Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2022 – 02:26 PM EDT

PDB ID	:	7TIF
Title	:	2.85 Angstroem 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:

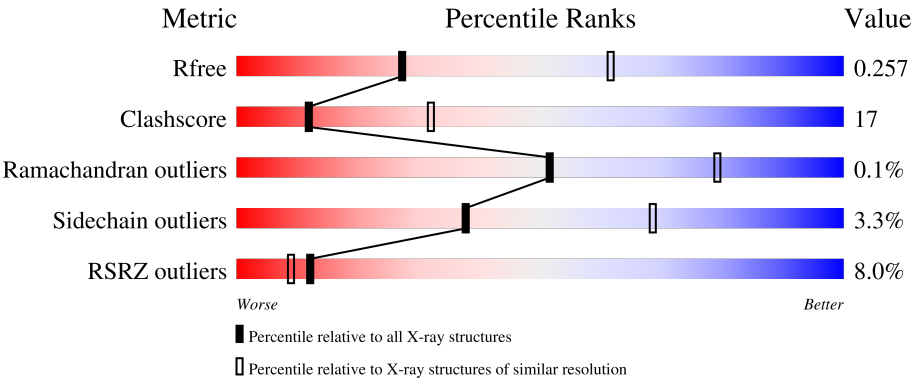
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 <=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	4% 65% 24% • 10%
1	B	518	5% 64% 24% • 10%
1	C	518	6% 65% 22% • 10%
1	D	518	5% 59% 27% • 12%
1	E	518	5% 65% 23% • 10%

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Mol	Chain	Length	Quality of chain
1	F	518	6% 59% 30% 10%
1	G	518	6% 56% 30% 12%
1	H	518	6% 59% 28% 12%
1	I	518	8% 58% 27% 13%
1	J	518	14% 48% 37% 13%
1	K	518	6% 59% 29% 11%
1	L	518	14% 46% 38% 15%

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	A	614	-	-	-	X
2	SO4	A	620	-	-	-	X
2	SO4	A	622	-	-	-	X
2	SO4	B	605	-	-	-	X
2	SO4	B	607	-	-	-	X
2	SO4	B	617	-	-	-	X
2	SO4	B	622	-	-	-	X
2	SO4	C	601	-	-	X	-
2	SO4	C	604	-	-	X	-
2	SO4	C	609	-	-	-	X
2	SO4	C	612	-	-	-	X
2	SO4	C	618	-	-	-	X
2	SO4	C	621	-	-	-	X
2	SO4	D	602	-	-	-	X
2	SO4	D	609	-	-	X	-
2	SO4	E	601	-	-	X	-
2	SO4	E	611	-	-	-	X
2	SO4	E	612	-	-	X	-
2	SO4	F	613	-	-	-	X
2	SO4	G	608	-	-	X	-
2	SO4	G	610	-	-	-	X
2	SO4	G	611	-	-	-	X
2	SO4	G	617	-	-	X	-
2	SO4	H	601	-	-	X	-
2	SO4	H	605	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	H	608	-	-	-	X
2	SO4	H	610	-	-	-	X
2	SO4	H	612	-	-	X	-
2	SO4	H	613	-	-	-	X
2	SO4	I	602	-	-	X	X
2	SO4	I	603	-	-	-	X
2	SO4	I	611	-	-	X	-
2	SO4	J	601	-	-	-	X
2	SO4	J	603	-	-	X	-
2	SO4	K	605	-	-	X	X
2	SO4	K	608	-	-	-	X
2	SO4	L	604	-	-	X	-
2	SO4	L	611	-	-	X	-
3	GOL	A	625	-	-	X	-
3	GOL	D	624	-	-	-	X
3	GOL	D	625	-	-	-	X
3	GOL	D	626	-	-	-	X
3	GOL	F	615	-	-	-	X
3	GOL	H	616	-	-	-	X

2 Entry composition (i)

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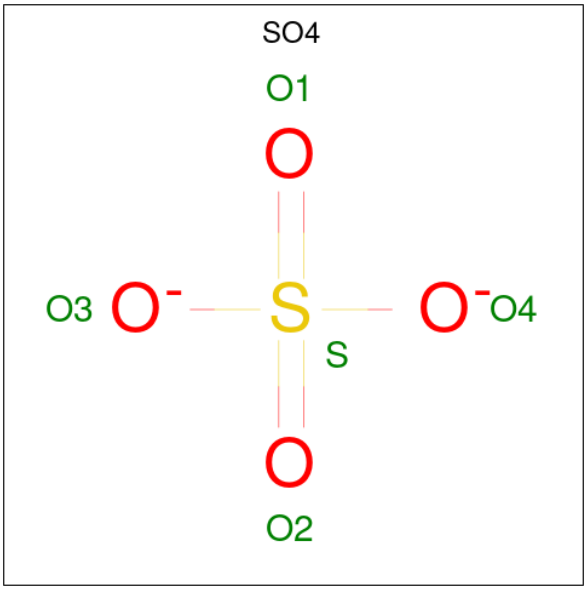
Chain	Residue	Modelled	Actual	Comment	Reference
L	512	GLU	-	expression tag	UNP P16639
L	513	HIS	-	expression tag	UNP P16639
L	514	HIS	-	expression tag	UNP P16639
L	515	HIS	-	expression tag	UNP P16639
L	516	HIS	-	expression tag	UNP P16639
L	517	HIS	-	expression tag	UNP P16639
L	518	HIS	-	expression tag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

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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

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

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

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

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

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

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

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

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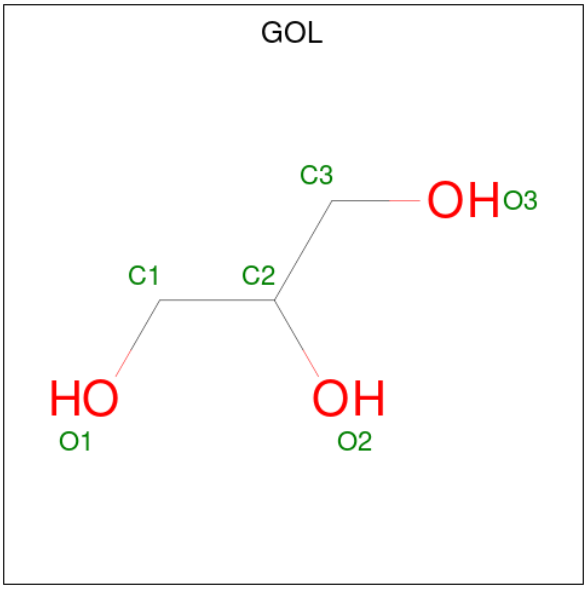
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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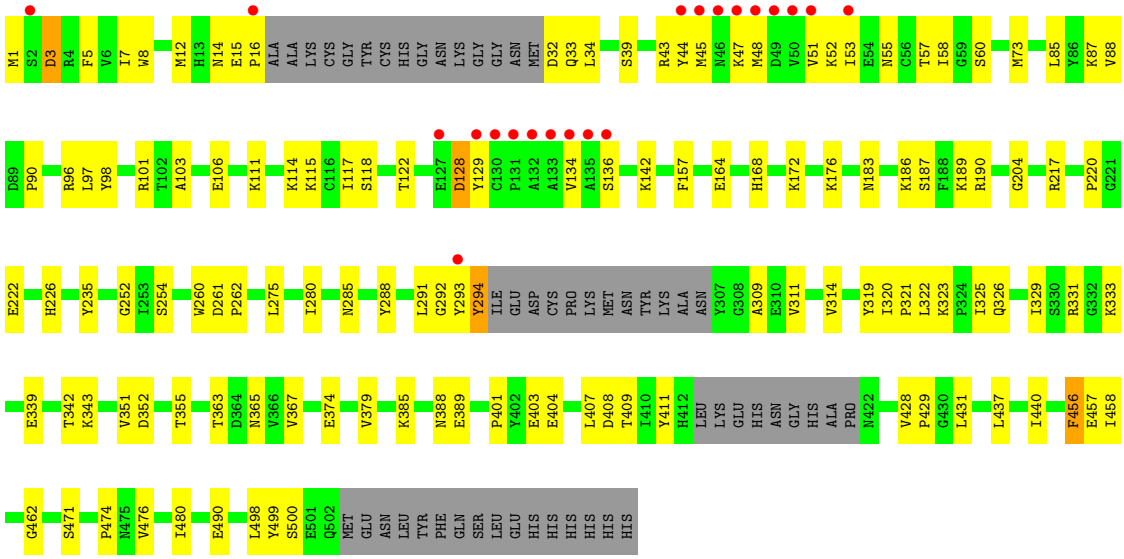
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	9	Total O 9 9	0	0
4	F	5	Total O 5 5	0	0
4	G	7	Total O 7 7	0	0
4	H	3	Total O 3 3	0	0
4	I	2	Total O 2 2	0	0
4	J	2	Total O 2 2	0	0
4	K	5	Total O 5 5	0	0
4	L	2	Total O 2 2	0	0

3 Residue-property plots (i)

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

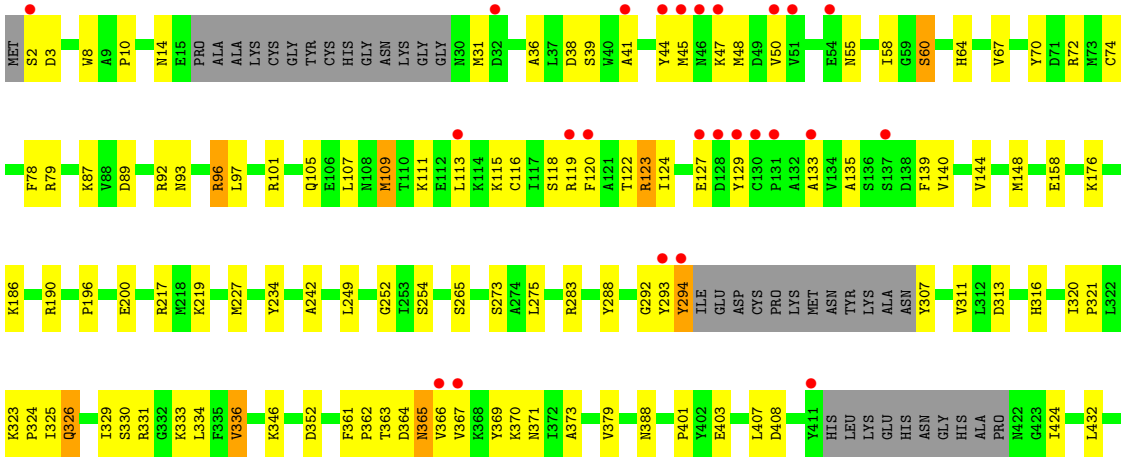
• Molecule 1: Arginyl-tRNA--protein transferase 1

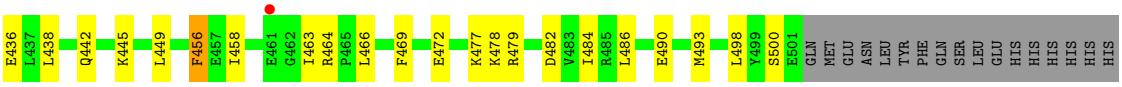
Chain A:



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

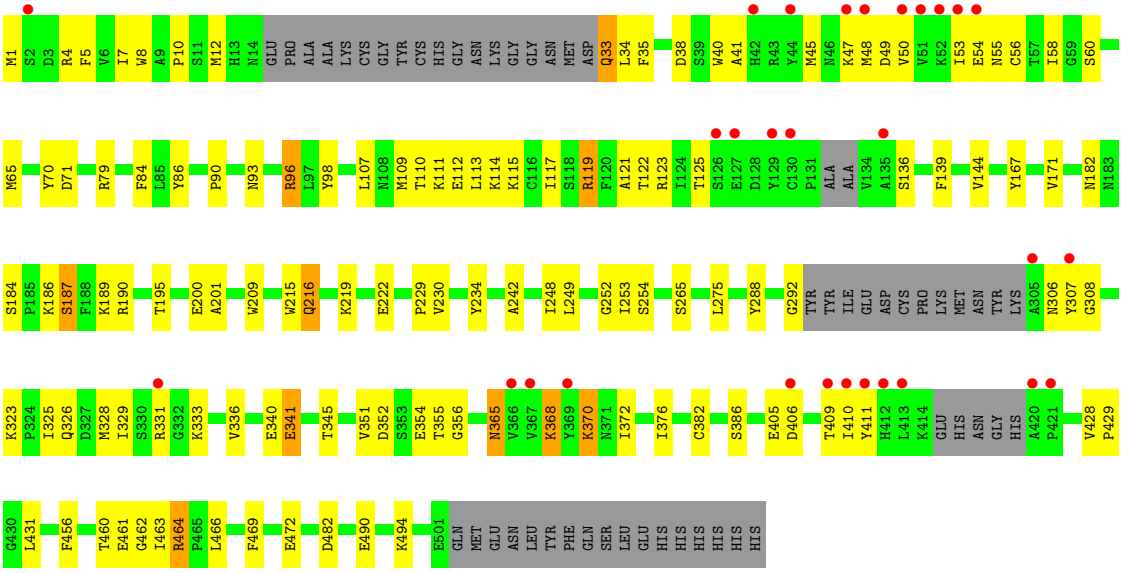
Chain B:





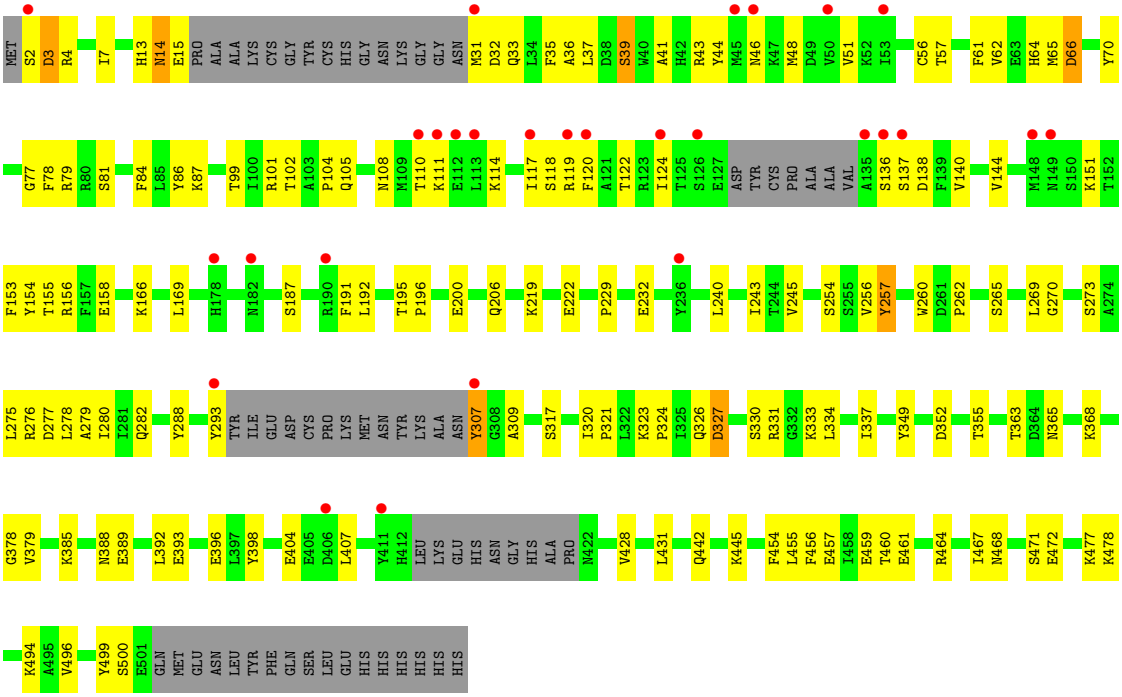
• Molecule 1: Arginyl-tRNA--protein transferase 1

