1:C:462:GLY:H	1.65	0.62
1:L:76:MET:HE3	2:L:604:SO4:O4	1.98	0.62
1:J:468:ASN:ND2	1:L:341:GLU:OE1	2.32	0.62
1:D:330:SER:OG	1:D:331:ARG:N	2.33	0.62
1:E:78:PHE:CZ	1:E:486:LEU:CD1	2.82	0.62
1:F:111:LYS:H	1:F:111:LYS:HD2	1.65	0.62
1:I:428:VAL:HB	1:I:431:LEU:HD22	1.82	0.62
1:L:195:THR:HG21	1:L:229:PRO:HG3	1.81	0.62
1:D:117:ILE:HD11	1:D:275:LEU:HD13	1.82	0.62
1:F:3:ASP:HB2	1:H:200:GLU:CD	2.25	0.62
1:I:388:ASN:O	1:I:392:LEU:HD12	1.99	0.62
1:D:407:LEU:N	1:D:407:LEU:HD12	2.15	0.62
1:L:93:ASN:O	1:L:96:ARG:NH1	2.30	0.62
1:A:1:MET:H2	1:C:200:GLU:H	1.46	0.62
1:B:388:ASN:HD22	1:B:407:LEU:HD21	1.65	0.62
1:E:38:ASP:OD1	1:E:333:LYS:CE	2.48	0.62
1:D:105:GLN:O	1:D:105:GLN:HG2	2.00	0.61
1:B:388:ASN:ND2	1:B:407:LEU:HD21	2.15	0.61
1:J:124:ILE:HD12	1:J:125:THR:H	1.64	0.61
1:C:48:MET:HG3	1:C:49:ASP:N	2.15	0.61
1:L:113:LEU:HD23	1:L:113:LEU:H	1.65	0.61
1:D:140:VAL:HG22	1:D:279:ALA:HA	1.83	0.61
1:F:35:PHE:HE1	1:F:48:MET:HE2	1.63	0.61
1:I:234:TYR:HB2	1:I:242:ALA:HB3	1.81	0.61
1:A:186:LYS:HE2	1:A:190:ARG:NH1	2.14	0.61
1:K:115:LYS:HG2	1:K:118:SER:CB	2.31	0.61
1:L:468:ASN:HB2	1:L:471:SER:OG	2.01	0.61
1:A:428:VAL:HB	1:A:431:LEU:HD22	1.81	0.61
1:B:463:ILE:HD11	1:E:203:LEU:HD21	1.82	0.61
1:J:439:ASP:O	1:J:443:SER:CB	2.48	0.61
1:C:56:CYS:N	1:C:93:ASN:OD1	2.33	0.61
1:D:14:ASN:N	1:D:14:ASN:ND2	2.48	0.61
1:B:135:ALA:H	1:G:132:ALA:HB2	1.65	0.61
1:I:206:GLN:O	1:I:210:GLU:HG3	2.01	0.61
1:E:232:GLU:HB3	1:E:244:THR:HG23	1.82	0.61
1:I:105:GLN:HG3	1:I:105:GLN:O	1.99	0.61
1:J:344:VAL:HG11	1:J:348:LEU:HD21	1.83	0.61
1:K:243:ILE:HD12	1:K:259:ILE:HD11	1.83	0.61
1:C:323:LYS:HA	1:C:326:GLN:HB2	1.82	0.61
1:C:351:VAL:HG13	1:C:354:GLU:HB2	1.82	0.61
1:E:334:LEU:CD2	1:E:373:ALA:CB	2.77	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:479:ARG:NH2	1:F:502:GLN:HA	2.16	0.61
1:H:78:PHE:CE1	1:H:87:LYS:HD2	2.36	0.61
1:J:144:VAL:O	1:J:148:MET:N	2.33	0.61
1:J:391:ALA:HB1	1:J:402:TYR:HB3	1.83	0.61
1:D:232:GLU:OE1	1:D:276:ARG:NH1	2.33	0.60
1:F:325:ILE:HB	1:F:328:MET:HE3	1.82	0.60
1:G:284:THR:HG23	1:G:286:LEU:HG	1.82	0.60
1:H:140:VAL:HG21	1:H:282:GLN:OE1	2.01	0.60
1:L:101:ARG:HG3	1:L:288:TYR:HB3	1.83	0.60
1:A:87:LYS:HE2	3:A:625:GOL:H2	1.82	0.60
1:D:2:SER:OG	1:D:64:HIS:NE2	2.29	0.60
1:E:486:LEU:CD2	1:E:487:PHE:CZ	2.83	0.60
1:H:164:GLU:CG	3:H:617:GOL:H31	2.32	0.60
1:B:111:LYS:H	1:B:111:LYS:HE2	1.66	0.60
1:E:79:ARG:NH1	4:E:702:HOH:O	2.33	0.60
1:E:134:VAL:HG21	1:E:142:LYS:HZ1	1.66	0.60
1:F:393:GLU:CB	1:F:397:LEU:HD13	2.25	0.60
1:H:125:THR:HB	1:H:150:SER:HB2	1.83	0.60
1:J:460:THR:HG23	1:J:462:GLY:H	1.65	0.60
1:A:32:ASP:N	1:A:45:MET:CE	2.63	0.60
1:C:167:TYR:O	1:C:171:VAL:HG12	2.01	0.60
1:C:190:ARG:NH1	2:C:601:SO4:O3	2.34	0.60
1:G:336:VAL:HG23	1:G:372:ILE:HG13	1.83	0.60
1:I:113:LEU:CD2	1:I:114:LYS:HD2	2.30	0.60
1:J:351:VAL:HG21	1:L:445:LYS:HD2	1.84	0.60
1:J:445:LYS:HA	1:L:349:TYR:CE1	2.37	0.60
1:C:328:MET:HE2	1:C:371:ASN:ND2	2.17	0.60
1:A:320:ILE:HD12	1:A:321:PRO:HD2	1.83	0.60
1:D:78:PHE:CE1	1:D:87:LYS:HD2	2.37	0.60
1:G:134:VAL:HG12	1:G:134:VAL:O	2.01	0.60
1:J:431:LEU:HD22	1:J:486:LEU:HA	1.83	0.60
1:H:8:TRP:CH2	1:H:458:ILE:HG21	2.36	0.60
1:K:80:ARG:HH12	1:K:195:THR:HG22	1.67	0.60
1:C:325:ILE:HG23	1:C:325:ILE:O	2.02	0.60
1:C:489:PHE:CD2	1:C:493:MET:HE2	2.37	0.60
1:F:352:ASP:OD1	1:F:490:GLU:HG3	2.02	0.60
1:H:112:GLU:CD	1:H:271:LYS:NZ	2.59	0.60
1:H:227:MET:HE1	1:H:250:PRO:CD	2.31	0.60
1:J:313:ASP:O	1:J:317:SER:N	2.35	0.60
1:L:209:TRP:CH2	1:L:230:VAL:HG12	2.37	0.60
1:F:35:PHE:CE1	1:F:48:MET:HE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:TYR:HD1	1:G:326:GLN:NE2	1.99	0.59
1:D:192:LEU:HD11	1:D:257:TYR:HD2	1.67	0.59
1:F:445:LYS:HA	3:F:615:GOL:H32	1.84	0.59
1:H:405:GLU:OE2	1:H:426:ASN:N	2.20	0.59
1:K:80:ARG:NH1	1:K:195:THR:HG22	2.18	0.59
1:L:320:ILE:HD12	1:L:321:PRO:HD2	1.83	0.59
1:D:363:THR:C	1:D:365:ASN:H	2.09	0.59
1:E:2:SER:N	1:E:64:HIS:HE2	2.00	0.59
1:F:2:SER:HA	1:F:64:HIS:NE2	2.17	0.59
1:H:117:ILE:O	1:H:120:PHE:HB3	2.02	0.59
1:H:252:GLY:HA2	1:H:286:LEU:HB3	1.83	0.59
1:B:39:SER:HB3	1:B:379:VAL:HG13	1.83	0.59
1:F:10:PRO:HG2	1:F:482:ASP:HB3	1.84	0.59
1:H:79:ARG:NH1	1:H:255:SER:O	2.36	0.59
1:L:112:GLU:CD	1:L:112:GLU:H	2.08	0.59
1:A:403:GLU:OE1	1:A:403:GLU:HA	2.03	0.59
1:G:195:THR:HG21	1:G:229:PRO:HG3	1.84	0.59
1:I:78:PHE:CE1	1:I:87:LYS:HD2	2.37	0.59
1:K:244:THR:HG22	1:K:258:PHE:CE1	2.38	0.59
1:E:78:PHE:CZ	1:E:486:LEU:HD11	2.37	0.59
1:E:468:ASN:OD1	1:F:367:VAL:HG21	2.02	0.59
1:J:37:LEU:HB3	1:J:374:GLU:OE1	2.02	0.59
1:K:98:TYR:OH	1:K:333:LYS:O	2.13	0.59
1:E:121:ALA:O	1:E:125:THR:HG22	2.03	0.59
1:E:172:LYS:HE2	1:E:262:PRO:HD2	1.84	0.59
1:G:214:ASN:OD1	1:G:217:ARG:HD2	2.02	0.59
1:I:440:ILE:HD13	1:I:445:LYS:HD3	1.84	0.59
1:L:374:GLU:HG2	1:L:378:GLY:HA3	1.83	0.59
1:K:110:THR:HG22	1:K:113:LEU:HD12	1.85	0.59
1:K:115:LYS:CG	1:K:118:SER:CB	2.80	0.59
1:G:325:ILE:O	1:G:325:ILE:HG22	2.02	0.59
1:H:112:GLU:OE1	1:H:271:LYS:NZ	2.31	0.59
1:H:120:PHE:O	1:H:124:ILE:HG12	2.03	0.59
1:I:408:ASP:HA	2:I:611:SO4:O3	2.02	0.59
1:J:39:SER:HB2	1:J:374:GLU:OE2	2.02	0.59
1:J:336:VAL:HG13	1:J:372:ILE:H	1.67	0.59
1:L:66:ASP:OD1	1:L:69:THR:OG1	2.18	0.59
1:C:93:ASN:O	1:C:96:ARG:NH1	2.35	0.58
1:F:452:ARG:HE	1:F:493:MET:HE2	1.67	0.58
1:K:5:PHE:CE2	1:K:7:ILE:HD13	2.38	0.58
1:B:325:ILE:HB	1:B:328:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ILE:HG12	1:B:500:SER:HB3	1.85	0.58
1:C:466:LEU:HD21	1:C:469:PHE:HB2	1.85	0.58
1:D:104:PRO:HA	1:D:278:LEU:HD22	1.84	0.58
1:L:484:ILE:HG22	1:L:489:PHE:HA	1.84	0.58
1:A:32:ASP:HB2	1:A:333:LYS:NZ	2.17	0.58
1:C:56:CYS:O	1:C:93:ASN:ND2	2.36	0.58
1:H:266:LYS:NZ	2:H:601:SO4:O1	2.36	0.58
1:I:67:VAL:HG21	1:I:227:MET:HB3	1.84	0.58
1:I:113:LEU:HD23	1:I:114:LYS:HG3	1.84	0.58
1:J:326:GLN:O	1:J:329:ILE:N	2.29	0.58
1:L:281:ILE:HD13	1:L:289:TYR:HB2	1.84	0.58
1:B:8:TRP:O	1:B:60:SER:OG	2.22	0.58
1:D:2:SER:HB3	1:D:66:ASP:HB3	1.85	0.58
1:H:53:ILE:CD1	1:H:94:CYS:HB3	2.32	0.58
1:I:113:LEU:HD21	1:I:275:LEU:HD11	1.86	0.58
1:I:313:ASP:OD2	1:I:316:HIS:HD2	1.87	0.58
1:I:325:ILE:CG1	1:I:328:MET:HE1	2.33	0.58
1:K:54:GLU:HB2	1:K:56:CYS:SG	2.43	0.58
1:C:195:THR:HG21	1:C:229:PRO:HG3	1.85	0.58
1:G:322:LEU:HG	1:G:326:GLN:HB2	1.83	0.58
1:K:452:ARG:NH1	1:L:207:GLU:OE1	2.36	0.58
1:L:387:ALA:HB1	1:L:434:LEU:HD13	1.85	0.58
1:L:424:ILE:HD12	1:L:424:ILE:H	1.68	0.58
1:G:322:LEU:CG	1:G:326:GLN:HB2	2.33	0.58
1:I:120:PHE:CE1	1:I:124:ILE:HD11	2.39	0.58
1:E:38:ASP:CG	1:E:333:LYS:HZ3	2.11	0.58
1:E:134:VAL:HG21	1:E:142:LYS:NZ	2.18	0.58
1:G:307:TYR:CD1	1:G:326:GLN:NE2	2.70	0.58
1:K:224:LEU:HD23	1:K:286:LEU:HD11	1.85	0.58
1:C:144:VAL:HG12	1:C:148:MET:HE2	1.85	0.58
1:F:398:TYR:O	1:F:477:LYS:NZ	2.37	0.58
1:I:211:GLN:NE2	1:I:224:LEU:HA	2.18	0.58
1:D:79:ARG:NH2	1:D:254:SER:OG	2.37	0.58
1:G:48:MET:HG3	1:G:49:ASP:OD1	2.03	0.58
1:K:109:MET:HE3	1:K:114:LYS:HA	1.85	0.57
1:L:231:HIS:CD2	1:L:245:VAL:HG12	2.39	0.57
1:G:375:GLU:N	1:G:375:GLU:OE2	2.37	0.57
1:I:113:LEU:HD21	1:I:275:LEU:CD2	2.34	0.57
1:E:475:ASN:O	1:E:479:ARG:HG3	2.04	0.57
1:J:69:THR:O	1:J:73:MET:HG2	2.04	0.57
1:C:110:THR:HG21	1:C:306:ASN:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:ASN:ND2	1:C:368:LYS:HA	2.20	0.57
1:H:115:LYS:O	1:H:119:ARG:HG3	2.04	0.57
1:H:208:SER:HB2	1:H:226:HIS:HB2	1.87	0.57
1:L:38:ASP:HA	1:L:41:ALA:HB3	1.87	0.57
1:C:65:MET:HE3	1:C:70:TYR:HB2	1.87	0.57
1:L:291:LEU:HD21	1:L:293:TYR:CD1	2.39	0.57
1:L:403:GLU:CG	1:L:404:GLU:H	2.16	0.57
1:H:2:SER:O	1:H:2:SER:OG	2.11	0.57
1:L:312:LEU:HG	1:L:319:TYR:CE1	2.40	0.57
1:L:347:GLU:HB2	1:L:433:PRO:HB3	1.86	0.57
1:I:280:ILE:O	1:I:284:THR:OG1	2.23	0.57
1:J:113:LEU:HD11	1:J:275:LEU:HD21	1.87	0.57
1:F:3:ASP:HB2	1:H:200:GLU:OE1	2.04	0.56
1:G:190:ARG:HG3	1:G:190:ARG:HH11	1.69	0.56
1:D:37:LEU:HD12	1:D:378:GLY:HA2	1.85	0.56
1:G:129:TYR:CZ	1:G:131:PRO:CG	2.87	0.56
1:I:50:VAL:O	1:I:50:VAL:HG13	2.05	0.56
1:L:323:LYS:HB3	1:L:324:PRO:HD3	1.85	0.56
1:C:186:LYS:HE2	1:C:186:LYS:H	1.69	0.56
1:D:151:LYS:HD3	1:D:151:LYS:O	2.05	0.56
1:E:269:LEU:HD23	1:E:272:LEU:HD23	1.86	0.56
1:I:339:GLU:O	1:I:370:LYS:NZ	2.38	0.56
1:J:437:LEU:HD11	1:J:481:CYS:SG	2.45	0.56
1:L:192:LEU:HD22	1:L:245:VAL:HG21	1.87	0.56
1:L:313:ASP:OD1	1:L:314:VAL:N	2.38	0.56
1:C:84:PHE:CE2	1:C:86:TYR:HB3	2.40	0.56
1:C:325:ILE:HG23	1:C:329:ILE:HD13	1.87	0.56
1:D:200:GLU:CD	1:G:3:ASP:HB2	2.31	0.56
1:F:343:LYS:NZ	1:F:344:VAL:H	2.03	0.56
1:F:385:LYS:O	1:F:389:GLU:HG3	2.06	0.56
1:I:479:ARG:NH1	2:I:602:SO4:O3	2.38	0.56
1:A:1:MET:N	1:C:201:ALA:H	2.04	0.56
1:B:36:ALA:HB2	1:B:96:ARG:HD2	1.87	0.56
1:J:455:LEU:HD11	1:J:466:LEU:HD23	1.88	0.56
1:J:475:ASN:O	1:J:479:ARG:NH1	2.39	0.56
1:L:318:LYS:HD3	1:L:359:GLU:HB2	1.87	0.56
1:E:486:LEU:HD23	1:E:487:PHE:CZ	2.40	0.56
1:A:39:SER:CB	1:A:379:VAL:HG23	2.35	0.56
1:K:200:GLU:HG3	1:L:3:ASP:CB	2.34	0.56
1:A:457:GLU:HG2	1:A:499:TYR:CE2	2.40	0.56
1:E:73:MET:HE2	1:E:487:PHE:CD1	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:120:PHE:O	1:J:124:ILE:HG13	2.05	0.56
1:K:130:CYS:HB2	1:K:131:PRO:HD2	1.86	0.56
1:L:464:ARG:NH2	1:L:472:GLU:OE1	2.35	0.56
1:L:469:PHE:CE2	1:L:477:LYS:HD2	2.41	0.56
1:A:200:GLU:HB3	1:C:1:MET:H2	1.70	0.56
1:B:320:ILE:HG13	1:B:321:PRO:HD2	1.88	0.56
1:I:409:THR:HG23	1:I:411:TYR:N	2.15	0.56
1:J:380:GLY:HA2	1:J:407:LEU:CD2	2.28	0.56
1:D:36:ALA:O	1:D:37:LEU:HD23	2.06	0.56
1:J:343:LYS:CG	1:J:344:VAL:H	2.19	0.56
1:A:118:SER:O	1:A:122:THR:HG23	2.06	0.55
1:C:219:LYS:O	1:C:222:GLU:HG2	2.06	0.55
1:L:440:ILE:HG23	1:L:445:LYS:HB3	1.88	0.55
1:L:447:THR:O	1:L:450:GLU:HG2	2.05	0.55
1:E:311:VAL:HG11	1:E:329:ILE:CD1	2.32	0.55
1:I:222:GLU:O	1:I:285:ASN:ND2	2.39	0.55
1:K:320:ILE:HD13	1:K:337:ILE:HD11	1.87	0.55
1:L:71:ASP:HA	1:L:249:LEU:HD13	1.87	0.55
1:L:318:LYS:NZ	1:L:359:GLU:OE1	2.37	0.55
1:E:365:ASN:HD22	1:E:365:ASN:C	2.07	0.55
1:J:407:LEU:O	1:J:407:LEU:CG	2.48	0.55
1:A:67:VAL:H	1:C:1:MET:HE2	1.71	0.55
1:J:397:LEU:HB3	1:J:398:TYR:CD2	2.42	0.55
1:L:126:SER:HB3	1:L:128:ASP:H	1.72	0.55
1:C:464:ARG:NH2	1:C:472:GLU:OE2	2.40	0.55
1:L:123:ARG:O	1:L:123:ARG:HG2	2.06	0.55
1:C:54:GLU:HG2	1:C:55:ASN:H	1.72	0.55
1:D:169:LEU:HD23	1:D:243:ILE:HG13	1.88	0.55
1:E:234:TYR:HB2	1:E:242:ALA:HB3	1.89	0.55
1:G:440:ILE:HG23	1:G:445:LYS:HB3	1.88	0.55
1:H:115:LYS:HG3	1:H:119:ARG:HD2	1.89	0.55
1:J:445:LYS:O	1:J:445:LYS:HG3	2.07	0.55
1:K:326:GLN:HA	1:K:329:ILE:HG22	1.89	0.55
1:L:394:LEU:CG	1:L:438:LEU:HD13	2.35	0.55
1:F:32:ASP:O	1:F:333:LYS:NZ	2.40	0.55
1:G:106:GLU:HB3	1:G:308:GLY:O	2.07	0.55
1:D:102:THR:HG22	1:D:309:ALA:HB2	1.88	0.55
1:A:157:PHE:HZ	1:A:280:ILE:HD13	1.72	0.55
1:B:135:ALA:HB2	1:G:132:ALA:CB	2.25	0.55
1:F:117:ILE:HA	1:F:120:PHE:HB3	1.89	0.55
1:F:322:LEU:C	1:F:322:LEU:HD23	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:400:ILE:HD13	1:K:481:CYS:SG	2.47	0.55
1:L:291:LEU:HD23	1:L:293:TYR:H	1.72	0.54
1:K:218:MET:HE2	1:K:284:THR:HG22	1.89	0.54
1:K:33:GLN:HG3	1:K:34:LEU:N	2.21	0.54
1:K:124:ILE:HD11	1:K:146:ALA:HB1	1.89	0.54
1:A:14:ASN:O	1:A:15:GLU:HG3	2.07	0.54
1:C:489:PHE:HD2	1:C:493:MET:HE2	1.73	0.54
1:D:39:SER:HB3	1:D:379:VAL:H	1.72	0.54
1:E:99:THR:HA	1:E:292:GLY:HA2	1.89	0.54
1:F:352:ASP:OD2	1:F:489:PHE:HB3	2.07	0.54
1:H:322:LEU:HD11	1:H:329:ILE:HG12	1.87	0.54
1:I:500:SER:N	2:I:602:SO4:O2	2.40	0.54
1:C:456:PHE:CE1	1:C:462:GLY:HA2	2.43	0.54
1:D:65:MET:HE2	1:D:196:PRO:HG2	1.90	0.54
1:D:120:PHE:CE1	1:D:124:ILE:HD11	2.42	0.54
1:F:195:THR:CG2	1:F:197:PHE:H	2.20	0.54
