Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:09 PM GMT

PDB ID	:	4KK1
Title	:	Crystal Structure of TSC1 core domain from S. pombe
Authors	:	Sun, W.; Zhu, Y.; Wang, Z.Z.; Zhong, Q.; Gao, F.; Lou, J.Z.; Gong, W.M.; Xu, W.Q.
Deposited on	:	2013-05-05
Resolution	:	3.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

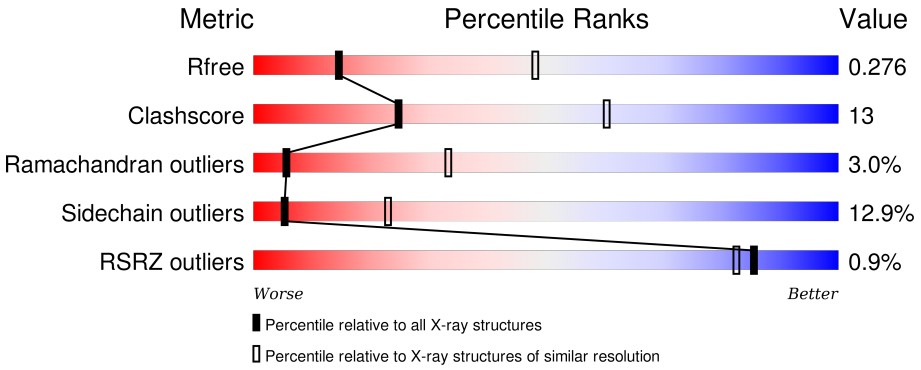
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	434	% 53% 33% 7% 7%
1	B	434	58% 27% • • 10%
1	C	434	% 59% 26% 5% 10%
1	D	434	% 60% 26% • 10%
1	E	434	54% 30% 6% 10%

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Mol	Chain	Length	Quality of chain
1	F	434	57% 29% • 10%
1	G	434	56% 30% • 10%
1	H	434	% 49% 35% 6% 10%
1	I	434	56% 26% 8% 10%
1	J	434	52% 32% 6% 10%
1	K	434	2% 57% 31% • 7%
1	L	434	58% 28% • 10%
1	M	434	% 57% 27% 6% 10%
1	N	434	54% 30% 6% 10%
1	O	434	54% 29% 6% 10%
1	P	434	% 59% 25% 7% 10%
1	Q	434	3% 55% 31% • 10%
1	R	434	60% 26% • 10%
1	S	434	% 59% 26% 5% 10%
1	T	434	% 59% 27% • 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 63794 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 Tuberous sclerosis 1 protein homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	Se	0	0	0
			3268	2116	548	591	8	5			
1	B	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	C	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	D	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	E	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	F	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	G	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	H	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	I	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	J	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	K	403	Total	C	N	O	S	Se	0	0	0
			3268	2116	548	591	8	5			
1	L	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	M	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	N	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	O	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	P	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	R	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	S	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	T	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q09778
A	-1	HIS	-	EXPRESSION TAG	UNP Q09778
A	0	MSE	-	EXPRESSION TAG	UNP Q09778
B	-2	SER	-	EXPRESSION TAG	UNP Q09778
B	-1	HIS	-	EXPRESSION TAG	UNP Q09778
B	0	MSE	-	EXPRESSION TAG	UNP Q09778
C	-2	SER	-	EXPRESSION TAG	UNP Q09778
C	-1	HIS	-	EXPRESSION TAG	UNP Q09778
C	0	MSE	-	EXPRESSION TAG	UNP Q09778
D	-2	SER	-	EXPRESSION TAG	UNP Q09778
D	-1	HIS	-	EXPRESSION TAG	UNP Q09778
D	0	MSE	-	EXPRESSION TAG	UNP Q09778
E	-2	SER	-	EXPRESSION TAG	UNP Q09778
E	-1	HIS	-	EXPRESSION TAG	UNP Q09778
E	0	MSE	-	EXPRESSION TAG	UNP Q09778
F	-2	SER	-	EXPRESSION TAG	UNP Q09778
F	-1	HIS	-	EXPRESSION TAG	UNP Q09778
F	0	MSE	-	EXPRESSION TAG	UNP Q09778
G	-2	SER	-	EXPRESSION TAG	UNP Q09778
G	-1	HIS	-	EXPRESSION TAG	UNP Q09778
G	0	MSE	-	EXPRESSION TAG	UNP Q09778
H	-2	SER	-	EXPRESSION TAG	UNP Q09778
H	-1	HIS	-	EXPRESSION TAG	UNP Q09778
H	0	MSE	-	EXPRESSION TAG	UNP Q09778
I	-2	SER	-	EXPRESSION TAG	UNP Q09778
I	-1	HIS	-	EXPRESSION TAG	UNP Q09778
I	0	MSE	-	EXPRESSION TAG	UNP Q09778
J	-2	SER	-	EXPRESSION TAG	UNP Q09778
J	-1	HIS	-	EXPRESSION TAG	UNP Q09778
J	0	MSE	-	EXPRESSION TAG	UNP Q09778
K	-2	SER	-	EXPRESSION TAG	UNP Q09778

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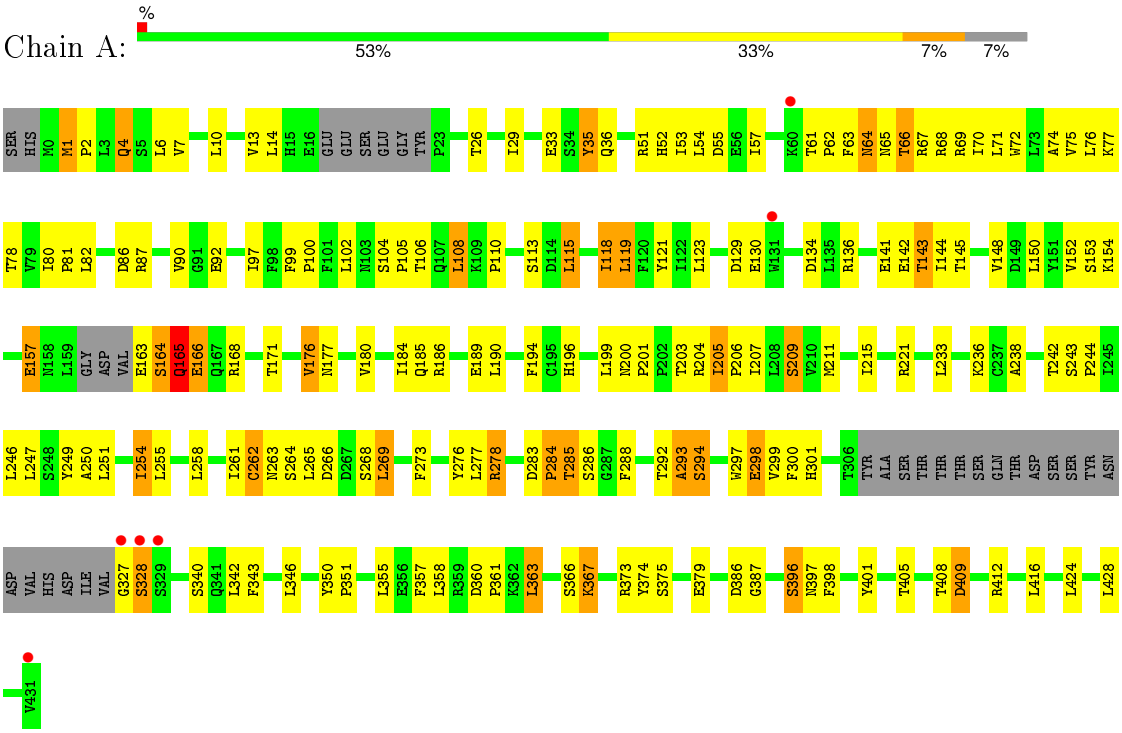
Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	EXPRESSION TAG	UNP Q09778
K	0	MSE	-	EXPRESSION TAG	UNP Q09778
L	-2	SER	-	EXPRESSION TAG	UNP Q09778
L	-1	HIS	-	EXPRESSION TAG	UNP Q09778
L	0	MSE	-	EXPRESSION TAG	UNP Q09778
M	-2	SER	-	EXPRESSION TAG	UNP Q09778
M	-1	HIS	-	EXPRESSION TAG	UNP Q09778
M	0	MSE	-	EXPRESSION TAG	UNP Q09778
N	-2	SER	-	EXPRESSION TAG	UNP Q09778
N	-1	HIS	-	EXPRESSION TAG	UNP Q09778
N	0	MSE	-	EXPRESSION TAG	UNP Q09778
O	-2	SER	-	EXPRESSION TAG	UNP Q09778
O	-1	HIS	-	EXPRESSION TAG	UNP Q09778
O	0	MSE	-	EXPRESSION TAG	UNP Q09778
P	-2	SER	-	EXPRESSION TAG	UNP Q09778
P	-1	HIS	-	EXPRESSION TAG	UNP Q09778
P	0	MSE	-	EXPRESSION TAG	UNP Q09778
Q	-2	SER	-	EXPRESSION TAG	UNP Q09778
Q	-1	HIS	-	EXPRESSION TAG	UNP Q09778
Q	0	MSE	-	EXPRESSION TAG	UNP Q09778
R	-2	SER	-	EXPRESSION TAG	UNP Q09778
R	-1	HIS	-	EXPRESSION TAG	UNP Q09778
R	0	MSE	-	EXPRESSION TAG	UNP Q09778
S	-2	SER	-	EXPRESSION TAG	UNP Q09778
S	-1	HIS	-	EXPRESSION TAG	UNP Q09778
S	0	MSE	-	EXPRESSION TAG	UNP Q09778
T	-2	SER	-	EXPRESSION TAG	UNP Q09778
T	-1	HIS	-	EXPRESSION TAG	UNP Q09778
T	0	MSE	-	EXPRESSION TAG	UNP Q09778

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

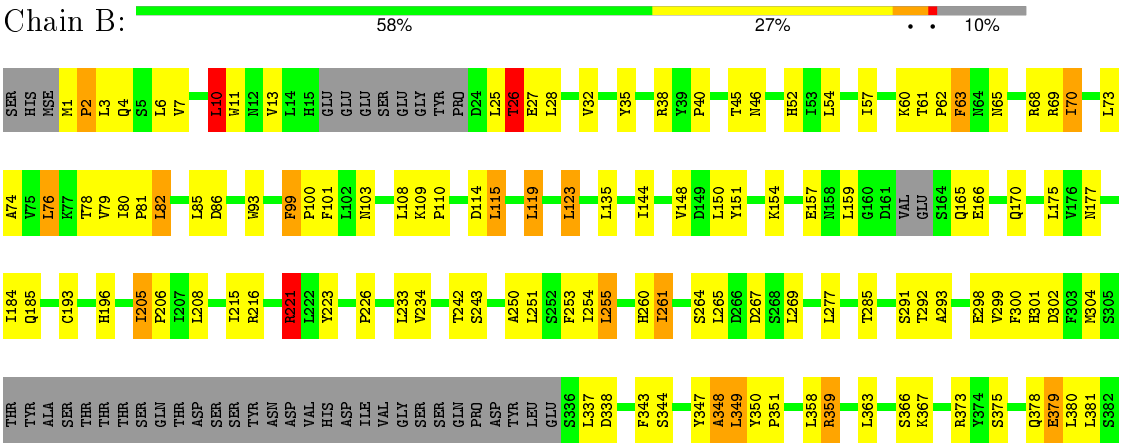
- Molecule 1: Tuberous sclerosis 1 protein homolog