Chain C:



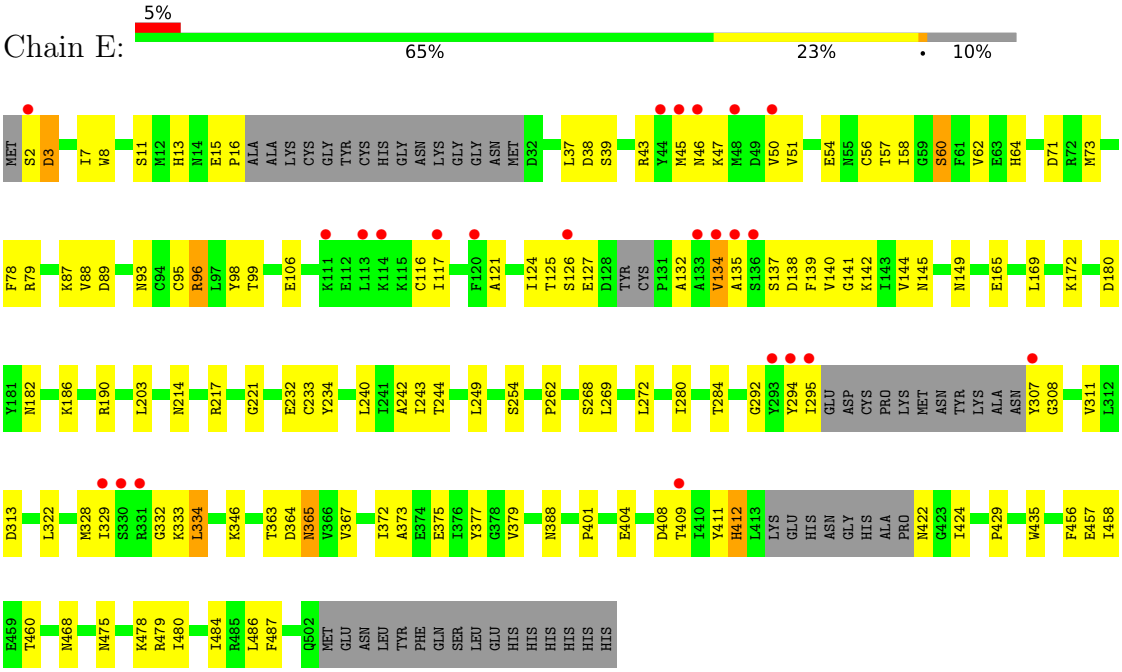
• Molecule 1: Arginyl-tRNA--protein transferase 1

Chain D:



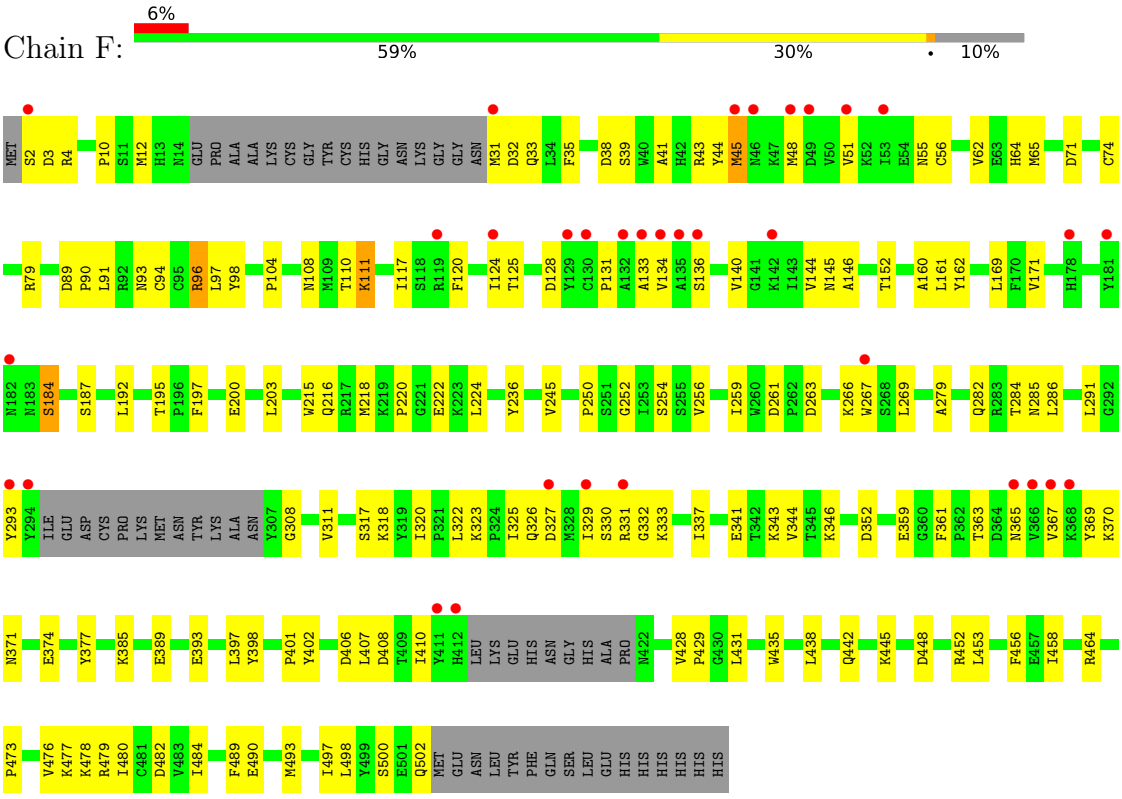
• Molecule 1: Arginyl-tRNA--protein transferase 1

Chain E:



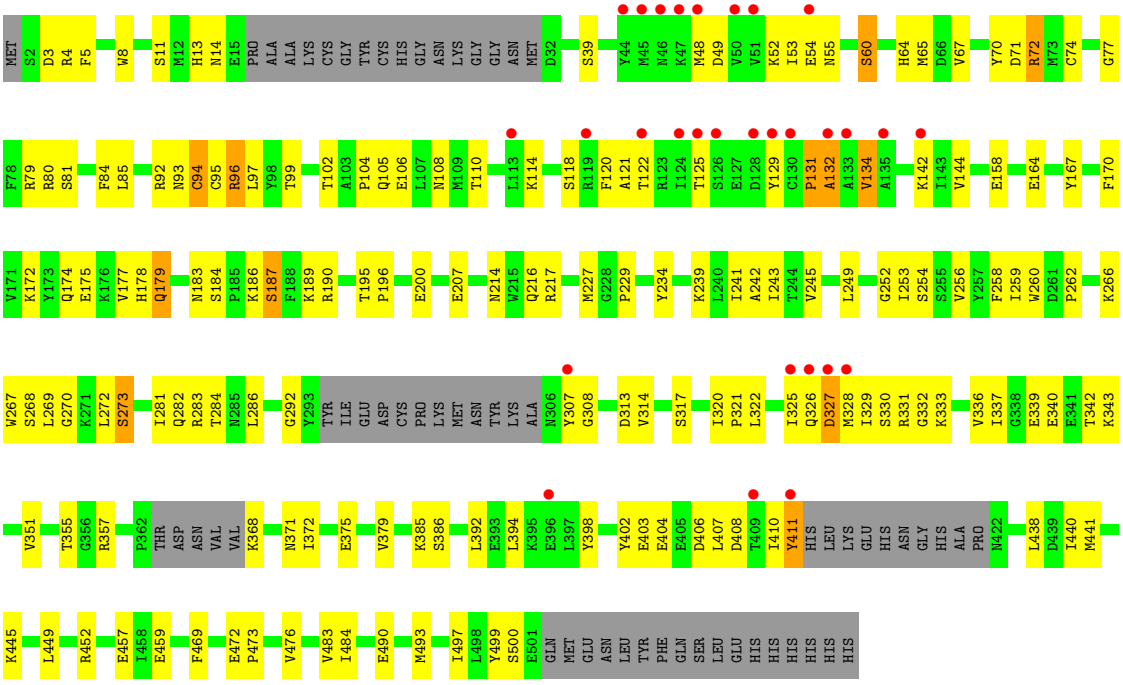
• Molecule 1: Arginyl-tRNA--protein transferase 1

Chain F:



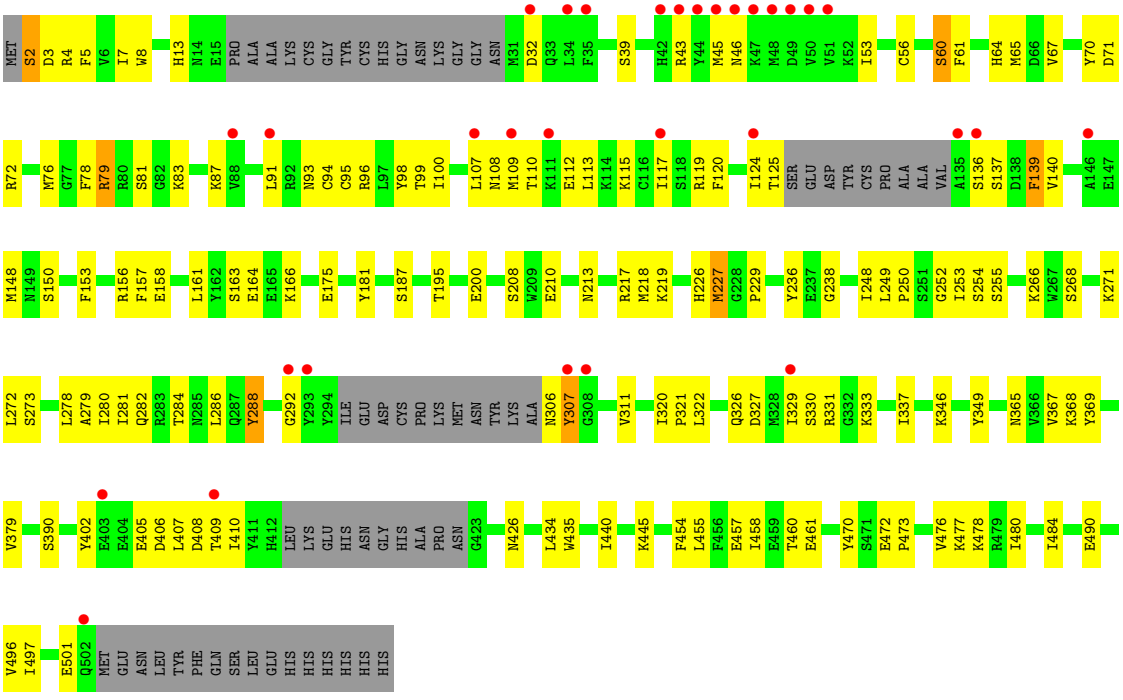
• Molecule 1: Arginyl-tRNA--protein transferase 1

Chain G:



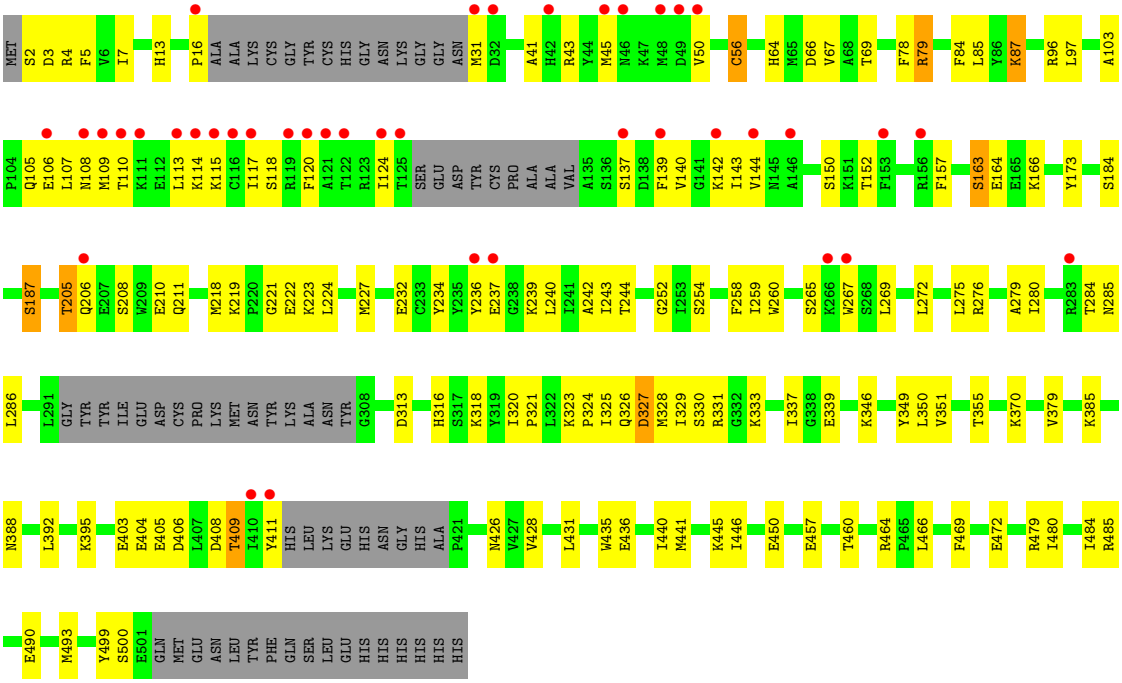
• Molecule 1: Arginyl-tRNA--protein transferase 1

Chain H:



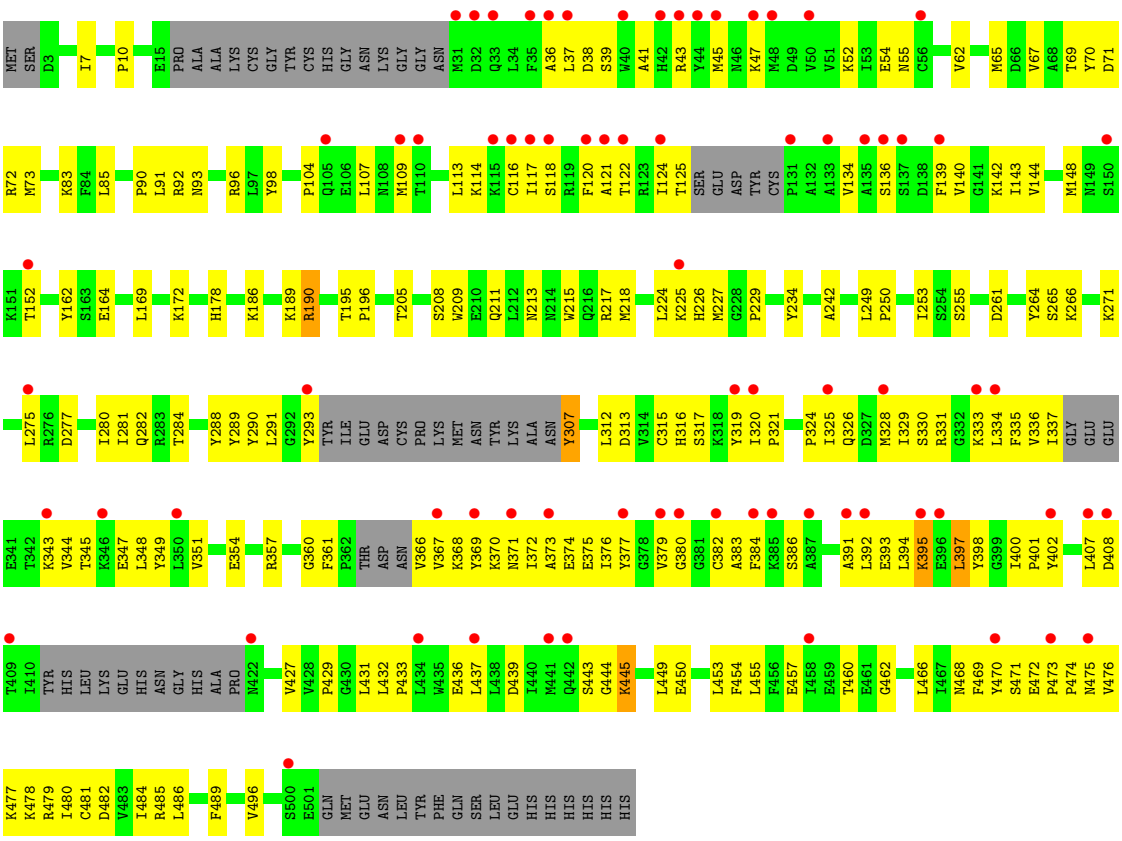
• Molecule 1: Arginyl-tRNA--protein transferase 1

Chain I:



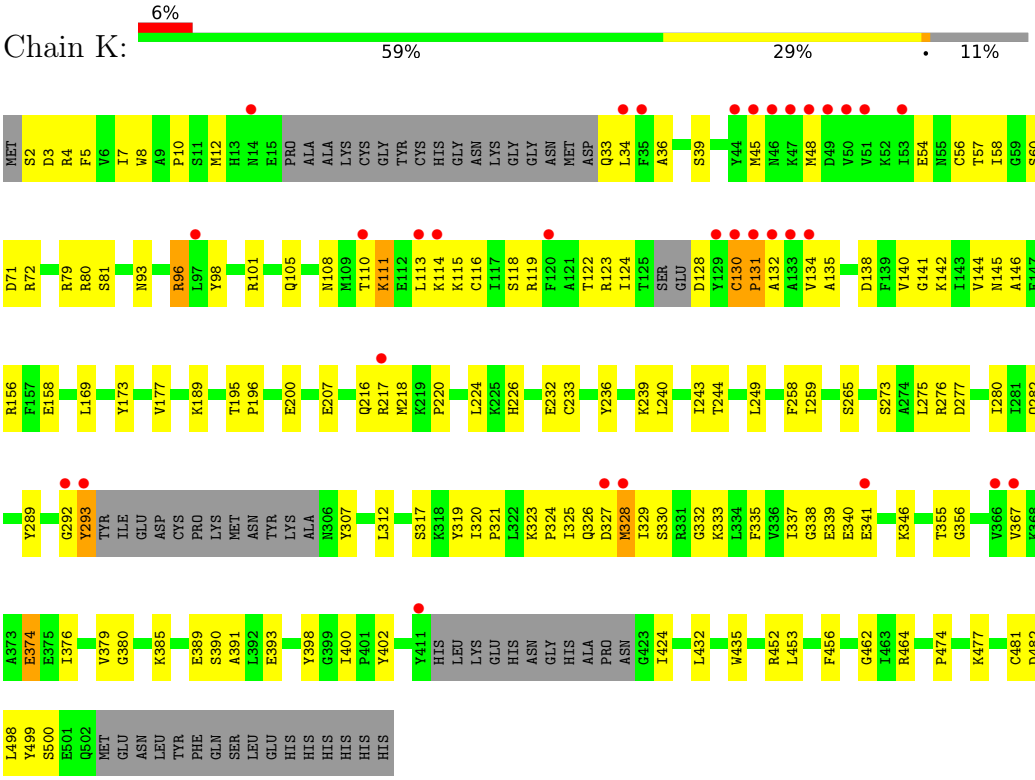
• Molecule 1: Arginyl-tRNA--protein transferase 1

Chain J:



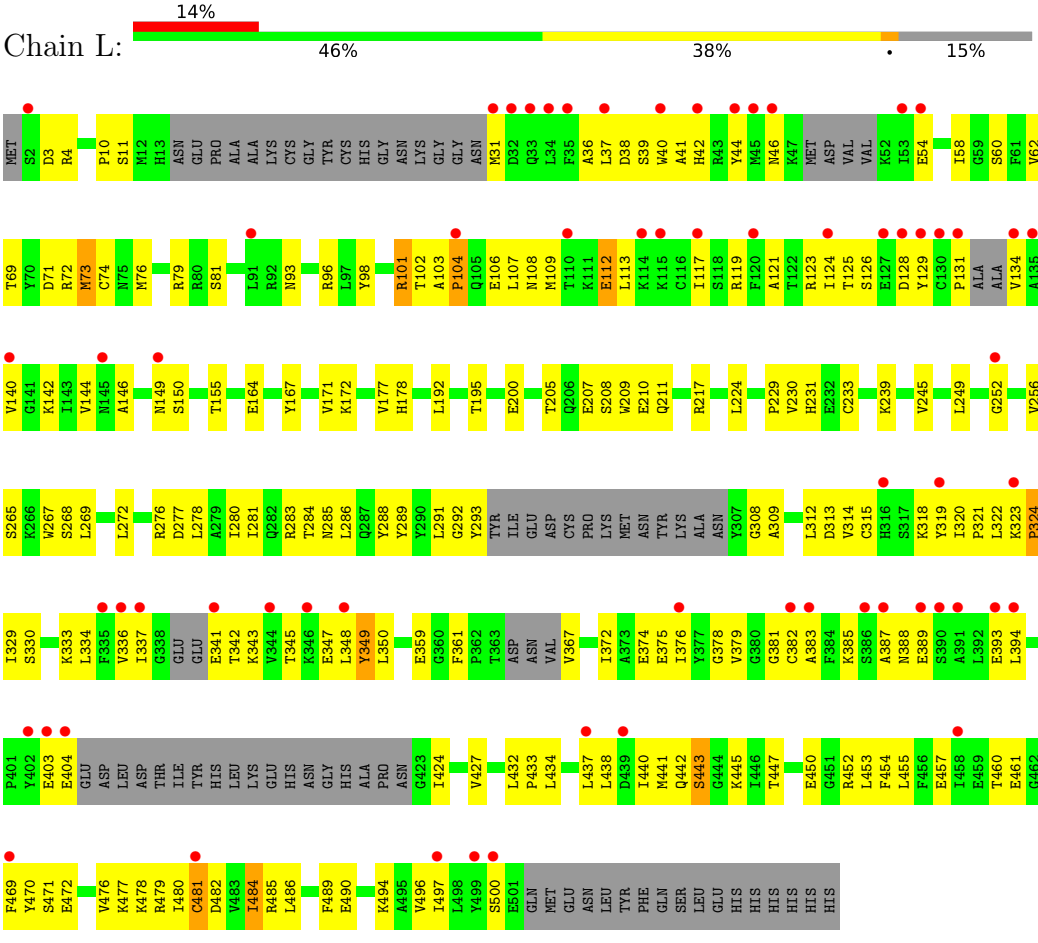
• Molecule 1: Arginyl-tRNA--protein transferase 1

Chain K:



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

Chain L:



4 Data and refinement statistics (i)

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) 100.0 (65.25-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.200 , 0.257 0.200 , 0.257	Depositor DCC
R_{free} test set	10891 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 , 84.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, SO4

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	0.53	0/3898	0.68	0/5269
1	B	0.53	1/3867 (0.0%)	0.71	0/5226
1	C	0.55	0/3871	0.70	0/5229
1	D	0.50	0/3804	0.66	1/5136 (0.0%)
1	E	0.51	0/3875	0.67	1/5236 (0.0%)
1	F	0.52	1/3870 (0.0%)	0.66	0/5230
1	G	0.49	0/3808	0.65	2/5143 (0.0%)
1	H	0.48	0/3811	0.66	2/5146 (0.0%)
1	I	0.50	0/3764	0.67	1/5083 (0.0%)
1	J	0.48	0/3737	0.69	2/5043 (0.0%)
1	K	0.51	0/3823	0.70	3/5165 (0.1%)
1	L	0.49	0/3675	0.70	1/4956 (0.0%)
All	All	0.51	2/45803 (0.0%)	0.68	13/61862 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	VAL	CB-CG1	-5.58	1.41	1.52
1	F	74	CYS	CB-SG	-5.09	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	220	PRO	N-CA-C	6.72	129.57	112.10
1	H	288	TYR	CB-CA-C	-6.17	98.06	110.40
1	G	132	ALA	N-CA-C	5.83	126.73	111.00
1	K	220	PRO	CB-CA-C	-5.74	97.65	112.00
1	G	102	THR	C-N-CA	5.57	135.63	121.70
1	E	137	SER	N-CA-C	-5.56	95.99	111.00
1	I	205	THR	C-N-CA	5.53	135.53	121.70
1	L	481	CYS	CB-CA-C	-5.52	99.35	110.40
1	K	328	MET	CG-SD-CE	5.30	108.67	100.20
1	D	66	ASP	CB-CG-OD1	5.28	123.05	118.30
1	J	190	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	H	227	MET	CG-SD-CE	-5.17	91.92	100.20
1	J	397	LEU	CA-CB-CG	5.11	127.05	115.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3800	0	3733	103	2
1	B	3775	0	3707	102	0
1	C	3776	0	3727	110	0
1	D	3715	0	3654	116	0
1	E	3783	0	3722	122	0
1	F	3777	0	3710	129	0
1	G	3718	0	3653	164	0
1	H	3721	0	3660	123	0
1	I	3676	0	3629	132	2
1	J	3651	0	3615	183	0
1	K	3733	0	3675	140	0
1	L	3589	0	3546	206	3
2	A	115	0	0	2	1
2	B	125	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	10	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	4	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
4	B	12	0	0	2	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	1563	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 17.

All (1563) 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
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:J:104:PRO:HG2	1:J:282:GLN:HB2	1.44	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:C:38:ASP:CG	1:C:331:ARG:NH2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:284:THR:HG23	1:H:286:LEU:HG	1.47	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: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: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: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:L:478:LYS:C	1:L:481:CYS:SG	2.51	0.88
1:J:444:GLY:O	1:L:349:TYR:CE1	2.26	0.88
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:352:ASP:CG	1:F:490:GLU:HG3	1.99	0.82
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
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:L:325:ILE:HG23	1:L:328:MET:HE2	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:G:490:GLU:HA	1:G:493:MET:HE2	1.67	0.76
1:K:115:LYS:HG3	1:K:118:SER:HB3	1.65	0.76
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:L:69:THR:HG22	1:L:73:MET:HE1	1.66	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: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: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:F:43:ARG:HE	1:F:44:TYR:HE1	1.32	0.74
1:F:341:GLU:O	1:F:341:GLU:CD	2.26	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:I:325:ILE:HG13	1:I:328:MET:HE1	1.69	0.73
1:E:87:LYS:NZ	4:E:701:HOH:O	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:65:MET:HE1	1:J:85:LEU:HD22	1.70	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
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: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: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: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:B:148:MET:HE3	1:B:217:ARG:HH11	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:37:LEU:HD21	1:D:334:LEU:HD23	1.73	0.69
1:I:218:MET:HE2	1:I:284:THR:HA	1.74	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:E:334:LEU:C	1:E:334:LEU:HD23	2.13	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: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: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:D:65:MET:HE2	1:D:196:PRO:HG2	1.77	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:I:110:THR:H	1:I:114:LYS:HZ2	1.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:L:106:GLU:O	1:L:106:GLU:HG2	1.96	0.66
1:B:45:MET:HA	1:B:48:MET:HE2	1.76	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:11:SER:OG	1:E:13:HIS:NE2	2.30	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
1:B:78:PHE:CE2	1:B:87:LYS:HD2	2.33	0.64
1:K:218:MET:HE2	1:K:284:THR:HA	1.79	0.64
1:C:35:PHE:HD2	1:C:411:TYR:HH	1.44	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: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:A:1:MET:H2	1:C:200:GLU:H	1.44	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:E:294:TYR:CG	1:E:295:ILE:N	2.67	0.63
1:G:457:GLU:HG3	1:G:499:TYR:CE1	2.33	0.63
1:H:406:ASP:HB3	1:H:408:ASP:OD1	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:460:THR:HG22	1:C:462:GLY:H	1.65	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: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: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:A:32:ASP:N	1:A:45:MET:CE	2.63	0.61
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:E:73:MET:HE1	1:E:487:PHE:HA	1.84	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:F:352:ASP:OD1	1:F:490:GLU:HG3	2.02	0.60
1:J:313:ASP:O	1:J:317:SER:N	2.35	0.60
1:L:93:ASN:C	1:L:96:ARG:HH12	2.04	0.60
1:L:209:TRP:CH2	1:L:230:VAL:HG12	2.37	0.60