1:I:243:ILE:HD12	1:I:259:ILE:HD11	1.89	0.54
1:I:327:ASP:HA	1:I:330:SER:OG	2.08	0.54
1:E:15:GLU:CB	1:E:16:PRO:CD	2.75	0.54
1:F:134:VAL:O	1:F:136:SER:OG	2.20	0.54
1:H:158:GLU:OE1	3:H:614:GOL:H2	2.07	0.54
1:I:223:LYS:NZ	1:I:285:ASN:O	2.22	0.54
1:K:148:MET:SD	1:K:149:ASN:CG	2.91	0.54
1:A:437:LEU:HA	1:A:440:ILE:HD12	1.89	0.54
1:B:331:ARG:NH1	1:B:333:LYS:HE3	2.22	0.54
1:D:219:LYS:HB2	1:D:222:GLU:HG3	1.88	0.54
1:H:72:ARG:HG2	1:H:76:MET:HE3	1.90	0.54
1:A:172:LYS:HE2	1:A:262:PRO:HD2	1.90	0.54
1:G:79:ARG:NH2	1:G:254:SER:OG	2.41	0.54
1:L:125:THR:HG21	1:L:129:TYR:CG	2.43	0.54
1:L:284:THR:OG1	1:L:286:LEU:HD12	2.07	0.54
1:H:227:MET:HE1	1:H:250:PRO:N	2.22	0.54
1:L:347:GLU:N	1:L:347:GLU:OE1	2.41	0.54
1:L:385:LYS:O	1:L:389:GLU:HG3	2.08	0.54
1:A:44:TYR:OH	1:A:409:THR:HG21	2.08	0.54
1:E:294:TYR:CG	1:E:295:ILE:N	2.67	0.54
1:J:38:ASP:N	1:J:38:ASP:OD1	2.41	0.54
1:J:92:ARG:HH22	1:J:427:VAL:HG23	1.72	0.54
1:J:319:TYR:H	1:J:360:GLY:HA2	1.73	0.54
1:D:102:THR:HG22	1:D:309:ALA:CB	2.38	0.53
1:E:313:ASP:HA	3:E:628:GOL:H12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:TYR:CD1	1:H:461:GLU:HG3	2.44	0.53
1:C:79:ARG:HD2	1:C:292:GLY:HA3	1.91	0.53
1:F:43:ARG:NE	1:F:44:TYR:HE1	2.05	0.53
1:G:175:GLU:O	1:G:179:GLN:HA	2.09	0.53
1:I:113:LEU:CD1	1:I:275:LEU:HD11	2.37	0.53
1:D:320:ILE:HD13	1:D:337:ILE:CD1	2.38	0.53
1:E:78:PHE:HE2	1:E:486:LEU:HD11	1.71	0.53
1:F:322:LEU:HD23	1:F:326:GLN:HB2	1.90	0.53
1:G:234:TYR:HB2	1:G:242:ALA:HB3	1.90	0.53
1:G:325:ILE:O	1:G:325:ILE:CG2	2.56	0.53
1:H:480:ILE:O	1:H:484:ILE:HG13	2.08	0.53
1:L:376:ILE:O	1:L:381:GLY:HA3	2.09	0.53
1:B:464:ARG:NH2	1:B:472:GLU:OE2	2.34	0.53
1:G:129:TYR:CZ	1:G:131:PRO:CB	2.89	0.53
1:G:402:TYR:C	1:G:403:GLU:HG3	2.33	0.53
1:H:281:ILE:HG23	1:H:286:LEU:HB2	1.90	0.53
1:J:109:MET:HE2	1:J:114:LYS:HG2	1.89	0.53
1:B:478:LYS:NZ	2:B:613:SO4:O4	2.38	0.53
1:C:111:LYS:HG3	1:C:112:GLU:H	1.72	0.53
1:D:110:THR:CG2	1:D:111:LYS:H	2.21	0.53
1:H:110:THR:OG1	1:H:112:GLU:HG2	2.08	0.53
1:I:109:MET:H	1:I:114:LYS:NZ	2.06	0.53
1:I:115:LYS:HA	1:I:118:SER:OG	2.09	0.53
1:K:327:ASP:O	1:K:330:SER:OG	2.26	0.53
1:A:1:MET:H2	1:C:200:GLU:N	2.07	0.53
1:D:392:LEU:CD1	1:D:404:GLU:HG3	2.39	0.53
1:K:115:LYS:HG2	1:K:118:SER:HG	1.74	0.53
1:F:97:LEU:CD1	1:F:293:TYR:HA	2.39	0.53
1:I:323:LYS:HE3	1:I:326:GLN:OE1	2.08	0.53
1:B:135:ALA:H	1:G:132:ALA:CB	2.22	0.53
1:G:129:TYR:CZ	1:G:131:PRO:HG3	2.41	0.53
1:C:340:GLU:HB2	1:C:370:LYS:HD2	1.90	0.53
1:I:450:GLU:HA	1:I:466:LEU:HD12	1.91	0.53
1:L:76:MET:CE	2:L:604:SO4:O4	2.56	0.53
1:C:34:LEU:HD21	1:C:53:ILE:HG21	1.90	0.53
1:C:54:GLU:HG2	1:C:55:ASN:N	2.24	0.53
1:E:54:GLU:HB2	1:E:56:CYS:SG	2.49	0.53
1:F:363:THR:C	1:F:365:ASN:H	2.17	0.53
1:H:161:LEU:O	1:H:166:LYS:NZ	2.42	0.53
1:I:173:TYR:HE2	1:I:260:TRP:CZ3	2.27	0.52
1:L:322:LEU:C	1:L:322:LEU:HD12	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:THR:OG1	1:C:123:ARG:HG3	2.10	0.52
1:A:456:PHE:HB3	1:A:498:LEU:HD12	1.91	0.52
1:F:97:LEU:HD12	1:F:293:TYR:HA	1.90	0.52
1:J:343:LYS:CG	1:J:344:VAL:N	2.70	0.52
1:J:445:LYS:HE3	1:J:489:PHE:CZ	2.45	0.52
1:C:48:MET:HG3	1:C:49:ASP:H	1.74	0.52
1:E:38:ASP:OD1	1:E:333:LYS:HE2	2.09	0.52
1:H:67:VAL:CG2	2:H:612:SO4:O3	2.55	0.52
1:I:113:LEU:CD2	1:I:114:LYS:HG3	2.40	0.52
1:K:341:GLU:O	1:K:341:GLU:CD	2.52	0.52
1:A:45:MET:C	1:A:47:LYS:N	2.67	0.52
1:C:113:LEU:HD22	1:C:275:LEU:HD11	1.91	0.52
1:E:480:ILE:O	1:E:484:ILE:HG13	2.09	0.52
1:F:327:ASP:O	1:F:330:SER:OG	2.25	0.52
1:H:454:PHE:O	1:H:496:VAL:HA	2.09	0.52
1:J:208:SER:HB2	1:J:226:HIS:HB2	1.92	0.52
1:J:347:GLU:HG3	1:J:383:ALA:CB	2.39	0.52
1:B:135:ALA:N	1:G:132:ALA:HB2	2.24	0.52
1:G:105:GLN:CD	1:G:105:GLN:H	2.18	0.52
1:D:110:THR:CG2	1:D:111:LYS:N	2.73	0.52
1:D:155:THR:HG21	1:D:276:ARG:NH1	2.24	0.52
1:E:47:LYS:O	1:E:50:VAL:HG12	2.09	0.52
1:E:311:VAL:HG21	1:E:329:ILE:HD13	1.91	0.52
1:F:252:GLY:HA2	1:F:286:LEU:HB3	1.92	0.52
1:I:321:PRO:HB2	1:I:324:PRO:HG2	1.90	0.52
1:J:134:VAL:CG2	1:J:142:LYS:HE2	2.40	0.52
1:L:177:VAL:HG12	1:L:178:HIS:CD2	2.45	0.52
1:F:308:GLY:H	1:F:323:LYS:HE2	1.75	0.52
1:F:311:VAL:HG21	1:F:329:ILE:HD11	1.91	0.52
1:G:459:GLU:OE1	1:G:500:SER:HB2	2.10	0.52
1:I:110:THR:N	1:I:114:LYS:HZ3	2.06	0.52
1:J:55:ASN:HA	1:J:93:ASN:OD1	2.10	0.52
1:F:245:VAL:HG12	1:F:256:VAL:HB	1.91	0.52
1:G:283:ARG:NH1	2:G:617:SO4:O4	2.43	0.52
1:G:325:ILE:O	1:G:329:ILE:CG2	2.58	0.52
1:G:441:MET:HE1	1:G:469:PHE:HE2	1.75	0.52
1:I:350:LEU:HD22	1:I:355:THR:HG22	1.92	0.52
1:A:222:GLU:O	1:A:285:ASN:ND2	2.41	0.52
1:B:352:ASP:OD2	1:B:490:GLU:HB2	2.10	0.52
1:B:364:ASP:O	1:B:367:VAL:HG22	2.10	0.52
1:F:402:TYR:CE1	1:F:478:LYS:HE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:325:ILE:O	1:J:325:ILE:HG22	2.09	0.52
1:J:469:PHE:CZ	1:J:477:LYS:HB3	2.45	0.52
1:K:385:LYS:O	1:K:389:GLU:HG2	2.10	0.52
1:K:391:ALA:HB1	1:K:402:TYR:HB3	1.92	0.52
1:A:45:MET:O	1:A:48:MET:HG2	2.10	0.51
1:A:314:VAL:HG22	3:A:624:GOL:H32	1.91	0.51
1:C:47:LYS:HB3	1:C:50:VAL:HB	1.92	0.51
1:G:336:VAL:CG2	1:G:372:ILE:HG13	2.40	0.51
1:H:110:THR:HG1	1:H:113:LEU:H	1.58	0.51
1:A:32:ASP:HB2	1:A:333:LYS:HZ1	1.75	0.51
1:A:73:MET:HE1	1:A:487:PHE:HB3	1.91	0.51
1:B:365:ASN:C	1:B:367:VAL:N	2.68	0.51
1:E:58:ILE:HD11	1:E:89:ASP:HB2	1.92	0.51
1:H:331:ARG:O	1:H:333:LYS:NZ	2.43	0.51
1:E:8:TRP:O	1:E:60:SER:OG	2.28	0.51
1:F:352:ASP:OD2	1:F:490:GLU:N	2.43	0.51
1:K:134:VAL:HG12	1:K:135:ALA:N	2.25	0.51
1:A:88:VAL:CG2	1:A:97:LEU:HB3	2.41	0.51
1:C:119:ARG:HG2	1:C:122:THR:HG21	1.92	0.51
1:E:145:ASN:O	1:E:149:ASN:ND2	2.44	0.51
1:G:329:ILE:HG13	1:G:333:LYS:HD3	1.92	0.51
1:H:8:TRP:O	1:H:60:SER:OG	2.28	0.51
1:I:105:GLN:OE1	1:I:108:ASN:ND2	2.30	0.51
1:J:72:ARG:HD2	1:J:357:ARG:HD3	1.92	0.51
1:K:338:GLY:HA3	1:K:372:ILE:HG12	1.92	0.51
1:C:328:MET:HE2	1:C:371:ASN:HD22	1.75	0.51
1:E:127:GLU:H	1:E:127:GLU:CD	2.19	0.51
1:F:91:LEU:HD13	1:F:377:TYR:HB3	1.92	0.51
1:H:124:ILE:HG23	1:H:153:PHE:HB3	1.91	0.51
1:I:320:ILE:HD13	1:I:337:ILE:HG13	1.92	0.51
1:I:388:ASN:O	1:I:392:LEU:CD1	2.58	0.51
1:I:460:THR:HG22	1:I:460:THR:O	2.11	0.51
1:L:437:LEU:HD13	1:L:484:ILE:CD1	2.40	0.51
1:A:32:ASP:O	1:A:34:LEU:HD12	2.11	0.51
1:E:106:GLU:OE1	1:H:217:ARG:HD2	2.11	0.51
1:H:311:VAL:HG21	1:H:322:LEU:HD13	1.93	0.51
1:L:40:TRP:CZ2	1:L:379:VAL:HB	2.46	0.51
1:L:398:TYR:HE2	1:L:438:LEU:HD11	1.75	0.51
1:A:88:VAL:HG21	1:A:97:LEU:HB3	1.93	0.51
1:B:293:TYR:O	1:B:294:TYR:HB2	2.10	0.51
1:A:476:VAL:O	1:A:480:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:MET:HG2	1:C:113:LEU:HB3	1.92	0.51
1:C:308:GLY:HA3	1:C:323:LYS:HE2	1.93	0.51
1:C:331:ARG:HH21	1:C:333:LYS:HD2	1.75	0.51
1:F:145:ASN:OD1	1:F:146:ALA:N	2.44	0.51
1:H:227:MET:HE1	1:H:250:PRO:HD3	1.92	0.51
1:L:113:LEU:N	1:L:113:LEU:CD2	2.73	0.51
1:A:3:ASP:HB2	1:C:200:GLU:OE1	2.11	0.51
1:B:47:LYS:HB3	1:B:50:VAL:HG21	1.92	0.51
1:D:455:LEU:HB3	1:D:499:TYR:HE1	1.75	0.51
1:F:134:VAL:HG12	1:F:134:VAL:O	2.09	0.51
1:H:455:LEU:HD23	1:H:497:ILE:HB	1.92	0.51
1:H:457:GLU:O	1:H:460:THR:HG22	2.10	0.51
1:L:101:ARG:HB3	1:L:319:TYR:CE1	2.45	0.51
1:L:267:TRP:HB2	1:L:269:LEU:HG	1.92	0.51
1:A:456:PHE:CE1	1:A:462:GLY:HA2	2.46	0.51
1:C:123:ARG:CZ	2:C:604:SO4:O3	2.59	0.51
1:E:372:ILE:O	1:E:375:GLU:HG2	2.11	0.51
1:A:45:MET:C	1:A:47:LYS:H	2.18	0.50
1:B:67:VAL:HG21	1:B:227:MET:HB3	1.92	0.50
1:E:117:ILE:O	1:E:121:ALA:N	2.39	0.50
1:F:263:ASP:HB2	1:I:239:LYS:HZ3	1.76	0.50
1:G:186:LYS:HA	1:G:189:LYS:HE3	1.92	0.50
1:K:57:THR:O	1:K:58:ILE:HD13	2.11	0.50
1:L:309:ALA:O	1:L:322:LEU:N	2.44	0.50
1:B:109:MET:SD	1:B:139:PHE:CD1	3.04	0.50
1:G:253:ILE:HB	1:G:281:ILE:HD11	1.92	0.50
1:I:124:ILE:HG23	1:I:152:THR:HB	1.92	0.50
1:K:8:TRP:O	1:K:60:SER:OG	2.29	0.50
1:L:79:ARG:CZ	1:L:292:GLY:O	2.59	0.50
1:L:172:LYS:HE2	1:L:262:PRO:HD2	1.92	0.50
1:A:51:VAL:CG2	1:A:411:TYR:HB3	2.41	0.50
1:D:270:GLY:O	1:D:273:SER:HB3	2.11	0.50
1:K:325:ILE:HA	1:K:327:ASP:HB2	1.91	0.50
1:K:339:GLU:CD	1:K:367:VAL:HG21	2.37	0.50
1:L:108:ASN:H	1:L:308:GLY:N	2.09	0.50
1:L:455:LEU:HD23	1:L:497:ILE:HB	1.94	0.50
1:A:351:VAL:O	1:A:355:THR:HG23	2.12	0.50
1:B:70:TYR:HD2	1:B:249:LEU:HD21	1.77	0.50
1:B:219:LYS:HD3	1:F:220:PRO:HB3	1.93	0.50
1:D:154:TYR:HE2	1:D:156:ARG:HE	1.59	0.50
1:H:93:ASN:O	1:H:96:ARG:NH1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:SER:N	1:B:64:HIS:HE2	2.08	0.50
1:G:322:LEU:CD1	1:G:326:GLN:HG3	2.41	0.50
1:H:13:HIS:O	1:H:56:CYS:HB2	2.11	0.50
1:J:261:ASP:HB3	1:J:264:TYR:HD1	1.77	0.50
1:B:93:ASN:O	1:B:96:ARG:NH1	2.45	0.50
1:B:438:LEU:O	1:B:442:GLN:HG3	2.12	0.50
1:D:365:ASN:OD1	1:D:368:LYS:HA	2.12	0.50
1:F:401:PRO:HD2	1:F:478:LYS:HB2	1.92	0.50
1:L:463:ILE:HD12	1:L:463:ILE:H	1.76	0.50
1:C:4:ARG:HD3	1:C:494:LYS:O	2.12	0.50
1:D:457:GLU:HG2	1:D:460:THR:HG23	1.93	0.50
1:E:57:THR:HG22	1:E:88:VAL:HG12	1.93	0.50
1:G:322:LEU:O	1:G:326:GLN:N	2.45	0.50
1:G:339:GLU:HG3	1:G:340:GLU:N	2.27	0.50
1:H:109:MET:SD	1:H:139:PHE:HB3	2.52	0.50
1:L:432:LEU:O	1:L:485:ARG:NH2	2.45	0.50
1:A:252:GLY:HA3	1:A:288:TYR:O	2.12	0.50
1:B:479:ARG:NH1	2:B:604:SO4:O4	2.44	0.50
1:C:119:ARG:HA	1:C:122:THR:CG2	2.39	0.50
1:B:39:SER:HB3	1:B:379:VAL:H	1.77	0.50
1:B:326:GLN:OE1	1:B:330:SER:OG	2.29	0.50
1:D:320:ILE:HG13	1:D:321:PRO:CD	2.39	0.50
1:E:364:ASP:CB	1:H:156:ARG:NE	2.75	0.50
1:F:291:LEU:HD12	1:F:291:LEU:H	1.76	0.50
1:H:107:LEU:HD13	1:H:278:LEU:HD11	1.94	0.50
1:H:195:THR:HG21	1:H:229:PRO:HG3	1.94	0.50
1:I:211:GLN:HE22	1:I:224:LEU:HA	1.76	0.50
1:I:265:SER:C	1:I:267:TRP:H	2.20	0.50
1:J:321:PRO:O	1:J:324:PRO:HD2	2.11	0.50
1:L:62:VAL:HG11	1:L:65:MET:CE	2.41	0.50
1:C:38:ASP:OD1	1:C:331:ARG:CZ	2.60	0.49
1:D:158:GLU:OE2	1:D:166:LYS:HE2	2.11	0.49
1:G:408:ASP:OD1	1:G:408:ASP:N	2.38	0.49
1:K:134:VAL:HG11	1:K:142:LYS:HD3	1.93	0.49
1:F:352:ASP:OD1	1:F:490:GLU:CG	2.60	0.49
1:F:479:ARG:HH22	1:F:502:GLN:HA	1.76	0.49
1:F:480:ILE:O	1:F:484:ILE:HG13	2.11	0.49
1:A:293:TYR:CG	1:A:293:TYR:O	2.65	0.49
1:B:200:GLU:OE2	1:E:3:ASP:HB2	2.12	0.49
1:B:445:LYS:HE2	1:D:349:TYR:CD2	2.47	0.49
1:E:37:LEU:HD21	1:E:334:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:VAL:HG21	1:E:322:LEU:HD13	1.95	0.49
1:E:334:LEU:HD23	1:E:334:LEU:O	2.11	0.49
1:G:394:LEU:HD21	1:G:438:LEU:HA	1.93	0.49
1:J:118:SER:O	1:J:122:THR:HG23	2.12	0.49
1:J:326:GLN:HE22	1:J:330:SER:HB3	1.77	0.49
1:L:102:THR:HG22	1:L:103:ALA:O	2.11	0.49
1:C:352:ASP:OD2	1:C:490:GLU:N	2.44	0.49
1:G:52:LYS:CE	1:G:54:GLU:HG2	2.42	0.49
1:G:283:ARG:CZ	2:G:617:SO4:O4	2.60	0.49
1:J:195:THR:HG21	1:J:229:PRO:HG3	1.95	0.49
1:D:15:GLU:HB3	1:D:57:THR:CG2	2.41	0.49
1:E:401:PRO:HD2	1:E:478:LYS:HB2	1.93	0.49
1:E:409:THR:C	1:E:411:TYR:N	2.70	0.49
1:G:55:ASN:HB3	1:G:94:CYS:HB3	1.93	0.49
1:G:110:THR:O	1:G:114:LYS:HG3	2.13	0.49
1:G:473:PRO:HB2	1:G:476:VAL:HG12	1.94	0.49
1:L:54:GLU:HG3	1:L:54:GLU:O	2.13	0.49
1:L:336:VAL:O	1:L:372:ILE:HG12	2.12	0.49
1:A:43:ARG:HH22	1:A:409:THR:CG2	2.14	0.49
1:C:209:TRP:CH2	1:C:230:VAL:HG12	2.46	0.49
1:C:234:TYR:HB2	1:C:242:ALA:HB3	1.94	0.49
1:F:311:VAL:HG11	1:F:325:ILE:HD11	1.94	0.49
1:I:16:PRO:HG3	1:I:84:PHE:HE2	1.78	0.49
1:I:113:LEU:HD22	1:I:114:LYS:CE	2.42	0.49
1:I:331:ARG:NH2	1:I:333:LYS:HE3	2.27	0.49
1:J:83:LYS:HA	1:J:196:PRO:HD3	1.95	0.49
1:A:103:ALA:H	1:A:106:GLU:HG2	1.76	0.49
1:B:109:MET:SD	1:B:139:PHE:HB3	2.53	0.49
1:C:372:ILE:HD12	1:C:376:ILE:HD11	1.95	0.49
1:D:245:VAL:O	1:D:256:VAL:HG22	2.12	0.49
1:F:124:ILE:HG13	1:F:125:THR:N	2.27	0.49
1:G:108:ASN:OD1	1:G:308:GLY:HA3	2.13	0.49
1:J:10:PRO:HG2	1:J:482:ASP:HB3	1.94	0.49
1:J:65:MET:SD	1:J:70:TYR:HB2	2.52	0.49