Chain A:



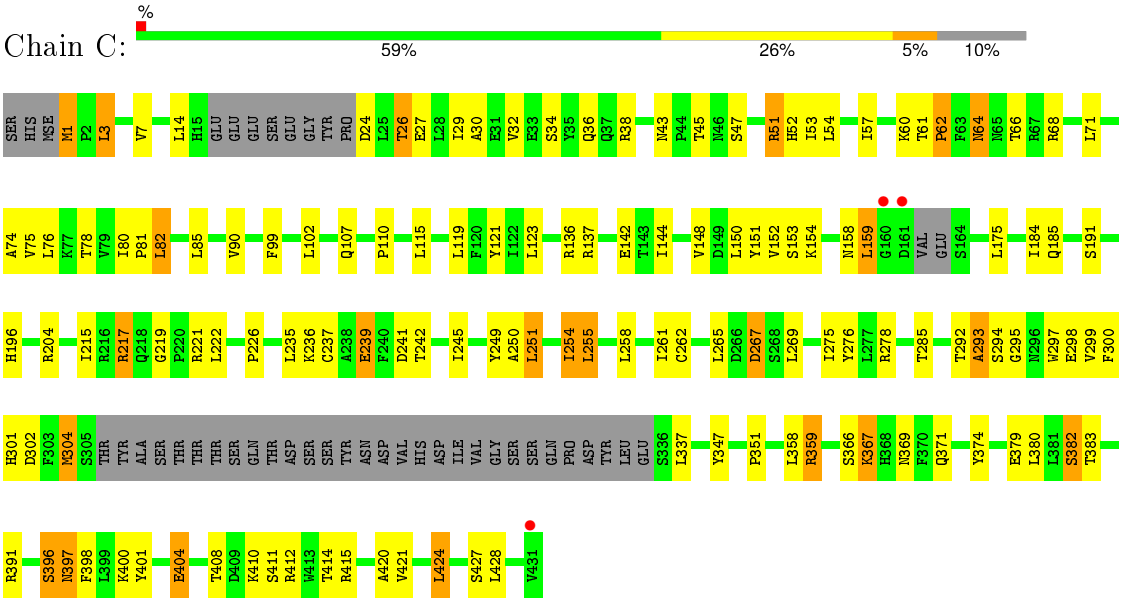
- Molecule 1: Tuberous sclerosis 1 protein homolog

Chain B:



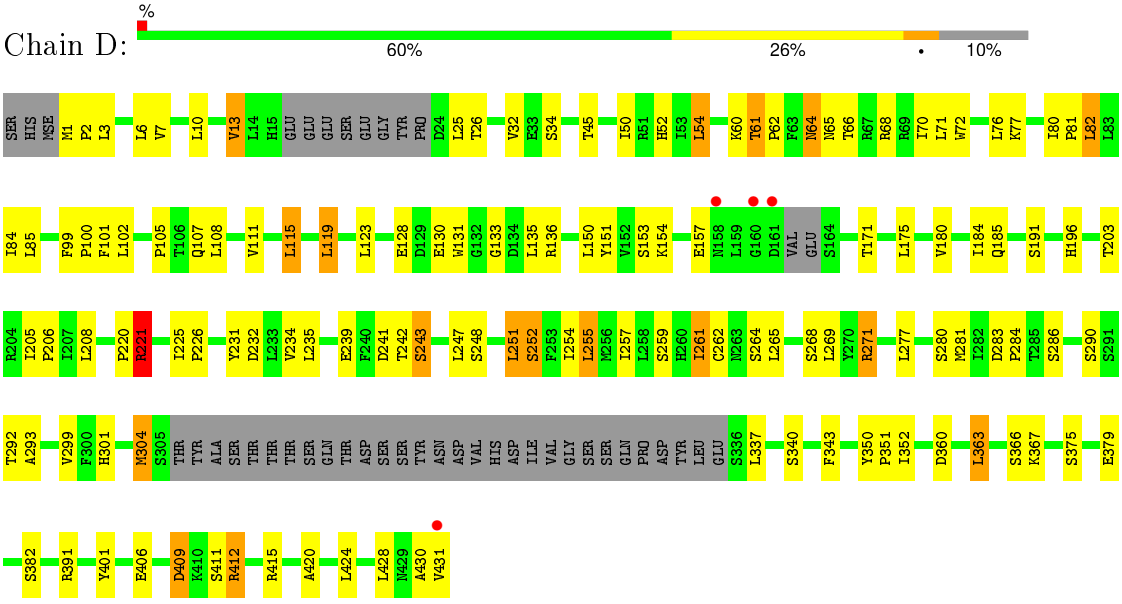
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain C:



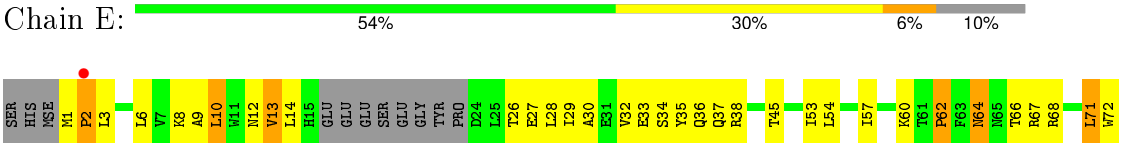
• Molecule 1: Tuberous sclerosis 1 protein homolog

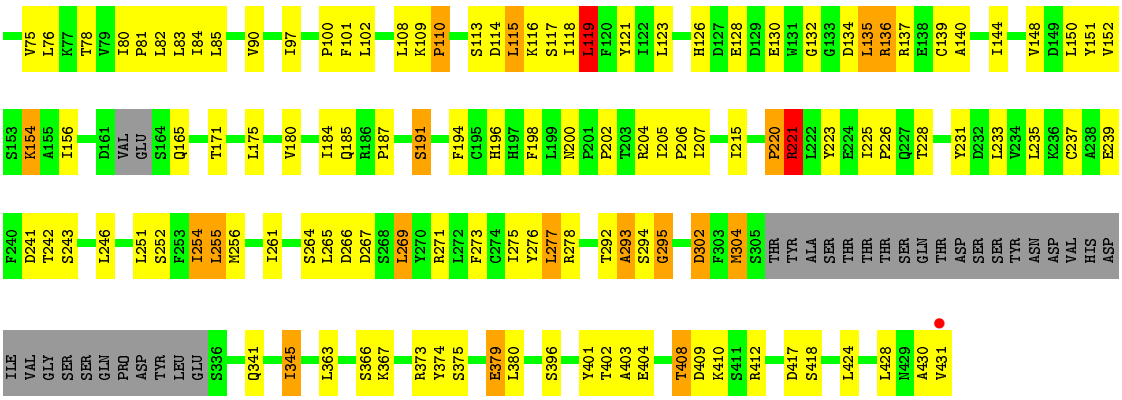
Chain D:



• Molecule 1: Tuberous sclerosis 1 protein homolog

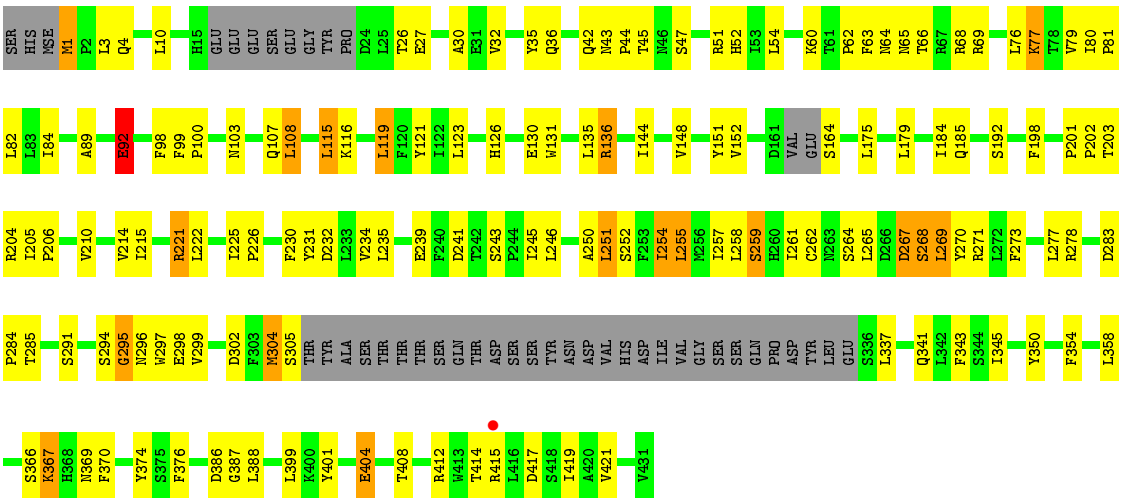
Chain E:





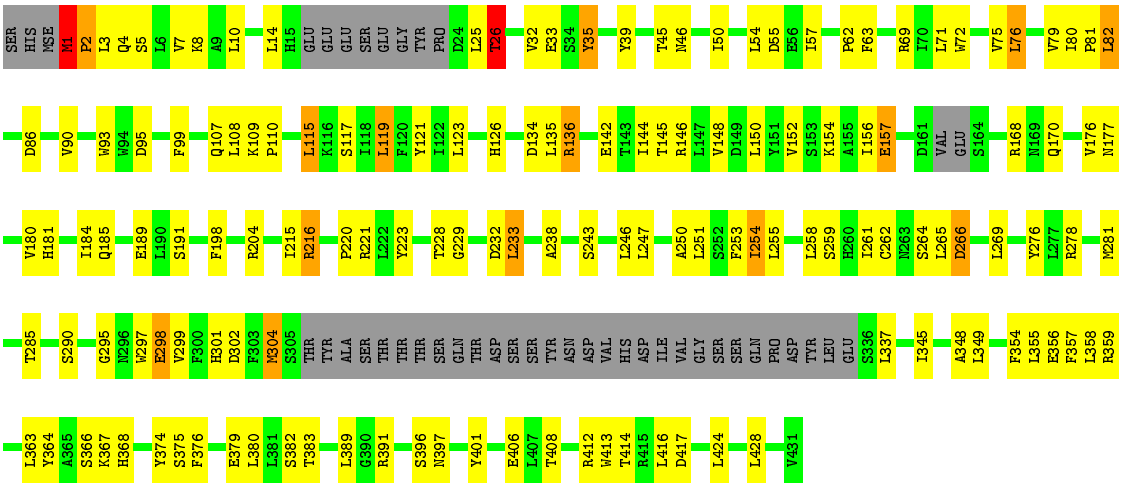
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain F:



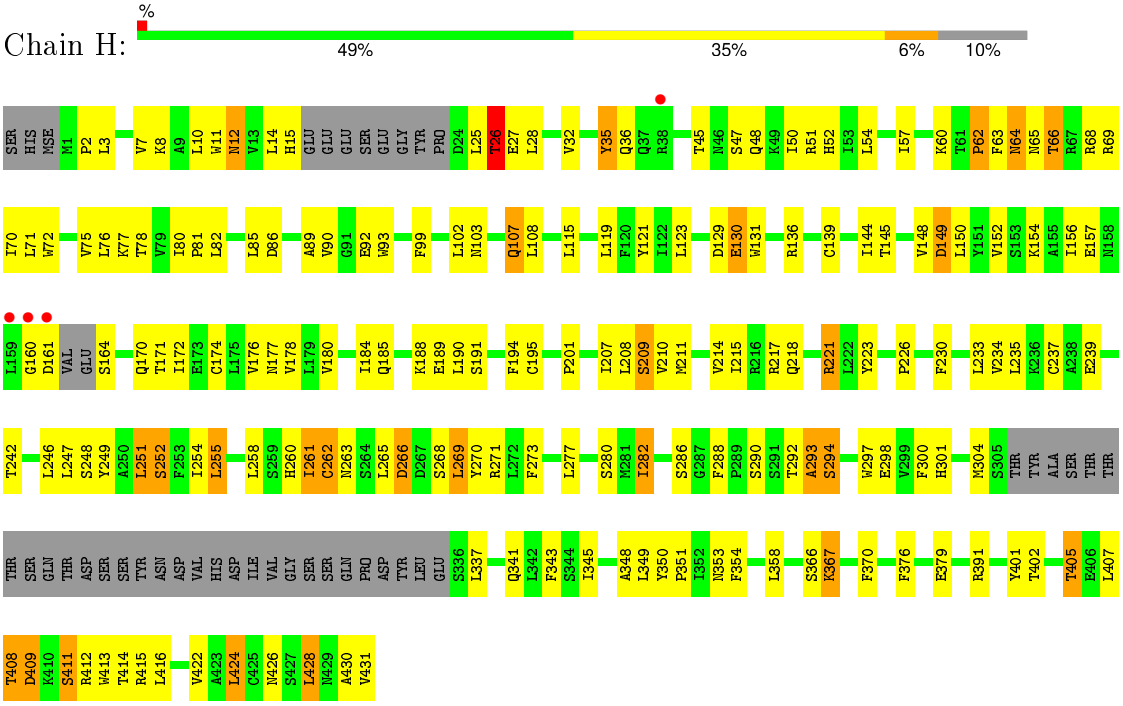
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain G:



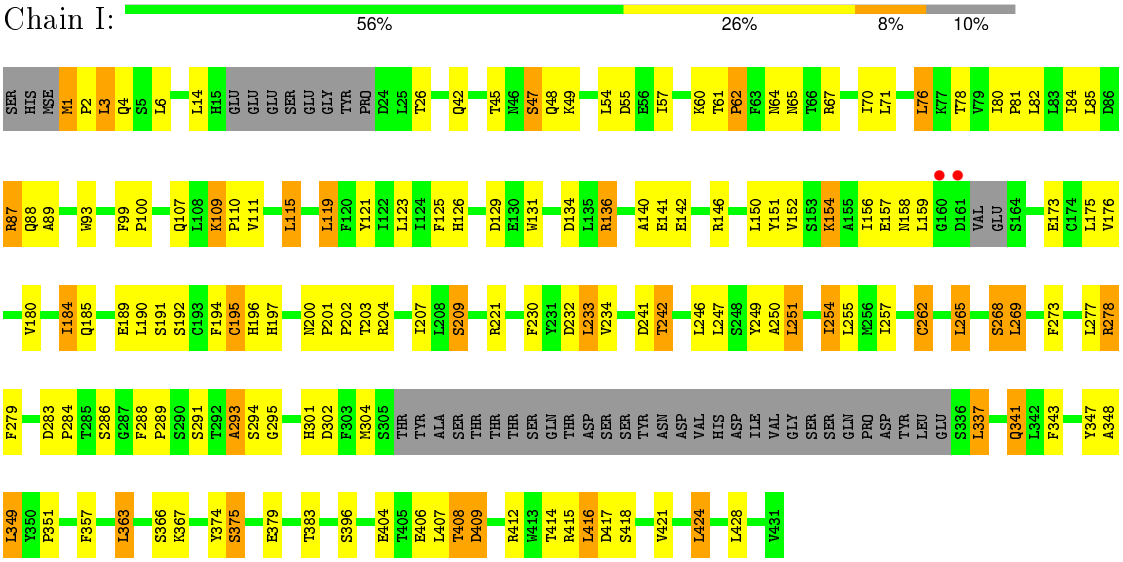
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain H:



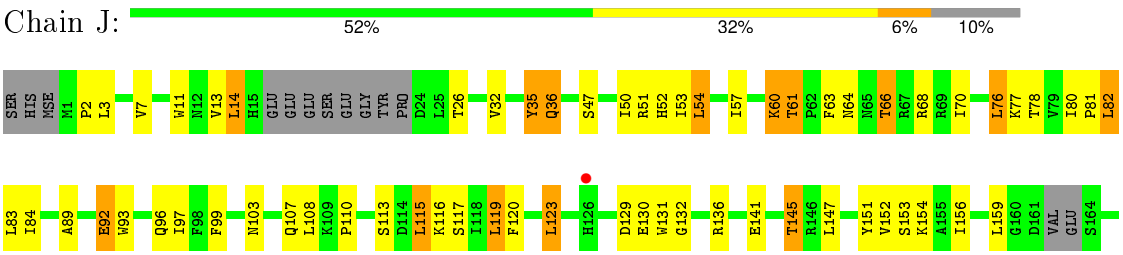
• Molecule 1: Tuberous sclerosis 1 protein homolog

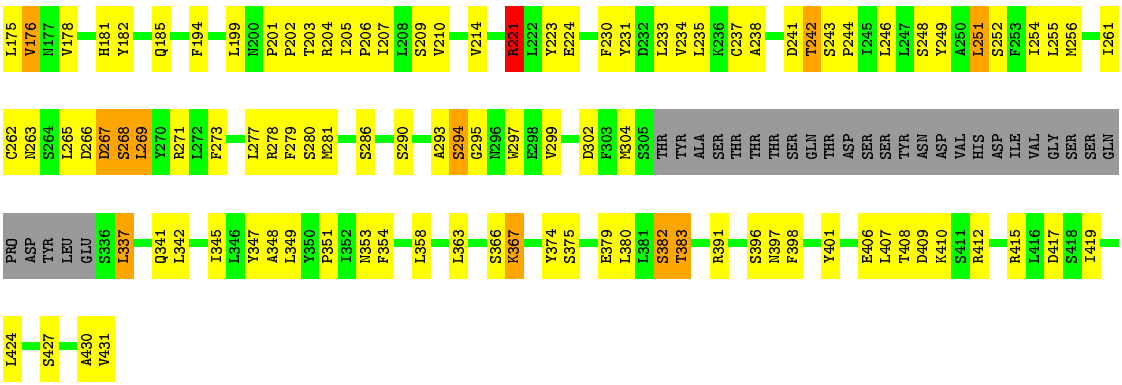
Chain I:



• Molecule 1: Tuberous sclerosis 1 protein homolog

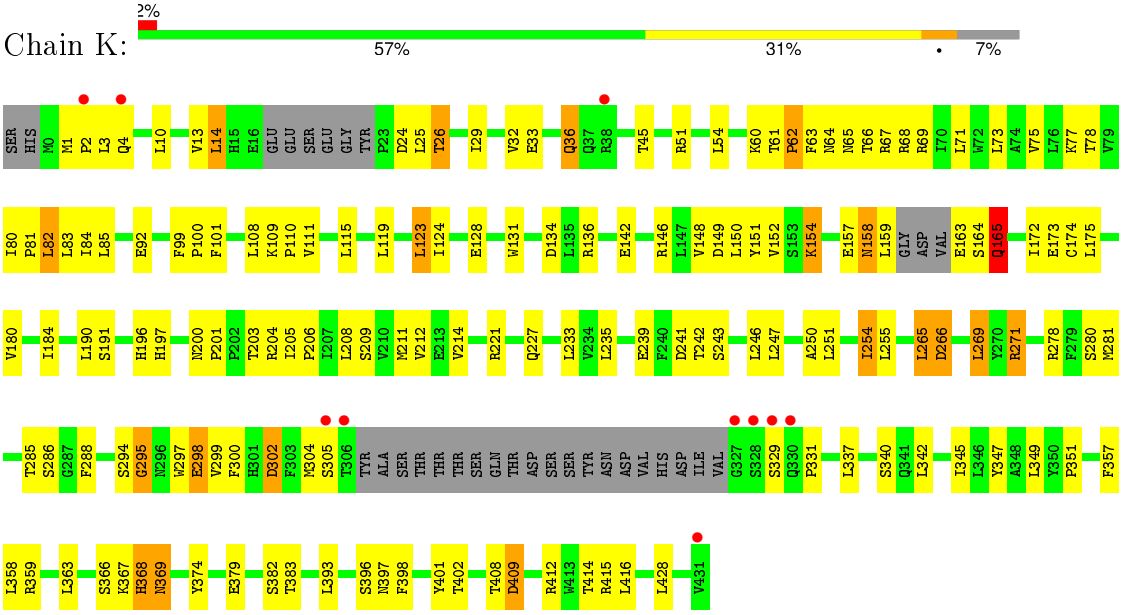
Chain J:





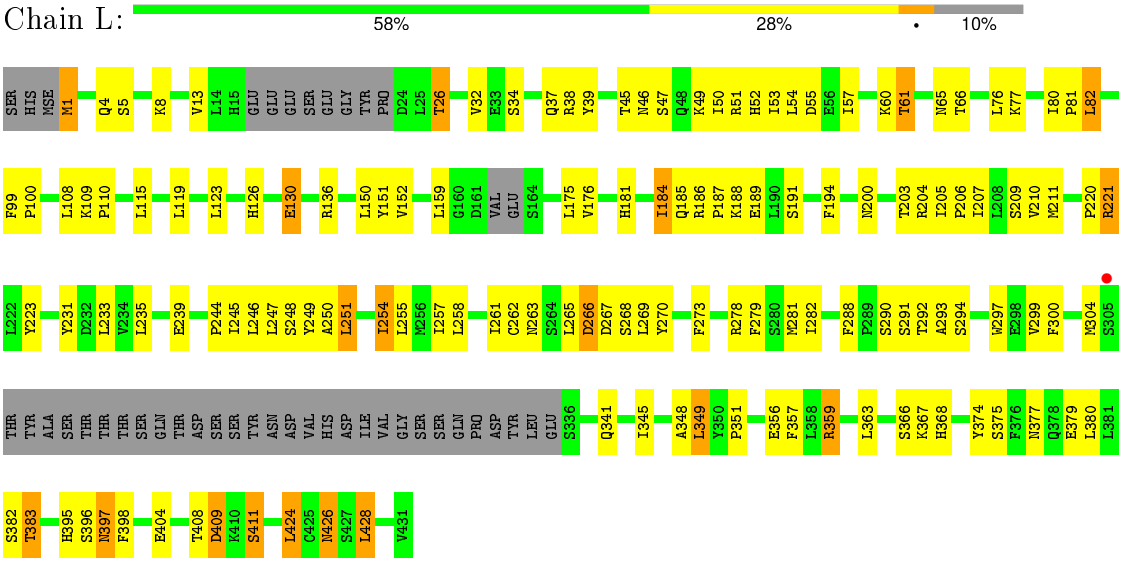
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain K:



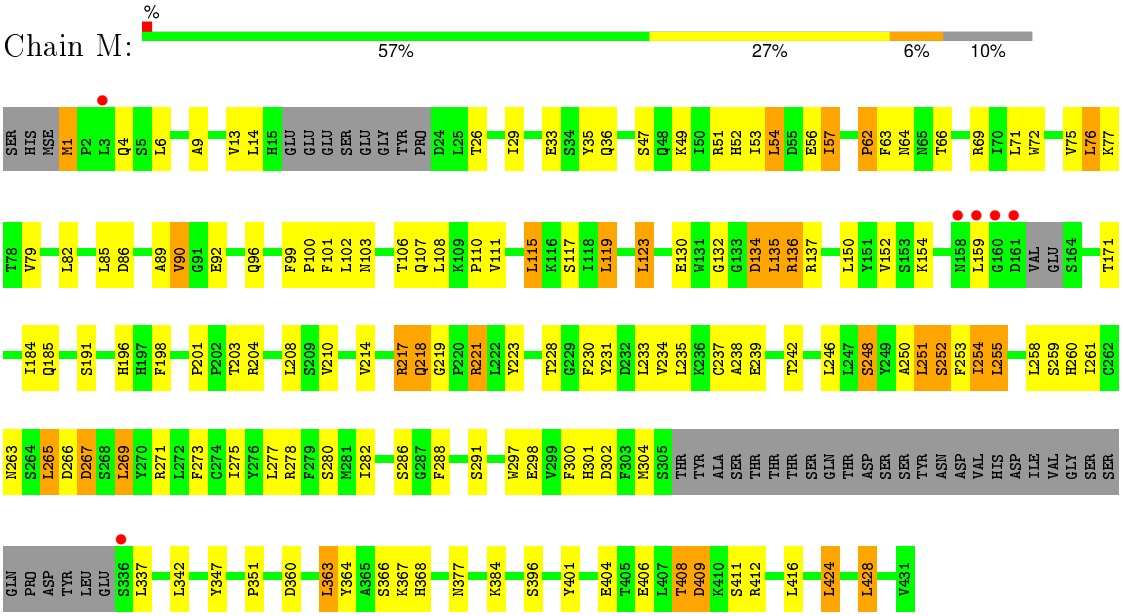
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain L:



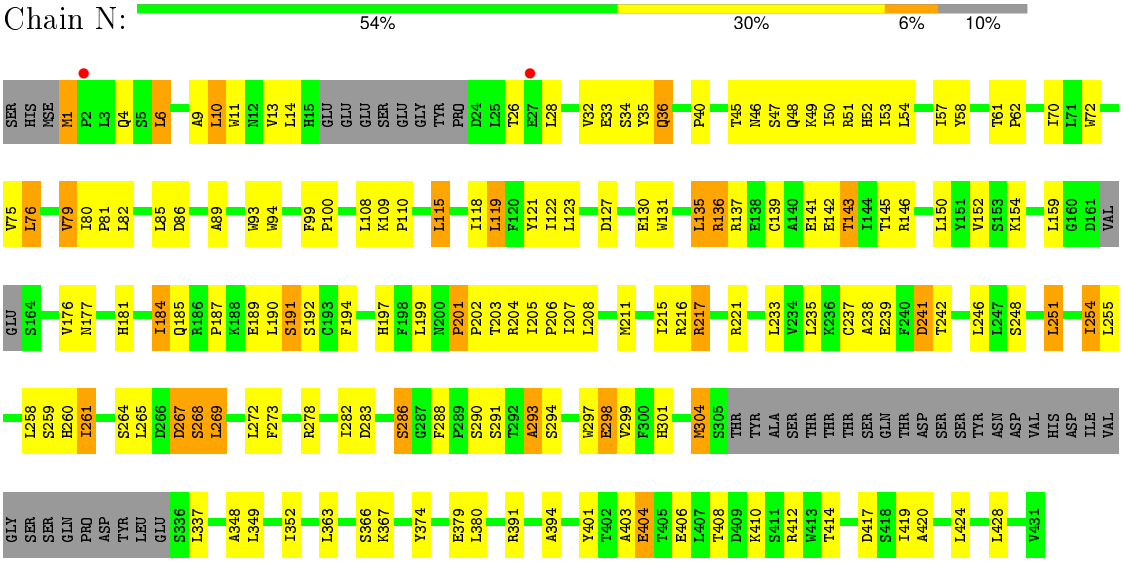
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain M:



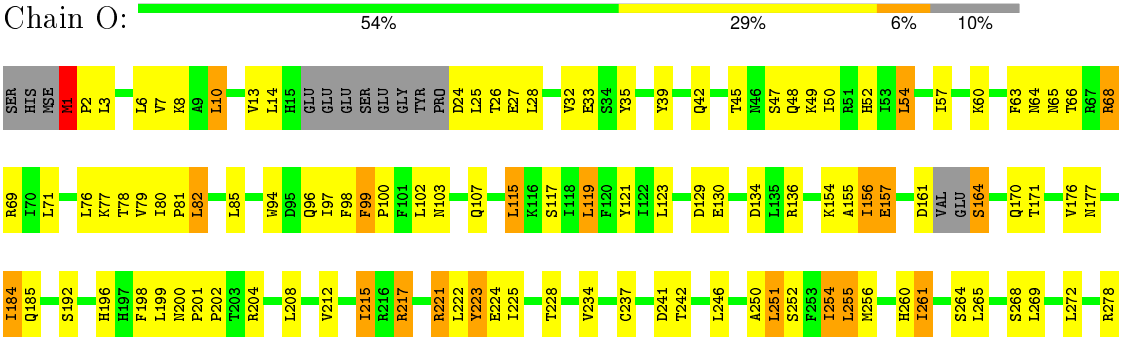
• Molecule 1: Tuberous sclerosis 1 protein homolog

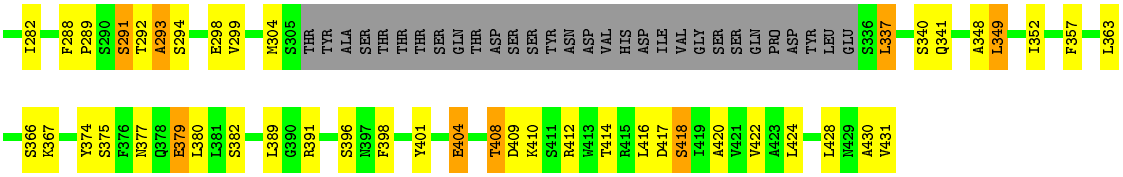
Chain N:

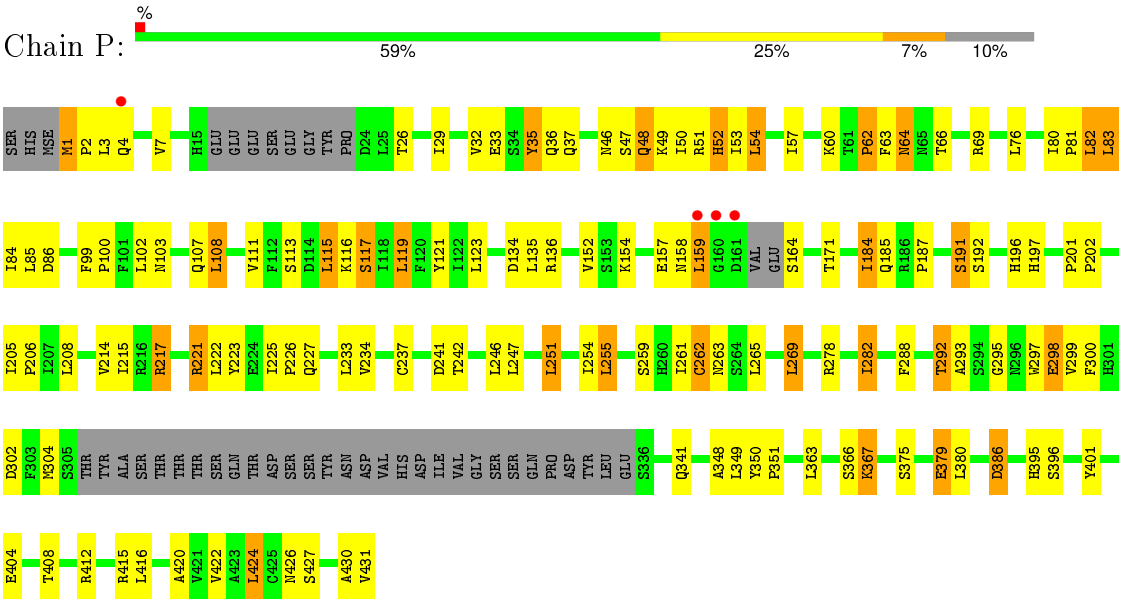


• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain O:





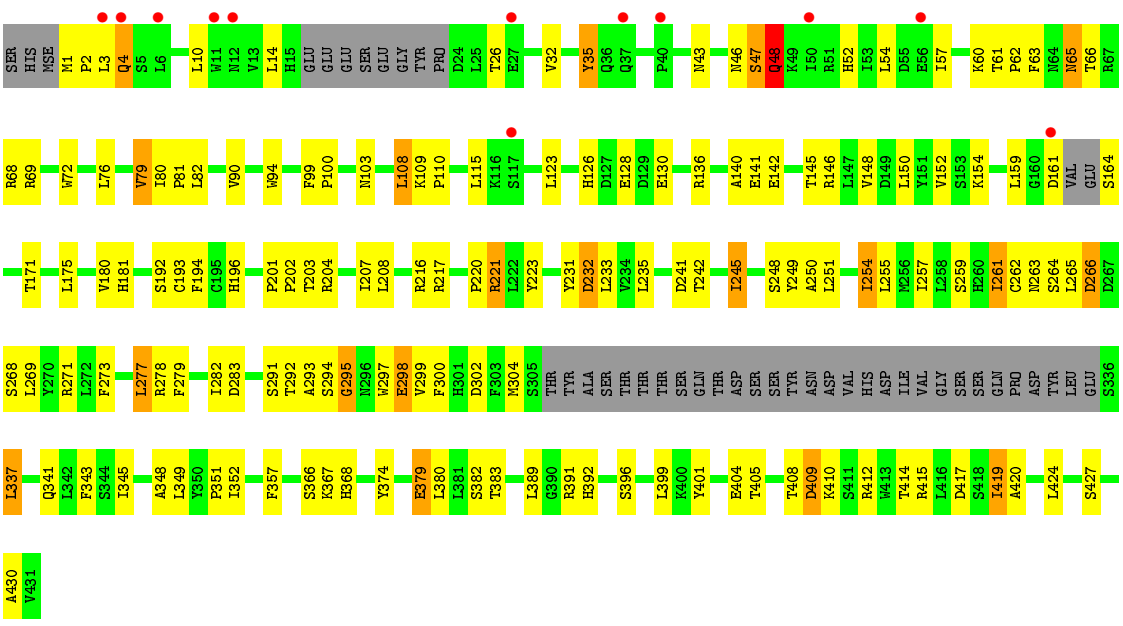


• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain P:

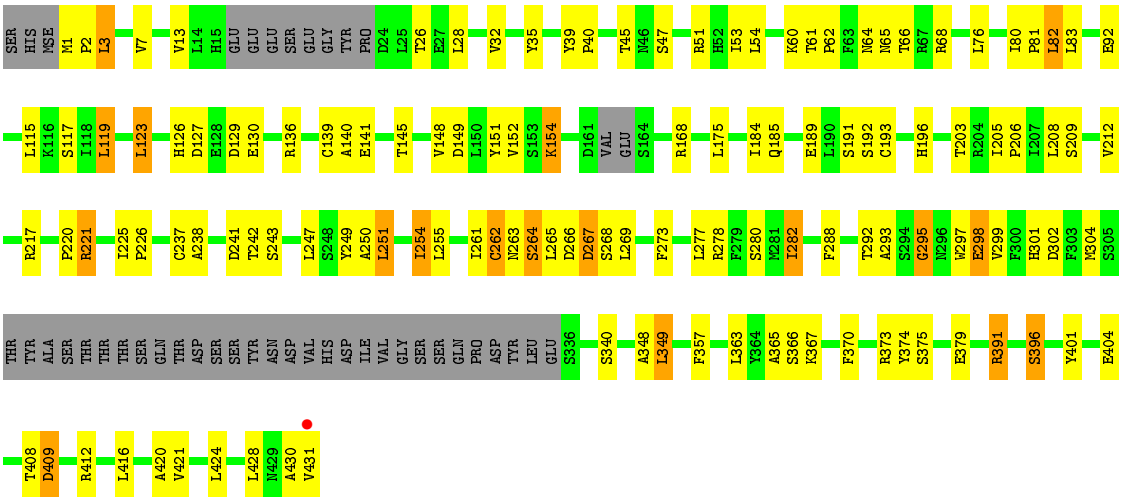
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain Q:



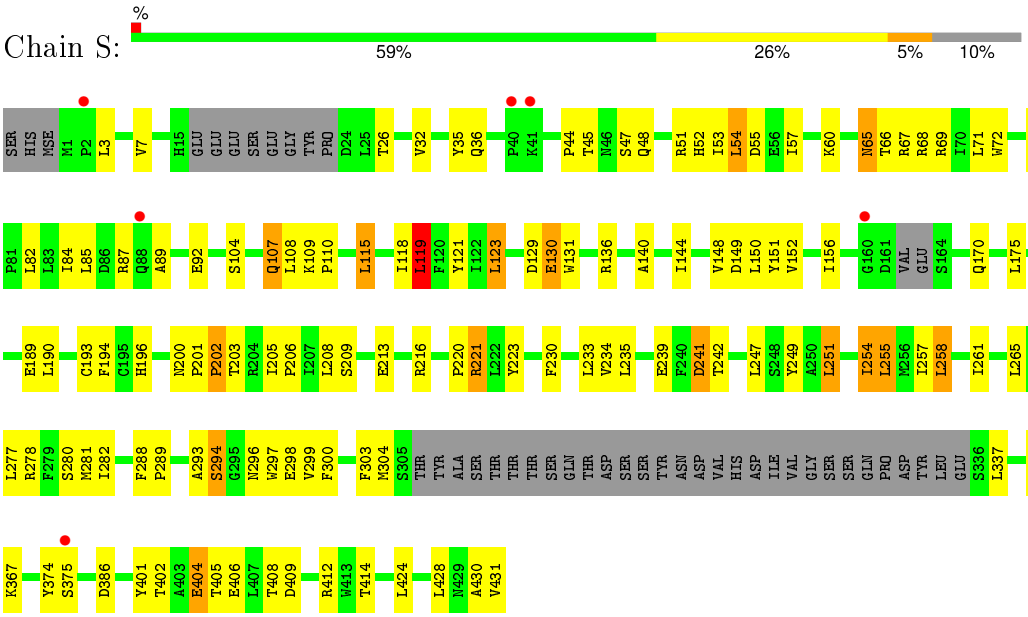
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain R:



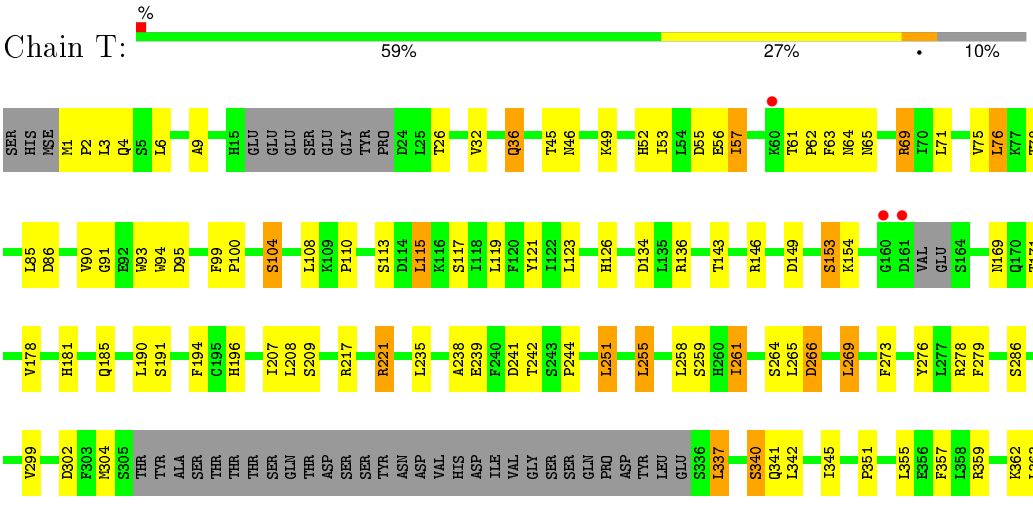
• Molecule 1: Tuberous sclerosis 1 protein homolog

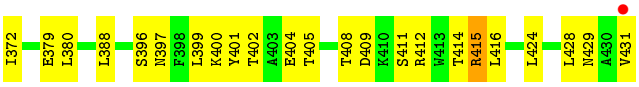
Chain S:



• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain T:




I372
E379
L380
L388
S396
N397
F398
L399
K400
Y401
T402
A403
E404
T405
T408
D409
K410
S411
R412
K413
T414
R415
L416
L424
L428
N429
A430
V431

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.32Å 254.83Å 228.47Å 90.00° 99.71° 90.00°	Depositor
Resolution (Å)	39.82 – 3.30 39.79 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.82-3.30) 96.2 (39.79-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.186 , 0.268 0.187 , 0.276	Depositor DCC
R_{free} test set	9230 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	85.9	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 198889 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	63794	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.63	0/3343	0.86	1/4535 (0.0%)
1	B	0.64	0/3257	0.85	1/4421 (0.0%)
1	C	0.65	0/3257	0.85	3/4421 (0.1%)
1	D	0.65	0/3257	0.85	4/4421 (0.1%)
1	E	0.62	0/3257	0.87	3/4421 (0.1%)
1	F	0.61	1/3257 (0.0%)	0.83	1/4421 (0.0%)
1	G	0.65	0/3257	0.88	5/4421 (0.1%)
1	H	0.61	0/3257	0.81	0/4421
1	I	0.66	0/3257	0.87	2/4421 (0.0%)
1	J	0.63	0/3257	0.86	2/4421 (0.0%)
1	K	0.61	0/3343	0.85	1/4535 (0.0%)
1	L	0.66	0/3257	0.86	0/4421
1	M	0.65	0/3257	0.88	1/4421 (0.0%)
1	N	0.68	0/3257	0.88	2/4421 (0.0%)
1	O	0.71	0/3257	0.91	3/4421 (0.1%)
1	P	0.64	0/3257	0.86	3/4421 (0.1%)
1	Q	0.64	0/3257	0.84	1/4421 (0.0%)
1	R	0.64	0/3257	0.86	2/4421 (0.0%)
1	S	0.58	0/3257	0.79	0/4421
1	T	0.60	0/3257	0.82	2/4421 (0.0%)
All	All	0.64	1/65312 (0.0%)	0.85	37/88648 (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	E	0	1
1	F	0	1
1	I	0	1
1	K	0	1
1	O	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	92	GLU	CG-CD	5.12	1.59	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	304	MSE	CB-CA-C	9.11	128.63	110.40
1	C	1	MSE	CG-SE-CE	7.77	116.00	98.90
1	J	221	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	E	304	MSE	CB-CA-C	6.98	124.36	110.40
1	G	337	LEU	CA-CB-CG	6.82	130.99	115.30
1	G	1	MSE	CG-SE-CE	6.69	113.63	98.90
1	C	51	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	P	217	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	M	237	CYS	CA-CB-SG	-6.17	102.90	114.00
1	G	216	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	G	428	LEU	CA-CB-CG	5.87	128.80	115.30
1	D	304	MSE	CB-CA-C	5.82	122.04	110.40
1	E	221	ARG	N-CA-C	-5.73	95.52	111.00
1	B	221	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	O	217	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	278	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	409	ASP	N-CA-C	-5.42	96.37	111.00
1	Q	337	LEU	CA-CB-CG	5.40	127.71	115.30
1	G	233	LEU	CA-CB-CG	5.29	127.45	115.30
1	O	1	MSE	CG-SE-CE	5.28	110.51	98.90
1	D	221	ARG	N-CA-C	-5.27	96.78	111.00
1	J	337	LEU	CA-CB-CG	5.27	127.42	115.30
1	D	337	LEU	CA-CB-CG	5.26	127.41	115.30
1	E	373	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	217	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	O	25	LEU	N-CA-C	5.17	124.95	111.00
1	R	92	GLU	CA-CB-CG	5.16	124.75	113.40
1	K	123	LEU	CA-CB-CG	5.14	127.13	115.30
1	F	92	GLU	CA-CB-CG	5.09	124.59	113.40
1	N	217	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	P	227	GLN	CB-CA-C	-5.06	100.28	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	92	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	T	217	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	T	123	LEU	CA-CB-CG	5.03	126.87	115.30
1	P	217	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	I	278	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	I	337	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	220	PRO	Peptide
1	F	164	SER	Peptide
1	I	3	LEU	Peptide
1	K	368	HIS	Peptide
1	O	164	SER	Peptide
1	O	24	ASP	Peptide
1	P	164	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3268	0	3216	108	0
1	B	3181	0	3145	81	0
1	C	3181	0	3145	73	0
1	D	3181	0	3145	74	0
1	E	3181	0	3145	80	0
1	F	3181	0	3145	80	0
1	G	3181	0	3145	81	0
1	H	3181	0	3145	114	0
1	I	3181	0	3145	78	0
1	J	3181	0	3145	99	0
1	K	3268	0	3216	81	0
1	L	3181	0	3145	83	0
1	M	3181	0	3145	95	0
1	N	3181	0	3145	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3181	0	3145	89	0
1	P	3181	0	3145	79	0
1	Q	3181	0	3145	84	0
1	R	3181	0	3145	74	0
1	S	3181	0	3145	85	0
1	T	3181	0	3145	73	0
All	All	63794	0	63042	1624	0

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 13.