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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: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: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:I:325:ILE:CG1	1:I:328:MET:HE1	2.33	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:221:GLY:C	2:E:612:SO4:O3	2.41	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:D:3:ASP:HB2	1:G:200:GLU:CD	2.22	0.58
1:K:5:PHE:CE2	1:K:7:ILE:HD13	2.38	0.58
1:B:458:ILE:HG12	1:B:500:SER:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:134:VAL:O	1:F:136:SER:OG	2.20	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: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:K:156:ARG:HH22	1:K:158:GLU:CD	2.01	0.58
1:I:120:PHE:CE1	1:I:124:ILE:HD11	2.39	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: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:L:441:MET:HE1	1:L:469:PHE:CE2	2.39	0.58
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
1:F:3:ASP:HB2	1:H:200:GLU:CD	2.25	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:109:MET:HE2	1:J:114:LYS:HG2	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:134:VAL:HG21	1:E:142:LYS:HZ1	1.70	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:I:223:LYS:NZ	1:I:285:ASN:O	2.22	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:D:65:MET:HE2	1:D:196:PRO:CG	2.35	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:469:PHE:CE2	1:L:477:LYS:HD2	2.41	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:J:407:LEU:O	1:J:407:LEU:CG	2.48	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:H:112:GLU:CD	1:H:271:LYS:NZ	2.59	0.55
1:I:339:GLU:O	1:I:370:LYS:NZ	2.38	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:D:363:THR:C	1:D:365:ASN:H	2.09	0.55
1:F:117:ILE:HA	1:F:120:PHE:HB3	1.89	0.55
1:K:400:ILE:HD13	1:K:481:CYS:SG	2.47	0.55
1:A:32:ASP:N	1:A:45:MET:HE1	2.22	0.54
1:L:112:GLU:H	1:L:112:GLU:CD	2.08	0.54
1:L:291:LEU:HD23	1:L:293:TYR:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:137:SER:O	1:D:137:SER:OG	2.25	0.54
1:E:15:GLU:CB	1:E:16:PRO:CD	2.75	0.54
1:F:31:MET:N	1:F:48:MET:CE	2.70	0.54
1:H:158:GLU:OE1	3:H:614:GOL:H2	2.07	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: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:A:1:MET:H2	1:C:200:GLU:N	2.06	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:H:65:MET:HE3	1:H:70:TYR:HB2	1.90	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
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:H:227:MET:HE1	1:H:250:PRO:CD	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:281:ILE:HG23	1:H:286:LEU:HB2	1.90	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: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:B:176:LYS:NZ	4:B:702:HOH:O	2.33	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:C:65:MET:HE3	1:C:70:TYR:HB2	1.91	0.53
1:E:54:GLU:HB2	1:E:56:CYS:SG	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:325:ILE:HD12	1:L:328:MET:HE1	1.92	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:I:325:ILE:CD1	1:I:328:MET:HE1	2.39	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: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: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
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:D:200:GLU:CD	1:G:3:ASP:HB2	2.31	0.51
1:E:58:ILE:HD11	1:E:89:ASP:HB2	1.92	0.51
1:G:5:PHE:HE1	1:G:65:MET:HE2	1.75	0.51
1:H:331:ARG:O	1:H:333:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:490:GLU:HA	1:I:493:MET:HE2	1.91	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:372:ILE:O	1:E:375:GLU:HG2	2.11	0.51
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:E:365:ASN:HD22	1:E:365:ASN:C	2.07	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:K:218:MET:HE1	1:K:284:THR:HA	1.90	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:H:110:THR:HG1	1:H:113:LEU:H	1.59	0.50
1:K:325:ILE:HA	1:K:327:ASP:HB2	1.91	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
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:322:LEU:HD23	1:F:322:LEU:C	2.32	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:E:334:LEU:HD23	1:E:334:LEU:O	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:69:THR:O	1:L:73:MET:HE2	2.11	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: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:H:72:ARG:HG2	1:H:76:MET:HE3	1.94	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:C:109:MET:HE1	1:C:114:LYS:HB2	1.94	0.49
1:E:37:LEU:HD21	1:E:334:LEU:HD22	1.94	0.49
1:E:311:VAL:HG21	1:E:322:LEU:HD13	1.95	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:K:148:MET:SD	1:K:149:ASN:CG	2.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:398:TYR:O	1:F:477:LYS:NZ	2.37	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
1:F:12:MET:HE2	1:F:56:CYS:HB3	1.96	0.48
1:J:397:LEU:HB3	1:J:398:TYR:CE2	2.48	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: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:G:402:TYR:C	1:G:403:GLU:HG3	2.33	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:322:LEU:C	1:L:322:LEU:HD12	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:129:TYR:HH	1:G:131:PRO:HB3	1.70	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:L:172:LYS:HZ3	1:L:261:ASP:CG	2.16	0.48
1:D:388:ASN:CB	1:D:404:GLU:HG2	2.39	0.48
1:F:363:THR:C	1:F:365:ASN:H	2.17	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: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:A:45:MET:C	1:A:47:LYS:N	2.67	0.47
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:69:THR:HG22	1:L:73:MET:CE	2.38	0.47
1:L:367:VAL:HG12	1:L:367:VAL:O	2.14	0.47
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:K:341:GLU:O	1:K:341:GLU:CD	2.52	0.47
1:C:10:PRO:HG2	1:C:482:ASP:HB3	1.97	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:G:105:GLN:H	1:G:105:GLN:CD	2.18	0.47
1:J:398:TYR:O	1:J:400:ILE:HG13	2.15	0.47
1:K:398:TYR:O	1:K:477:LYS:NZ	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:65:MET:HE3	1:G:85:LEU:HD22	1.97	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:L:76:MET:HE3	2:L:604:SO4:O4	2.14	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
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: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:B:365:ASN:C	1:B:367:VAL:N	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:139:PHE:O	1:I:142:LYS:HB2	2.15	0.47
1:J:62:VAL:HG11	1:J:65:MET:HE2	1.96	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: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: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: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: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:E:127:GLU:H	1:E:127:GLU:CD	2.19	0.46
1:E:221:GLY:CA	2:E:612:SO4:O3	2.64	0.46
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:H:227:MET:HE1	1:H:250:PRO:HG3	1.96	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:110:THR:H	1:I:114:LYS:HZ3	1.61	0.46
1:I:450:GLU:CA	1:I:466:LEU:HD12	2.46	0.46
1:K:56:CYS:N	1:K:93:ASN:OD1	2.41	0.46
1:L:109:MET:HE1	1:L:139:PHE:HB3	1.98	0.46
1:A:117:ILE:HD11	1:A:275:LEU:HD13	1.98	0.46
1:H:470:TYR:O	1:H:477:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:172:LYS:HZ3	1:A:261:ASP:CG	2.19	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: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:I:66:ASP:OD1	1:I:69:THR:N	2.28	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:A:32:ASP:N	1:A:45:MET:HE3	2.31	0.46
1:A:45:MET:C	1:A:47:LYS:H	2.18	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
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: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:K:339:GLU:CD	1:K:367:VAL:HG21	2.37	0.46
1:B:127:GLU:C	1:B:129:TYR:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:65:MET:CE	1:G:85:LEU:HD22	2.47	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
1:L:337:ILE:HD13	1:L:361:PHE:CZ	2.52	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: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: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:I:265:SER:C	1:I:267:TRP:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:438:LEU:O	1:F:442:GLN:HG3	2.17	0.45
1:F:452:ARG:HE	1:F:493:MET:CE	2.29	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: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: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: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: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:A:88:VAL:O	3:A:625:GOL:O2	2.27	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:G:5:PHE:CE1	1:G:65:MET:HE2	2.52	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:E:409:THR:C	1:E:411:TYR:N	2.70	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: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:B:365:ASN:C	1:B:367:VAL:H	2.19	0.44
1:D:48:MET:HA	1:D:51:VAL:HG12	1.99	0.44
1:D:65:MET:CE	1:D:70:TYR:HB2	2.47	0.44
1:D:240:LEU:HD21	1:D:243:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:LEU:CD1	1:D:407:LEU:H	2.31	0.44
1:E:328:MET:HE2	1:E:328:MET:HB2	1.72	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:L:107:LEU:C	1:L:107:LEU:HD23	2.38	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: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:E:457:GLU:O	1:E:460:THR:OG1	2.33	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
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:I:464:ARG:HH12	1:I:472:GLU:CD	2.21	0.44
1:L:73:MET:HE3	1:L:73:MET:HB2	1.67	0.44
1:L:239:LYS:HA	1:L:239:LYS:HD2	1.68	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:L:209:TRP:CZ3	1:L:230:VAL:HG12	2.53	0.44
1:L:374:GLU:C	1:L:376:ILE:H	2.20	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:H:93:ASN:HB3	1:H:95:CYS:O	2.18	0.44
1:H:148:MET:CE	1:H:217:ARG:HD3	2.48	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:E:73:MET:CE	1:E:487:PHE:HD1	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:65:MET:HE2	1:K:196:PRO:CG	2.48	0.44
1:K:258:PHE:CE1	1:K:273:SER:HB3	2.53	0.44
1:L:76:MET:HE1	2:L:604:SO4:O4	2.17	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: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: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:D:478:LYS:HZ2	3:D:626:GOL:H11	1.83	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
1:K:328:MET:HG2	1:K:371:ASN:HD22	1.83	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:164:GLU:CD	1:L:164:GLU:H	2.22	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: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: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:31:MET:N	1:F:48:MET:HE1	2.34	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: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: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: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:F:31:MET:N	1:F:48:MET:HE3	2.34	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:101:ARG:HG2	1:A:319:TYR:CE2	2.54	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:115:LYS:HA	1:B:118:SER:OG	2.20	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: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:G:398:TYR:HB3	1:G:441:MET:HE2	2.02	0.42
1:J:205:THR:HG1	1:J:208:SER:H	1.66	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: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: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:I:441:MET:HE1	1:I:446:ILE:HG12	2.01	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: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:D:464:ARG:HH22	1:D:472:GLU:CD	2.22	0.42
1:F:2:SER:C	1:F:4:ARG:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:169:LEU:HD12	1:J:169:LEU:HA	1.82	0.42
1:J:392:LEU:HA	1:J:395:LYS:CD	2.49	0.42
1:K:156:ARG:NH2	1:K:158:GLU:CD	2.65	0.42
1:L:372:ILE:O	1:L:375:GLU:HG2	2.19	0.42
1:D:124:ILE:HG21	1:D:153:PHE:HB3	2.01	0.42
1:E:134:VAL:O	1:E:135:ALA:C	2.58	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: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:D:2:SER:C	1:D:4:ARG:H	2.23	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:L:62:VAL:HG11	1:L:65:MET:HE3	2.01	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:F:452:ARG:HE	1:F:493:MET:HE2	1.84	0.41
1:G:11:SER:OG	1:G:13:HIS:NE2	2.52	0.41
1:G:207:GLU:H	1:G:207:GLU:CD	2.22	0.41
1:H:99:THR:HA	1:H:292:GLY:HA2	2.02	0.41
1:H:227:MET:HE1	1:H:250:PRO:CG	2.50	0.41
1:H:368:LYS:HB2	1:H:368:LYS:HE2	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:388:ASN:CG	1:L:404:GLU:HG3	2.40	0.41
1:L:469:PHE:HE1	1:L:480:ILE:HG21	1.85	0.41
1:B:463:ILE:HD13	1:B:463:ILE:HG21	1.76	0.41
1:E:45:MET:HG3	1:E:46:ASN:H	1.86	0.41
1:E:409:THR:C	1:E:411:TYR:H	2.23	0.41
1:F:346:LYS:HE3	1:F:435:TRP:CZ2	2.55	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: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: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:I:395:LYS:NZ	1:I:403:GLU:OE2	2.50	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: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:136:SER:OG	1:H:137:SER:N	2.53	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:390:SER:OG	2:K:603:SO4:O3	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:406:ASP:C	1:I:408:ASP:H	2.24	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:A:32:ASP:HB2	1:A:333:LYS:HZ3	1.83	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: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: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: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: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: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:323:LYS:O	1:B:324:PRO:C	2.60	0.41
1:B:432:LEU:HD21	1:B:436:GLU:HG2	2.03	0.41
1:D:35:PHE:O	1:D:333:LYS:HE3	2.21	0.41
1:G:53:ILE:HG22	1:G:411:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:MET:HE2	1:G:65:MET:HB3	1.99	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:I:441:MET:HE1	1:I:469:PHE:CE2	2.55	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:K:328:MET:C	1:K:330:SER:N	2.74	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:L:62:VAL:HG11	1:L:65:MET:HE2	2.02	0.41
1:D:65:MET:HE3	1:D:70:TYR:HB2	2.03	0.40
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:131:PRO:C	1:F:133:ALA:N	2.74	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:HG2	1:K:326:GLN:O	2.21	0.40
1:K:372:ILE:HD12	1:K:376:ILE:HD11	2.03	0.40
1:B:31:MET:HE3	1:B:31:MET:HB3	1.75	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:177:VAL:C	1:G:179:GLN:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:PHE:N	1:H:213:ASN:OD1	2.49	0.40
1:H:236:TYR:C	1:H:238:GLY:H	2.25	0.40
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: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:F:263:ASP:HB2	1:I:239:LYS:HZ3	1.87	0.40
1:F:456:PHE:HB3	1:F:498:LEU:HD12	2.04	0.40
1:G:441:MET:HE1	1:G:469:PHE:HE2	1.86	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: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:280:ILE:O	1:E:284:THR:OG1	2.32	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:337:ILE:HG23	1:H:369:TYR:HB3	2.03	0.40
1:I:219:LYS:C	1:I:221:GLY:H	2.24	0.40
1:J:121:ALA:HA	1:J:124:ILE:HD11	2.03	0.40
1:J:148:MET:HE1	1:J:217:ARG:HE	1.86	0.40
1:K:39:SER:HG	1:K:374:GLU:CD	2.18	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:B:148:MET:HE3	1:B:217:ARG:NH1	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:TYR:O	1:G:170:PHE:HB3	2.21	0.40
1:J:316:HIS:NE2	1:J:337:ILE:O	2.48	0.40
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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	47	75
1	F	456/518 (88%)	423 (93%)	33 (7%)	0	100	100
1	G	447/518 (86%)	417 (93%)	28 (6%)	2 (0%)	34	62
1	H	446/518 (86%)	424 (95%)	22 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	K	449/518 (87%)	415 (92%)	32 (7%)	2 (0%)	34 62
1	L	425/518 (82%)	385 (91%)	39 (9%)	1 (0%)	47 75
All	All	5371/6216 (86%)	4997 (93%)	368 (7%)	6 (0%)	51 79

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)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	418/460 (91%)	409 (98%)	9 (2%)	52 79
1	B	415/460 (90%)	397 (96%)	18 (4%)	29 59
1	C	416/460 (90%)	401 (96%)	15 (4%)	35 66
1	D	409/460 (89%)	394 (96%)	15 (4%)	34 65
1	E	416/460 (90%)	399 (96%)	17 (4%)	30 61
1	F	415/460 (90%)	408 (98%)	7 (2%)	60 83
1	G	408/460 (89%)	392 (96%)	16 (4%)	32 63
1	H	409/460 (89%)	395 (97%)	14 (3%)	37 67
1	I	406/460 (88%)	394 (97%)	12 (3%)	41 72
1	J	401/460 (87%)	392 (98%)	9 (2%)	52 79
1	K	410/460 (89%)	399 (97%)	11 (3%)	44 74
1	L	394/460 (86%)	375 (95%)	19 (5%)	25 55
All	All	4917/5520 (89%)	4755 (97%)	162 (3%)	38 68