1:J:315:CYS:SG	1:J:429:PRO:HB3	2.53	0.49
1:K:330:SER:O	1:K:332:GLY:N	2.45	0.49
1:L:36:ALA:O	1:L:333:LYS:HB3	2.13	0.49
1:L:211:GLN:OE1	1:L:224:LEU:HD12	2.13	0.49
1:A:401:PRO:HD3	1:A:474:PRO:HB3	1.95	0.49
1:B:118:SER:O	1:B:122:THR:HG23	2.13	0.49
2:G:601:SO4:O3	1:H:349:TYR:OH	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:351:VAL:O	1:I:355:THR:HG23	2.13	0.49
1:K:101:ARG:HA	1:K:289:TYR:O	2.13	0.49
1:L:36:ALA:O	1:L:37:LEU:HG	2.13	0.49
1:A:103:ALA:H	1:A:106:GLU:CG	2.26	0.49
1:B:41:ALA:O	1:B:45:MET:HG3	2.13	0.49
1:B:456:PHE:HB3	1:B:498:LEU:HD12	1.94	0.49
1:D:195:THR:HG21	1:D:229:PRO:HG3	1.95	0.49
1:F:200:GLU:HB2	1:H:3:ASP:O	2.13	0.49
1:G:325:ILE:CD1	1:G:337:ILE:HD11	2.43	0.49
1:H:252:GLY:HA3	1:H:288:TYR:O	2.12	0.49
1:I:464:ARG:HH12	1:I:472:GLU:CD	2.21	0.49
1:J:37:LEU:HD13	1:J:374:GLU:HG2	1.94	0.49
1:J:90:PRO:HD2	1:J:429:PRO:HD2	1.95	0.49
1:E:134:VAL:HB	1:E:142:LYS:HD2	1.95	0.49
1:G:67:VAL:HG21	1:G:227:MET:HB3	1.94	0.49
1:G:406:ASP:OD1	1:G:410:ILE:HA	2.13	0.49
1:H:472:GLU:OE2	1:H:473:PRO:HD2	2.12	0.49
1:J:368:LYS:HD3	1:J:369:TYR:CD2	2.48	0.49
1:L:109:MET:HE1	1:L:139:PHE:HB3	1.95	0.49
1:A:43:ARG:O	1:A:43:ARG:HG3	2.12	0.48
1:B:363:THR:O	1:B:363:THR:HG22	2.13	0.48
1:B:365:ASN:C	1:B:367:VAL:H	2.19	0.48
1:G:325:ILE:O	1:G:329:ILE:HG23	2.12	0.48
1:H:112:GLU:HG3	1:H:113:LEU:HD23	1.95	0.48
1:L:11:SER:HA	1:L:424:ILE:HD11	1.94	0.48
1:L:107:LEU:C	1:L:107:LEU:HD23	2.38	0.48
1:L:374:GLU:C	1:L:376:ILE:H	2.20	0.48
1:A:52:LYS:HG2	1:A:53:ILE:H	1.78	0.48
1:D:61:PHE:CE2	3:D:624:GOL:H32	2.47	0.48
1:E:50:VAL:HG13	1:E:51:VAL:HG23	1.94	0.48
1:F:458:ILE:HD11	1:F:500:SER:HB3	1.95	0.48
1:G:167:TYR:OH	1:G:183:ASN:O	2.30	0.48
1:H:115:LYS:HE3	1:H:119:ARG:CZ	2.43	0.48
1:J:316:HIS:CD2	1:J:361:PHE:HZ	2.31	0.48
1:J:337:ILE:HD12	1:J:361:PHE:CD2	2.48	0.48
1:J:431:LEU:HD13	1:J:486:LEU:HD12	1.95	0.48
1:L:309:ALA:HB3	1:L:322:LEU:HD21	1.95	0.48
1:E:221:GLY:HA2	2:E:612:SO4:O3	2.13	0.48
1:G:172:LYS:CE	2:G:608:SO4:O1	2.60	0.48
1:I:450:GLU:HG2	1:I:466:LEU:HD12	1.94	0.48
1:D:468:ASN:OD1	1:D:471:SER:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:397:LEU:HB3	1:J:398:TYR:CE2	2.48	0.48
1:L:172:LYS:HZ3	1:L:261:ASP:CG	2.21	0.48
1:L:393:GLU:O	1:L:397:LEU:HB2	2.14	0.48
1:A:292:GLY:O	1:A:294:TYR:N	2.46	0.48
1:C:328:MET:HE1	1:C:333:LYS:HE2	1.95	0.48
1:E:58:ILE:HG23	1:E:424:ILE:HD12	1.95	0.48
1:F:330:SER:OG	1:F:331:ARG:HG3	2.12	0.48
1:H:98:TYR:CE2	1:H:329:ILE:HG22	2.48	0.48
1:I:139:PHE:HA	1:I:142:LYS:HG3	1.96	0.48
1:H:175:GLU:HB3	1:H:181:TYR:CZ	2.49	0.48
1:H:281:ILE:HA	1:H:284:THR:HG22	1.95	0.48
1:K:500:SER:N	2:K:601:SO4:O3	2.45	0.48
1:L:101:ARG:O	1:L:309:ALA:HB1	2.13	0.48
1:L:325:ILE:HD12	1:L:328:MET:HE1	1.95	0.48
1:A:134:VAL:HG11	1:A:142:LYS:HG2	1.95	0.48
1:C:5:PHE:CZ	1:C:7:ILE:HG21	2.49	0.48
1:E:98:TYR:CD2	1:E:329:ILE:HG12	2.49	0.48
1:H:326:GLN:HA	1:H:329:ILE:HG13	1.94	0.48
1:B:186:LYS:O	1:B:190:ARG:HG3	2.14	0.48
1:C:336:VAL:CG2	1:C:372:ILE:HG13	2.42	0.48
1:F:41:ALA:O	1:F:45:MET:HB3	2.13	0.48
1:F:343:LYS:HZ1	1:F:344:VAL:H	1.62	0.48
1:G:328:MET:HG2	1:G:331:ARG:HE	1.78	0.48
1:I:140:VAL:O	1:I:144:VAL:HG23	2.13	0.48
1:J:449:LEU:CD1	1:J:480:ILE:HD11	2.44	0.48
1:K:398:TYR:O	1:K:477:LYS:NZ	2.41	0.48
1:L:164:GLU:CD	1:L:164:GLU:H	2.22	0.48
1:D:388:ASN:CB	1:D:404:GLU:HG2	2.39	0.48
1:F:365:ASN:ND2	1:F:369:TYR:CZ	2.81	0.48
1:F:473:PRO:HB2	1:F:476:VAL:HG12	1.96	0.48
1:K:36:ALA:HA	1:K:96:ARG:HD3	1.96	0.48
1:K:108:ASN:HB2	1:K:307:TYR:HA	1.96	0.48
1:L:454:PHE:O	1:L:496:VAL:HA	2.14	0.48
1:B:326:GLN:O	1:B:329:ILE:N	2.26	0.48
1:D:81:SER:HB2	1:D:191:PHE:CE1	2.49	0.48
1:G:207:GLU:H	1:G:207:GLU:CD	2.22	0.48
1:K:156:ARG:HH12	1:K:158:GLU:CG	2.24	0.48
1:L:469:PHE:CZ	1:L:477:LYS:HD2	2.49	0.48
1:K:244:THR:HG22	1:K:258:PHE:HD1	1.77	0.47
1:K:323:LYS:O	1:K:326:GLN:N	2.47	0.47
1:L:367:VAL:HG12	1:L:367:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:TYR:HD2	1:F:51:VAL:CG1	2.27	0.47
1:F:108:ASN:O	1:F:110:THR:HG23	2.14	0.47
1:F:322:LEU:CD2	1:F:326:GLN:HB2	2.43	0.47
1:G:39:SER:OG	1:G:379:VAL:HG23	2.13	0.47
1:J:7:ILE:HG22	1:J:62:VAL:HG22	1.96	0.47
1:K:39:SER:OG	1:K:374:GLU:OE2	2.20	0.47
1:B:127:GLU:C	1:B:129:TYR:N	2.70	0.47
1:C:10:PRO:HG2	1:C:482:ASP:HB3	1.97	0.47
1:C:109:MET:HE3	1:C:113:LEU:HB3	1.96	0.47
1:L:119:ARG:O	1:L:123:ARG:CB	2.62	0.47
1:L:313:ASP:OD2	1:L:337:ILE:HG22	2.14	0.47
1:B:105:GLN:OE1	1:G:217:ARG:HD3	2.15	0.47
1:J:398:TYR:O	1:J:400:ILE:HG13	2.15	0.47
1:K:453:LEU:HD11	1:K:497:ILE:HG13	1.95	0.47
1:B:38:ASP:HA	1:B:41:ALA:HB3	1.95	0.47
1:B:362:PRO:O	1:B:369:TYR:OH	2.31	0.47
1:D:407:LEU:N	1:D:407:LEU:CD1	2.77	0.47
1:F:169:LEU:HD11	1:F:261:ASP:HA	1.96	0.47
1:K:321:PRO:HB2	1:K:324:PRO:HG2	1.97	0.47
1:E:294:TYR:CD2	1:E:295:ILE:N	2.80	0.47
1:H:408:ASP:OD1	1:H:409:THR:HG22	2.13	0.47
1:J:98:TYR:CE1	1:J:329:ILE:HG23	2.49	0.47
1:J:271:LYS:O	1:J:275:LEU:HG	2.14	0.47
1:J:437:LEU:HD21	1:J:481:CYS:HB3	1.97	0.47
1:K:2:SER:OG	1:L:200:GLU:HB2	2.14	0.47
1:L:272:LEU:O	1:L:276:ARG:HG3	2.13	0.47
1:B:14:ASN:ND2	1:B:55:ASN:O	2.46	0.47
1:C:54:GLU:CG	1:C:55:ASN:H	2.28	0.47
1:C:345:THR:O	1:C:382:CYS:HB2	2.15	0.47
1:D:35:PHE:HB2	1:D:41:ALA:HB2	1.96	0.47
1:D:124:ILE:CG2	1:D:153:PHE:HB3	2.44	0.47
1:D:392:LEU:HD13	1:D:404:GLU:HG3	1.96	0.47
1:F:62:VAL:HG11	1:F:65:MET:HG2	1.97	0.47
1:F:124:ILE:HG13	1:F:125:THR:HG23	1.96	0.47
1:G:252:GLY:HA2	1:G:286:LEU:HB3	1.97	0.47
1:H:53:ILE:HD13	1:H:94:CYS:HB3	1.95	0.47
1:J:334:LEU:HD12	1:J:335:PHE:N	2.29	0.47
1:A:16:PRO:HD2	1:A:57:THR:OG1	2.15	0.47
1:A:323:LYS:O	1:A:326:GLN:HG2	2.14	0.47
1:A:407:LEU:HD12	1:A:407:LEU:H	1.80	0.47
1:E:140:VAL:O	1:E:144:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:GLN:O	1:F:330:SER:HB3	2.15	0.47
1:H:329:ILE:HD12	1:H:330:SER:N	2.29	0.47
1:I:328:MET:HE3	1:I:328:MET:HB2	1.53	0.47
1:J:472:GLU:O	1:J:477:LYS:HD3	2.14	0.47
1:A:1:MET:N	1:C:200:GLU:HB3	2.30	0.47
1:A:189:LYS:HG3	1:C:461:GLU:OE2	2.14	0.47
1:A:309:ALA:HB3	1:A:322:LEU:HD22	1.97	0.47
1:A:365:ASN:ND2	1:A:367:VAL:HB	2.30	0.47
1:B:331:ARG:NH1	1:B:333:LYS:HG3	2.29	0.47
1:D:464:ARG:HH22	1:D:472:GLU:CD	2.22	0.47
1:F:152:THR:HB	1:F:236:TYR:CE1	2.50	0.47
1:G:4:ARG:HA	1:G:4:ARG:HD3	1.58	0.47
1:H:91:LEU:HG	1:H:410:ILE:HD11	1.97	0.47
1:H:476:VAL:O	1:H:480:ILE:HG13	2.15	0.47
1:I:12:MET:HE2	1:I:12:MET:HB3	1.74	0.47
1:I:139:PHE:O	1:I:142:LYS:HB2	2.15	0.47
1:A:343:LYS:O	1:A:343:LYS:HG3	2.14	0.47
1:D:4:ARG:HD3	1:D:494:LYS:O	2.15	0.47
1:D:43:ARG:NH2	1:D:44:TYR:HH	2.12	0.47
1:G:131:PRO:HG2	1:G:134:VAL:HG22	1.97	0.47
1:H:3:ASP:O	1:H:4:ARG:HG2	2.15	0.47
1:I:326:GLN:O	1:I:329:ILE:HG12	2.14	0.47
1:I:441:MET:HE1	1:I:446:ILE:HG12	1.96	0.47
1:J:450:GLU:HA	1:J:466:LEU:HD12	1.96	0.47
1:K:10:PRO:HG2	1:K:482:ASP:HB3	1.97	0.47
1:K:156:ARG:NH2	1:K:158:GLU:CD	2.65	0.47
1:L:345:THR:HB	1:L:382:CYS:SG	2.55	0.47
1:A:98:TYR:CE2	1:A:329:ILE:HG12	2.50	0.46
1:A:352:ASP:OD2	1:A:490:GLU:HG3	2.15	0.46
1:B:79:ARG:CZ	1:B:292:GLY:HA2	2.45	0.46
1:B:96:ARG:O	1:B:97:LEU:HD23	2.15	0.46
1:D:140:VAL:O	1:D:144:VAL:HG12	2.15	0.46
1:E:134:VAL:O	1:E:135:ALA:C	2.58	0.46
1:E:233:CYS:HB3	1:E:240:LEU:CD1	2.45	0.46
1:I:79:ARG:NH2	1:I:254:SER:OG	2.48	0.46
1:J:445:LYS:HD2	1:L:349:TYR:HD2	1.75	0.46
1:A:458:ILE:HG22	1:A:500:SER:HB3	1.96	0.46
1:B:388:ASN:ND2	1:B:407:LEU:CD2	2.78	0.46
1:D:2:SER:C	1:D:4:ARG:H	2.23	0.46
1:E:221:GLY:CA	2:E:612:SO4:O3	2.64	0.46
1:I:72:ARG:HG2	1:I:76:MET:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:312:LEU:HB2	1:K:319:TYR:CE1	2.50	0.46
1:L:125:THR:OG1	1:L:129:TYR:HB2	2.15	0.46
1:A:320:ILE:CD1	1:A:321:PRO:HD2	2.44	0.46
1:B:36:ALA:HB1	1:B:334:LEU:HB2	1.97	0.46
1:C:405:GLU:CA	1:C:409:THR:HG21	2.46	0.46
1:E:47:LYS:HB3	1:E:50:VAL:CG1	2.46	0.46
1:E:93:ASN:HB3	1:E:95:CYS:O	2.15	0.46
1:F:90:PRO:HG2	1:F:429:PRO:HB2	1.98	0.46
1:F:479:ARG:NH1	2:F:604:SO4:O2	2.48	0.46
1:I:346:LYS:HD3	1:I:435:TRP:CD2	2.50	0.46
1:K:115:LYS:HG2	1:K:118:SER:HB3	1.93	0.46
1:L:403:GLU:CG	1:L:404:GLU:N	2.76	0.46
1:I:450:GLU:CA	1:I:466:LEU:HD12	2.46	0.46
1:I:490:GLU:HA	1:I:493:MET:HE2	1.96	0.46
1:K:56:CYS:N	1:K:93:ASN:OD1	2.41	0.46
1:A:117:ILE:HD11	1:A:275:LEU:HD13	1.98	0.46
1:E:457:GLU:O	1:E:460:THR:OG1	2.33	0.46
1:H:470:TYR:O	1:H:477:LYS:NZ	2.49	0.46
1:J:394:LEU:HD13	1:J:402:TYR:HD2	1.81	0.46
1:K:328:MET:HG2	1:K:371:ASN:ND2	2.30	0.46
1:L:388:ASN:CG	1:L:404:GLU:HG3	2.40	0.46
1:B:120:PHE:CZ	1:B:124:ILE:HD13	2.50	0.46
1:C:252:GLY:HA3	1:C:288:TYR:O	2.16	0.46
1:G:71:ASP:HA	1:G:249:LEU:HD13	1.98	0.46
1:G:267:TRP:HB2	1:G:269:LEU:HG	1.97	0.46
1:G:314:VAL:HG22	3:G:623:GOL:H12	1.96	0.46
1:H:65:MET:HE2	1:H:196:PRO:CG	2.45	0.46
1:I:16:PRO:HG3	1:I:84:PHE:CE2	2.51	0.46
1:I:41:ALA:O	1:I:45:MET:HG3	2.16	0.46
1:J:372:ILE:HD12	1:J:376:ILE:HD11	1.97	0.46
1:A:43:ARG:NH2	1:A:409:THR:HG23	2.20	0.46
1:D:84:PHE:CE2	1:D:86:TYR:HB3	2.51	0.46
1:E:124:ILE:HG13	1:E:125:THR:N	2.30	0.46
1:G:64:HIS:HA	1:G:196:PRO:O	2.16	0.46
1:G:398:TYR:HB3	1:G:441:MET:HE2	1.98	0.46
1:I:66:ASP:OD1	1:I:69:THR:N	2.28	0.46
1:I:406:ASP:C	1:I:408:ASP:H	2.24	0.46
1:J:291:LEU:O	1:J:293:TYR:N	2.43	0.46
1:K:138:ASP:OD2	1:K:141:GLY:HA3	2.14	0.46
1:D:393:GLU:O	1:D:396:GLU:O	2.34	0.46
1:E:346:LYS:NZ	1:F:442:GLN:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:61:PHE:CZ	1:H:83:LYS:HD3	2.50	0.46
1:J:43:ARG:HH12	1:J:408:ASP:HA	1.80	0.46
1:L:140:VAL:O	1:L:144:VAL:HG23	2.16	0.46
1:L:432:LEU:HD13	1:L:484:ILE:O	2.15	0.46
1:L:437:LEU:O	1:L:441:MET:HG2	2.15	0.46
1:A:220:PRO:HA	1:A:285:ASN:OD1	2.16	0.46
1:I:325:ILE:CD1	1:I:328:MET:HE1	2.46	0.46
1:J:109:MET:HE2	1:J:109:MET:HB3	1.73	0.46
1:J:134:VAL:HG11	1:J:142:LYS:HG2	1.97	0.46
1:J:288:TYR:HB2	1:J:290:TYR:CE1	2.51	0.46
1:J:454:PHE:O	1:J:496:VAL:HA	2.16	0.46
1:J:473:PRO:O	1:J:477:LYS:HE2	2.16	0.46
1:C:331:ARG:NH2	1:C:333:LYS:HD3	2.28	0.46
1:D:101:ARG:HD2	1:D:288:TYR:CD1	2.50	0.46
1:D:269:LEU:O	1:D:273:SER:HB2	2.16	0.46
1:D:478:LYS:NZ	3:D:626:GOL:H11	2.31	0.46
1:G:449:LEU:HD11	1:G:484:ILE:HD11	1.98	0.46
1:I:113:LEU:CD2	1:I:114:LYS:CD	2.91	0.46
1:I:113:LEU:HD21	1:I:275:LEU:CG	2.46	0.46
1:I:31:MET:SD	1:I:31:MET:N	2.89	0.45
1:I:269:LEU:HD23	1:I:272:LEU:HD23	1.98	0.45
1:J:52:LYS:HB2	1:J:52:LYS:HE3	1.70	0.45
1:L:172:LYS:HD2	2:L:611:SO4:O4	2.16	0.45
1:L:387:ALA:O	1:L:434:LEU:HD22	2.16	0.45
1:L:388:ASN:HB3	1:L:404:GLU:HG3	1.97	0.45
1:A:73:MET:HG3	1:A:85:LEU:HD21	1.97	0.45
1:B:313:ASP:HA	3:B:627:GOL:H11	1.99	0.45
1:C:71:ASP:HA	1:C:249:LEU:HD13	1.98	0.45
1:D:13:HIS:HB2	1:D:57:THR:OG1	2.17	0.45
1:D:472:GLU:O	1:D:477:LYS:HE3	2.17	0.45
1:G:329:ILE:HD11	1:G:371:ASN:HD21	1.75	0.45
1:L:112:GLU:OE1	1:L:112:GLU:N	2.30	0.45
1:A:87:LYS:HB2	3:A:625:GOL:H2	1.98	0.45
1:F:39:SER:HB3	1:F:374:GLU:OE1	2.16	0.45
1:J:433:PRO:O	1:J:436:GLU:N	2.38	0.45
1:K:110:THR:O	1:K:114:LYS:HB2	2.17	0.45
1:L:38:ASP:OD1	1:L:38:ASP:N	2.49	0.45
1:D:114:LYS:HD3	1:D:137:SER:HB2	1.99	0.45
1:E:364:ASP:CB	1:H:156:ARG:HE	2.29	0.45
1:F:160:ALA:O	1:F:161:LEU:HD23	2.17	0.45
1:J:277:ASP:HB3	1:J:289:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:337:ILE:HD13	1:L:361:PHE:CZ	2.52	0.45
1:A:88:VAL:O	3:A:625:GOL:O2	2.27	0.45
1:C:12:MET:SD	1:C:58:ILE:HG12	2.56	0.45
1:F:169:LEU:HD12	1:F:169:LEU:O	2.17	0.45
1:G:177:VAL:C	1:G:179:GLN:H	2.25	0.45
1:H:365:ASN:HB2	1:H:367:VAL:HG23	1.97	0.45
1:I:140:VAL:O	1:I:143:ILE:HG12	2.16	0.45
1:I:205:THR:HG21	1:I:208:SER:HB3	1.98	0.45
1:K:119:ARG:HA	1:K:119:ARG:NE	2.32	0.45