All (1624) 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:G:115:LEU:HD22	1:G:119:LEU:HD22	1.43	0.98
1:M:401:TYR:CZ	1:M:412:ARG:HG3	1.99	0.96
1:A:121:TYR:O	1:A:136:ARG:NH2	2.05	0.90
1:I:142:GLU:OE2	1:I:146:ARG:NH1	2.08	0.86
1:Q:279:PHE:O	1:Q:282:ILE:HG22	1.76	0.85
1:E:235:LEU:O	1:E:239:GLU:HG3	1.77	0.85
1:F:250:ALA:O	1:F:254:ILE:HG23	1.77	0.85
1:T:185:GLN:O	1:T:221:ARG:NH2	2.09	0.85
1:J:32:VAL:HG13	1:J:82:LEU:HD21	1.59	0.85
1:L:130:GLU:OE1	1:L:136:ARG:NH1	2.11	0.83
1:R:401:TYR:CZ	1:R:412:ARG:HG3	2.13	0.83
1:R:379:GLU:HG3	1:T:185:GLN:HA	1.58	0.82
1:M:185:GLN:HA	1:O:379:GLU:HG3	1.60	0.82
1:G:299:VAL:HG11	1:G:301:HIS:CE1	2.15	0.81
1:J:89:ALA:O	1:J:92:GLU:HB2	1.81	0.81
1:P:379:GLU:HG3	1:R:185:GLN:HA	1.60	0.81
1:L:379:GLU:HG3	1:N:185:GLN:HA	1.63	0.80
1:B:406:GLU:O	1:B:412:ARG:NH2	2.13	0.80
1:H:251:LEU:HD22	1:H:255:LEU:HD22	1.64	0.80
1:R:299:VAL:HG11	1:R:301:HIS:CE1	2.18	0.79
1:N:199:LEU:O	1:N:201:PRO:HD3	1.84	0.78
1:S:401:TYR:CZ	1:S:412:ARG:HG3	2.19	0.78
1:B:366:SER:O	1:B:367:LYS:HB2	1.83	0.78
1:S:44:PRO:O	1:S:48:GLN:HG2	1.84	0.77
1:L:409:ASP:OD1	1:L:411:SER:OG	2.01	0.77
1:L:282:ILE:HD12	1:L:288:PHE:CZ	2.20	0.77
1:T:402:THR:OG1	1:T:405:THR:HG23	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LEU:O	1:C:239:GLU:HG3	1.85	0.76
1:M:115:LEU:HD22	1:M:119:LEU:HD22	1.68	0.76
1:P:50:ILE:O	1:P:54:LEU:HD22	1.86	0.76
1:N:115:LEU:HD22	1:N:119:LEU:HD22	1.66	0.76
1:H:366:SER:O	1:H:367:LYS:HB2	1.85	0.76
1:M:71:LEU:O	1:M:75:VAL:HG23	1.85	0.76
1:G:185:GLN:HA	1:I:379:GLU:HG3	1.68	0.76
1:I:14:LEU:HD23	1:I:71:LEU:HD23	1.67	0.75
1:S:32:VAL:O	1:S:36:GLN:HG3	1.86	0.75
1:J:278:ARG:HD2	1:J:374:TYR:CZ	2.20	0.75
1:H:89:ALA:O	1:H:92:GLU:N	2.19	0.75
1:O:222:LEU:O	1:O:224:GLU:N	2.20	0.75
1:O:401:TYR:CZ	1:O:412:ARG:HG3	2.21	0.75
1:J:115:LEU:HD22	1:J:119:LEU:HD22	1.68	0.75
1:K:180:VAL:HG13	1:K:214:VAL:HG22	1.67	0.74
1:Q:278:ARG:HD2	1:Q:374:TYR:CE1	2.22	0.74
1:Q:152:VAL:HG13	1:Q:203:THR:HG22	1.69	0.74
1:A:379:GLU:HG3	1:I:185:GLN:HA	1.68	0.74
1:H:99:PHE:O	1:H:103:ASN:HB2	1.88	0.74
1:J:130:GLU:OE1	1:J:136:ARG:NH1	2.21	0.74
1:J:280:SER:O	1:J:281:MSE:HE2	1.87	0.73
1:L:366:SER:O	1:L:367:LYS:HB2	1.89	0.73
1:L:185:GLN:HA	1:T:379:GLU:HG3	1.70	0.73
1:O:102:LEU:O	1:O:171:THR:HG23	1.88	0.73
1:N:121:TYR:O	1:N:136:ARG:NH2	2.21	0.73
1:G:3:LEU:O	1:G:7:VAL:HG23	1.89	0.73
1:O:185:GLN:HA	1:Q:379:GLU:HG3	1.69	0.73
1:L:404:GLU:O	1:L:408:THR:HG22	1.88	0.73
1:P:47:SER:O	1:P:51:ARG:HG3	1.89	0.73
1:J:152:VAL:HG13	1:J:203:THR:HG22	1.69	0.72
1:K:250:ALA:O	1:K:254:ILE:HG23	1.89	0.72
1:G:401:TYR:CZ	1:G:412:ARG:HG3	2.24	0.72
1:T:404:GLU:O	1:T:408:THR:HG22	1.88	0.72
1:N:261:ILE:HG21	1:N:264:SER:HB2	1.70	0.72
1:O:161:ASP:CB	1:O:164:SER:CB	2.67	0.72
1:M:255:LEU:HD23	1:M:337:LEU:HB3	1.70	0.72
1:N:51:ARG:HA	1:N:54:LEU:HD23	1.70	0.71
1:G:150:LEU:O	1:G:154:LYS:HB2	1.90	0.71
1:T:255:LEU:HD23	1:T:337:LEU:HD12	1.73	0.71
1:M:235:LEU:O	1:M:239:GLU:HG3	1.91	0.71
1:L:278:ARG:HD2	1:L:374:TYR:CZ	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:293:ALA:HB3	1:R:373:ARG:NE	2.06	0.71
1:S:151:TYR:HA	1:S:175:LEU:HD13	1.72	0.70
1:H:211:MSE:O	1:H:215:ILE:HG12	1.92	0.70
1:N:10:LEU:O	1:N:13:VAL:HG12	1.92	0.70
1:G:414:THR:HG21	1:H:223:TYR:CE2	2.27	0.69
1:P:430:ALA:O	1:P:431:VAL:HB	1.92	0.69
1:K:158:ASN:N	1:K:158:ASN:OD1	2.25	0.69
1:G:71:LEU:O	1:G:75:VAL:HG23	1.91	0.69
1:N:235:LEU:O	1:N:239:GLU:HG3	1.92	0.69
1:A:278:ARG:HD2	1:A:374:TYR:CE1	2.27	0.69
1:C:250:ALA:O	1:C:254:ILE:HG23	1.92	0.69
1:I:1:MSE:HE2	1:I:4:GLN:HB2	1.74	0.69
1:A:238:ALA:O	1:A:278:ARG:NH1	2.26	0.69
1:Q:32:VAL:HG13	1:Q:82:LEU:HD21	1.75	0.68
1:M:251:LEU:HD22	1:M:255:LEU:HD22	1.75	0.68
1:P:401:TYR:OH	1:P:412:ARG:HG3	1.94	0.68
1:J:401:TYR:CZ	1:J:412:ARG:HG3	2.28	0.68
1:B:358:LEU:O	1:B:359:ARG:CB	2.42	0.68
1:G:406:GLU:O	1:G:412:ARG:NH2	2.27	0.68
1:R:243:SER:OG	1:R:302:ASP:OD1	2.09	0.68
1:P:247:LEU:HD12	1:P:288:PHE:CD1	2.29	0.67
1:A:29:ILE:O	1:A:33:GLU:HG3	1.95	0.67
1:C:404:GLU:O	1:C:408:THR:HG22	1.95	0.67
1:R:293:ALA:HB3	1:R:373:ARG:HE	1.60	0.67
1:L:247:LEU:HD12	1:L:288:PHE:CD1	2.29	0.67
1:R:250:ALA:O	1:R:254:ILE:HG23	1.95	0.67
1:H:194:PHE:CD1	1:H:207:ILE:HG23	2.29	0.67
1:C:235:LEU:O	1:C:239:GLU:CG	2.43	0.67
1:G:32:VAL:HG13	1:G:82:LEU:HD21	1.76	0.67
1:D:102:LEU:O	1:D:105:PRO:HD3	1.95	0.66
1:E:401:TYR:CZ	1:E:412:ARG:HG3	2.31	0.66
1:S:408:THR:O	1:S:408:THR:HG23	1.96	0.66
1:B:401:TYR:CZ	1:B:412:ARG:HG3	2.31	0.66
1:H:255:LEU:HD23	1:H:337:LEU:HB3	1.77	0.66
1:J:96:GLN:O	1:J:97:ILE:HD13	1.97	0.65
1:I:241:ASP:O	1:I:278:ARG:NH2	2.27	0.65
1:T:241:ASP:HA	1:T:299:VAL:HG13	1.77	0.65
1:L:1:MSE:HE2	1:L:4:GLN:HB2	1.78	0.65
1:B:348:ALA:O	1:B:350:TYR:N	2.29	0.65
1:F:401:TYR:CZ	1:F:412:ARG:HG3	2.32	0.65
1:H:401:TYR:CZ	1:H:412:ARG:HG3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD22	1:B:119:LEU:HD22	1.77	0.65
1:O:156:ILE:HG22	1:O:157:GLU:H	1.62	0.65
1:E:243:SER:OG	1:E:302:ASP:OD1	2.15	0.65
1:S:89:ALA:O	1:S:92:GLU:HB2	1.96	0.65
1:C:47:SER:O	1:C:51:ARG:HG3	1.97	0.65
1:O:250:ALA:O	1:O:254:ILE:HG23	1.95	0.65
1:C:278:ARG:HD2	1:C:374:TYR:CZ	2.32	0.65
1:L:379:GLU:CG	1:N:185:GLN:HA	2.26	0.65
1:R:238:ALA:O	1:R:278:ARG:NH1	2.30	0.65
1:H:180:VAL:O	1:H:184:ILE:HG23	1.95	0.65
1:E:27:GLU:O	1:E:30:ALA:HB3	1.97	0.64
1:O:80:ILE:N	1:O:81:PRO:HD2	2.12	0.64
1:H:366:SER:O	1:H:367:LYS:CB	2.45	0.64
1:E:71:LEU:O	1:E:75:VAL:HG23	1.98	0.64
1:K:24:ASP:OD1	1:K:26:THR:OG1	2.13	0.64