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	96	ARG
1	A	128	ASP
1	A	129	TYR
1	A	187	SER
1	A	254	SER
1	A	294	TYR
1	A	456	PHE
1	A	471	SER
1	B	3	ASP
1	B	60	SER
1	B	72	ARG
1	B	74	CYS
1	B	96	ARG
1	B	109	MET
1	B	116	CYS
1	B	123	ARG
1	B	158	GLU
1	B	254	SER
1	B	265	SER
1	B	273	SER
1	B	294	TYR
1	B	326	GLN
1	B	365	ASN
1	B	403	GLU
1	B	408	ASP
1	B	456	PHE
1	C	1	MET
1	C	33	GLN
1	C	96	ARG
1	C	119	ARG
1	C	136	SER
1	C	187	SER
1	C	216	GLN
1	C	265	SER
1	C	307	TYR
1	C	341	GLU
1	C	365	ASN
1	C	368	LYS
1	C	370	LYS
1	C	386	SER
1	C	464	ARG

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Mol	Chain	Res	Type
1	D	3	ASP
1	D	14	ASN
1	D	32	ASP
1	D	39	SER
1	D	46	ASN
1	D	136	SER
1	D	187	SER
1	D	257	TYR
1	D	265	SER
1	D	293	TYR
1	D	307	TYR
1	D	317	SER
1	D	327	ASP
1	D	456	PHE
1	D	500	SER
1	E	3	ASP
1	E	43	ARG
1	E	60	SER
1	E	96	ARG
1	E	116	CYS
1	E	134	VAL
1	E	214	ASN
1	E	217	ARG
1	E	254	SER
1	E	268	SER
1	E	307	TYR
1	E	334	LEU
1	E	365	ASN
1	E	408	ASP
1	E	412	HIS
1	E	422	ASN
1	E	456	PHE
1	F	45	MET
1	F	96	ARG
1	F	111	LYS
1	F	128	ASP
1	F	184	SER
1	F	317	SER
1	F	408	ASP
1	G	14	ASN
1	G	60	SER
1	G	72	ARG

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Mol	Chain	Res	Type
1	G	74	CYS
1	G	81	SER
1	G	94	CYS
1	G	95	CYS
1	G	96	ARG
1	G	179	GLN
1	G	187	SER
1	G	273	SER
1	G	327	ASP
1	G	330	SER
1	G	385	LYS
1	G	386	SER
1	G	411	TYR
1	H	2	SER
1	H	32	ASP
1	H	46	ASN
1	H	60	SER
1	H	79	ARG
1	H	81	SER
1	H	139	PHE
1	H	163	SER
1	H	187	SER
1	H	268	SER
1	H	273	SER
1	H	307	TYR
1	H	327	ASP
1	H	501	GLU
1	I	3	ASP
1	I	56	CYS
1	I	79	ARG
1	I	87	LYS
1	I	96	ARG
1	I	107	LEU
1	I	137	SER
1	I	163	SER
1	I	187	SER
1	I	327	ASP
1	I	385	LYS
1	I	409	THR
1	J	47	LYS
1	J	178	HIS
1	J	255	SER

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Mol	Chain	Res	Type
1	J	265	SER
1	J	307	TYR
1	J	354	GLU
1	J	386	SER
1	J	395	LYS
1	J	445	LYS
1	K	3	ASP
1	K	81	SER
1	K	96	ARG
1	K	105	GLN
1	K	111	LYS
1	K	116	CYS
1	K	128	ASP
1	K	265	SER
1	K	282	GLN
1	K	293	TYR
1	K	374	GLU
1	L	31	MET
1	L	73	MET
1	L	74	CYS
1	L	81	SER
1	L	101	ARG
1	L	112	GLU
1	L	117	ILE
1	L	136	SER
1	L	138	ASP
1	L	149	ASN
1	L	265	SER
1	L	268	SER
1	L	283	ARG
1	L	326	GLN
1	L	349	TYR
1	L	443	SER
1	L	470	TYR
1	L	484	ILE
1	L	500	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	14	ASN
1	F	178	HIS

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Mol	Chain	Res	Type
1	G	145	ASN
1	K	365	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	D	618	-	4,4,4	0.17	0	6,6,6	0.12	0
2	SO4	K	610	-	4,4,4	0.63	0	6,6,6	0.13	0
2	SO4	K	604	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	C	619	-	4,4,4	0.41	0	6,6,6	0.05	0
2	SO4	J	602	-	4,4,4	0.52	0	6,6,6	0.08	0
2	SO4	E	619	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	H	602	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	A	618	-	4,4,4	0.44	0	6,6,6	0.06	0
2	SO4	E	613	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	K	601	-	4,4,4	0.17	0	6,6,6	0.26	0
3	GOL	A	627	-	5,5,5	0.90	0	5,5,5	0.93	0
2	SO4	F	611	-	4,4,4	0.17	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	E	609	-	4,4,4	0.17	0	6,6,6	0.26	0
2	SO4	A	609	-	4,4,4	0.18	0	6,6,6	0.20	0
2	SO4	A	602	-	4,4,4	0.12	0	6,6,6	0.41	0
3	GOL	D	623	-	5,5,5	1.18	0	5,5,5	0.76	0
2	SO4	H	604	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	I	603	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	C	604	-	4,4,4	0.46	0	6,6,6	0.07	0
2	SO4	B	617	-	4,4,4	0.15	0	6,6,6	0.14	0
3	GOL	A	631	-	5,5,5	0.09	0	5,5,5	0.27	0
2	SO4	I	601	-	4,4,4	0.45	0	6,6,6	0.07	0
2	SO4	A	616	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	C	611	-	4,4,4	0.52	0	6,6,6	0.09	0
2	SO4	D	621	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	603	-	4,4,4	0.09	0	6,6,6	0.26	0
2	SO4	A	601	-	4,4,4	0.20	0	6,6,6	0.48	0
3	GOL	J	609	-	5,5,5	1.26	1 (20%)	5,5,5	0.78	0
2	SO4	L	602	-	4,4,4	0.11	0	6,6,6	0.15	0
3	GOL	G	621	-	5,5,5	0.94	0	5,5,5	1.15	0
2	SO4	B	616	-	4,4,4	0.47	0	6,6,6	0.06	0
2	SO4	G	607	-	4,4,4	0.43	0	6,6,6	0.06	0
2	SO4	J	601	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	C	617	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	G	603	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	B	618	-	4,4,4	0.42	0	6,6,6	0.05	0
2	SO4	D	617	-	4,4,4	0.49	0	6,6,6	0.08	0
2	SO4	E	625	-	4,4,4	0.15	0	6,6,6	0.22	0
3	GOL	H	616	-	5,5,5	0.88	0	5,5,5	1.13	0
2	SO4	A	613	-	4,4,4	0.42	0	6,6,6	0.04	0
2	SO4	G	613	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	F	606	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	L	608	-	4,4,4	0.49	0	6,6,6	0.08	0
2	SO4	G	616	-	4,4,4	0.17	0	6,6,6	0.12	0
2	SO4	I	612	-	4,4,4	0.45	0	6,6,6	0.05	0
2	SO4	L	601	-	4,4,4	0.48	0	6,6,6	0.08	0
2	SO4	E	608	-	4,4,4	0.13	0	6,6,6	0.45	0
2	SO4	F	602	-	4,4,4	0.14	0	6,6,6	0.15	0
3	GOL	H	617	-	5,5,5	1.67	2 (40%)	5,5,5	1.00	0
2	SO4	G	601	-	4,4,4	0.21	0	6,6,6	0.37	0
2	SO4	B	623	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	I	610	-	4,4,4	0.57	0	6,6,6	0.09	0
3	GOL	G	618	-	5,5,5	0.78	0	5,5,5	1.14	1 (20%)
2	SO4	B	609	-	4,4,4	0.17	0	6,6,6	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	615	-	4,4,4	0.14	0	6,6,6	0.08	0
3	GOL	G	620	-	5,5,5	1.09	0	5,5,5	0.90	0
2	SO4	H	609	-	4,4,4	0.13	0	6,6,6	0.26	0
2	SO4	C	612	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	B	610	-	4,4,4	0.51	0	6,6,6	0.05	0
3	GOL	B	626	-	5,5,5	1.09	0	5,5,5	0.91	0
2	SO4	C	622	-	4,4,4	0.14	0	6,6,6	0.12	0
3	GOL	F	614	-	5,5,5	1.09	0	5,5,5	0.97	0
2	SO4	B	620	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	I	613	-	4,4,4	0.45	0	6,6,6	0.06	0
2	SO4	G	615	-	4,4,4	0.47	0	6,6,6	0.08	0
2	SO4	E	605	-	4,4,4	0.19	0	6,6,6	0.14	0
2	SO4	C	614	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	I	604	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	D	610	-	4,4,4	0.13	0	6,6,6	0.18	0
2	SO4	B	613	-	4,4,4	0.13	0	6,6,6	0.11	0
3	GOL	B	628	-	5,5,5	1.26	1 (20%)	5,5,5	1.04	0
2	SO4	F	603	-	4,4,4	0.19	0	6,6,6	0.23	0
2	SO4	D	611	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	H	603	-	4,4,4	0.15	0	6,6,6	0.19	0
2	SO4	F	608	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	C	608	-	4,4,4	0.11	0	6,6,6	0.19	0
2	SO4	D	607	-	4,4,4	0.15	0	6,6,6	0.43	0
2	SO4	F	612	-	4,4,4	0.14	0	6,6,6	0.11	0
3	GOL	B	627	-	5,5,5	1.16	1 (20%)	5,5,5	1.15	0
2	SO4	B	604	-	4,4,4	0.18	0	6,6,6	0.13	0
2	SO4	E	620	-	4,4,4	0.13	0	6,6,6	0.19	0
2	SO4	G	606	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	E	618	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	J	608	-	4,4,4	0.12	0	6,6,6	0.08	0
2	SO4	B	601	-	4,4,4	0.19	0	6,6,6	0.22	0
2	SO4	J	604	-	4,4,4	0.49	0	6,6,6	0.06	0
2	SO4	I	602	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	E	611	-	4,4,4	0.23	0	6,6,6	0.49	0
2	SO4	D	615	-	4,4,4	0.50	0	6,6,6	0.07	0
2	SO4	H	601	-	4,4,4	0.45	0	6,6,6	0.07	0
2	SO4	A	623	-	4,4,4	0.48	0	6,6,6	0.07	0
2	SO4	I	607	-	4,4,4	0.12	0	6,6,6	0.12	0
3	GOL	E	627	-	5,5,5	0.85	0	5,5,5	0.94	0
2	SO4	B	624	-	4,4,4	0.12	0	6,6,6	0.10	0
2	SO4	C	618	-	4,4,4	0.52	0	6,6,6	0.09	0
3	GOL	A	629	-	5,5,5	0.79	0	5,5,5	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	G	605	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	L	607	-	4,4,4	0.18	0	6,6,6	0.14	0
2	SO4	E	617	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	B	607	-	4,4,4	0.12	0	6,6,6	0.24	0
2	SO4	G	614	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	A	612	-	4,4,4	0.49	0	6,6,6	0.06	0
3	GOL	A	626	-	5,5,5	1.17	1 (20%)	5,5,5	0.80	0
2	SO4	F	605	-	4,4,4	0.13	0	6,6,6	0.25	0
2	SO4	I	606	-	4,4,4	0.55	0	6,6,6	0.09	0
2	SO4	H	607	-	4,4,4	0.12	0	6,6,6	0.17	0
2	SO4	L	611	-	4,4,4	0.48	0	6,6,6	0.08	0
3	GOL	E	626	-	5,5,5	1.28	1 (20%)	5,5,5	0.88	0
2	SO4	A	606	-	4,4,4	0.12	0	6,6,6	0.22	0
2	SO4	D	616	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	C	606	-	4,4,4	0.17	0	6,6,6	0.17	0
2	SO4	C	609	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	B	612	-	4,4,4	0.55	0	6,6,6	0.13	0
2	SO4	G	609	-	4,4,4	0.12	0	6,6,6	0.14	0
2	SO4	D	609	-	4,4,4	0.49	0	6,6,6	0.09	0
2	SO4	A	611	-	4,4,4	0.50	0	6,6,6	0.06	0
2	SO4	B	606	-	4,4,4	0.11	0	6,6,6	0.50	0
2	SO4	G	602	-	4,4,4	0.11	0	6,6,6	0.47	0
2	SO4	A	607	-	4,4,4	0.15	0	6,6,6	0.29	0
2	SO4	B	619	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	K	606	-	4,4,4	0.12	0	6,6,6	0.17	0
3	GOL	B	630	-	5,5,5	1.06	0	5,5,5	0.89	0
2	SO4	C	607	-	4,4,4	0.15	0	6,6,6	0.22	0
2	SO4	C	621	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	H	612	-	4,4,4	0.52	0	6,6,6	0.06	0
3	GOL	E	628	-	5,5,5	0.77	0	5,5,5	0.99	0
2	SO4	H	606	-	4,4,4	0.18	0	6,6,6	0.30	0
2	SO4	I	605	-	4,4,4	0.16	0	6,6,6	0.21	0
2	SO4	E	616	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	F	613	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	K	607	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	D	606	-	4,4,4	0.17	0	6,6,6	0.09	0
2	SO4	D	622	-	4,4,4	0.46	0	6,6,6	0.06	0
2	SO4	C	613	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	H	613	-	4,4,4	0.17	0	6,6,6	0.16	0
3	GOL	D	626	-	5,5,5	1.04	0	5,5,5	0.86	0
2	SO4	K	605	-	4,4,4	0.42	0	6,6,6	0.05	0
2	SO4	L	610	-	4,4,4	0.44	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	F	604	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	F	609	-	4,4,4	0.43	0	6,6,6	0.05	0
2	SO4	C	603	-	4,4,4	0.19	0	6,6,6	0.40	0
3	GOL	F	615	-	5,5,5	1.33	1 (20%)	5,5,5	1.11	0
2	SO4	E	601	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SO4	A	610	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	A	615	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	A	622	-	4,4,4	0.10	0	6,6,6	0.29	0
2	SO4	E	607	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	B	605	-	4,4,4	0.49	0	6,6,6	0.07	0
2	SO4	E	614	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	F	601	-	4,4,4	0.20	0	6,6,6	0.44	0
2	SO4	C	615	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	K	603	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	E	606	-	4,4,4	0.13	0	6,6,6	0.22	0
3	GOL	I	614	-	5,5,5	0.89	0	5,5,5	1.08	0
2	SO4	D	605	-	4,4,4	0.15	0	6,6,6	0.09	0
3	GOL	K	612	-	5,5,5	0.99	0	5,5,5	0.88	0
2	SO4	J	605	-	4,4,4	0.43	0	6,6,6	0.06	0
2	SO4	C	616	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	H	605	-	4,4,4	0.59	0	6,6,6	0.10	0
2	SO4	G	611	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	A	620	-	4,4,4	0.51	0	6,6,6	0.09	0
2	SO4	C	601	-	4,4,4	0.47	0	6,6,6	0.08	0
2	SO4	C	620	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	D	612	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	E	615	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	L	604	-	4,4,4	0.52	0	6,6,6	0.09	0
2	SO4	A	608	-	4,4,4	0.57	0	6,6,6	0.09	0
2	SO4	D	601	-	4,4,4	0.18	0	6,6,6	0.41	0
2	SO4	D	603	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	B	625	-	4,4,4	0.16	0	6,6,6	0.11	0
3	GOL	L	612	-	5,5,5	1.02	0	5,5,5	1.19	1 (20%)
3	GOL	H	614	-	5,5,5	1.41	0	5,5,5	0.66	0
3	GOL	K	611	-	5,5,5	1.41	1 (20%)	5,5,5	0.54	0
2	SO4	K	602	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	B	602	-	4,4,4	0.09	0	6,6,6	0.42	0
2	SO4	J	603	-	4,4,4	0.55	0	6,6,6	0.05	0
2	SO4	D	619	-	4,4,4	0.13	0	6,6,6	0.25	0
2	SO4	E	623	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SO4	F	610	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	D	613	-	4,4,4	0.44	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	K	608	-	4,4,4	0.14	0	6,6,6	0.33	0
2	SO4	E	622	-	4,4,4	0.16	0	6,6,6	0.08	0
3	GOL	K	613	-	5,5,5	1.17	0	5,5,5	0.90	0
2	SO4	B	622	-	4,4,4	0.44	0	6,6,6	0.06	0
2	SO4	A	617	-	4,4,4	0.53	0	6,6,6	0.07	0
2	SO4	A	621	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	D	620	-	4,4,4	0.55	0	6,6,6	0.05	0
2	SO4	L	603	-	4,4,4	0.50	0	6,6,6	0.07	0
2	SO4	C	605	-	4,4,4	0.21	0	6,6,6	0.23	0
2	SO4	H	608	-	4,4,4	0.51	0	6,6,6	0.06	0
2	SO4	K	609	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	C	610	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	I	611	-	4,4,4	0.54	0	6,6,6	0.08	0
2	SO4	A	603	-	4,4,4	0.48	0	6,6,6	0.07	0
2	SO4	C	623	-	4,4,4	0.15	0	6,6,6	0.08	0
3	GOL	C	626	-	5,5,5	1.05	0	5,5,5	1.19	0
2	SO4	E	602	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	E	603	-	4,4,4	0.45	0	6,6,6	0.05	0
2	SO4	B	621	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SO4	B	614	-	4,4,4	0.20	0	6,6,6	0.22	0
2	SO4	B	611	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	I	608	-	4,4,4	0.17	0	6,6,6	0.11	0
3	GOL	H	615	-	5,5,5	0.88	0	5,5,5	0.98	0
3	GOL	G	622	-	5,5,5	1.16	0	5,5,5	0.97	0
3	GOL	G	619	-	5,5,5	0.86	0	5,5,5	1.11	0
3	GOL	A	628	-	5,5,5	1.10	0	5,5,5	0.95	0
3	GOL	A	630	-	5,5,5	1.09	0	5,5,5	0.76	0
2	SO4	E	604	-	4,4,4	0.19	0	6,6,6	0.28	0
2	SO4	G	610	-	4,4,4	0.46	0	6,6,6	0.07	0
2	SO4	H	611	-	4,4,4	0.44	0	6,6,6	0.05	0
2	SO4	J	607	-	4,4,4	0.43	0	6,6,6	0.05	0
3	GOL	C	624	-	5,5,5	0.99	0	5,5,5	0.90	0
2	SO4	J	606	-	4,4,4	0.56	0	6,6,6	0.07	0
2	SO4	L	606	-	4,4,4	0.12	0	6,6,6	0.12	0
2	SO4	B	608	-	4,4,4	0.61	0	6,6,6	0.14	0
2	SO4	D	602	-	4,4,4	0.14	0	6,6,6	0.11	0
3	GOL	D	624	-	5,5,5	0.93	0	5,5,5	0.84	0
2	SO4	D	608	-	4,4,4	0.12	0	6,6,6	0.15	0
2	SO4	A	614	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	E	610	-	4,4,4	0.16	0	6,6,6	0.11	0
3	GOL	B	629	-	5,5,5	1.23	0	5,5,5	0.88	0
3	GOL	A	625	-	5,5,5	1.51	1 (20%)	5,5,5	0.67	0
2	SO4	L	609	-	4,4,4	0.14	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	D	604	-	4,4,4	0.14	0	6,6,6	0.11	0
3	GOL	G	623	-	5,5,5	0.66	0	5,5,5	1.33	1 (20%)
2	SO4	G	608	-	4,4,4	0.47	0	6,6,6	0.06	0
2	SO4	L	605	-	4,4,4	0.16	0	6,6,6	0.45	0
2	SO4	F	607	-	4,4,4	0.19	0	6,6,6	0.32	0
2	SO4	G	604	-	4,4,4	0.13	0	6,6,6	0.20	0
2	SO4	E	624	-	4,4,4	0.46	0	6,6,6	0.07	0
2	SO4	H	610	-	4,4,4	0.15	0	6,6,6	0.17	0
3	GOL	A	624	-	5,5,5	1.16	0	5,5,5	1.02	0
2	SO4	I	609	-	4,4,4	0.44	0	6,6,6	0.06	0
2	SO4	A	605	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	E	621	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	G	612	-	4,4,4	0.17	0	6,6,6	0.10	0
2	SO4	G	617	-	4,4,4	0.44	0	6,6,6	0.06	0
2	SO4	D	614	-	4,4,4	0.13	0	6,6,6	0.14	0
3	GOL	C	625	-	5,5,5	1.07	0	5,5,5	0.97	0
2	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	E	612	-	4,4,4	0.52	0	6,6,6	0.09	0
3	GOL	D	625	-	5,5,5	1.16	0	5,5,5	0.86	0
2	SO4	C	602	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	A	619	-	4,4,4	0.16	0	6,6,6	0.14	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	G	620	-	-	3/4/4/4	-
3	GOL	E	626	-	-	3/4/4/4	-
3	GOL	A	627	-	-	0/4/4/4	-
3	GOL	B	626	-	-	1/4/4/4	-
3	GOL	C	626	-	-	2/4/4/4	-
3	GOL	F	614	-	-	1/4/4/4	-
3	GOL	D	623	-	-	2/4/4/4	-
3	GOL	B	630	-	-	1/4/4/4	-
3	GOL	E	628	-	-	2/4/4/4	-
3	GOL	H	615	-	-	2/4/4/4	-
3	GOL	G	622	-	-	0/4/4/4	-
3	GOL	G	619	-	-	4/4/4/4	-
3	GOL	A	628	-	-	0/4/4/4	-