1:L:131:PRO:HB2	1:L:142:LYS:NZ	2.32	0.45
1:L:226:HIS:O	1:L:227:MET:HE2	2.16	0.45
1:L:342:THR:HG23	1:L:343:LYS:O	2.16	0.45
1:E:71:ASP:HA	1:E:249:LEU:HD13	1.98	0.45
1:F:195:THR:HG23	1:F:197:PHE:CD2	2.52	0.45
1:I:124:ILE:HG22	1:I:150:SER:OG	2.16	0.45
1:K:110:THR:OG1	1:K:111:LYS:N	2.50	0.45
1:K:155:THR:HG21	1:K:276:ARG:NH2	2.32	0.45
1:L:101:ARG:HD3	1:L:319:TYR:CZ	2.51	0.45
1:A:186:LYS:HE2	1:A:190:ARG:HH12	1.78	0.45
1:B:325:ILE:HD12	1:B:325:ILE:O	2.16	0.45
1:C:121:ALA:O	1:C:125:THR:OG1	2.31	0.45
1:C:351:VAL:O	1:C:355:THR:HG23	2.16	0.45
1:D:120:PHE:CZ	1:D:124:ILE:HD11	2.52	0.45
1:F:31:MET:N	1:F:48:MET:CE	2.70	0.45
1:F:438:LEU:O	1:F:442:GLN:HG3	2.17	0.45
1:G:52:LYS:HE2	1:G:54:GLU:CG	2.44	0.45
1:G:351:VAL:HG11	1:H:445:LYS:HE3	1.97	0.45
1:I:219:LYS:C	1:I:221:GLY:H	2.24	0.45
1:I:395:LYS:NZ	1:I:403:GLU:OE2	2.50	0.45
1:J:72:ARG:HB3	1:J:357:ARG:NH1	2.32	0.45
1:J:392:LEU:HA	1:J:395:LYS:HD3	1.98	0.45
1:K:39:SER:HG	1:K:374:GLU:CD	2.18	0.45
1:L:315:CYS:HB2	1:L:348:LEU:HD12	1.99	0.45
1:B:449:LEU:HD11	1:B:484:ILE:HD11	1.98	0.45
1:E:409:THR:C	1:E:411:TYR:H	2.23	0.45
1:F:169:LEU:HG	1:F:259:ILE:HG22	1.99	0.45
1:G:8:TRP:O	1:G:60:SER:OG	2.35	0.45
1:G:53:ILE:HD12	1:G:53:ILE:O	2.17	0.45
1:H:440:ILE:HG23	1:H:445:LYS:HB3	1.98	0.45
1:J:41:ALA:O	1:J:45:MET:HG3	2.17	0.45
1:K:35:PHE:CZ	1:K:48:MET:HE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:200:GLU:CG	1:L:3:ASP:HB3	2.37	0.45
1:L:36:ALA:HB2	1:L:96:ARG:HD3	1.99	0.45
1:L:325:ILE:HA	1:L:328:MET:SD	2.57	0.45
1:A:15:GLU:N	1:A:16:PRO:HD3	2.32	0.45
1:D:352:ASP:O	1:D:355:THR:HG22	2.16	0.45
1:E:98:TYR:CE2	1:E:329:ILE:HG12	2.52	0.45
1:F:452:ARG:HE	1:F:493:MET:CE	2.29	0.45
1:J:349:TYR:O	1:L:443:SER:OG	2.26	0.45
1:K:115:LYS:HG3	1:K:118:SER:CB	2.42	0.45
1:G:368:LYS:HA	1:G:368:LYS:HD3	1.70	0.45
1:H:71:ASP:HA	1:H:249:LEU:HD13	1.99	0.45
1:J:394:LEU:HD13	1:J:402:TYR:CD2	2.52	0.45
1:B:89:ASP:OD2	1:B:92:ARG:NH1	2.47	0.44
1:C:331:ARG:HE	1:C:333:LYS:HD3	1.81	0.44
1:D:200:GLU:OE2	1:G:3:ASP:HB2	2.16	0.44
1:F:131:PRO:C	1:F:133:ALA:N	2.74	0.44
1:F:171:VAL:HB	1:I:164:GLU:HG2	1.99	0.44
1:G:268:SER:HA	3:G:621:GOL:H32	1.99	0.44
1:K:169:LEU:HD22	1:K:240:LEU:HG	1.99	0.44
1:L:478:LYS:HD2	1:L:481:CYS:SG	2.57	0.44
1:A:326:GLN:C	1:A:328:MET:H	2.25	0.44
1:D:48:MET:HA	1:D:51:VAL:HG12	1.99	0.44
1:D:240:LEU:HD21	1:D:243:ILE:HD11	1.99	0.44
1:D:407:LEU:CD1	1:D:407:LEU:H	2.31	0.44
1:I:346:LYS:HD3	1:I:435:TRP:CE2	2.53	0.44
1:J:54:GLU:HG3	1:J:55:ASN:N	2.32	0.44
1:J:218:MET:CE	1:J:284:THR:HA	2.48	0.44
1:J:476:VAL:O	1:J:480:ILE:HG22	2.17	0.44
1:K:325:ILE:C	1:K:327:ASP:N	2.73	0.44
1:B:252:GLY:HA3	1:B:288:TYR:O	2.17	0.44
1:E:412:HIS:ND1	1:E:412:HIS:N	2.60	0.44
1:F:367:VAL:HG12	1:F:367:VAL:O	2.16	0.44
1:J:331:ARG:O	1:J:333:LYS:N	2.50	0.44
1:J:474:PRO:HA	1:J:477:LYS:NZ	2.32	0.44
1:B:464:ARG:HH22	1:B:472:GLU:CD	2.21	0.44
1:C:189:LYS:CE	2:C:601:SO4:O1	2.59	0.44
1:E:39:SER:OG	1:E:379:VAL:HG23	2.17	0.44
1:F:2:SER:C	1:F:4:ARG:H	2.26	0.44
1:I:5:PHE:CZ	1:I:7:ILE:HG21	2.52	0.44
1:J:37:LEU:HD11	1:J:373:ALA:HB1	1.99	0.44
1:B:320:ILE:HB	1:B:361:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:LYS:HD2	1:E:190:ARG:NH2	2.32	0.44
1:H:280:ILE:O	1:H:284:THR:HG22	2.17	0.44
1:I:457:GLU:HB2	1:I:499:TYR:CZ	2.52	0.44
1:L:239:LYS:HA	1:L:239:LYS:HD2	1.68	0.44
1:H:236:TYR:C	1:H:238:GLY:H	2.25	0.44
1:I:234:TYR:CE2	1:I:276:ARG:HD3	2.52	0.44
1:J:253:ILE:HD12	1:J:281:ILE:HG13	2.00	0.44
1:K:328:MET:C	1:K:330:SER:N	2.74	0.44
1:L:108:ASN:HB2	1:L:307:TYR:C	2.42	0.44
1:L:209:TRP:CZ3	1:L:230:VAL:HG12	2.53	0.44
1:L:218:MET:HE3	1:L:222:GLU:HG2	2.00	0.44
1:C:356:GLY:O	2:C:611:SO4:O4	2.36	0.44
1:D:323:LYS:O	1:D:326:GLN:HG2	2.17	0.44
1:F:195:THR:HG23	1:F:197:PHE:HD2	1.83	0.44
1:G:320:ILE:HG13	1:G:321:PRO:HD2	1.99	0.44
1:G:441:MET:HE1	1:G:469:PHE:CE2	2.52	0.44
1:H:93:ASN:HB3	1:H:95:CYS:O	2.18	0.44
1:J:474:PRO:HA	1:J:477:LYS:CE	2.48	0.44
1:K:346:LYS:HE3	1:K:435:TRP:CD2	2.53	0.44
1:C:325:ILE:HG13	1:C:328:MET:HB2	1.99	0.44
1:D:327:ASP:HA	1:D:330:SER:CB	2.45	0.44
1:F:56:CYS:N	1:F:93:ASN:OD1	2.38	0.44
1:G:118:SER:O	1:G:122:THR:HG23	2.18	0.44
1:G:472:GLU:HB3	1:G:476:VAL:HG13	1.99	0.44
1:I:163:SER:HB3	1:I:166:LYS:HD3	2.00	0.44
1:K:258:PHE:CE1	1:K:273:SER:HB3	2.53	0.44
1:L:482:ASP:O	1:L:485:ARG:HB2	2.18	0.44
1:C:122:THR:CB	1:C:123:ARG:HG3	2.48	0.44
1:C:428:VAL:HB	1:C:431:LEU:HD22	2.00	0.44
1:F:109:MET:HE1	1:F:113:LEU:O	2.18	0.44
1:G:120:PHE:CD1	1:G:272:LEU:HD21	2.52	0.44
1:H:284:THR:HG21	1:H:286:LEU:CD1	2.48	0.44
1:I:485:ARG:HE	1:I:485:ARG:HB3	1.51	0.44
1:J:111:LYS:C	1:J:113:LEU:H	2.25	0.44
1:C:323:LYS:O	1:C:326:GLN:CB	2.66	0.43
1:C:365:ASN:ND2	1:C:368:LYS:HG3	2.33	0.43
1:D:260:TRP:CZ3	1:D:262:PRO:HA	2.53	0.43
1:F:2:SER:C	1:F:4:ARG:N	2.73	0.43
1:G:5:PHE:HE1	1:G:65:MET:CE	2.31	0.43
1:G:313:ASP:O	1:G:317:SER:N	2.51	0.43
1:J:468:ASN:OD1	1:J:471:SER:OG	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:328:MET:HG2	1:K:371:ASN:HD22	1.83	0.43
1:L:73:MET:HE2	1:L:73:MET:HB2	1.51	0.43
1:B:44:TYR:O	1:B:48:MET:HG3	2.18	0.43
1:F:406:ASP:OD2	1:F:410:ILE:HG22	2.18	0.43
1:F:489:PHE:O	1:F:493:MET:HG3	2.19	0.43
1:G:340:GLU:H	1:G:340:GLU:HG2	1.61	0.43
1:H:45:MET:H	1:H:45:MET:HG2	1.67	0.43
1:I:2:SER:HA	1:I:64:HIS:NE2	2.34	0.43
1:I:406:ASP:C	1:I:408:ASP:N	2.75	0.43
1:J:218:MET:C	1:J:219:LYS:HG3	2.42	0.43
1:B:107:LEU:HD12	1:B:307:TYR:N	2.32	0.43
1:C:494:LYS:HB2	1:C:494:LYS:HE2	1.80	0.43
1:J:320:ILE:HG21	1:J:337:ILE:CD1	2.45	0.43
1:K:115:LYS:O	1:K:118:SER:N	2.51	0.43
1:L:42:HIS:O	1:L:42:HIS:ND1	2.45	0.43
1:B:283:ARG:HD3	1:B:283:ARG:HA	1.71	0.43
1:D:154:TYR:HE2	1:D:156:ARG:NE	2.17	0.43
1:G:144:VAL:HG13	1:G:216:GLN:HB3	2.01	0.43
1:H:390:SER:HB2	1:H:434:LEU:HB3	2.01	0.43
1:I:205:THR:OG1	1:I:208:SER:N	2.51	0.43
1:K:52:LYS:NZ	1:K:411:TYR:O	2.47	0.43
1:K:119:ARG:NH2	1:K:122:THR:OG1	2.47	0.43
1:A:114:LYS:HE2	1:A:136:SER:O	2.19	0.43
1:E:232:GLU:HB3	1:E:244:THR:CG2	2.48	0.43
1:F:12:MET:HE2	1:F:12:MET:HB3	1.80	0.43
1:F:428:VAL:HB	1:F:431:LEU:HD22	2.01	0.43
1:H:72:ARG:HH22	1:H:490:GLU:HB2	1.83	0.43
1:H:164:GLU:HG2	3:H:617:GOL:C3	2.46	0.43
1:I:252:GLY:HA2	1:I:286:LEU:HB3	2.00	0.43
1:K:456:PHE:HB3	1:K:498:LEU:HD22	2.00	0.43
1:L:453:LEU:HD11	1:L:497:ILE:HG12	2.00	0.43
1:A:12:MET:SD	1:A:58:ILE:HG12	2.58	0.43
1:B:10:PRO:HG2	1:B:482:ASP:HB3	2.00	0.43
1:E:138:ASP:O	1:E:141:GLY:N	2.48	0.43
1:F:89:ASP:CG	1:F:92:ARG:HB2	2.44	0.43
1:F:203:LEU:HD22	1:H:454:PHE:CE2	2.54	0.43
1:H:139:PHE:HD1	1:H:139:PHE:H	1.66	0.43
1:J:186:LYS:HE2	1:J:190:ARG:NE	2.32	0.43
1:J:211:GLN:HE22	1:J:224:LEU:HA	1.82	0.43
1:J:453:LEU:HD22	1:J:480:ILE:HD12	2.01	0.43
1:J:468:ASN:HD22	1:L:341:GLU:CD	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:456:PHE:CE1	1:K:462:GLY:HA2	2.53	0.43
1:E:365:ASN:HB2	1:E:367:VAL:O	2.18	0.43
1:F:144:VAL:HG13	1:F:216:GLN:HG2	1.99	0.43
1:F:341:GLU:O	1:F:341:GLU:CG	2.67	0.43
1:H:227:MET:HB3	1:H:227:MET:HE3	1.29	0.43
1:J:107:LEU:HD12	1:J:307:TYR:N	2.33	0.43
1:J:261:ASP:HB3	1:J:264:TYR:CD1	2.53	0.43
1:J:394:LEU:CD1	1:J:402:TYR:HD2	2.31	0.43
1:L:58:ILE:CG2	1:L:486:LEU:HD21	2.46	0.43
1:L:62:VAL:HG11	1:L:65:MET:HE3	1.99	0.43
1:B:226:HIS:O	1:B:227:MET:HE2	2.19	0.43
1:B:466:LEU:HD11	1:B:469:PHE:HA	2.01	0.43
1:D:31:MET:HA	1:D:33:GLN:OE1	2.19	0.43
1:E:132:ALA:O	1:E:134:VAL:HG12	2.17	0.43
1:F:448:ASP:OD1	3:F:615:GOL:H12	2.19	0.43
1:H:65:MET:HE2	1:H:196:PRO:HG2	2.00	0.43
1:K:123:ARG:NE	1:K:236:TYR:OH	2.45	0.43
1:L:98:TYR:OH	1:L:333:LYS:N	2.51	0.43
1:C:106:GLU:CD	1:C:309:ALA:HA	2.44	0.43
1:F:224:LEU:HD22	1:F:284:THR:HB	2.00	0.43
1:G:97:LEU:HD22	1:G:292:GLY:O	2.18	0.43
1:I:113:LEU:HD22	1:I:114:LYS:HE3	2.00	0.43
1:J:36:ALA:O	1:J:333:LYS:HB3	2.18	0.43
1:J:43:ARG:HH22	1:J:408:ASP:CG	2.27	0.43
1:J:117:ILE:HD12	1:J:117:ILE:H	1.84	0.43
1:K:145:ASN:HA	1:K:148:MET:CB	2.39	0.43
1:K:320:ILE:CD1	1:K:337:ILE:HD11	2.49	0.43
1:K:379:VAL:HG23	1:K:380:GLY:N	2.34	0.43
1:L:146:ALA:O	1:L:150:SER:HB2	2.19	0.43
1:L:252:GLY:HA2	1:L:286:LEU:HB3	2.01	0.43
1:A:90:PRO:HG2	1:A:429:PRO:HB2	2.00	0.43
1:C:218:MET:HE3	1:C:222:GLU:HG3	2.01	0.43
1:C:331:ARG:HE	1:C:333:LYS:CD	2.32	0.43
1:E:134:VAL:HB	1:E:142:LYS:CD	2.49	0.43
1:J:136:SER:HB2	1:K:132:ALA:HB2	2.01	0.43
1:K:339:GLU:OE2	1:K:367:VAL:HG21	2.17	0.43
1:L:134:VAL:O	1:L:142:LYS:HE3	2.19	0.43
1:F:71:ASP:OD2	1:F:250:PRO:HD2	2.19	0.42
1:G:121:ALA:O	1:G:125:THR:HG23	2.19	0.42
1:G:239:LYS:HE3	1:G:241:ILE:HG22	2.01	0.42
1:G:314:VAL:HG22	3:G:623:GOL:C1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:406:ASP:HB3	1:H:408:ASP:CG	2.43	0.42
1:J:98:TYR:CZ	1:J:329:ILE:HG23	2.53	0.42
1:J:481:CYS:HA	1:J:484:ILE:CG1	2.38	0.42
1:K:320:ILE:HD11	1:K:335:PHE:CE2	2.53	0.42
1:L:374:GLU:C	1:L:376:ILE:N	2.77	0.42
1:A:101:ARG:HG2	1:A:319:TYR:CE2	2.54	0.42
1:B:31:MET:HE3	1:B:31:MET:HB3	1.86	0.42
1:B:101:ARG:NH1	4:B:701:HOH:O	2.31	0.42
1:B:336:VAL:HG12	1:B:373:ALA:HB2	2.01	0.42
1:D:7:ILE:HG22	1:D:62:VAL:HG22	2.00	0.42
1:I:405:GLU:HG3	1:I:426:ASN:ND2	2.34	0.42
1:J:326:GLN:O	1:J:328:MET:N	2.51	0.42
1:J:470:TYR:CE1	1:L:342:THR:HG21	2.54	0.42
1:K:148:MET:SD	1:K:149:ASN:OD1	2.76	0.42
1:L:79:ARG:HD2	1:L:292:GLY:HA3	2.02	0.42
1:A:101:ARG:HD2	1:A:288:TYR:CD1	2.54	0.42
1:B:96:ARG:C	1:B:97:LEU:HD23	2.44	0.42
1:B:115:LYS:HA	1:B:118:SER:OG	2.20	0.42
1:B:323:LYS:O	1:B:324:PRO:C	2.60	0.42
1:C:464:ARG:HH21	1:C:472:GLU:CD	2.27	0.42
1:E:388:ASN:HB3	1:E:404:GLU:HG3	2.01	0.42
1:F:104:PRO:HG2	1:F:282:GLN:HB2	2.02	0.42
1:F:195:THR:HG22	1:F:197:PHE:N	2.27	0.42
1:H:248:ILE:HG12	1:H:253:ILE:CD1	2.45	0.42
1:J:189:LYS:HB2	1:J:189:LYS:HE2	1.74	0.42
1:K:48:MET:C	1:K:50:VAL:H	2.27	0.42
1:K:130:CYS:HB2	1:K:131:PRO:CD	2.37	0.42
1:K:217:ARG:O	1:K:217:ARG:CG	2.66	0.42
1:K:432:LEU:HB2	1:K:485:ARG:HA	2.00	0.42
1:A:385:LYS:O	1:A:389:GLU:HG3	2.20	0.42
1:C:40:TRP:CE2	1:C:410:ILE:HG13	2.55	0.42
1:E:486:LEU:HD21	1:E:487:PHE:CZ	2.54	0.42
1:F:464:ARG:HG3	1:F:464:ARG:HH11	1.83	0.42
1:I:110:THR:HA	1:I:114:LYS:HD3	2.00	0.42
1:J:312:LEU:HB2	1:J:319:TYR:CE2	2.55	0.42
1:J:453:LEU:CD2	1:J:480:ILE:HD12	2.49	0.42
1:K:4:ARG:HA	1:K:4:ARG:HD3	1.73	0.42
1:K:39:SER:CB	1:K:379:VAL:HG13	2.48	0.42
1:A:408:ASP:OD1	1:A:408:ASP:N	2.53	0.42
1:D:78:PHE:CZ	1:D:87:LYS:HD2	2.54	0.42
1:E:88:VAL:H	3:E:626:GOL:H12	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:TRP:HB3	1:F:269:LEU:CD2	2.49	0.42
1:G:80:ARG:HA	1:G:84:PHE:O	2.19	0.42
1:G:322:LEU:HD11	1:G:326:GLN:HG3	2.01	0.42
1:G:325:ILE:CD1	1:G:337:ILE:CD1	2.97	0.42
1:J:477:LYS:HE3	1:J:477:LYS:HB2	1.69	0.42
1:K:173:TYR:O	1:K:177:VAL:HB	2.19	0.42
1:K:226:HIS:HA	2:K:607:SO4:O2	2.20	0.42
1:K:292:GLY:O	1:K:293:TYR:HB2	2.20	0.42
1:K:389:GLU:O	1:K:393:GLU:HG2	2.19	0.42
1:L:167:TYR:O	1:L:171:VAL:HG23	2.20	0.42
1:A:45:MET:O	1:A:48:MET:N	2.52	0.42
1:E:7:ILE:HG22	1:E:62:VAL:HG22	2.00	0.42
1:E:38:ASP:CG	1:E:333:LYS:NZ	2.74	0.42
1:E:45:MET:HG3	1:E:46:ASN:N	2.34	0.42
1:E:106:GLU:HB3	1:E:308:GLY:O	2.19	0.42
1:E:334:LEU:HD23	1:E:373:ALA:CB	2.49	0.42
1:E:346:LYS:HD3	1:E:435:TRP:CE2	2.54	0.42
1:F:79:ARG:NH2	1:F:254:SER:OG	2.53	0.42
1:G:62:VAL:HG11	1:G:65:MET:HE3	2.00	0.42
1:H:326:GLN:C	1:H:328:MET:H	2.26	0.42
1:H:346:LYS:HD3	1:H:435:TRP:CE2	2.54	0.42
1:I:13:HIS:O	1:I:56:CYS:CB	2.68	0.42
1:J:344:VAL:CG1	1:L:442:GLN:OE1	2.62	0.42
1:J:370:LYS:HG2	1:J:371:ASN:N	2.33	0.42
1:K:189:LYS:HD2	1:L:461:GLU:HB3	2.01	0.42
1:L:155:THR:HA	1:L:233:CYS:O	2.19	0.42
1:A:164:GLU:HG3	1:A:168[A]:HIS:NE2	2.34	0.42