1:G:191:SER:HB2	1:G:228:THR:HG21	1.78	0.64
1:N:264:SER:O	1:N:268:SER:OG	2.16	0.64
1:K:278:ARG:HD2	1:K:374:TYR:CE1	2.33	0.64
1:I:109:LYS:HB2	1:I:110:PRO:HD3	1.77	0.64
1:C:366:SER:O	1:C:367:LYS:HB2	1.98	0.64
1:O:3:LEU:O	1:O:7:VAL:HG23	1.99	0.63
1:I:150:LEU:HG	1:I:175:LEU:HD11	1.81	0.63
1:M:134:ASP:O	1:M:136:ARG:N	2.31	0.63
1:K:99:PHE:HB3	1:K:100:PRO:HD3	1.80	0.63
1:B:115:LEU:HD22	1:B:119:LEU:CD2	2.28	0.63
1:T:273:PHE:HB3	1:T:357:PHE:CE2	2.33	0.63
1:L:366:SER:O	1:L:367:LYS:CB	2.45	0.63
1:H:102:LEU:O	1:H:171:THR:HG23	1.99	0.63
1:K:347:TYR:O	1:K:351:PRO:HB3	1.99	0.63
1:L:291:SER:OG	1:L:292:THR:N	2.31	0.63
1:J:406:GLU:O	1:J:412:ARG:NH2	2.31	0.63
1:I:76:LEU:HG	1:I:93:TRP:CZ3	2.34	0.63
1:M:401:TYR:OH	1:M:412:ARG:CG	2.47	0.63
1:O:156:ILE:HG22	1:O:157:GLU:N	2.13	0.63
1:E:115:LEU:HD22	1:E:119:LEU:HD22	1.80	0.63
1:M:53:ILE:O	1:M:57:ILE:HG13	1.99	0.63
1:B:379:GLU:HG3	1:D:185:GLN:HA	1.81	0.63
1:C:144:ILE:O	1:C:148:VAL:HG23	1.98	0.63
1:E:200:ASN:OD1	1:E:202:PRO:HD2	1.99	0.63
1:Q:278:ARG:HD2	1:Q:374:TYR:CZ	2.34	0.62
1:K:163:GLU:C	1:K:165:GLN:N	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:32:VAL:HG13	1:L:82:LEU:HD21	1.80	0.62
1:P:1:MSE:HE2	1:P:4:GLN:HB2	1.81	0.62
1:L:200:ASN:O	1:L:203:THR:OG1	2.15	0.62
1:K:379:GLU:HG3	1:S:185:GLN:HA	1.81	0.62
1:S:404:GLU:O	1:S:408:THR:HG22	2.00	0.62
1:N:70:ILE:HD11	1:N:108:LEU:HD12	1.82	0.62
1:N:142:GLU:OE2	1:N:146:ARG:NH1	2.32	0.62
1:R:152:VAL:HG13	1:R:203:THR:HG22	1.79	0.62
1:J:366:SER:O	1:J:367:LYS:HB2	2.00	0.62
1:F:404:GLU:O	1:F:408:THR:HG22	1.99	0.62
1:R:148:VAL:HG21	1:R:193:CYS:HB3	1.82	0.62
1:B:366:SER:O	1:B:367:LYS:CB	2.47	0.62
1:K:280:SER:O	1:K:281:MSE:HE2	1.99	0.62
1:P:215:ILE:HD12	1:P:222:LEU:HD22	1.82	0.62
1:P:366:SER:O	1:P:367:LYS:HB2	1.99	0.62
1:A:144:ILE:O	1:A:148:VAL:HG23	2.00	0.62
1:F:262:CYS:HA	1:F:265:LEU:HD12	1.81	0.62
1:M:198:PHE:CE1	1:M:204:ARG:HG2	2.35	0.61
1:J:293:ALA:O	1:J:294:SER:HB3	1.98	0.61
1:N:86:ASP:H	1:N:89:ALA:HB3	1.65	0.61
1:F:239:GLU:O	1:F:278:ARG:NH1	2.34	0.61
1:I:152:VAL:HG13	1:I:203:THR:HG22	1.80	0.61
1:T:340:SER:HB2	1:T:388:LEU:HD21	1.83	0.61
1:H:64:ASN:OD1	1:H:64:ASN:N	2.30	0.61
1:E:410:LYS:N	1:E:410:LYS:HD3	2.15	0.61
1:E:366:SER:O	1:E:367:LYS:HB2	2.01	0.61
1:L:396:SER:O	1:L:398:PHE:N	2.33	0.61
1:B:148:VAL:HG21	1:B:193:CYS:HB3	1.81	0.61
1:I:406:GLU:O	1:I:412:ARG:NH2	2.34	0.61
1:K:63:PHE:CE1	1:K:69:ARG:HA	2.36	0.61
1:N:28:LEU:O	1:N:32:VAL:HG23	2.01	0.61
1:D:277:LEU:HD23	1:D:277:LEU:C	2.21	0.61
1:O:184:ILE:HD11	1:Q:380:LEU:HB2	1.83	0.61
1:K:66:THR:O	1:K:67:ARG:C	2.39	0.61
1:A:366:SER:O	1:A:367:LYS:HB2	2.01	0.61
1:R:366:SER:O	1:R:367:LYS:HB2	2.01	0.61
1:R:130:GLU:OE1	1:R:136:ARG:NH1	2.33	0.61
1:M:401:TYR:OH	1:M:412:ARG:HG3	2.00	0.61
1:F:278:ARG:HD2	1:F:374:TYR:CE1	2.36	0.61
1:S:430:ALA:O	1:S:431:VAL:HB	2.01	0.61
1:A:262:CYS:SG	1:B:421:VAL:HG21	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:141:GLU:O	1:R:145:THR:OG1	2.17	0.61
1:A:194:PHE:CD1	1:A:207:ILE:HG23	2.36	0.61
1:O:255:LEU:HD23	1:O:337:LEU:HB3	1.82	0.60
1:T:235:LEU:O	1:T:239:GLU:HG3	2.00	0.60
1:N:150:LEU:O	1:N:154:LYS:HB2	2.01	0.60
1:A:401:TYR:CZ	1:A:412:ARG:HG3	2.36	0.60
1:D:283:ASP:OD1	1:D:284:PRO:CD	2.49	0.60
1:H:130:GLU:OE1	1:H:136:ARG:NH1	2.34	0.60
1:I:250:ALA:O	1:I:254:ILE:HG23	2.02	0.60
1:H:239:GLU:OE2	1:H:271:ARG:NE	2.31	0.60
1:D:360:ASP:OD2	1:D:363:LEU:HB2	2.01	0.60
1:J:205:ILE:HB	1:J:206:PRO:HD3	1.84	0.60
1:O:32:VAL:HG13	1:O:82:LEU:HD21	1.84	0.60
1:I:151:TYR:HA	1:I:175:LEU:HD13	1.84	0.60
1:B:76:LEU:HG	1:B:93:TRP:CZ3	2.36	0.60
1:L:49:LYS:O	1:L:53:ILE:HG12	2.01	0.60
1:L:282:ILE:HD12	1:L:288:PHE:CE2	2.36	0.60
1:J:64:ASN:OD1	1:J:68:ARG:NH1	2.35	0.60
1:C:184:ILE:HD11	1:E:380:LEU:HB2	1.83	0.60
1:N:348:ALA:O	1:N:349:LEU:HB2	2.01	0.60
1:A:7:VAL:HG13	1:A:53:ILE:HG21	1.83	0.60
1:A:141:GLU:O	1:A:145:THR:OG1	2.18	0.60
1:J:151:TYR:HA	1:J:175:LEU:HD13	1.83	0.60
1:J:382:SER:O	1:J:383:THR:C	2.40	0.60
1:H:3:LEU:HD23	1:H:3:LEU:O	2.02	0.60
1:M:29:ILE:O	1:M:33:GLU:HG3	2.01	0.60
1:C:424:LEU:O	1:C:427:SER:OG	2.19	0.60
1:H:174:CYS:O	1:H:178:VAL:HG23	2.02	0.60
1:E:225:ILE:O	1:E:228:THR:OG1	2.16	0.60
1:A:190:LEU:HD11	1:A:194:PHE:CE2	2.37	0.60
1:A:408:THR:O	1:A:409:ASP:HB2	2.00	0.60
1:B:184:ILE:HD11	1:J:380:LEU:HB2	1.83	0.60
1:K:414:THR:O	1:K:416:LEU:N	2.35	0.60
1:H:293:ALA:O	1:H:294:SER:HB3	2.01	0.60
1:C:3:LEU:O	1:C:7:VAL:HG23	2.01	0.60
1:D:401:TYR:CZ	1:D:412:ARG:HG3	2.37	0.59
1:S:220:PRO:HB2	1:S:221:ARG:HG3	1.84	0.59
1:H:379:GLU:HG2	1:J:185:GLN:HG2	1.84	0.59
1:B:69:ARG:O	1:B:70:ILE:C	2.40	0.59
1:I:64:ASN:OD1	1:I:65:ASN:N	2.34	0.59
1:J:7:VAL:O	1:J:11:TRP:HD1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:LEU:O	1:D:239:GLU:HG3	2.02	0.59
1:E:84:ILE:C	1:E:85:LEU:HD12	2.23	0.59
1:J:89:ALA:O	1:J:93:TRP:HD1	1.86	0.59
1:B:404:GLU:O	1:B:408:THR:HG22	2.02	0.59
1:S:235:LEU:O	1:S:239:GLU:HG3	2.02	0.59
1:C:24:ASP:N	1:C:26:THR:HG1	2.00	0.59
1:C:278:ARG:HD2	1:C:374:TYR:CE1	2.37	0.59
1:C:241:ASP:HA	1:C:299:VAL:HG13	1.84	0.59
1:M:408:THR:O	1:M:408:THR:OG1	2.18	0.59
1:O:13:VAL:HG13	1:O:14:LEU:HG	1.83	0.59
1:L:299:VAL:HG12	1:L:300:PHE:N	2.18	0.59
1:H:28:LEU:O	1:H:28:LEU:HD12	2.03	0.59
1:H:66:THR:O	1:H:70:ILE:HD12	2.02	0.59
1:H:131:TRP:HZ3	1:H:139:CYS:HG	1.51	0.59
1:T:401:TYR:CZ	1:T:412:ARG:HG3	2.38	0.59
1:M:242:THR:HB	1:M:301:HIS:HA	1.85	0.59
1:A:247:LEU:HD12	1:A:288:PHE:CE1	2.38	0.59
1:N:278:ARG:HD2	1:N:374:TYR:CE1	2.38	0.59