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	617	GOL	C1-C2	2.64	1.62	1.51
3	H	617	GOL	C3-C2	2.54	1.62	1.51
3	B	628	GOL	O2-C2	-2.47	1.36	1.43
3	A	625	GOL	C3-C2	2.40	1.61	1.51
3	E	626	GOL	C3-C2	2.17	1.60	1.51
3	K	611	GOL	C3-C2	2.12	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	627	GOL	C1-C2	2.09	1.60	1.51
3	F	615	GOL	C3-C2	2.07	1.60	1.51
3	A	626	GOL	C3-C2	2.02	1.60	1.51
3	J	609	GOL	C3-C2	2.02	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	612	GOL	C3-C2-C1	-2.18	103.21	111.70
3	G	618	GOL	C3-C2-C1	-2.14	103.40	111.70
3	G	623	GOL	C3-C2-C1	-2.13	103.44	111.70

There are no chirality outliers.

All (73) 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
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	G	623	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

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

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Mol	Chain	Res	Type	Atoms
3	E	626	GOL	O2-C2-C3-O3
3	E	627	GOL	O1-C1-C2-O2
3	A	626	GOL	C1-C2-C3-O3
3	C	624	GOL	C1-C2-C3-O3
3	H	617	GOL	O2-C2-C3-O3

There are no ring outliers.

49 monomers are involved in 86 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	601	SO4	1	0
2	C	604	SO4	2	0
3	A	631	GOL	2	0
2	A	616	SO4	1	0
2	C	611	SO4	1	0
2	L	602	SO4	1	0
3	G	621	GOL	2	0
3	H	617	GOL	3	0
2	G	601	SO4	1	0
2	I	610	SO4	1	0
2	B	610	SO4	1	0
2	B	613	SO4	1	0
3	B	628	GOL	1	0
3	B	627	GOL	1	0
2	B	604	SO4	1	0
2	I	602	SO4	2	0
2	H	601	SO4	4	0
3	E	627	GOL	1	0
3	A	629	GOL	1	0
2	A	612	SO4	0	1
2	L	611	SO4	3	0
3	E	626	GOL	1	0
2	D	609	SO4	2	0
2	H	612	SO4	2	0
3	E	628	GOL	1	0
2	K	607	SO4	1	0
3	D	626	GOL	2	0
2	K	605	SO4	2	0
2	F	604	SO4	1	0
3	F	615	GOL	2	0
2	E	601	SO4	3	0
2	K	603	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	SO4	3	0
2	L	604	SO4	6	0
2	A	608	SO4	1	0
3	H	614	GOL	1	0
3	K	611	GOL	1	0
2	J	603	SO4	2	0
2	I	611	SO4	2	0
3	G	619	GOL	1	0
2	G	610	SO4	1	0
3	D	624	GOL	1	0
3	A	625	GOL	5	0
3	G	623	GOL	2	0
2	G	608	SO4	2	0
3	A	624	GOL	1	0
2	G	617	SO4	3	0
2	E	612	SO4	3	0
3	D	625	GOL	1	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, 95^{th} 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%)	0.19	21 (4%) 33 28	37, 65, 138, 195	0
1	B	464/518 (89%)	0.31	26 (5%) 24 20	42, 65, 138, 195	0
1	C	464/518 (89%)	0.29	29 (6%) 20 15	38, 67, 153, 188	0
1	D	456/518 (88%)	0.29	28 (6%) 21 17	40, 72, 143, 195	0
1	E	465/518 (89%)	0.24	24 (5%) 27 22	30, 67, 146, 216	0
1	F	464/518 (89%)	0.34	33 (7%) 16 12	30, 73, 152, 216	0
1	G	457/518 (88%)	0.39	29 (6%) 20 15	30, 74, 146, 202	0
1	H	456/518 (88%)	0.35	31 (6%) 17 13	30, 78, 146, 223	0
1	I	452/518 (87%)	0.47	40 (8%) 10 6	30, 80, 155, 186	0
1	J	449/518 (86%)	0.83	75 (16%) 1 1	55, 108, 166, 205	0
1	K	459/518 (88%)	0.36	33 (7%) 15 11	30, 79, 163, 228	0
1	L	441/518 (85%)	0.76	70 (15%) 1 1	30, 110, 171, 221	0
All	All	5493/6216 (88%)	0.40	439 (7%) 12 9	30, 77, 154, 228	0

All (439) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	129	TYR	10.1
1	B	46	ASN	9.2
1	I	113	LEU	8.5
1	F	133	ALA	8.4
1	H	46	ASN	8.2
1	G	130	CYS	7.6
1	L	130	CYS	7.4
1	C	366	VAL	6.9
1	I	120	PHE	6.8
1	H	45	MET	6.8
1	I	49	ASP	6.7