1:B:135:ALA:CA	1:G:132:ALA:HB2	2.49	0.42
1:B:144:VAL:O	1:B:148:MET:HB2	2.19	0.42
1:B:352:ASP:OD2	1:B:490:GLU:N	2.35	0.42
1:F:44:TYR:HD2	1:F:51:VAL:HG11	1.84	0.42
1:H:284:THR:HG21	1:H:286:LEU:HD12	2.02	0.42
1:I:97:LEU:HD13	1:I:97:LEU:HA	1.94	0.42
1:J:215:TRP:CD2	1:J:280:ILE:HG12	2.55	0.42
1:L:476:VAL:O	1:L:480:ILE:HD12	2.20	0.42
1:B:65:MET:HE2	1:B:196:PRO:CG	2.49	0.42
1:D:119:ARG:O	1:D:119:ARG:HG2	2.20	0.42
1:D:454:PHE:HB2	1:D:496:VAL:HG22	2.01	0.42
1:H:473:PRO:HB2	1:H:476:VAL:HG23	2.01	0.42
1:I:117:ILE:HG13	1:I:275:LEU:HD23	2.01	0.42
1:J:169:LEU:HD12	1:J:169:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:392:LEU:HA	1:J:395:LYS:CD	2.49	0.42
1:L:372:ILE:O	1:L:375:GLU:HG2	2.19	0.42
1:C:89:ASP:OD1	1:C:89:ASP:C	2.62	0.42
1:D:124:ILE:HG21	1:D:153:PHE:HB3	2.01	0.42
1:F:89:ASP:HA	1:F:90:PRO:HD3	1.95	0.42
1:G:392:LEU:HD21	1:G:404:GLU:OE1	2.20	0.42
1:H:218:MET:O	1:H:219:LYS:HG2	2.20	0.42
1:I:347:GLU:CD	1:I:433:PRO:HB3	2.44	0.42
1:J:209:TRP:O	1:J:213:ASN:ND2	2.52	0.42
1:L:320:ILE:HG13	1:L:325:ILE:HD11	2.02	0.42
1:A:388:ASN:CB	1:A:404:GLU:HG2	2.48	0.42
1:B:140:VAL:O	1:B:144:VAL:HG23	2.20	0.42
1:C:182:ASN:ND2	1:D:459:GLU:HB3	2.35	0.42
1:F:35:PHE:O	1:F:333:LYS:NZ	2.50	0.42
1:L:323:LYS:N	1:L:324:PRO:CD	2.83	0.42
1:A:32:ASP:OD1	1:A:33:GLN:HG2	2.20	0.41
1:B:64:HIS:HA	1:B:196:PRO:O	2.20	0.41
1:B:320:ILE:HG13	1:B:321:PRO:CD	2.51	0.41
1:C:122:THR:HB	1:C:123:ARG:HG3	2.02	0.41
1:C:368:LYS:H	1:C:368:LYS:HE2	1.84	0.41
1:D:105:GLN:O	1:D:105:GLN:CG	2.67	0.41
1:F:266:LYS:HG3	1:F:267:TRP:HD1	1.85	0.41
1:I:85:LEU:HD12	1:I:85:LEU:HA	1.92	0.41
1:I:236:TYR:O	1:I:237:GLU:HB3	2.20	0.41
1:K:379:VAL:HG23	1:K:380:GLY:H	1.83	0.41
1:L:40:TRP:HE1	1:L:378:GLY:HA2	1.85	0.41
1:A:183:ASN:O	1:K:474:PRO:HD3	2.21	0.41
1:B:200:GLU:HB2	1:E:2:SER:HB3	2.01	0.41
1:B:401:PRO:HD2	1:B:478:LYS:HB2	2.02	0.41
1:C:79:ARG:NH2	1:C:254:SER:OG	2.52	0.41
1:E:126:SER:OG	1:E:127:GLU:N	2.53	0.41
1:F:98:TYR:CZ	1:F:329:ILE:HG12	2.55	0.41
1:G:11:SER:OG	1:G:13:HIS:NE2	2.52	0.41
1:H:99:THR:HA	1:H:292:GLY:HA2	2.02	0.41
1:H:236:TYR:C	1:H:238:GLY:N	2.77	0.41
1:H:368:LYS:HB2	1:H:368:LYS:HE2	1.61	0.41
1:H:402:TYR:CZ	1:H:478:LYS:HE2	2.55	0.41
1:J:186:LYS:HE2	1:J:190:ARG:CZ	2.50	0.41
1:J:367:VAL:O	1:J:368:LYS:HB2	2.20	0.41
1:K:148:MET:SD	1:K:149:ASN:ND2	2.93	0.41
1:L:469:PHE:HE1	1:L:480:ILE:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASP:OD1	1:A:89:ASP:C	2.63	0.41
1:B:463:ILE:HD13	1:B:463:ILE:HG21	1.76	0.41
1:D:207:GLU:CD	1:D:207:GLU:H	2.28	0.41
1:E:45:MET:HG3	1:E:46:ASN:H	1.86	0.41
1:F:346:LYS:HE3	1:F:435:TRP:CZ2	2.55	0.41
1:F:354:GLU:HG2	1:F:359:GLU:CD	2.45	0.41
1:G:322:LEU:CD1	1:G:326:GLN:CG	2.98	0.41
1:H:458:ILE:H	1:H:458:ILE:HG23	1.61	0.41
1:I:7:ILE:O	1:I:7:ILE:HG13	2.21	0.41
1:J:162:TYR:OH	1:J:164:GLU:HG2	2.21	0.41
1:L:121:ALA:O	1:L:125:THR:HG22	2.21	0.41
1:C:33:GLN:N	1:C:33:GLN:OE1	2.54	0.41
1:C:117:ILE:CD1	1:C:139:PHE:HB2	2.49	0.41
1:C:326:GLN:C	1:C:326:GLN:CD	2.85	0.41
1:D:323:LYS:HB2	1:D:324:PRO:HD3	2.02	0.41
1:D:398:TYR:OH	1:D:442:GLN:HA	2.20	0.41
1:E:8:TRP:CH2	1:E:458:ILE:HD13	2.44	0.41
1:H:291:LEU:C	1:H:293:TYR:H	2.28	0.41
1:I:157:PHE:HZ	1:I:280:ILE:HD13	1.84	0.41
1:I:349:TYR:HA	1:I:436:GLU:OE1	2.19	0.41
1:J:91:LEU:CD1	1:J:377:TYR:HB3	2.51	0.41
1:K:33:GLN:CG	1:K:34:LEU:H	2.25	0.41
1:K:341:GLU:O	1:K:341:GLU:CG	2.69	0.41
1:L:103:ALA:O	1:L:104:PRO:C	2.63	0.41
1:L:125:THR:HG21	1:L:129:TYR:CD2	2.56	0.41
1:B:234:TYR:HB2	1:B:242:ALA:HB3	2.03	0.41
1:C:171:VAL:HG13	1:G:164:GLU:HG2	2.03	0.41
1:C:248:ILE:HD13	1:C:253:ILE:HG12	2.03	0.41
1:F:453:LEU:HD11	1:F:497:ILE:HG13	2.03	0.41
1:G:55:ASN:HA	1:G:93:ASN:OD1	2.21	0.41
1:G:177:VAL:HG12	1:G:178:HIS:ND1	2.35	0.41
1:G:327:ASP:OD1	1:G:327:ASP:N	2.52	0.41
1:H:406:ASP:OD1	1:H:407:LEU:N	2.54	0.41
1:I:4:ARG:HA	1:I:4:ARG:HD3	1.71	0.41
1:I:78:PHE:CZ	1:I:87:LYS:HD2	2.55	0.41
1:J:113:LEU:O	1:J:116:CYS:HB3	2.20	0.41
1:J:457:GLU:O	1:J:460:THR:HG22	2.21	0.41
1:K:218:MET:HE1	1:K:284:THR:HA	1.95	0.41
1:K:390:SER:OG	2:K:603:SO4:O3	2.38	0.41
1:A:128:ASP:OD1	1:A:128:ASP:N	2.53	0.41
1:D:385:LYS:HE3	1:D:389:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:VAL:HB	1:E:142:LYS:CG	2.51	0.41
1:F:370:LYS:HG2	1:F:371:ASN:N	2.35	0.41
1:G:72:ARG:HG3	1:G:357:ARG:NH1	2.35	0.41
1:H:39:SER:OG	1:H:379:VAL:HG23	2.21	0.41
1:I:480:ILE:O	1:I:484:ILE:HG13	2.20	0.41
1:J:312:LEU:HD11	1:J:317:SER:HA	2.01	0.41
1:J:449:LEU:HD12	1:J:480:ILE:HD11	2.03	0.41
1:K:71:ASP:HA	1:K:249:LEU:HD13	2.03	0.41
1:K:134:VAL:HG12	1:K:135:ALA:H	1.86	0.41
1:L:44:TYR:HB2	1:L:46:ASN:OD1	2.20	0.41
1:L:72:ARG:NH2	1:L:490:GLU:OE2	2.48	0.41
1:L:276:ARG:O	1:L:280:ILE:HG13	2.21	0.41
1:L:309:ALA:C	1:L:322:LEU:HG	2.45	0.41
1:A:331:ARG:O	1:A:333:LYS:HG2	2.21	0.41
1:D:461:GLU:HG3	1:G:189:LYS:HE2	2.03	0.41
1:G:2:SER:C	1:G:4:ARG:N	2.77	0.41
1:G:104:PRO:HG2	1:G:282:GLN:HB2	2.02	0.41
1:H:5:PHE:CE2	1:H:7:ILE:HG21	2.54	0.41
1:I:152:THR:HG22	1:I:236:TYR:CE1	2.56	0.41
1:J:71:ASP:HB2	1:J:250:PRO:HD2	2.02	0.41
1:K:65:MET:HE2	1:K:65:MET:HB3	1.84	0.41
1:K:134:VAL:HG11	1:K:142:LYS:CD	2.51	0.41
1:L:106:GLU:HG2	1:L:308:GLY:O	2.21	0.41
1:C:144:VAL:HG13	1:C:216:GLN:HB3	2.02	0.41
1:C:215:TRP:CE2	1:C:216:GLN:HG2	2.56	0.41
1:E:328:MET:HE2	1:E:328:MET:HB2	1.80	0.41
1:F:90:PRO:HD2	1:F:429:PRO:HD2	2.01	0.41
1:F:222:GLU:O	1:F:285:ASN:ND2	2.50	0.41
1:F:407:LEU:HD12	1:F:407:LEU:HA	1.93	0.41
1:G:65:MET:CE	1:G:85:LEU:HD22	2.47	0.41
1:I:13:HIS:O	1:I:56:CYS:HB3	2.21	0.41
1:I:276:ARG:O	1:I:279:ALA:HB3	2.20	0.41
1:I:316:HIS:O	1:I:318:LYS:HG3	2.21	0.41
1:J:45:MET:HB2	1:J:45:MET:HE3	1.71	0.41
1:J:366:VAL:O	1:J:366:VAL:HG23	2.20	0.41
1:A:5:PHE:CZ	1:A:7:ILE:HG21	2.56	0.41
1:A:176:LYS:HB2	1:A:262:PRO:HG2	2.01	0.41
1:B:58:ILE:HG23	1:B:424:ILE:HG12	2.03	0.41
1:B:97:LEU:HD13	1:B:293:TYR:HB2	2.02	0.41
1:B:432:LEU:HD21	1:B:436:GLU:HG2	2.03	0.41
1:C:405:GLU:C	1:C:409:THR:HG21	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:PHE:O	1:D:333:LYS:HE3	2.21	0.41
1:E:89:ASP:C	1:E:89:ASP:OD1	2.64	0.41
1:E:456:PHE:C	1:E:456:PHE:CD1	2.99	0.41
1:F:148:MET:HE1	1:F:217:ARG:HG2	2.02	0.41
1:G:53:ILE:HG22	1:G:411:TYR:CD1	2.56	0.41
1:G:170:PHE:O	1:G:174:GLN:HB2	2.20	0.41
1:G:258:PHE:CE1	1:G:273:SER:HB2	2.56	0.41
1:G:260:TRP:CZ3	1:G:262:PRO:HA	2.56	0.41
1:G:351:VAL:O	1:G:355:THR:HG23	2.21	0.41
1:H:120:PHE:CD1	1:H:272:LEU:HD21	2.56	0.41
1:J:211:GLN:OE1	1:J:224:LEU:HD12	2.21	0.41
1:J:316:HIS:CG	1:J:361:PHE:HZ	2.39	0.41
1:L:4:ARG:HD2	1:L:494:LYS:O	2.21	0.41
1:L:98:TYR:CE2	1:L:329:ILE:HG21	2.56	0.41
1:L:172:LYS:CE	2:L:611:SO4:O4	2.69	0.41
1:A:235:TYR:OH	2:A:616:SO4:O3	2.38	0.41
1:C:107:LEU:HD12	1:C:107:LEU:HA	1.81	0.41
1:C:113:LEU:HD23	1:C:113:LEU:HA	1.82	0.41
1:C:341:GLU:O	1:C:341:GLU:HG3	2.19	0.41
1:G:92:ARG:HG2	1:G:410:ILE:HD12	2.03	0.41
1:K:111:LYS:H	1:K:111:LYS:HD2	1.86	0.41
1:K:323:LYS:N	1:K:324:PRO:HD2	2.36	0.41
1:D:269:LEU:HD23	1:D:269:LEU:HA	1.77	0.40
1:D:428:VAL:HB	1:D:431:LEU:HD22	2.03	0.40
1:F:215:TRP:O	1:F:218:MET:HB2	2.21	0.40
1:H:326:GLN:HG3	1:H:329:ILE:CD1	2.42	0.40
1:I:409:THR:O	1:I:409:THR:HG22	2.21	0.40
1:J:208:SER:HB3	1:J:225:LYS:CG	2.51	0.40
1:K:207:GLU:OE2	1:L:452:ARG:NH1	2.54	0.40
1:K:326:GLN:O	1:K:326:GLN:HG2	2.21	0.40
1:K:372:ILE:HD12	1:K:376:ILE:HD11	2.03	0.40
1:L:79:ARG:NH1	1:L:292:GLY:C	2.73	0.40
1:B:486:LEU:HD12	1:B:486:LEU:HA	1.95	0.40
1:F:318:LYS:HA	1:F:359:GLU:O	2.22	0.40
1:F:393:GLU:CB	1:F:397:LEU:CD1	2.98	0.40
1:G:131:PRO:HG2	1:G:134:VAL:CG2	2.51	0.40
1:G:245:VAL:HG12	1:G:256:VAL:HB	2.03	0.40
1:G:407:LEU:HD12	1:G:407:LEU:H	1.87	0.40
1:G:483:VAL:HG21	1:G:497:ILE:CD1	2.51	0.40
1:H:136:SER:OG	1:H:137:SER:N	2.53	0.40
1:H:157:PHE:N	1:H:213:ASN:OD1	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:426:ASN:HB3	1:H:434:LEU:HD22	2.02	0.40
1:I:330:SER:OG	1:I:331:ARG:N	2.54	0.40
1:J:162:TYR:CD1	1:J:162:TYR:C	2.99	0.40
1:L:337:ILE:HG21	1:L:361:PHE:CZ	2.56	0.40
1:A:260:TRP:CZ3	1:A:262:PRO:HA	2.56	0.40
1:A:291:LEU:HD13	1:A:291:LEU:HA	1.84	0.40
1:B:472:GLU:O	1:B:477:LYS:HE2	2.21	0.40
1:E:169:LEU:HD23	1:E:243:ILE:HG13	2.03	0.40
1:E:437:LEU:HD11	1:E:441:MET:HE1	2.04	0.40
1:F:456:PHE:HB3	1:F:498:LEU:HD12	2.04	0.40
1:H:311:VAL:CG2	1:H:322:LEU:HD13	2.50	0.40
1:J:344:VAL:HG11	1:J:348:LEU:HD23	2.04	0.40
1:J:367:VAL:O	1:J:368:LYS:HE2	2.21	0.40
1:K:12:MET:HE2	1:K:56:CYS:HB3	2.02	0.40
1:K:12:MET:HG2	1:K:58:ILE:CD1	2.52	0.40
1:A:15:GLU:HG2	1:A:55:ASN:HB3	2.03	0.40
1:B:113:LEU:HD22	1:B:275:LEU:HD11	2.03	0.40
1:B:331:ARG:O	1:B:333:LYS:N	2.55	0.40
1:D:464:ARG:NH2	1:D:472:GLU:OE2	2.46	0.40
1:E:78:PHE:HZ	1:E:486:LEU:HD12	1.83	0.40
1:E:377:TYR:CZ	1:E:429:PRO:HG3	2.56	0.40
1:F:98:TYR:CD2	1:F:329:ILE:HG23	2.56	0.40
1:F:266:LYS:HB2	1:F:266:LYS:HE3	1.78	0.40
1:F:393:GLU:O	1:F:397:LEU:HB2	2.21	0.40
1:G:158:GLU:OE2	3:G:619:GOL:O3	2.24	0.40
1:H:43:ARG:HD2	1:H:379:VAL:HG21	2.02	0.40
1:H:45:MET:O	1:H:48:MET:HE3	2.22	0.40
1:H:227:MET:HE1	1:H:249:LEU:C	2.46	0.40
1:H:337:ILE:HG23	1:H:369:TYR:HB3	2.03	0.40
1:J:121:ALA:HA	1:J:124:ILE:HD11	2.03	0.40
1:K:70:TYR:OH	1:K:80:ARG:HG2	2.21	0.40
1:K:155:THR:HA	1:K:233:CYS:O	2.22	0.40
1:K:323:LYS:O	1:K:325:ILE:N	2.54	0.40
1:L:10:PRO:HB3	1:L:60:SER:OG	2.21	0.40
1:L:320:ILE:CG1	1:L:325:ILE:HD11	2.51	0.40
1:L:441:MET:HE1	1:L:469:PHE:CE2	2.56	0.40
1:F:33:GLN:O	1:F:96:ARG:NH2	2.54	0.40
1:F:192:LEU:HD13	1:F:245:VAL:HG21	2.04	0.40
1:G:167:TYR:O	1:G:170:PHE:HB3	2.21	0.40
1:I:109:MET:H	1:I:114:LYS:HZ2	1.68	0.40
1:J:316:HIS:NE2	1:J:337:ILE:O	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:432:LEU:HD22	1:J:436:GLU:HG2	2.03	0.40
1:J:445:LYS:HB2	1:L:349:TYR:CB	2.46	0.40

All (4) 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:L:217:ARG:NH1	2:A:612:SO4:O3[4_555]	1.42	0.78
1:A:363:THR:CG2	1:L:210:GLU:OE2[3_554]	2.02	0.18
1:I:219:LYS:NZ	1:L:285:ASN:ND2[1_554]	2.14	0.06
1:A:217:ARG:CG	1:I:106:GLU:OE2[3_555]	2.15	0.05

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	459/518 (89%)	435 (95%)	24 (5%)	0	100	100
1	B	456/518 (88%)	436 (96%)	20 (4%)	0	100	100
1	C	455/518 (88%)	425 (93%)	30 (7%)	0	100	100
1	D	446/518 (86%)	420 (94%)	26 (6%)	0	100	100
1	E	455/518 (88%)	428 (94%)	26 (6%)	1 (0%)	43	62
1	F	456/518 (88%)	423 (93%)	33 (7%)	0	100	100
1	G	447/518 (86%)	417 (93%)	28 (6%)	2 (0%)	30	48
1	H	348/518 (67%)	331 (95%)	17 (5%)	0	100	100
1	I	442/518 (85%)	395 (89%)	47 (11%)	0	100	100
1	J	435/518 (84%)	394 (91%)	41 (9%)	0	100	100
1	K	449/518 (87%)	415 (92%)	32 (7%)	2 (0%)	30	48
1	L	425/518 (82%)	385 (91%)	39 (9%)	1 (0%)	43	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5273/6216 (85%)	4904 (93%)	363 (7%)	6 (0%)	48 68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	130	CYS
1	K	131	PRO
1	E	139	PHE
1	G	131	PRO
1	G	134	VAL
1	L	324	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

244 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	613	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	A	617	-	4,4,4	0.44	0	6,6,6	0.11	0
2	SO4	E	603	-	4,4,4	0.38	0	6,6,6	0.06	0
2	SO4	C	612	-	4,4,4	0.24	0	6,6,6	0.27	0
2	SO4	C	621	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	K	605	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	E	619	-	4,4,4	0.23	0	6,6,6	0.17	0
2	SO4	C	610	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	F	610	-	4,4,4	0.26	0	6,6,6	0.14	0
2	SO4	G	607	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	F	601	-	4,4,4	0.30	0	6,6,6	0.44	0