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Mol	Chain	Res	Type	RSRZ
1	E	48	MET	6.6
1	K	46	ASN	6.5
1	K	129	TYR	6.4
1	H	51	VAL	6.4
1	F	367	VAL	6.4
1	J	384	PHE	6.2
1	G	132	ALA	6.2
1	G	46	ASN	6.2
1	L	42	HIS	6.1
1	G	51	VAL	6.0
1	K	131	PRO	6.0
1	J	392	LEU	5.9
1	G	45	MET	5.9
1	E	294	TYR	5.7
1	L	128	ASP	5.6
1	J	385	LYS	5.6
1	G	129	TYR	5.5
1	K	130	CYS	5.3
1	L	327	ASP	5.2
1	I	110	THR	5.2
1	F	366	VAL	5.1
1	G	50	VAL	5.1
1	C	129	TYR	5.1
1	F	135	ALA	5.1
1	E	133	ALA	5.0
1	L	135	ALA	5.0
1	I	125	THR	5.0
1	I	114	LYS	5.0
1	J	377	TYR	4.9
1	G	128	ASP	4.9
1	I	48	MET	4.9
1	G	126	SER	4.9
1	A	131	PRO	4.8
1	E	135	ALA	4.8
1	B	130	CYS	4.8
1	J	391	ALA	4.8
1	L	387	ALA	4.7
1	B	411	TYR	4.7
1	L	45	MET	4.7
1	F	45	MET	4.7
1	D	50	VAL	4.7
1	I	283	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	J	293	TYR	4.7
1	K	44	TYR	4.7
1	J	437	LEU	4.6
1	D	293	TYR	4.6
1	L	44	TYR	4.6
1	J	44	TYR	4.6
1	J	434	LEU	4.5
1	C	51	VAL	4.5
1	A	50	VAL	4.5
1	A	129	TYR	4.5
1	H	293	TYR	4.5
1	K	366	VAL	4.4
1	B	44	TYR	4.4
1	G	133	ALA	4.4
1	J	133	ALA	4.4
1	G	125	THR	4.3
1	L	344	VAL	4.3
1	L	323	LYS	4.3
1	H	35	PHE	4.3
1	I	121	ALA	4.2
1	B	294	TYR	4.2
1	L	383	ALA	4.2
1	I	267	TRP	4.2
1	L	131	PRO	4.2
1	J	37	LEU	4.2
1	D	149	ASN	4.2
1	L	34	LEU	4.1
1	I	50	VAL	4.1
1	F	130	CYS	4.1
1	E	50	VAL	4.1
1	J	48	MET	4.1
1	J	45	MET	4.1
1	L	394	LEU	4.1
1	L	54	GLU	4.0
1	G	326	GLN	4.0
1	G	328	MET	4.0
1	B	129	TYR	4.0
1	D	112	GLU	4.0
1	I	45	MET	4.0
1	L	31	MET	4.0
1	I	122	THR	4.0
1	K	48	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	I	146	ALA	4.0
1	J	334	LEU	4.0
1	G	54	GLU	4.0
1	C	406	ASP	3.9
1	C	305	ALA	3.9
1	L	46	ASN	3.9
1	I	411	TYR	3.9
1	I	137	SER	3.9
1	J	47	LYS	3.9
1	J	422	ASN	3.9
1	I	116	CYS	3.8
1	L	403	GLU	3.8
1	H	42	HIS	3.8
1	C	50	VAL	3.8
1	I	16	PRO	3.8
1	D	137	SER	3.8
1	J	367	VAL	3.7
1	K	97	LEU	3.7
1	J	408	ASP	3.7
1	D	110	THR	3.7
1	C	331	ARG	3.7
1	G	47	LYS	3.7
1	I	139	PHE	3.7
1	J	470	TYR	3.7
1	C	410	ILE	3.7
1	H	50	VAL	3.7
1	C	2	SER	3.7
1	J	40	TRP	3.6
1	J	442	GLN	3.6
1	J	136	SER	3.6
1	D	111	LYS	3.6
1	J	407	LEU	3.6
1	L	481	CYS	3.6
1	J	43	ARG	3.6
1	J	139	PHE	3.6
1	K	328	MET	3.5
1	I	124	ILE	3.5
1	K	14	ASN	3.5
1	K	50	VAL	3.5
1	C	367	VAL	3.5
1	I	410	ILE	3.5
1	J	379	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	307	TYR	3.5
1	H	43	ARG	3.5
1	G	135	ALA	3.5
1	L	134	VAL	3.5
1	B	2	SER	3.5
1	J	346	LYS	3.5
1	L	437	LEU	3.5
1	K	45	MET	3.4
1	K	120	PHE	3.4
1	E	46	ASN	3.4
1	J	50	VAL	3.4
1	L	149	ASN	3.4
1	J	35	PHE	3.4
1	A	45	MET	3.4
1	C	130	CYS	3.4
1	C	413	LEU	3.4
1	D	126	SER	3.4
1	E	136	SER	3.4
1	F	132	ALA	3.4
1	A	133	ALA	3.4
1	F	129	TYR	3.4
1	E	113	LEU	3.4
1	A	130	CYS	3.4
1	B	113	LEU	3.3
1	L	127	GLU	3.3
1	H	409	THR	3.3
1	D	136	SER	3.3
1	K	49	ASP	3.3
1	G	409	THR	3.3
1	A	134	VAL	3.3
1	J	319	TYR	3.3
1	F	182	ASN	3.3
1	B	367	VAL	3.3
1	K	134	VAL	3.3
1	J	124	ILE	3.3
1	L	346	LYS	3.3
1	G	44	TYR	3.2
1	J	395	LYS	3.2
1	F	411	TYR	3.2
1	G	142	LYS	3.2
1	F	53	ILE	3.2
1	L	53	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	120	PHE	3.2
1	B	128	ASP	3.2
1	A	132	ALA	3.2
1	C	369	TYR	3.2
1	I	236	TYR	3.2
1	A	293	TYR	3.1
1	D	117	ILE	3.1
1	A	127	GLU	3.1
1	D	124	ILE	3.1
1	J	409	THR	3.1
1	F	31	MET	3.1
1	E	409	THR	3.1
1	G	411	TYR	3.1
1	H	502	GLN	3.1
1	H	135	ALA	3.1
1	F	119	ARG	3.1
1	L	400	ILE	3.1
1	K	341	GLU	3.0
1	J	475	ASN	3.0
1	F	2	SER	3.0
1	K	327	ASP	3.0
1	B	127	GLU	3.0
1	D	148	MET	3.0
1	H	146	ALA	3.0
1	B	131	PRO	3.0
1	F	134	VAL	3.0
1	H	44	TYR	3.0
1	A	46	ASN	3.0
1	E	329	ILE	3.0
1	H	307	TYR	3.0
1	J	380	GLY	3.0
1	J	33	GLN	3.0
1	D	113	LEU	2.9
1	K	369	TYR	2.9
1	L	35	PHE	2.9
1	I	106	GLU	2.9
1	J	320	ILE	2.9
1	D	120	PHE	2.9
1	D	236	TYR	2.9
1	C	127	GLU	2.9
1	A	53	ILE	2.9
1	E	126	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	40	TRP	2.9
1	E	134	VAL	2.9
1	L	316	HIS	2.9
1	I	42	HIS	2.9
1	A	2	SER	2.9
1	E	114	LYS	2.9
1	H	49	ASP	2.9
1	G	122	THR	2.9
1	H	124	ILE	2.9
1	I	117	ILE	2.9
1	I	142	LYS	2.9
1	E	45	MET	2.9
1	H	109	MET	2.9
1	I	119	ARG	2.9
1	L	376	ILE	2.8
1	D	45	MET	2.8
1	H	329	ILE	2.8
1	A	49	ASP	2.8
1	A	48	MET	2.8
1	B	41	ALA	2.8
1	J	373	ALA	2.8
1	H	47	LYS	2.8
1	L	458	ILE	2.8
1	L	328	MET	2.8
1	L	469	PHE	2.8
1	I	144	VAL	2.8
1	C	54	GLU	2.8
1	E	293	TYR	2.8
1	J	121	ALA	2.8
1	L	33	GLN	2.8
1	L	348	LEU	2.7
1	F	368	LYS	2.7
1	E	295	ILE	2.7
1	A	16	PRO	2.7
1	L	124	ILE	2.7
1	L	404	GLU	2.7
1	C	126	SER	2.7
1	H	136	SER	2.7
1	C	307	TYR	2.7
1	I	46	ASN	2.7
1	L	110	THR	2.7
1	F	142	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	111	LYS	2.7
1	L	252	GLY	2.7
1	J	42	HIS	2.7
1	H	117	ILE	2.7
1	L	337	ILE	2.7
1	F	365	ASN	2.7
1	D	307	TYR	2.6
1	C	44	TYR	2.6
1	K	114	LYS	2.6
1	J	369	TYR	2.6
1	C	48	MET	2.6
1	F	136	SER	2.6
1	J	110	THR	2.6
1	D	53	ILE	2.6
1	I	206	GLN	2.6
1	J	402	TYR	2.6
1	L	439	ASP	2.6
1	B	133	ALA	2.6
1	D	46	ASN	2.6
1	J	36	ALA	2.6
1	G	327	ASP	2.6
1	J	500	SER	2.6
1	K	367	VAL	2.6
1	C	52	LYS	2.6
1	J	343	LYS	2.6
1	C	412	HIS	2.5
1	B	32	ASP	2.5
1	L	32	ASP	2.5
1	C	420	ALA	2.5
1	K	132	ALA	2.5
1	J	31	MET	2.5
1	K	293	TYR	2.5
1	H	403	GLU	2.5
1	H	34	LEU	2.5
1	J	275	LEU	2.5
1	I	108	ASN	2.5
1	L	117	ILE	2.5
1	B	45	MET	2.5
1	F	294	TYR	2.5
1	L	393	GLU	2.5
1	J	458	ILE	2.5
1	F	51	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	293	TYR	2.5
1	H	292	GLY	2.5
1	F	329	ILE	2.5
1	J	325	ILE	2.5
1	L	136	SER	2.5
1	C	42	HIS	2.5
1	L	2	SER	2.5
1	B	50	VAL	2.5
1	J	396	GLU	2.4
1	F	49	ASP	2.4
1	C	411	TYR	2.4
1	J	350	LEU	2.4
1	B	47	LYS	2.4
1	J	135	ALA	2.4
1	J	387	ALA	2.4
1	B	120	PHE	2.4
1	L	140	VAL	2.4
1	L	386	SER	2.4
1	J	371	ASN	2.4
1	B	54	GLU	2.4
1	C	53	ILE	2.4
1	G	48	MET	2.4
1	E	44	TYR	2.4
1	H	88	VAL	2.4
1	L	402	TYR	2.4
1	L	115	LYS	2.4
1	K	411	TYR	2.4
1	G	325	ILE	2.4
1	J	333	LYS	2.4
1	H	48	MET	2.4
1	F	181	TYR	2.3
1	A	47	LYS	2.3
1	J	441	MET	2.3
1	D	31	MET	2.3
1	D	119	ARG	2.3
1	E	117	ILE	2.3
1	J	56	CYS	2.3
1	B	366	VAL	2.3
1	J	115	LYS	2.3
1	J	109	MET	2.3
1	F	124	ILE	2.3
1	G	396	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	152	THR	2.3
1	L	390	SER	2.3
1	C	47	LYS	2.3
1	A	44	TYR	2.3
1	D	411	TYR	2.3
1	K	133	ALA	2.3
1	F	267	TRP	2.3
1	F	412	HIS	2.3
1	C	135	ALA	2.3
1	I	31	MET	2.3
1	J	122	THR	2.3
1	J	225	LYS	2.3
1	J	116	CYS	2.3
1	D	406	ASP	2.3
1	L	382	CYS	2.3
1	L	468	ASN	2.3
1	H	32	ASP	2.3
1	L	137	SER	2.2
1	J	131	PRO	2.2
1	I	109	MET	2.2
1	B	461	GLU	2.2
1	I	32	ASP	2.2
1	I	115	LYS	2.2
1	L	114	LYS	2.2
1	L	391	ALA	2.2
1	K	35	PHE	2.2
1	J	105	GLN	2.2
1	A	51	VAL	2.2
1	L	145	ASN	2.2
1	J	473	PRO	2.2
1	J	137	SER	2.2
1	K	34	LEU	2.2
1	K	53	ILE	2.2
1	L	319	TYR	2.2
1	K	292	GLY	2.2
1	L	341	GLU	2.2
1	A	135	ALA	2.2
1	C	421	PRO	2.2
1	J	32	ASP	2.2
1	E	2	SER	2.2
1	K	47	LYS	2.2
1	J	382	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	137	SER	2.2
1	J	150	SER	2.2
1	L	37	LEU	2.2
1	I	156	ARG	2.2
1	K	51	VAL	2.2
1	G	113	LEU	2.1
1	H	91	LEU	2.1
1	E	331	ARG	2.1
1	F	331	ARG	2.1
1	E	120	PHE	2.1
1	J	328	MET	2.1
1	H	107	LEU	2.1
1	D	190	ARG	2.1
1	C	409	THR	2.1
1	B	293	TYR	2.1
1	L	499	TYR	2.1
1	I	266	LYS	2.1
1	K	113	LEU	2.1
1	J	117	ILE	2.1
1	L	497	ILE	2.1
1	J	120	PHE	2.1
1	L	91	LEU	2.1
1	K	110	THR	2.1
1	D	135	ALA	2.1
1	I	153	PHE	2.1
1	L	335	PHE	2.1
1	E	307	TYR	2.1
1	F	327	ASP	2.1
1	G	119	ARG	2.1
1	B	51	VAL	2.1
1	D	182	ASN	2.1
1	E	111	LYS	2.1
1	F	46	ASN	2.1
1	L	500	SER	2.0
1	H	308	GLY	2.0
1	F	178	HIS	2.0
1	A	136	SER	2.0
1	E	330	SER	2.0
1	L	389	GLU	2.0
1	B	119	ARG	2.0
1	D	178	HIS	2.0
1	H	111	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	118	SER	2.0
1	F	48	MET	2.0
1	G	124	ILE	2.0
1	I	237	GLU	2.0
1	D	2	SER	2.0
1	K	217	ARG	2.0
1	L	336	VAL	2.0
1	L	104	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	C	612	5/5	0.44	0.51	188,189,191,191	0
2	SO4	H	601	5/5	0.49	0.27	190,193,193,194	0
3	GOL	F	614	6/6	0.49	0.29	102,116,120,121	0
3	GOL	D	625	6/6	0.50	0.47	109,115,120,122	0
2	SO4	A	620	5/5	0.53	0.66	201,202,202,203	0
2	SO4	G	611	5/5	0.55	0.49	192,193,194,195	0
2	SO4	B	622	5/5	0.55	0.53	196,196,197,197	0
2	SO4	G	607	5/5	0.56	0.33	177,178,180,180	0
2	SO4	A	623	5/5	0.59	0.22	198,199,200,201	0
2	SO4	F	613	5/5	0.60	0.44	184,185,187,188	0
2	SO4	J	607	5/5	0.61	0.28	192,192,193,194	0
2	SO4	B	618	5/5	0.61	0.32	214,215,216,216	0
2	SO4	D	617	5/5	0.61	0.18	155,159,163,166	0
2	SO4	F	609	5/5	0.62	0.28	180,185,186,188	0
2	SO4	G	610	5/5	0.63	0.54	206,206,207,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	601	5/5	0.63	0.21	157,159,161,161	0
2	SO4	A	618	5/5	0.63	0.29	181,182,183,184	0
2	SO4	H	611	5/5	0.64	0.22	185,187,187,188	0
2	SO4	A	621	5/5	0.66	0.29	195,196,197,197	0
2	SO4	E	623	5/5	0.66	0.21	185,185,186,187	0
2	SO4	D	609	5/5	0.67	0.31	184,186,187,188	0
3	GOL	D	626	6/6	0.67	0.44	123,126,128,130	0
2	SO4	E	624	5/5	0.67	0.19	192,197,198,199	0
2	SO4	I	602	5/5	0.68	0.44	185,188,189,190	0
2	SO4	H	613	5/5	0.68	0.44	174,178,178,182	0
2	SO4	L	603	5/5	0.68	0.21	172,173,174,177	0
2	SO4	C	604	5/5	0.69	0.25	190,191,192,192	0
2	SO4	D	616	5/5	0.69	0.37	165,169,171,171	0
2	SO4	B	617	5/5	0.69	0.52	182,184,185,186	0
2	SO4	E	612	5/5	0.69	0.28	154,154,158,160	0
2	SO4	D	602	5/5	0.69	0.41	180,181,181,181	0
3	GOL	A	627	6/6	0.70	0.32	107,114,120,127	0
2	SO4	C	616	5/5	0.70	0.33	164,164,166,166	0
2	SO4	G	608	5/5	0.71	0.18	175,176,177,178	0
2	SO4	H	612	5/5	0.71	0.36	161,161,164,168	0
2	SO4	F	610	5/5	0.71	0.34	173,174,175,177	0
2	SO4	A	622	5/5	0.71	0.46	156,159,161,166	0
2	SO4	C	619	5/5	0.71	0.38	167,167,169,169	0
2	SO4	C	615	5/5	0.72	0.33	182,184,184,185	0
3	GOL	A	628	6/6	0.72	0.30	98,110,112,112	0
2	SO4	K	605	5/5	0.72	0.40	203,205,206,207	0
2	SO4	K	609	5/5	0.72	0.22	184,185,185,185	0
2	SO4	H	608	5/5	0.72	0.45	174,178,178,179	0
3	GOL	H	616	6/6	0.72	0.64	125,129,134,140	0
2	SO4	L	609	5/5	0.73	0.25	185,185,186,188	0
2	SO4	I	610	5/5	0.73	0.27	175,176,177,179	0
2	SO4	J	605	5/5	0.73	0.38	171,171,173,174	0
3	GOL	A	630	6/6	0.73	0.23	99,106,111,111	0
2	SO4	C	618	5/5	0.73	0.41	164,164,166,167	0
2	SO4	A	614	5/5	0.73	0.47	166,166,169,171	0
2	SO4	A	612	5/5	0.73	0.21	190,192,193,194	0
2	SO4	D	618	5/5	0.73	0.16	167,169,169,169	0
2	SO4	C	609	5/5	0.74	0.43	149,152,157,158	0
2	SO4	A	613	5/5	0.74	0.30	159,161,162,164	0
2	SO4	I	606	5/5	0.74	0.29	154,157,159,160	0
2	SO4	C	621	5/5	0.74	0.72	183,183,185,187	0
2	SO4	J	601	5/5	0.74	0.40	156,156,159,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	G	616	5/5	0.74	0.27	185,185,187,188	0
3	GOL	H	617	6/6	0.74	0.27	80,86,94,95	0
2	SO4	C	622	5/5	0.75	0.14	181,182,184,185	0
3	GOL	A	626	6/6	0.75	0.17	84,88,90,91	0
2	SO4	E	601	5/5	0.75	0.30	173,174,175,178	0
2	SO4	J	602	5/5	0.75	0.37	168,170,173,173	0
2	SO4	B	623	5/5	0.75	0.28	164,165,167,168	0
2	SO4	C	611	5/5	0.75	0.37	146,149,154,155	0
2	SO4	K	604	5/5	0.75	0.23	163,165,166,166	0
2	SO4	B	605	5/5	0.75	0.42	183,184,184,185	0
3	GOL	F	615	6/6	0.75	0.44	78,92,107,114	0
2	SO4	F	605	5/5	0.75	0.37	150,154,156,159	0
2	SO4	A	603	5/5	0.75	0.28	170,170,171,172	0
2	SO4	K	607	5/5	0.76	0.35	157,159,163,165	0
2	SO4	H	602	5/5	0.76	0.25	145,147,149,150	0
2	SO4	D	615	5/5	0.76	0.17	166,169,170,171	0
2	SO4	I	604	5/5	0.76	0.35	145,150,151,153	0
2	SO4	D	610	5/5	0.76	0.23	175,176,178,180	0
2	SO4	I	609	5/5	0.76	0.26	162,164,166,168	0
2	SO4	E	614	5/5	0.76	0.23	154,157,158,160	0
2	SO4	L	602	5/5	0.77	0.32	146,147,149,154	0
2	SO4	E	617	5/5	0.77	0.33	155,156,158,160	0
2	SO4	H	605	5/5	0.77	0.50	171,173,176,177	0
2	SO4	I	612	5/5	0.77	0.38	171,173,177,177	0
2	SO4	E	620	5/5	0.77	0.34	161,164,167,167	0
2	SO4	B	616	5/5	0.77	0.33	180,181,184,184	0
2	SO4	E	603	5/5	0.77	0.21	187,188,189,190	0
3	GOL	D	624	6/6	0.77	0.42	116,127,129,133	0
2	SO4	E	611	5/5	0.77	0.45	151,156,159,160	0
2	SO4	J	608	5/5	0.77	0.31	178,179,179,180	0
2	SO4	G	614	5/5	0.77	0.39	171,172,174,176	0
2	SO4	B	624	5/5	0.77	0.38	177,178,182,182	0
2	SO4	B	625	5/5	0.77	0.21	168,169,172,173	0
2	SO4	I	608	5/5	0.77	0.23	166,167,167,168	0
2	SO4	D	612	5/5	0.78	0.34	162,164,165,166	0
2	SO4	A	604	5/5	0.78	0.22	153,154,155,157	0
3	GOL	B	630	6/6	0.78	0.23	93,99,100,104	0
2	SO4	K	608	5/5	0.78	0.45	137,139,141,143	0
2	SO4	A	615	5/5	0.78	0.21	166,167,168,168	0
2	SO4	A	617	5/5	0.78	0.31	186,187,191,194	0
2	SO4	H	604	5/5	0.78	0.18	171,172,172,173	0
2	SO4	E	613	5/5	0.78	0.29	173,173,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	605	5/5	0.78	0.29	134,138,142,142	0
2	SO4	H	610	5/5	0.78	0.55	172,173,174,176	0
3	GOL	K	611	6/6	0.78	0.25	93,114,118,121	0
2	SO4	D	614	5/5	0.79	0.22	168,170,171,175	0
2	SO4	I	603	5/5	0.79	0.57	159,163,166,167	0
2	SO4	E	608	5/5	0.79	0.20	122,131,133,133	0
3	GOL	G	620	6/6	0.79	0.28	78,99,104,110	0
2	SO4	E	622	5/5	0.79	0.28	163,164,165,168	0
2	SO4	C	623	5/5	0.79	0.25	194,195,196,197	0
2	SO4	J	604	5/5	0.79	0.23	154,156,158,160	0
2	SO4	G	615	5/5	0.80	0.29	180,182,183,183	0
2	SO4	D	613	5/5	0.80	0.20	165,167,170,170	0
2	SO4	B	603	5/5	0.80	0.28	135,138,140,144	0
2	SO4	B	607	5/5	0.80	0.56	186,187,188,190	0
2	SO4	E	621	5/5	0.80	0.32	154,156,160,163	0
2	SO4	B	614	5/5	0.80	0.33	152,153,157,159	0
2	SO4	F	612	5/5	0.80	0.26	155,156,157,159	0
2	SO4	H	609	5/5	0.80	0.29	147,147,153,156	0
3	GOL	K	613	6/6	0.80	0.27	108,110,112,115	0
3	GOL	L	612	6/6	0.80	0.41	131,134,136,137	0
2	SO4	E	616	5/5	0.81	0.30	166,170,171,172	0
3	GOL	G	621	6/6	0.81	0.22	92,102,106,111	0
3	GOL	H	614	6/6	0.81	0.23	78,90,94,99	0
3	GOL	A	625	6/6	0.81	0.42	73,87,90,92	0
2	SO4	F	602	5/5	0.81	0.14	151,157,158,159	0
2	SO4	D	620	5/5	0.81	0.27	163,164,166,166	0
2	SO4	C	607	5/5	0.81	0.26	167,169,170,172	0
2	SO4	K	606	5/5	0.81	0.36	144,146,148,153	0
2	SO4	B	613	5/5	0.82	0.30	194,196,197,199	0
2	SO4	D	608	5/5	0.82	0.24	146,148,149,152	0
2	SO4	E	605	5/5	0.82	0.30	152,155,159,159	0
2	SO4	E	615	5/5	0.82	0.27	143,145,148,154	0
3	GOL	I	614	6/6	0.82	0.33	105,111,114,115	0
2	SO4	C	613	5/5	0.82	0.27	165,166,167,169	0
2	SO4	C	608	5/5	0.82	0.15	162,162,164,164	0
2	SO4	K	602	5/5	0.82	0.20	139,139,144,149	0
2	SO4	E	619	5/5	0.83	0.25	186,187,188,188	0
2	SO4	B	606	5/5	0.83	0.26	127,134,135,140	0
2	SO4	F	608	5/5	0.83	0.31	160,161,163,163	0
2	SO4	I	607	5/5	0.83	0.21	151,152,152,153	0
2	SO4	G	613	5/5	0.83	0.68	204,205,206,207	0
3	GOL	B	626	6/6	0.83	0.19	75,101,103,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	J	606	5/5	0.83	0.32	137,141,144,145	0
3	GOL	C	625	6/6	0.83	0.30	90,98,100,101	0
2	SO4	G	605	5/5	0.83	0.34	155,159,161,163	0
2	SO4	C	617	5/5	0.83	0.22	164,164,167,168	0
2	SO4	I	611	5/5	0.83	0.58	178,178,180,180	0
2	SO4	J	603	5/5	0.84	0.18	195,195,196,198	0
2	SO4	C	620	5/5	0.84	0.25	162,163,164,165	0
2	SO4	D	603	5/5	0.84	0.18	193,194,195,198	0
2	SO4	D	604	5/5	0.84	0.38	208,209,210,211	0
3	GOL	E	627	6/6	0.84	0.30	115,115,117,121	0
2	SO4	L	608	5/5	0.84	0.17	154,158,161,163	0
2	SO4	D	605	5/5	0.84	0.24	162,162,163,167	0
2	SO4	B	609	5/5	0.84	0.26	125,130,138,140	0
2	SO4	E	610	5/5	0.84	0.21	147,149,152,154	0
2	SO4	K	603	5/5	0.84	0.30	149,152,153,154	0
3	GOL	H	615	6/6	0.84	0.27	88,97,109,115	0
2	SO4	A	616	5/5	0.84	0.26	193,194,196,196	0
2	SO4	B	619	5/5	0.84	0.49	167,169,169,169	0
3	GOL	A	631	6/6	0.84	0.38	20,20,20,20	0
3	GOL	J	609	6/6	0.84	0.20	95,98,100,101	0
2	SO4	G	602	5/5	0.84	0.26	119,128,137,138	0
3	GOL	K	612	6/6	0.84	0.17	91,114,115,120	0
3	GOL	B	629	6/6	0.84	0.26	99,103,107,107	0
2	SO4	D	619	5/5	0.84	0.34	158,159,160,164	0
2	SO4	A	606	5/5	0.85	0.30	127,131,134,135	0
2	SO4	I	601	5/5	0.85	0.25	174,174,176,179	0
3	GOL	G	622	6/6	0.85	0.24	85,88,94,98	0
2	SO4	D	621	5/5	0.85	0.28	176,177,178,180	0
2	SO4	L	604	5/5	0.85	0.37	184,187,189,190	0
2	SO4	L	606	5/5	0.85	0.19	155,156,158,160	0
2	SO4	L	607	5/5	0.85	0.19	141,143,150,151	0
2	SO4	B	610	5/5	0.85	0.17	162,164,165,166	0
2	SO4	E	625	5/5	0.85	0.41	158,158,160,163	0
2	SO4	D	607	5/5	0.85	0.29	115,120,123,127	0
2	SO4	D	611	5/5	0.85	0.25	148,151,159,160	0
2	SO4	G	606	5/5	0.85	0.22	138,141,143,145	0
2	SO4	E	606	5/5	0.85	0.23	136,143,144,146	0
2	SO4	E	602	5/5	0.86	0.16	176,177,178,178	0
2	SO4	F	611	5/5	0.86	0.22	165,166,167,168	0
2	SO4	C	606	5/5	0.86	0.24	128,134,135,139	0
3	GOL	A	624	6/6	0.86	0.40	74,86,91,91	0
3	GOL	G	618	6/6	0.86	0.26	98,100,101,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	620	5/5	0.86	0.16	159,162,163,166	0
2	SO4	F	606	5/5	0.86	0.14	162,163,165,165	0
2	SO4	B	612	5/5	0.86	0.61	180,181,184,186	0
2	SO4	E	607	5/5	0.86	0.23	137,140,144,148	0
2	SO4	H	606	5/5	0.87	0.27	128,131,132,132	0
2	SO4	H	603	5/5	0.87	0.29	134,137,137,141	0
2	SO4	B	615	5/5	0.87	0.21	154,156,158,160	0
2	SO4	G	609	5/5	0.87	0.14	158,161,162,162	0
2	SO4	L	601	5/5	0.88	0.13	177,180,180,182	0
2	SO4	D	606	5/5	0.88	0.29	166,167,167,167	0
2	SO4	A	610	5/5	0.88	0.34	157,163,165,166	0
2	SO4	A	619	5/5	0.88	0.27	167,167,170,171	0
2	SO4	L	605	5/5	0.88	0.17	87,119,127,128	0
2	SO4	G	603	5/5	0.88	0.27	139,143,144,148	0
2	SO4	F	603	5/5	0.88	0.28	139,139,141,141	0
2	SO4	B	611	5/5	0.88	0.19	169,170,171,173	0
3	GOL	C	626	6/6	0.89	0.50	120,120,122,123	0
2	SO4	F	604	5/5	0.89	0.25	137,138,142,146	0
3	GOL	G	619	6/6	0.89	0.24	112,114,115,117	0
2	SO4	C	610	5/5	0.89	0.27	163,165,166,167	0
2	SO4	A	611	5/5	0.89	0.35	174,174,175,175	0
3	GOL	A	629	6/6	0.89	0.34	95,99,103,103	0
3	GOL	E	628	6/6	0.89	0.39	105,107,108,108	0
2	SO4	A	605	5/5	0.89	0.14	144,144,147,149	0
2	SO4	A	607	5/5	0.90	0.28	118,123,128,129	0
3	GOL	B	627	6/6	0.90	0.45	87,98,104,105	0
2	SO4	G	612	5/5	0.90	0.14	152,154,155,156	0
2	SO4	F	607	5/5	0.90	0.38	135,139,140,141	0
3	GOL	E	626	6/6	0.90	0.32	68,72,83,84	0
2	SO4	L	611	5/5	0.90	0.54	30,30,30,30	0
2	SO4	A	608	5/5	0.91	0.28	136,144,146,148	0
2	SO4	A	609	5/5	0.91	0.23	127,131,134,138	0
2	SO4	D	601	5/5	0.91	0.38	118,121,125,134	0
2	SO4	C	614	5/5	0.91	0.34	160,161,162,165	0
2	SO4	B	608	5/5	0.91	0.33	142,147,148,148	0
3	GOL	G	623	6/6	0.91	0.57	87,93,100,111	0
2	SO4	A	601	5/5	0.91	0.34	96,102,116,116	0
2	SO4	E	609	5/5	0.91	0.34	121,135,138,139	0
2	SO4	I	605	5/5	0.92	0.22	140,143,143,143	0
2	SO4	E	618	5/5	0.92	0.28	135,139,142,143	0
2	SO4	B	621	5/5	0.92	0.33	156,157,159,159	0
2	SO4	D	622	5/5	0.92	0.50	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	E	604	5/5	0.92	0.36	114,124,128,134	0
2	SO4	B	604	5/5	0.92	0.18	115,120,123,129	0
2	SO4	I	613	5/5	0.93	0.49	30,30,30,30	0
3	GOL	B	628	6/6	0.93	0.31	62,78,80,82	0
2	SO4	C	603	5/5	0.93	0.17	87,91,93,97	0
2	SO4	F	601	5/5	0.93	0.21	80,104,106,106	0
2	SO4	G	604	5/5	0.93	0.37	133,135,137,137	0
2	SO4	H	607	5/5	0.94	0.20	144,146,150,151	0
2	SO4	B	602	5/5	0.94	0.30	99,102,110,113	0
2	SO4	C	602	5/5	0.94	0.27	108,117,118,122	0
2	SO4	G	601	5/5	0.94	0.23	92,93,101,111	0
2	SO4	A	602	5/5	0.94	0.19	80,94,96,98	0
2	SO4	K	610	5/5	0.95	0.58	30,30,30,30	0
2	SO4	G	617	5/5	0.95	0.48	30,30,30,30	0
3	GOL	D	623	6/6	0.95	0.34	70,80,84,90	0
2	SO4	L	610	5/5	0.96	0.54	30,30,30,30	0
2	SO4	K	601	5/5	0.96	0.14	87,87,101,106	0
3	GOL	C	624	6/6	0.97	0.25	66,70,75,76	0
2	SO4	B	601	5/5	0.97	0.18	120,121,125,130	0

6.5 Other polymers (i)

There are no such residues in this entry.