2	SO4	H	609	-	4,4,4	0.22	0	6,6,6	0.27	0
2	SO4	H	602	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	D	607	-	4,4,4	0.26	0	6,6,6	0.35	0
2	SO4	A	615	-	4,4,4	0.25	0	6,6,6	0.16	0
2	SO4	B	615	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	D	619	-	4,4,4	0.22	0	6,6,6	0.22	0
2	SO4	L	608	-	4,4,4	0.42	0	6,6,6	0.10	0
2	SO4	E	611	-	4,4,4	0.32	0	6,6,6	0.36	0
2	SO4	I	603	-	4,4,4	0.23	0	6,6,6	0.21	0
2	SO4	B	605	-	4,4,4	0.42	0	6,6,6	0.08	0
2	SO4	K	606	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	B	622	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	H	605	-	4,4,4	0.50	0	6,6,6	0.11	0
2	SO4	A	614	-	4,4,4	0.26	0	6,6,6	0.19	0
2	SO4	I	611	-	4,4,4	0.46	0	6,6,6	0.11	0
2	SO4	H	612	-	4,4,4	0.45	0	6,6,6	0.10	0
2	SO4	G	606	-	4,4,4	0.26	0	6,6,6	0.24	0
3	GOL	H	616	-	5,5,5	0.91	0	5,5,5	1.21	1 (20%)
2	SO4	D	613	-	4,4,4	0.38	0	6,6,6	0.06	0
2	SO4	B	617	-	4,4,4	0.25	0	6,6,6	0.12	0
3	GOL	K	613	-	5,5,5	1.24	0	5,5,5	0.97	0
2	SO4	E	623	-	4,4,4	0.23	0	6,6,6	0.14	0
3	GOL	A	624	-	5,5,5	1.21	0	5,5,5	1.10	0
2	SO4	C	618	-	4,4,4	0.45	0	6,6,6	0.11	0
2	SO4	A	616	-	4,4,4	0.23	0	6,6,6	0.09	0
3	GOL	A	630	-	5,5,5	1.14	0	5,5,5	0.83	0
2	SO4	F	608	-	4,4,4	0.30	0	6,6,6	0.23	0
3	GOL	G	618	-	5,5,5	0.83	0	5,5,5	1.22	1 (20%)
3	GOL	G	623	-	5,5,5	0.69	0	5,5,5	1.42	1 (20%)
2	SO4	D	620	-	4,4,4	0.48	0	6,6,6	0.09	0
2	SO4	A	602	-	4,4,4	0.22	0	6,6,6	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	L	604	-	4,4,4	0.44	0	6,6,6	0.08	0
2	SO4	I	604	-	4,4,4	0.25	0	6,6,6	0.18	0
2	SO4	D	608	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	L	605	-	4,4,4	0.27	0	6,6,6	0.43	0
2	SO4	F	602	-	4,4,4	0.25	0	6,6,6	0.14	0
2	SO4	E	602	-	4,4,4	0.20	0	6,6,6	0.14	0
2	SO4	I	609	-	4,4,4	0.38	0	6,6,6	0.10	0
2	SO4	C	608	-	4,4,4	0.22	0	6,6,6	0.20	0
2	SO4	I	602	-	4,4,4	0.25	0	6,6,6	0.19	0
2	SO4	L	610	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	D	602	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	I	608	-	4,4,4	0.28	0	6,6,6	0.14	0
2	SO4	I	606	-	4,4,4	0.50	0	6,6,6	0.10	0
2	SO4	L	607	-	4,4,4	0.28	0	6,6,6	0.09	0
2	SO4	B	621	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	A	618	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	C	609	-	4,4,4	0.30	0	6,6,6	0.24	0
2	SO4	H	607	-	4,4,4	0.22	0	6,6,6	0.18	0
2	SO4	L	601	-	4,4,4	0.40	0	6,6,6	0.11	0
2	SO4	D	612	-	4,4,4	0.27	0	6,6,6	0.13	0
2	SO4	E	621	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	G	613	-	4,4,4	0.24	0	6,6,6	0.18	0
3	GOL	L	612	-	5,5,5	1.04	0	5,5,5	1.29	1 (20%)
2	SO4	C	606	-	4,4,4	0.28	0	6,6,6	0.19	0
2	SO4	H	601	-	4,4,4	0.39	0	6,6,6	0.10	0
2	SO4	D	621	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	G	616	-	4,4,4	0.27	0	6,6,6	0.16	0
2	SO4	B	616	-	4,4,4	0.41	0	6,6,6	0.08	0
2	SO4	D	601	-	4,4,4	0.29	0	6,6,6	0.38	0
2	SO4	K	609	-	4,4,4	0.25	0	6,6,6	0.18	0
2	SO4	E	616	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	C	616	-	4,4,4	0.25	0	6,6,6	0.10	0
3	GOL	D	623	-	5,5,5	1.25	0	5,5,5	0.82	0
2	SO4	A	622	-	4,4,4	0.21	0	6,6,6	0.29	0
3	GOL	E	626	-	5,5,5	1.36	1 (20%)	5,5,5	0.94	0
2	SO4	B	610	-	4,4,4	0.45	0	6,6,6	0.05	0
2	SO4	J	608	-	4,4,4	0.23	0	6,6,6	0.09	0
3	GOL	D	626	-	5,5,5	1.08	0	5,5,5	0.92	0
2	SO4	A	613	-	4,4,4	0.37	0	6,6,6	0.07	0
3	GOL	K	612	-	5,5,5	1.05	0	5,5,5	0.95	0
2	SO4	A	608	-	4,4,4	0.49	0	6,6,6	0.09	0
3	GOL	A	627	-	5,5,5	0.94	0	5,5,5	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	618	-	4,4,4	0.36	0	6,6,6	0.07	0
3	GOL	B	627	-	5,5,5	1.24	1 (20%)	5,5,5	1.22	0
3	GOL	A	625	-	5,5,5	1.60	1 (20%)	5,5,5	0.72	0
2	SO4	E	618	-	4,4,4	0.22	0	6,6,6	0.17	0
2	SO4	G	604	-	4,4,4	0.23	0	6,6,6	0.22	0
2	SO4	F	606	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	B	606	-	4,4,4	0.23	0	6,6,6	0.48	0
2	SO4	E	604	-	4,4,4	0.30	0	6,6,6	0.28	0
2	SO4	E	606	-	4,4,4	0.22	0	6,6,6	0.22	0
3	GOL	D	625	-	5,5,5	1.22	1 (20%)	5,5,5	0.92	0
2	SO4	L	602	-	4,4,4	0.20	0	6,6,6	0.15	0
2	SO4	I	601	-	4,4,4	0.39	0	6,6,6	0.10	0
2	SO4	J	601	-	4,4,4	0.24	0	6,6,6	0.27	0
2	SO4	E	617	-	4,4,4	0.26	0	6,6,6	0.17	0
2	SO4	D	606	-	4,4,4	0.27	0	6,6,6	0.13	0
3	GOL	C	625	-	5,5,5	1.12	0	5,5,5	1.04	0
2	SO4	L	611	-	4,4,4	0.42	0	6,6,6	0.11	0
2	SO4	B	624	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	C	617	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	J	605	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	D	617	-	4,4,4	0.42	0	6,6,6	0.07	0
2	SO4	D	615	-	4,4,4	0.43	0	6,6,6	0.11	0
2	SO4	L	609	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	E	607	-	4,4,4	0.24	0	6,6,6	0.17	0
2	SO4	A	621	-	4,4,4	0.24	0	6,6,6	0.16	0
2	SO4	C	602	-	4,4,4	0.23	0	6,6,6	0.22	0
2	SO4	B	609	-	4,4,4	0.27	0	6,6,6	0.35	0
2	SO4	H	613	-	4,4,4	0.27	0	6,6,6	0.15	0
2	SO4	G	609	-	4,4,4	0.22	0	6,6,6	0.16	0
2	SO4	D	609	-	4,4,4	0.41	0	6,6,6	0.12	0
2	SO4	B	608	-	4,4,4	0.53	0	6,6,6	0.17	0
2	SO4	A	604	-	4,4,4	0.25	0	6,6,6	0.16	0
2	SO4	G	614	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	B	614	-	4,4,4	0.30	0	6,6,6	0.22	0
2	SO4	D	614	-	4,4,4	0.23	0	6,6,6	0.17	0
2	SO4	C	611	-	4,4,4	0.45	0	6,6,6	0.12	0
2	SO4	H	610	-	4,4,4	0.24	0	6,6,6	0.17	0
2	SO4	F	613	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	K	602	-	4,4,4	0.25	0	6,6,6	0.26	0
2	SO4	A	601	-	4,4,4	0.30	0	6,6,6	0.44	0
2	SO4	A	610	-	4,4,4	0.25	0	6,6,6	0.16	0
2	SO4	E	613	-	4,4,4	0.23	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	623	-	4,4,4	0.25	0	6,6,6	0.07	0
3	GOL	B	629	-	5,5,5	1.29	0	5,5,5	0.95	0
3	GOL	H	617	-	5,5,5	1.78	2 (40%)	5,5,5	1.07	0
2	SO4	A	620	-	4,4,4	0.45	0	6,6,6	0.11	0
2	SO4	B	620	-	4,4,4	0.29	0	6,6,6	0.12	0
3	GOL	B	630	-	5,5,5	1.11	0	5,5,5	0.95	0
2	SO4	F	607	-	4,4,4	0.28	0	6,6,6	0.35	0
2	SO4	C	603	-	4,4,4	0.27	0	6,6,6	0.31	0
2	SO4	D	616	-	4,4,4	0.20	0	6,6,6	0.18	0
2	SO4	I	612	-	4,4,4	0.39	0	6,6,6	0.08	0
2	SO4	J	604	-	4,4,4	0.43	0	6,6,6	0.08	0
3	GOL	J	609	-	5,5,5	1.33	1 (20%)	5,5,5	0.83	0
3	GOL	A	628	-	5,5,5	1.17	0	5,5,5	1.02	0
3	GOL	G	620	-	5,5,5	1.16	0	5,5,5	0.97	0
2	SO4	E	609	-	4,4,4	0.28	0	6,6,6	0.28	0
2	SO4	K	601	-	4,4,4	0.28	0	6,6,6	0.27	0
3	GOL	A	631	-	5,5,5	0.09	0	5,5,5	0.26	0
3	GOL	B	628	-	5,5,5	1.29	1 (20%)	5,5,5	1.13	0
2	SO4	G	615	-	4,4,4	0.40	0	6,6,6	0.10	0
2	SO4	G	605	-	4,4,4	0.25	0	6,6,6	0.27	0
2	SO4	E	615	-	4,4,4	0.24	0	6,6,6	0.17	0
2	SO4	E	605	-	4,4,4	0.29	0	6,6,6	0.17	0
2	SO4	A	611	-	4,4,4	0.42	0	6,6,6	0.06	0
3	GOL	H	614	-	5,5,5	1.49	1 (20%)	5,5,5	0.72	0
2	SO4	B	612	-	4,4,4	0.48	0	6,6,6	0.15	0
2	SO4	J	603	-	4,4,4	0.47	0	6,6,6	0.04	0
2	SO4	G	612	-	4,4,4	0.28	0	6,6,6	0.08	0
2	SO4	F	604	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	A	623	-	4,4,4	0.42	0	6,6,6	0.05	0
2	SO4	C	604	-	4,4,4	0.40	0	6,6,6	0.09	0
2	SO4	F	612	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	B	625	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	A	619	-	4,4,4	0.27	0	6,6,6	0.18	0
2	SO4	K	603	-	4,4,4	0.27	0	6,6,6	0.18	0
2	SO4	D	618	-	4,4,4	0.27	0	6,6,6	0.15	0
2	SO4	B	601	-	4,4,4	0.29	0	6,6,6	0.18	0
2	SO4	C	601	-	4,4,4	0.40	0	6,6,6	0.05	0
2	SO4	A	603	-	4,4,4	0.41	0	6,6,6	0.07	0
2	SO4	B	603	-	4,4,4	0.19	0	6,6,6	0.25	0
2	SO4	H	603	-	4,4,4	0.25	0	6,6,6	0.20	0
2	SO4	I	607	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	J	602	-	4,4,4	0.45	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	J	607	-	4,4,4	0.38	0	6,6,6	0.07	0
2	SO4	D	610	-	4,4,4	0.23	0	6,6,6	0.20	0
3	GOL	B	626	-	5,5,5	1.14	0	5,5,5	0.98	0
2	SO4	D	603	-	4,4,4	0.23	0	6,6,6	0.10	0
3	GOL	F	614	-	5,5,5	1.16	0	5,5,5	1.04	0
3	GOL	G	619	-	5,5,5	0.88	0	5,5,5	1.19	1 (20%)
2	SO4	I	613	-	4,4,4	0.39	0	6,6,6	0.09	0
3	GOL	D	624	-	5,5,5	0.97	0	5,5,5	0.90	0
2	SO4	K	608	-	4,4,4	0.24	0	6,6,6	0.33	0
2	SO4	I	605	-	4,4,4	0.26	0	6,6,6	0.19	0
3	GOL	E	627	-	5,5,5	0.87	0	5,5,5	1.01	0
3	GOL	H	615	-	5,5,5	0.91	0	5,5,5	1.05	1 (20%)
2	SO4	F	603	-	4,4,4	0.29	0	6,6,6	0.19	0
2	SO4	H	611	-	4,4,4	0.38	0	6,6,6	0.08	0
3	GOL	G	622	-	5,5,5	1.21	0	5,5,5	1.04	0
2	SO4	F	611	-	4,4,4	0.28	0	6,6,6	0.10	0
2	SO4	E	624	-	4,4,4	0.40	0	6,6,6	0.11	0
2	SO4	L	603	-	4,4,4	0.43	0	6,6,6	0.08	0
2	SO4	B	619	-	4,4,4	0.26	0	6,6,6	0.14	0
3	GOL	F	615	-	5,5,5	1.41	1 (20%)	5,5,5	1.18	1 (20%)
2	SO4	G	610	-	4,4,4	0.39	0	6,6,6	0.08	0
2	SO4	C	614	-	4,4,4	0.26	0	6,6,6	0.19	0
2	SO4	E	610	-	4,4,4	0.26	0	6,6,6	0.13	0
2	SO4	G	601	-	4,4,4	0.31	0	6,6,6	0.33	0
2	SO4	E	601	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	K	604	-	4,4,4	0.25	0	6,6,6	0.18	0
2	SO4	L	606	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	G	603	-	4,4,4	0.21	0	6,6,6	0.17	0
3	GOL	A	629	-	5,5,5	0.82	0	5,5,5	1.18	0
2	SO4	H	608	-	4,4,4	0.44	0	6,6,6	0.08	0
3	GOL	C	626	-	5,5,5	1.09	0	5,5,5	1.28	1 (20%)
2	SO4	G	617	-	4,4,4	0.38	0	6,6,6	0.07	0
2	SO4	C	620	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	E	622	-	4,4,4	0.27	0	6,6,6	0.08	0
2	SO4	C	607	-	4,4,4	0.26	0	6,6,6	0.24	0
2	SO4	H	604	-	4,4,4	0.25	0	6,6,6	0.22	0
2	SO4	J	606	-	4,4,4	0.49	0	6,6,6	0.04	0
2	SO4	C	619	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	A	612	-	4,4,4	0.42	0	6,6,6	0.09	0
2	SO4	B	604	-	4,4,4	0.28	0	6,6,6	0.14	0
2	SO4	D	622	-	4,4,4	0.40	0	6,6,6	0.09	0
2	SO4	A	609	-	4,4,4	0.28	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	F	609	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	E	614	-	4,4,4	0.24	0	6,6,6	0.19	0
2	SO4	K	607	-	4,4,4	0.25	0	6,6,6	0.17	0
2	SO4	C	613	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	A	606	-	4,4,4	0.22	0	6,6,6	0.22	0
2	SO4	F	605	-	4,4,4	0.22	0	6,6,6	0.27	0
2	SO4	D	604	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	G	611	-	4,4,4	0.23	0	6,6,6	0.16	0
2	SO4	C	605	-	4,4,4	0.31	0	6,6,6	0.19	0
2	SO4	H	606	-	4,4,4	0.29	0	6,6,6	0.30	0
2	SO4	C	622	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	K	610	-	4,4,4	0.54	0	6,6,6	0.14	0
3	GOL	K	611	-	5,5,5	1.49	1 (20%)	5,5,5	0.58	0
2	SO4	D	605	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	E	620	-	4,4,4	0.22	0	6,6,6	0.21	0
2	SO4	I	610	-	4,4,4	0.48	0	6,6,6	0.09	0
2	SO4	G	608	-	4,4,4	0.41	0	6,6,6	0.06	0
3	GOL	G	621	-	5,5,5	1.00	0	5,5,5	1.23	0
2	SO4	B	623	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	E	608	-	4,4,4	0.23	0	6,6,6	0.43	0
3	GOL	I	614	-	5,5,5	0.93	0	5,5,5	1.16	1 (20%)
2	SO4	A	607	-	4,4,4	0.26	0	6,6,6	0.31	0
2	SO4	B	607	-	4,4,4	0.23	0	6,6,6	0.23	0
2	SO4	B	602	-	4,4,4	0.20	0	6,6,6	0.40	0
2	SO4	G	602	-	4,4,4	0.22	0	6,6,6	0.43	0
3	GOL	C	624	-	5,5,5	1.05	0	5,5,5	0.97	0
3	GOL	E	628	-	5,5,5	0.79	0	5,5,5	1.06	0
2	SO4	B	611	-	4,4,4	0.25	0	6,6,6	0.15	0
3	GOL	A	626	-	5,5,5	1.25	1 (20%)	5,5,5	0.86	0
2	SO4	C	615	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	A	605	-	4,4,4	0.25	0	6,6,6	0.16	0
2	SO4	E	612	-	4,4,4	0.43	0	6,6,6	0.10	0
2	SO4	D	611	-	4,4,4	0.26	0	6,6,6	0.18	0
2	SO4	E	625	-	4,4,4	0.25	0	6,6,6	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	L	612	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	F	615	-	-	3/4/4/4	-
3	GOL	H	617	-	-	1/4/4/4	-
3	GOL	B	629	-	-	2/4/4/4	-
3	GOL	D	623	-	-	2/4/4/4	-
3	GOL	E	626	-	-	3/4/4/4	-
3	GOL	B	630	-	-	1/4/4/4	-
3	GOL	A	629	-	-	2/4/4/4	-
3	GOL	C	626	-	-	2/4/4/4	-
3	GOL	D	626	-	-	2/4/4/4	-
3	GOL	J	609	-	-	0/4/4/4	-
3	GOL	A	628	-	-	0/4/4/4	-
3	GOL	G	620	-	-	3/4/4/4	-
3	GOL	B	628	-	-	3/4/4/4	-
3	GOL	A	631	-	-	0/4/4/4	-
3	GOL	K	612	-	-	4/4/4/4	-
3	GOL	A	627	-	-	0/4/4/4	-
3	GOL	B	627	-	-	2/4/4/4	-
3	GOL	H	614	-	-	4/4/4/4	-
3	GOL	A	625	-	-	2/4/4/4	-
3	GOL	K	611	-	-	2/4/4/4	-
3	GOL	H	616	-	-	2/4/4/4	-
3	GOL	D	625	-	-	0/4/4/4	-
3	GOL	K	613	-	-	0/4/4/4	-
3	GOL	G	621	-	-	2/4/4/4	-
3	GOL	A	624	-	-	0/4/4/4	-
3	GOL	A	630	-	-	0/4/4/4	-
3	GOL	C	625	-	-	4/4/4/4	-
3	GOL	G	618	-	-	3/4/4/4	-
3	GOL	I	614	-	-	0/4/4/4	-
3	GOL	G	623	-	-	1/4/4/4	-
3	GOL	C	624	-	-	1/4/4/4	-
3	GOL	B	626	-	-	1/4/4/4	-
3	GOL	F	614	-	-	1/4/4/4	-
3	GOL	G	619	-	-	4/4/4/4	-
3	GOL	E	628	-	-	2/4/4/4	-
3	GOL	D	624	-	-	1/4/4/4	-
3	GOL	A	626	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	627	-	-	3/4/4/4	-
3	GOL	H	615	-	-	2/4/4/4	-
3	GOL	G	622	-	-	0/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	617	GOL	C1-C2	2.83	1.62	1.51
3	H	617	GOL	C3-C2	2.73	1.62	1.51
3	A	625	GOL	C3-C2	2.57	1.61	1.51
3	B	628	GOL	O2-C2	-2.52	1.36	1.43
3	E	626	GOL	C3-C2	2.32	1.60	1.51
3	K	611	GOL	C3-C2	2.27	1.60	1.51
3	B	627	GOL	C1-C2	2.24	1.60	1.51
3	F	615	GOL	C3-C2	2.22	1.60	1.51
3	A	626	GOL	C3-C2	2.17	1.60	1.51
3	J	609	GOL	C3-C2	2.17	1.60	1.51
3	D	625	GOL	C1-C2	2.14	1.59	1.51
3	H	614	GOL	C3-C2	2.14	1.59	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	612	GOL	C3-C2-C1	-2.34	103.21	111.80
3	G	618	GOL	C3-C2-C1	-2.29	103.40	111.80
3	G	623	GOL	C3-C2-C1	-2.28	103.44	111.80
3	I	614	GOL	C3-C2-C1	-2.11	104.04	111.80
3	F	615	GOL	C3-C2-C1	-2.10	104.11	111.80
3	C	626	GOL	O3-C3-C2	-2.07	101.08	110.38
3	G	619	GOL	C3-C2-C1	-2.06	104.25	111.80
3	H	616	GOL	C3-C2-C1	-2.04	104.32	111.80
3	H	615	GOL	C3-C2-C1	-2.01	104.41	111.80

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	625	GOL	O1-C1-C2-C3
3	B	627	GOL	O1-C1-C2-C3
3	C	625	GOL	O1-C1-C2-C3
3	C	625	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	C	626	GOL	O1-C1-C2-C3
3	E	628	GOL	O1-C1-C2-O2
3	E	628	GOL	O1-C1-C2-C3
3	F	615	GOL	O1-C1-C2-O2
3	F	615	GOL	O1-C1-C2-C3
3	G	618	GOL	O1-C1-C2-C3
3	G	619	GOL	C1-C2-C3-O3
3	G	620	GOL	C1-C2-C3-O3
3	H	614	GOL	O1-C1-C2-C3
3	H	614	GOL	C1-C2-C3-O3
3	H	614	GOL	O2-C2-C3-O3
3	H	616	GOL	C1-C2-C3-O3
3	K	612	GOL	C1-C2-C3-O3
3	L	612	GOL	O1-C1-C2-O2
3	L	612	GOL	O1-C1-C2-C3
3	B	628	GOL	O1-C1-C2-O2
3	H	614	GOL	O1-C1-C2-O2
3	K	612	GOL	O2-C2-C3-O3
3	A	626	GOL	O1-C1-C2-C3
3	A	629	GOL	O1-C1-C2-C3
3	B	628	GOL	O1-C1-C2-C3
3	B	629	GOL	O1-C1-C2-C3
3	B	630	GOL	O1-C1-C2-C3
3	D	623	GOL	O1-C1-C2-C3
3	E	626	GOL	O1-C1-C2-C3
3	E	627	GOL	O1-C1-C2-C3
3	G	619	GOL	O1-C1-C2-C3
3	G	621	GOL	C1-C2-C3-O3
3	G	623	GOL	C1-C2-C3-O3
3	H	615	GOL	C1-C2-C3-O3
3	K	611	GOL	O1-C1-C2-C3
3	K	612	GOL	O1-C1-C2-C3
3	A	625	GOL	O1-C1-C2-O2
3	A	626	GOL	O1-C1-C2-O2
3	A	629	GOL	O1-C1-C2-O2
3	B	627	GOL	O1-C1-C2-O2
3	C	625	GOL	O1-C1-C2-O2
3	G	618	GOL	O1-C1-C2-O2
3	G	620	GOL	O2-C2-C3-O3
3	H	616	GOL	O2-C2-C3-O3
3	C	625	GOL	O2-C2-C3-O3
3	D	623	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	G	619	GOL	O2-C2-C3-O3
3	B	626	GOL	O1-C1-C2-O2
3	B	629	GOL	O1-C1-C2-O2
3	D	626	GOL	O2-C2-C3-O3
3	E	626	GOL	O1-C1-C2-O2
3	G	621	GOL	O2-C2-C3-O3
3	C	624	GOL	O2-C2-C3-O3
3	F	615	GOL	O2-C2-C3-O3
3	D	626	GOL	C1-C2-C3-O3
3	F	614	GOL	C1-C2-C3-O3
3	C	626	GOL	O1-C1-C2-O2
3	K	612	GOL	O1-C1-C2-O2
3	G	619	GOL	O1-C1-C2-O2
3	H	615	GOL	O2-C2-C3-O3
3	D	624	GOL	O1-C1-C2-C3
3	G	618	GOL	C1-C2-C3-O3
3	B	628	GOL	O2-C2-C3-O3
3	K	611	GOL	O1-C1-C2-O2
3	E	626	GOL	O2-C2-C3-O3
3	E	627	GOL	O1-C1-C2-O2
3	E	627	GOL	O2-C2-C3-O3
3	H	617	GOL	O2-C2-C3-O3
3	G	620	GOL	O1-C1-C2-C3

There are no ring outliers.

49 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	613	SO4	1	0
2	K	605	SO4	2	0
2	I	611	SO4	2	0
2	H	612	SO4	2	0
3	A	624	GOL	1	0
2	A	616	SO4	1	0
3	G	623	GOL	2	0
2	L	604	SO4	5	0
2	I	602	SO4	2	0
2	H	601	SO4	4	0
3	E	626	GOL	1	0
2	B	610	SO4	1	0
3	D	626	GOL	1	0
2	A	608	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	627	GOL	1	0
3	A	625	GOL	5	0
3	D	625	GOL	1	0
2	L	602	SO4	1	0
2	L	611	SO4	3	0
2	D	609	SO4	2	0
2	C	611	SO4	1	0
3	H	617	GOL	3	0
2	K	601	SO4	1	0
3	A	631	GOL	2	0
3	B	628	GOL	1	0
3	H	614	GOL	1	0
2	J	603	SO4	2	0
2	F	604	SO4	1	0
2	C	604	SO4	2	0
2	K	603	SO4	1	0
2	C	601	SO4	3	0
3	G	619	GOL	1	0
3	D	624	GOL	1	0
3	E	627	GOL	1	0
3	F	615	GOL	2	0
2	G	610	SO4	1	0
2	G	601	SO4	1	0
2	E	601	SO4	3	0
3	A	629	GOL	1	0
2	G	617	SO4	3	0
2	A	612	SO4	0	1
2	B	604	SO4	1	0
2	K	607	SO4	1	0
3	K	611	GOL	1	0
2	I	610	SO4	1	0
2	G	608	SO4	2	0
3	G	621	GOL	2	0
3	E	628	GOL	1	0
2	E	612	SO4	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	466/518 (89%)	-0.15	13 (2%)	55 46	33, 65, 138, 195	1 (0%)
1	B	464/518 (89%)	-0.08	19 (4%)	41 32	42, 65, 138, 195	0
1	C	464/518 (89%)	0.00	24 (5%)	33 25	25, 67, 153, 188	1 (0%)
1	D	456/518 (88%)	-0.06	17 (3%)	45 35	40, 72, 143, 195	0
1	E	465/518 (89%)	-0.08	21 (4%)	38 29	30, 67, 146, 216	0
1	F	464/518 (89%)	0.06	23 (4%)	34 27	30, 73, 152, 216	0
1	G	457/518 (88%)	0.07	26 (5%)	29 22	30, 74, 146, 202	0
1	H	456/518 (88%)	0.06	8 (1%)	67 61	30, 78, 146, 223	0
1	I	452/518 (87%)	0.23	31 (6%)	23 17	30, 80, 155, 186	0
1	J	449/518 (86%)	0.75	65 (14%)	6 4	55, 108, 166, 205	0
1	K	459/518 (88%)	0.16	25 (5%)	31 23	30, 79, 163, 228	0
1	L	441/518 (85%)	0.88	84 (19%)	3 3	30, 110, 171, 221	0
All	All	5493/6216 (88%)	0.15	356 (6%)	25 18	25, 77, 154, 228	2 (0%)

All (356) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	130	CYS	9.9
1	I	110	THR	7.1
1	C	292	GLY	5.8
1	I	113	LEU	5.4
1	F	341	GLU	5.3
1	F	367	VAL	5.2
1	J	442	GLN	5.2
1	L	2	SER	5.1
1	B	366	VAL	5.0
1	G	134	VAL	4.9
1	G	129	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	407	LEU	4.9
1	B	293	TYR	4.9
1	L	115	LYS	4.7
1	C	2	SER	4.7
1	K	125	THR	4.7
1	L	398	TYR	4.6
1	J	437	LEU	4.5
1	G	131	PRO	4.5
1	G	331	ARG	4.4
1	B	2	SER	4.4
1	I	407	LEU	4.4
1	L	324	PRO	4.3
1	H	292	GLY	4.3
1	H	287	GLN	4.3
1	D	293	TYR	4.2
1	A	307	TYR	4.2
1	L	394	LEU	4.2
1	I	308	GLY	4.2
1	J	225	LYS	4.1
1	L	393	GLU	4.1
1	H	407	LEU	4.0
1	K	97	LEU	4.0
1	F	307	TYR	4.0
1	L	349	TYR	4.0
1	E	409	THR	4.0
1	H	367	VAL	3.9
1	L	344	VAL	3.9
1	I	291	LEU	3.9
1	K	51	VAL	3.9
1	I	107	LEU	3.9
1	D	367	VAL	3.8
1	F	31	MET	3.8
1	C	366	VAL	3.8
1	I	109	MET	3.8
1	E	2	SER	3.7
1	K	220	PRO	3.7
1	L	316	HIS	3.7
1	C	406	ASP	3.7
1	J	354	GLU	3.7
1	G	54	GLU	3.7
1	E	333	LYS	3.7
1	J	471	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	293	TYR	3.7
1	F	132	ALA	3.6
1	G	328	MET	3.6
1	L	307	TYR	3.6
1	I	366	VAL	3.6
1	L	345	THR	3.6
1	K	341	GLU	3.6
1	G	135	ALA	3.6
1	C	331	ARG	3.6
1	J	325	ILE	3.6
1	C	1	MET	3.6
1	J	293	TYR	3.6
1	G	133	ALA	3.5
1	L	404	GLU	3.5
1	J	328	MET	3.5
1	F	135	ALA	3.5
1	J	344	VAL	3.5
1	J	444	GLY	3.5
1	B	411	TYR	3.4
1	I	48	MET	3.4
1	C	407	LEU	3.4
1	F	366	VAL	3.4
1	C	405	GLU	3.4
1	B	307	TYR	3.4
1	D	113	LEU	3.4
1	E	294	TYR	3.4
1	L	367	VAL	3.4
1	J	397	LEU	3.3
1	K	131	PRO	3.3
1	G	132	ALA	3.3
1	J	470	TYR	3.3
1	G	411	TYR	3.2
1	I	283	ARG	3.2
1	I	114	LYS	3.2
1	A	2	SER	3.2
1	A	293	TYR	3.2
1	A	131	PRO	3.2
1	L	148	MET	3.2
1	L	341	GLU	3.2
1	E	307	TYR	3.2
1	B	364	ASP	3.2
1	J	369	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	397	LEU	3.2
1	J	407	LEU	3.1
1	J	391	ALA	3.1
1	J	402	TYR	3.1
1	E	330	SER	3.1
1	F	2	SER	3.1
1	D	371	ASN	3.1
1	E	293	TYR	3.1
1	E	137	SER	3.1
1	J	439	ASP	3.1
1	L	481	CYS	3.1
1	L	348	LEU	3.1
1	L	400	ILE	3.0
1	E	131	PRO	3.0
1	K	366	VAL	3.0
1	A	129	TYR	3.0
1	F	293	TYR	3.0
1	G	501	GLU	3.0
1	A	97	LEU	3.0
1	C	412	HIS	3.0
1	L	314	VAL	3.0
1	L	402	TYR	3.0
1	I	367	VAL	3.0
1	L	467	ILE	2.9
1	L	491	THR	2.9
1	L	440	ILE	2.9
1	I	97	LEU	2.9
1	D	307	TYR	2.9
1	L	129	TYR	2.9
1	J	346	LYS	2.9
1	J	469	PHE	2.9
1	J	350	LEU	2.9
1	C	307	TYR	2.9
1	L	443	SER	2.9
1	C	367	VAL	2.9
1	F	133	ALA	2.9
1	J	377	TYR	2.8
1	E	367	VAL	2.8
1	G	32	ASP	2.8
1	J	352	ASP	2.8
1	H	125	THR	2.8
1	J	125	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.8
1	K	48	MET	2.8
1	K	219	LYS	2.8
1	L	384	PHE	2.8
1	B	46	ASN	2.8
1	A	136	SER	2.8
1	J	385	LYS	2.8
1	L	442	GLN	2.8
1	J	384	PHE	2.7
1	B	97	LEU	2.7
1	E	413	LEU	2.7
1	G	330	SER	2.7
1	C	421	PRO	2.7
1	I	206	GLN	2.7
1	B	461	GLU	2.7
1	L	337	ILE	2.7
1	C	409	THR	2.7
1	K	292	GLY	2.7
1	L	338	GLY	2.7
1	D	2	SER	2.7
1	J	134	VAL	2.7
1	L	346	LYS	2.7
1	J	362	PRO	2.7
1	I	2	SER	2.7
1	J	387	ALA	2.7
1	E	331	ARG	2.7
1	C	462	GLY	2.7
1	H	409	THR	2.7
1	J	409	THR	2.7
1	D	408	ASP	2.7
1	L	461	GLU	2.7
1	L	437	LEU	2.7
1	J	383	ALA	2.6
1	J	441	MET	2.6
1	L	470	TYR	2.6
1	L	426	ASN	2.6
1	L	327	ASP	2.6
1	I	42	HIS	2.6
1	K	221	GLY	2.6
1	F	142	LYS	2.6
1	J	434	LEU	2.6
1	G	329	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	341	GLU	2.6
1	L	54	GLU	2.6
1	D	150	SER	2.6
1	L	40	TRP	2.6
1	B	129	TYR	2.6
1	J	307	TYR	2.6
1	C	413	LEU	2.6
1	J	366	VAL	2.6
1	J	372	ILE	2.6
1	F	365	ASN	2.6
1	J	343	LYS	2.5
1	K	50	VAL	2.5
1	J	375	GLU	2.5
1	L	382	CYS	2.5
1	A	412	HIS	2.5
1	I	111	LYS	2.5
1	K	49	ASP	2.5
1	C	131	PRO	2.5
1	J	438	LEU	2.5
1	K	34	LEU	2.5
1	F	308	GLY	2.5
1	I	205	THR	2.5
1	L	387	ALA	2.5
1	I	55	ASN	2.5
1	I	49	ASP	2.5
1	C	308	GLY	2.5
1	D	156	ARG	2.5
1	J	49	ASP	2.4
1	K	129	TYR	2.4
1	L	135	ALA	2.4
1	G	441	MET	2.4
1	L	130	CYS	2.4
1	L	313	ASP	2.4
1	L	379	VAL	2.4
1	I	52	LYS	2.4
1	L	403	GLU	2.4
1	L	435	TRP	2.4
1	B	409	THR	2.4
1	E	412	HIS	2.4
1	J	392	LEU	2.4
1	K	14	ASN	2.4
1	I	95	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	406	ASP	2.4
1	E	366	VAL	2.4
1	L	373	ALA	2.4
1	K	44	TYR	2.4
1	J	491	THR	2.4
1	E	329	ILE	2.4
1	J	337	ILE	2.4
1	J	458	ILE	2.4
1	K	217	ARG	2.4
1	L	352	ASP	2.4
1	L	439	ASP	2.4
1	J	341	GLU	2.4
1	L	447	THR	2.4
1	L	97	LEU	2.4
1	L	392	LEU	2.4
1	A	365	ASN	2.3
1	B	32	ASP	2.3
1	I	120	PHE	2.3
1	I	45	MET	2.3
1	K	293	TYR	2.3
1	L	37	LEU	2.3
1	L	114	LYS	2.3
1	L	140	VAL	2.3
1	G	332	GLY	2.3
1	J	109	MET	2.3
1	E	295	ILE	2.3
1	J	398	TYR	2.3
1	L	458	ILE	2.3
1	L	425	PRO	2.3
1	B	367	VAL	2.3
1	D	308	GLY	2.3
1	J	139	PHE	2.3
1	B	132	ALA	2.3
1	E	461	GLU	2.3
1	D	48	MET	2.3
1	J	334	LEU	2.3
1	G	2	SER	2.3
1	L	500	SER	2.3
1	C	44	TYR	2.3
1	L	123	ARG	2.3
1	L	468	ASN	2.3
1	I	106	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	328	MET	2.3
1	C	408	ASP	2.3
1	F	352	ASP	2.3
1	G	326	GLN	2.3
1	J	351	VAL	2.3
1	J	292	GLY	2.3
1	K	216	GLN	2.2
1	C	410	ILE	2.2
1	J	410	ILE	2.2
1	L	116	CYS	2.2
1	L	351	VAL	2.2
1	E	48	MET	2.2
1	J	291	LEU	2.2
1	J	440	ILE	2.2
1	K	105	GLN	2.2
1	L	484	ILE	2.2
1	J	367	VAL	2.2
1	L	118	SER	2.2
1	A	292	GLY	2.2
1	L	385	LYS	2.2
1	F	340	GLU	2.2
1	A	16	PRO	2.2
1	I	220	PRO	2.2
1	L	444	GLY	2.2
1	B	368	LYS	2.2
1	K	172	LYS	2.2
1	L	370	LYS	2.2
1	G	407	LEU	2.2
1	J	348	LEU	2.2
1	D	135	ALA	2.2
1	G	340	GLU	2.2
1	C	46	ASN	2.2
1	E	328	MET	2.2
1	F	45	MET	2.2
1	G	122	THR	2.2
1	J	45	MET	2.2
1	L	317	SER	2.2
1	F	393	GLU	2.2
1	J	501	GLU	2.2
1	I	108	ASN	2.1
1	L	362	PRO	2.1
1	D	148	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	45	MET	2.1
1	C	330	SER	2.1
1	J	443	SER	2.1
1	K	147	GLU	2.1
1	L	347	GLU	2.1
1	L	376	ILE	2.1
1	D	178	HIS	2.1
1	L	13	HIS	2.1
1	C	50	VAL	2.1
1	D	31	MET	2.1
1	I	421	PRO	2.1
1	L	343	LYS	2.1
1	B	407	LEU	2.1
1	E	133	ALA	2.1
1	G	307	TYR	2.1
1	J	44	TYR	2.1
1	L	369	TYR	2.1
1	C	339	GLU	2.1
1	F	174	GLN	2.1
1	I	13	HIS	2.1
1	L	336	VAL	2.1
1	D	292	GLY	2.1
1	G	292	GLY	2.1
1	F	182	ASN	2.1
1	L	469	PHE	2.1
1	J	138	ASP	2.1
1	F	260	TRP	2.1
1	K	53	ILE	2.1
1	L	329	ILE	2.1
1	H	307	TYR	2.1
1	L	293	TYR	2.1
1	B	130	CYS	2.0
1	F	502	GLN	2.0
1	L	134	VAL	2.0
1	L	427	VAL	2.0
1	J	451	GLY	2.0
1	J	435	TRP	2.0
1	A	368	LYS	2.0
1	E	271	LYS	2.0
1	F	368	LYS	2.0
1	I	186	LYS	2.0
1	I	236	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	322	LEU	2.0
1	F	462	GLY	2.0
1	L	292	GLY	2.0
1	J	345	THR	2.0
1	J	393	GLU	2.0
1	B	31	MET	2.0
1	K	45	MET	2.0
1	L	109	MET	2.0
1	J	336	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	SO4	H	601	5/5	0.42	0.12	190,193,193,194	0
2	SO4	C	615	5/5	0.46	0.12	182,184,184,185	0
2	SO4	G	610	5/5	0.47	0.17	206,206,207,208	0
2	SO4	E	619	5/5	0.47	0.10	186,187,188,188	0
2	SO4	C	617	5/5	0.50	0.10	164,164,167,168	0
2	SO4	G	607	5/5	0.50	0.13	177,178,180,180	0
2	SO4	I	609	5/5	0.50	0.11	162,164,166,168	0
2	SO4	H	611	5/5	0.51	0.10	185,187,187,188	0
2	SO4	A	623	5/5	0.51	0.12	198,199,200,201	0
2	SO4	G	616	5/5	0.52	0.14	185,185,187,188	0
2	SO4	D	617	5/5	0.53	0.13	155,159,163,166	0
2	SO4	D	615	5/5	0.53	0.12	166,169,170,171	0
2	SO4	J	605	5/5	0.54	0.12	171,171,173,174	0
2	SO4	D	618	5/5	0.56	0.10	167,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	623	5/5	0.57	0.09	164,165,167,168	0
2	SO4	A	612	5/5	0.57	0.12	190,192,193,194	0
2	SO4	J	608	5/5	0.57	0.14	178,179,179,180	0
2	SO4	I	610	5/5	0.58	0.12	175,176,177,179	0
2	SO4	E	612	5/5	0.59	0.14	154,154,158,160	0
2	SO4	E	623	5/5	0.59	0.09	185,185,186,187	0
2	SO4	E	624	5/5	0.59	0.08	192,197,198,199	0
2	SO4	B	605	5/5	0.60	0.13	183,184,184,185	0
2	SO4	K	604	5/5	0.60	0.11	163,165,166,166	0
2	SO4	L	601	5/5	0.60	0.08	177,180,180,182	0
2	SO4	G	611	5/5	0.63	0.13	192,193,194,195	0
2	SO4	D	603	5/5	0.66	0.14	193,194,195,198	0
2	SO4	C	604	5/5	0.66	0.10	190,191,192,192	0
2	SO4	D	613	5/5	0.67	0.10	165,167,170,170	0
2	SO4	J	603	5/5	0.69	0.11	195,195,196,198	0
2	SO4	H	604	5/5	0.69	0.11	171,172,172,173	0
2	SO4	B	618	5/5	0.69	0.14	214,215,216,216	0
2	SO4	C	616	5/5	0.69	0.11	164,164,166,166	0
2	SO4	E	603	5/5	0.69	0.12	187,188,189,190	0
2	SO4	L	603	5/5	0.69	0.12	172,173,174,177	0
2	SO4	L	607	5/5	0.69	0.12	141,143,150,151	0
2	SO4	L	609	5/5	0.69	0.10	185,185,186,188	0
2	SO4	J	607	5/5	0.70	0.12	192,192,193,194	0
2	SO4	D	602	5/5	0.70	0.11	180,181,181,181	0
2	SO4	B	620	5/5	0.70	0.08	159,162,163,166	0
2	SO4	K	609	5/5	0.70	0.14	184,185,185,185	0
2	SO4	C	610	5/5	0.71	0.11	163,165,166,167	0
2	SO4	L	604	5/5	0.72	0.23	184,187,189,190	0
2	SO4	A	604	5/5	0.72	0.09	153,154,155,157	0
2	SO4	C	620	5/5	0.72	0.11	162,163,164,165	0
2	SO4	D	609	5/5	0.73	0.15	184,186,187,188	0
2	SO4	J	604	5/5	0.73	0.11	154,156,158,160	0
2	SO4	G	612	5/5	0.73	0.10	152,154,155,156	0
2	SO4	A	621	5/5	0.74	0.14	195,196,197,197	0
3	GOL	D	625	6/6	0.74	0.20	109,115,120,122	0
2	SO4	L	605	5/5	0.75	0.15	87,119,127,128	0
2	SO4	I	612	5/5	0.75	0.17	171,173,177,177	0
2	SO4	K	605	5/5	0.75	0.15	203,205,206,207	0
2	SO4	A	603	5/5	0.75	0.11	170,170,171,172	0
2	SO4	C	613	5/5	0.76	0.12	165,166,167,169	0
2	SO4	H	613	5/5	0.76	0.15	174,178,178,182	0
2	SO4	C	623	5/5	0.76	0.10	194,195,196,197	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	601	5/5	0.76	0.12	157,159,161,161	0
2	SO4	H	609	5/5	0.76	0.14	147,147,153,156	0
3	GOL	D	626	6/6	0.76	0.20	123,126,128,130	0
2	SO4	E	617	5/5	0.77	0.17	155,156,158,160	0
2	SO4	C	608	5/5	0.77	0.10	162,162,164,164	0
2	SO4	J	601	5/5	0.77	0.16	156,156,159,159	0
3	GOL	A	626	6/6	0.77	0.15	84,88,90,91	0
2	SO4	J	602	5/5	0.77	0.13	168,170,173,173	0
2	SO4	E	616	5/5	0.77	0.11	166,170,171,172	0
3	GOL	F	614	6/6	0.77	0.13	102,116,120,121	0
2	SO4	C	618	5/5	0.78	0.21	164,164,166,167	0
2	SO4	A	622	5/5	0.78	0.19	156,159,161,166	0
2	SO4	F	612	5/5	0.78	0.10	155,156,157,159	0
2	SO4	B	624	5/5	0.78	0.15	177,178,182,182	0
2	SO4	C	609	5/5	0.78	0.19	149,152,157,158	0
2	SO4	B	610	5/5	0.78	0.12	162,164,165,166	0
2	SO4	I	606	5/5	0.79	0.15	154,157,159,160	0
2	SO4	G	608	5/5	0.79	0.10	175,176,177,178	0
3	GOL	A	631	6/6	0.79	0.31	20,20,20,20	0
2	SO4	D	610	5/5	0.79	0.17	175,176,178,180	0
2	SO4	L	602	5/5	0.79	0.11	146,147,149,154	0
2	SO4	L	608	5/5	0.79	0.11	154,158,161,163	0
3	GOL	H	615	6/6	0.79	0.12	88,97,109,115	0
3	GOL	I	614	6/6	0.79	0.17	105,111,114,115	0
2	SO4	B	613	5/5	0.80	0.14	194,196,197,199	0
3	GOL	B	629	6/6	0.80	0.13	99,103,107,107	0
2	SO4	K	606	5/5	0.80	0.16	144,146,148,153	0
2	SO4	C	612	5/5	0.80	0.19	188,189,191,191	0
2	SO4	E	601	5/5	0.80	0.09	173,174,175,178	0
2	SO4	E	602	5/5	0.80	0.09	176,177,178,178	0
2	SO4	C	607	5/5	0.80	0.17	167,169,170,172	0
3	GOL	K	611	6/6	0.80	0.16	93,114,118,121	0
2	SO4	E	620	5/5	0.81	0.13	161,164,167,167	0
2	SO4	E	615	5/5	0.81	0.14	143,145,148,154	0
2	SO4	C	605	5/5	0.81	0.16	134,138,142,142	0
2	SO4	F	606	5/5	0.81	0.11	162,163,165,165	0
2	SO4	I	601	5/5	0.81	0.13	174,174,176,179	0
2	SO4	K	607	5/5	0.81	0.14	157,159,163,165	0
2	SO4	D	620	5/5	0.81	0.17	163,164,166,166	0
2	SO4	A	611	5/5	0.81	0.14	174,174,175,175	0
2	SO4	B	617	5/5	0.82	0.12	182,184,185,186	0
2	SO4	I	602	5/5	0.82	0.14	185,188,189,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	G	615	5/5	0.82	0.13	180,182,183,183	0
2	SO4	I	608	5/5	0.82	0.15	166,167,167,168	0
2	SO4	F	602	5/5	0.83	0.10	151,157,158,159	0
2	SO4	C	614	5/5	0.83	0.23	160,161,162,165	0
2	SO4	H	612	5/5	0.83	0.14	161,161,164,168	0
2	SO4	E	611	5/5	0.83	0.23	151,156,159,160	0
2	SO4	A	615	5/5	0.83	0.13	166,167,168,168	0
2	SO4	B	614	5/5	0.83	0.15	152,153,157,159	0
2	SO4	H	602	5/5	0.83	0.11	145,147,149,150	0
3	GOL	J	609	6/6	0.83	0.16	95,98,100,101	0
2	SO4	C	622	5/5	0.83	0.08	181,182,184,185	0
3	GOL	D	624	6/6	0.84	0.14	116,127,129,133	0
2	SO4	D	621	5/5	0.84	0.17	176,177,178,180	0
2	SO4	F	605	5/5	0.84	0.19	150,154,156,159	0
2	SO4	J	606	5/5	0.84	0.13	137,141,144,145	0
2	SO4	C	621	5/5	0.84	0.24	183,183,185,187	0
2	SO4	F	609	5/5	0.84	0.18	180,185,186,188	0
2	SO4	E	605	5/5	0.84	0.12	152,155,159,159	0
2	SO4	F	613	5/5	0.84	0.14	184,185,187,188	0
2	SO4	K	602	5/5	0.85	0.08	139,139,144,149	0
2	SO4	D	614	5/5	0.85	0.17	168,170,171,175	0
2	SO4	D	619	5/5	0.85	0.14	158,159,160,164	0
3	GOL	F	615	6/6	0.85	0.19	78,92,107,114	0
3	GOL	H	614	6/6	0.85	0.16	78,90,94,99	0
3	GOL	A	627	6/6	0.85	0.14	107,114,120,127	0
2	SO4	E	613	5/5	0.85	0.11	173,173,174,174	0
2	SO4	A	620	5/5	0.85	0.20	201,202,202,203	0
2	SO4	B	616	5/5	0.85	0.13	180,181,184,184	0
3	GOL	K	612	6/6	0.85	0.15	91,114,115,120	0
3	GOL	L	612	6/6	0.85	0.27	131,134,136,137	0
2	SO4	A	608	5/5	0.86	0.16	136,144,146,148	0
3	GOL	A	628	6/6	0.86	0.17	98,110,112,112	0
2	SO4	D	611	5/5	0.86	0.16	148,151,159,160	0
3	GOL	B	626	6/6	0.86	0.11	75,101,103,104	0
2	SO4	K	608	5/5	0.86	0.16	137,139,141,143	0
2	SO4	D	612	5/5	0.86	0.17	162,164,165,166	0
2	SO4	B	602	5/5	0.86	0.14	99,102,110,113	0
2	SO4	B	615	5/5	0.86	0.09	154,156,158,160	0
2	SO4	A	605	5/5	0.86	0.12	144,144,147,149	0
2	SO4	D	616	5/5	0.86	0.14	165,169,171,171	0
2	SO4	A	616	5/5	0.86	0.16	193,194,196,196	0
2	SO4	D	605	5/5	0.86	0.10	162,162,163,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	612	5/5	0.86	0.25	180,181,184,186	0
2	SO4	F	610	5/5	0.86	0.14	173,174,175,177	0
3	GOL	A	624	6/6	0.86	0.21	74,86,91,91	0
3	GOL	A	625	6/6	0.86	0.25	73,87,90,92	0
2	SO4	I	611	5/5	0.86	0.17	178,178,180,180	0
2	SO4	L	606	5/5	0.87	0.11	155,156,158,160	0
3	GOL	G	619	6/6	0.87	0.15	112,114,115,117	0
2	SO4	I	613	5/5	0.87	0.50	30,30,30,30	0
2	SO4	H	610	5/5	0.87	0.15	172,173,174,176	0
3	GOL	H	616	6/6	0.87	0.16	125,129,134,140	0
2	SO4	G	609	5/5	0.87	0.08	158,161,162,162	0
2	SO4	B	625	5/5	0.87	0.11	168,169,172,173	0
2	SO4	G	605	5/5	0.87	0.18	155,159,161,163	0
2	SO4	C	619	5/5	0.87	0.14	167,167,169,169	0
2	SO4	A	618	5/5	0.87	0.12	181,182,183,184	0
2	SO4	A	610	5/5	0.88	0.15	157,163,165,166	0
3	GOL	B	627	6/6	0.88	0.22	87,98,104,105	0
2	SO4	G	614	5/5	0.88	0.13	171,172,174,176	0
3	GOL	C	625	6/6	0.88	0.16	90,98,100,101	0
2	SO4	E	604	5/5	0.88	0.21	114,124,128,134	0
2	SO4	A	614	5/5	0.88	0.15	166,166,169,171	0
2	SO4	E	614	5/5	0.88	0.12	154,157,158,160	0
3	GOL	A	630	6/6	0.88	0.12	99,106,111,111	0
2	SO4	L	611	5/5	0.88	0.49	30,30,30,30	0
2	SO4	E	606	5/5	0.89	0.12	136,143,144,146	0
2	SO4	E	610	5/5	0.89	0.12	147,149,152,154	0
2	SO4	G	602	5/5	0.89	0.22	119,128,137,138	0
3	GOL	E	626	6/6	0.89	0.16	68,72,83,84	0
2	SO4	B	608	5/5	0.89	0.25	142,147,148,148	0
2	SO4	H	608	5/5	0.89	0.11	174,178,178,179	0
2	SO4	D	622	5/5	0.89	0.45	30,30,30,30	0
2	SO4	B	622	5/5	0.89	0.19	196,196,197,197	0
2	SO4	F	603	5/5	0.89	0.13	139,139,141,141	0
2	SO4	C	611	5/5	0.89	0.15	146,149,154,155	0
2	SO4	A	613	5/5	0.89	0.12	159,161,162,164	0
2	SO4	B	606	5/5	0.89	0.17	127,134,135,140	0
2	SO4	B	619	5/5	0.89	0.13	167,169,169,169	0
2	SO4	I	604	5/5	0.89	0.23	145,150,151,153	0
2	SO4	F	611	5/5	0.89	0.14	165,166,167,168	0
2	SO4	B	621	5/5	0.90	0.14	156,157,159,159	0
2	SO4	I	603	5/5	0.90	0.19	159,163,166,167	0
3	GOL	E	627	6/6	0.90	0.13	115,115,117,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	E	628	6/6	0.90	0.24	105,107,108,108	0
2	SO4	E	625	5/5	0.90	0.14	158,158,160,163	0
2	SO4	B	611	5/5	0.90	0.07	169,170,171,173	0
2	SO4	C	606	5/5	0.90	0.15	128,134,135,139	0
2	SO4	F	604	5/5	0.90	0.10	137,138,142,146	0
2	SO4	B	603	5/5	0.90	0.12	135,138,140,144	0
2	SO4	B	607	5/5	0.90	0.14	186,187,188,190	0
3	GOL	H	617	6/6	0.90	0.13	80,86,94,95	0
2	SO4	B	604	5/5	0.90	0.11	115,120,123,129	0
2	SO4	E	607	5/5	0.90	0.12	137,140,144,148	0
3	GOL	C	626	6/6	0.90	0.27	120,120,122,123	0
2	SO4	D	601	5/5	0.90	0.19	118,121,125,134	0
2	SO4	A	619	5/5	0.90	0.17	167,167,170,171	0
2	SO4	A	609	5/5	0.91	0.13	127,131,134,138	0
3	GOL	G	621	6/6	0.91	0.13	92,102,106,111	0
2	SO4	F	607	5/5	0.91	0.14	135,139,140,141	0
2	SO4	A	606	5/5	0.91	0.10	127,131,134,135	0
2	SO4	G	613	5/5	0.91	0.18	204,205,206,207	0
2	SO4	G	606	5/5	0.91	0.11	138,141,143,145	0
2	SO4	I	607	5/5	0.91	0.08	151,152,152,153	0
2	SO4	E	622	5/5	0.91	0.12	163,164,165,168	0
2	SO4	A	617	5/5	0.91	0.17	186,187,191,194	0
2	SO4	E	608	5/5	0.91	0.18	122,131,133,133	0
3	GOL	K	613	6/6	0.91	0.15	108,110,112,115	0
2	SO4	K	610	5/5	0.91	0.49	30,30,30,30	0
2	SO4	K	603	5/5	0.92	0.11	149,152,153,154	0
3	GOL	G	620	6/6	0.92	0.12	78,99,104,110	0
3	GOL	B	630	6/6	0.92	0.14	93,99,100,104	0
2	SO4	F	601	5/5	0.92	0.10	80,104,106,106	0
2	SO4	D	607	5/5	0.92	0.16	115,120,123,127	0
2	SO4	H	603	5/5	0.92	0.12	134,137,137,141	0
2	SO4	E	621	5/5	0.92	0.13	154,156,160,163	0
3	GOL	A	629	6/6	0.92	0.17	95,99,103,103	0
2	SO4	H	605	5/5	0.92	0.20	171,173,176,177	0
2	SO4	F	608	5/5	0.92	0.23	160,161,163,163	0
2	SO4	G	601	5/5	0.92	0.08	92,93,101,111	0
2	SO4	D	606	5/5	0.92	0.14	166,167,167,167	0
3	GOL	B	628	6/6	0.92	0.15	62,78,80,82	0
2	SO4	L	610	5/5	0.93	0.52	30,30,30,30	0
2	SO4	H	606	5/5	0.93	0.13	128,131,132,132	0
2	SO4	B	609	5/5	0.93	0.13	125,130,138,140	0
2	SO4	G	604	5/5	0.93	0.15	133,135,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	G	622	6/6	0.93	0.13	85,88,94,98	0
3	GOL	G	623	6/6	0.93	0.15	87,93,100,111	0
2	SO4	G	617	5/5	0.93	0.46	30,30,30,30	0
2	SO4	D	604	5/5	0.93	0.18	208,209,210,211	0
2	SO4	E	618	5/5	0.94	0.13	135,139,142,143	0
2	SO4	K	601	5/5	0.94	0.11	87,87,101,106	0
2	SO4	E	609	5/5	0.94	0.15	121,135,138,139	0
2	SO4	A	601	5/5	0.94	0.16	96,102,116,116	0
2	SO4	A	607	5/5	0.94	0.12	118,123,128,129	0
2	SO4	C	603	5/5	0.95	0.08	87,91,93,97	0
2	SO4	B	601	5/5	0.95	0.14	120,121,125,130	0
2	SO4	A	602	5/5	0.95	0.07	80,94,96,98	0
2	SO4	C	602	5/5	0.95	0.08	108,117,118,122	0
2	SO4	G	603	5/5	0.95	0.09	139,143,144,148	0
3	GOL	G	618	6/6	0.95	0.13	98,100,101,102	0
2	SO4	D	608	5/5	0.95	0.08	146,148,149,152	0
3	GOL	C	624	6/6	0.96	0.10	66,70,75,76	0
2	SO4	H	607	5/5	0.96	0.13	144,146,150,151	0
2	SO4	I	605	5/5	0.96	0.14	140,143,143,143	0
3	GOL	D	623	6/6	0.96	0.13	70,80,84,90	0

6.5 Other polymers

There are no such residues in this entry.