1:B:358:LEU:O	1:B:359:ARG:HB3	2.02	0.59
1:C:204:ARG:CZ	1:C:297:TRP:CZ2	2.85	0.59
1:D:220:PRO:HB2	1:D:221:ARG:HG3	1.85	0.59
1:A:102:LEU:O	1:A:171:THR:HG23	2.03	0.58
1:L:293:ALA:O	1:L:294:SER:HB3	2.03	0.58
1:I:424:LEU:HD13	1:J:348:ALA:HB1	1.84	0.58
1:Q:404:GLU:O	1:Q:408:THR:HG22	2.03	0.58
1:S:121:TYR:O	1:S:136:ARG:NH2	2.35	0.58
1:D:283:ASP:OD1	1:D:284:PRO:HD2	2.03	0.58
1:N:75:VAL:O	1:N:79:VAL:HG13	2.02	0.58
1:O:430:ALA:O	1:O:431:VAL:HB	2.03	0.58
1:G:198:PHE:CE1	1:G:204:ARG:HG2	2.38	0.58
1:B:119:LEU:O	1:B:123:LEU:HD22	2.03	0.58
1:H:161:ASP:HA	1:H:164:SER:HA	1.85	0.58
1:T:1:MSE:HE2	1:T:4:GLN:HB2	1.85	0.58
1:I:89:ALA:O	1:I:93:TRP:HD1	1.86	0.58
1:K:408:THR:O	1:K:409:ASP:HB2	2.03	0.58
1:L:426:ASN:OD1	1:L:426:ASN:N	2.36	0.58
1:P:401:TYR:CZ	1:P:412:ARG:HG3	2.39	0.58
1:B:243:SER:OG	1:B:302:ASP:OD1	2.14	0.58
1:R:282:ILE:HD12	1:R:288:PHE:CE1	2.38	0.58
1:O:99:PHE:HB3	1:O:100:PRO:HD3	1.86	0.58
1:E:220:PRO:HB2	1:E:221:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:217:ARG:HG2	1:P:217:ARG:HH11	1.68	0.58
1:H:80:ILE:HD12	1:H:93:TRP:CZ3	2.38	0.58
1:O:404:GLU:O	1:O:408:THR:HG23	2.03	0.58
1:E:85:LEU:O	1:E:135:LEU:HD22	2.03	0.58
1:Q:150:LEU:O	1:Q:154:LYS:HB2	2.03	0.58
1:E:293:ALA:O	1:E:294:SER:HB3	2.02	0.58
1:H:270:TYR:HB3	1:H:370:PHE:CE2	2.38	0.58
1:Q:72:TRP:O	1:Q:76:LEU:HD13	2.04	0.57
1:C:358:LEU:O	1:C:359:ARG:CB	2.50	0.57
1:E:231:TYR:CE2	1:E:235:LEU:HD11	2.39	0.57
1:T:414:THR:C	1:T:416:LEU:H	2.08	0.57
1:S:71:LEU:O	1:S:75:VAL:HG23	2.04	0.57
1:I:366:SER:O	1:I:367:LYS:HB2	2.05	0.57
1:F:267:ASP:OD1	1:F:267:ASP:N	2.37	0.57
1:H:150:LEU:O	1:H:154:LYS:HB2	2.05	0.57
1:G:142:GLU:OE2	1:G:146:ARG:NH1	2.38	0.57
1:H:185:GLN:O	1:H:221:ARG:NH2	2.38	0.57
1:H:144:ILE:O	1:H:148:VAL:HG23	2.05	0.57
1:H:129:ASP:O	1:H:131:TRP:N	2.38	0.57
1:D:50:ILE:O	1:D:54:LEU:HD22	2.05	0.57
1:D:203:THR:O	1:D:206:PRO:HD2	2.04	0.57
1:R:7:VAL:HG13	1:R:53:ILE:HG21	1.87	0.57
1:P:424:LEU:O	1:P:427:SER:OG	2.20	0.57
1:G:76:LEU:HG	1:G:93:TRP:CZ3	2.39	0.57
1:M:401:TYR:CZ	1:M:412:ARG:CG	2.84	0.57
1:I:278:ARG:HD2	1:I:374:TYR:CZ	2.40	0.57
1:A:247:LEU:HD12	1:A:288:PHE:CD1	2.40	0.57
1:I:115:LEU:HD22	1:I:119:LEU:HD22	1.86	0.57
1:A:150:LEU:O	1:A:154:LYS:HB2	2.05	0.57
1:J:36:GLN:HA	1:J:36:GLN:HE21	1.70	0.57
1:K:205:ILE:HB	1:K:206:PRO:HD3	1.87	0.57
1:F:89:ALA:O	1:F:92:GLU:HB2	2.05	0.57
1:O:408:THR:O	1:O:408:THR:OG1	2.17	0.56
1:M:47:SER:O	1:M:51:ARG:HG3	2.05	0.56
1:A:269:LEU:HD22	1:A:273:PHE:CE1	2.39	0.56
1:H:293:ALA:O	1:H:294:SER:CB	2.53	0.56
1:M:150:LEU:O	1:M:154:LYS:HB2	2.04	0.56
1:P:187:PRO:O	1:P:191:SER:OG	2.23	0.56
1:S:115:LEU:HD22	1:S:119:LEU:HD22	1.85	0.56
1:Q:273:PHE:HB3	1:Q:357:PHE:CE2	2.40	0.56
1:E:180:VAL:O	1:E:184:ILE:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:77:LYS:HD3	1:Q:292:THR:HG22	1.87	0.56
1:Q:231:TYR:CE2	1:Q:235:LEU:HD11	2.41	0.56
1:G:86:ASP:HB3	1:G:135:LEU:CD2	2.36	0.56
1:R:408:THR:O	1:R:409:ASP:HB2	2.05	0.56
1:H:148:VAL:O	1:H:152:VAL:HG23	2.06	0.56
1:B:86:ASP:HB3	1:B:135:LEU:HD22	1.87	0.56
1:O:366:SER:O	1:O:367:LYS:HB2	2.05	0.56
1:A:53:ILE:O	1:A:57:ILE:HG13	2.05	0.56
1:H:107:GLN:HE22	1:H:170:GLN:NE2	2.04	0.56
1:J:415:ARG:O	1:J:419:ILE:HG23	2.05	0.56
1:I:87:ARG:NH1	1:I:142:GLU:OE1	2.38	0.56
1:O:366:SER:O	1:O:367:LYS:CB	2.53	0.56
1:K:152:VAL:HG13	1:K:203:THR:HG22	1.85	0.56
1:K:25:LEU:O	1:K:26:THR:C	2.43	0.56
1:M:208:LEU:HD12	1:M:246:LEU:CD1	2.35	0.56
1:D:180:VAL:O	1:D:184:ILE:HG23	2.05	0.56
1:K:357:PHE:HD2	1:K:358:LEU:HD23	1.71	0.56
1:F:151:TYR:HA	1:F:175:LEU:HD13	1.88	0.56
1:O:241:ASP:HA	1:O:299:VAL:HG13	1.87	0.56
1:N:286:SER:HB3	1:P:116:LYS:HZ3	1.71	0.56
1:G:215:ILE:HD11	1:G:253:PHE:CE2	2.41	0.56
1:O:185:GLN:O	1:O:221:ARG:NH2	2.38	0.55
1:P:83:LEU:HD23	1:P:83:LEU:N	2.20	0.55
1:S:404:GLU:CD	1:S:404:GLU:H	2.09	0.55
1:Q:154:LYS:HG2	1:Q:171:THR:HG21	1.88	0.55
1:C:217:ARG:HH11	1:C:217:ARG:HG2	1.72	0.55
1:S:148:VAL:HG21	1:S:193:CYS:HB3	1.88	0.55
1:A:164:SER:O	1:A:166:GLU:N	2.39	0.55
1:R:365:ALA:HB1	1:R:370:PHE:O	2.06	0.55
1:H:261:ILE:C	1:H:263:ASN:H	2.09	0.55
1:L:203:THR:O	1:L:206:PRO:HD2	2.05	0.55
1:P:64:ASN:N	1:P:64:ASN:OD1	2.38	0.55
1:S:282:ILE:HD12	1:S:288:PHE:CZ	2.42	0.55
1:K:32:VAL:HG13	1:K:82:LEU:HD21	1.87	0.55
1:R:295:GLY:O	1:T:26:THR:HG23	2.06	0.55
1:I:80:ILE:N	1:I:81:PRO:HD2	2.21	0.55
1:R:80:ILE:N	1:R:81:PRO:HD2	2.22	0.55
1:P:35:TYR:C	1:P:35:TYR:CD1	2.80	0.55
1:H:35:TYR:CD1	1:H:35:TYR:C	2.79	0.55
1:P:366:SER:O	1:P:367:LYS:CB	2.55	0.55
1:A:250:ALA:O	1:A:254:ILE:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:237:CYS:SG	1:O:246:LEU:HD21	2.47	0.55
1:M:280:SER:O	1:M:384:LYS:NZ	2.34	0.55
1:M:132:GLY:O	1:M:135:LEU:HB2	2.07	0.55
1:E:223:TYR:CE2	1:F:414:THR:HG21	2.42	0.55
1:N:127:ASP:HB3	1:N:130:GLU:HB2	1.88	0.55
1:P:201:PRO:HB2	1:P:202:PRO:HD3	1.88	0.55
1:A:203:THR:C	1:A:206:PRO:HD2	2.25	0.55
1:E:35:TYR:CD1	1:E:35:TYR:C	2.79	0.55
1:N:50:ILE:O	1:N:54:LEU:HD22	2.06	0.55
1:D:203:THR:C	1:D:206:PRO:HD2	2.27	0.55
1:T:174:CYS:O	1:T:178:VAL:HG23	2.06	0.55
1:A:66:THR:O	1:A:69:ARG:N	2.39	0.55
1:Q:250:ALA:O	1:Q:254:ILE:HG23	2.07	0.55
1:R:242:THR:HG21	1:T:110:PRO:HG3	1.89	0.55
1:H:8:LYS:HG2	1:H:12:ASN:HD21	1.72	0.55
1:O:199:LEU:O	1:O:201:PRO:HD3	2.06	0.55
1:J:430:ALA:O	1:J:431:VAL:HB	2.07	0.55
1:T:71:LEU:O	1:T:75:VAL:HG23	2.06	0.55
1:O:121:TYR:O	1:O:136:ARG:NH2	2.40	0.55
1:A:51:ARG:HH21	1:A:92:GLU:CD	2.11	0.55
1:M:185:GLN:HA	1:O:379:GLU:CG	2.32	0.54
1:R:278:ARG:HD2	1:R:374:TYR:CZ	2.41	0.54
1:N:283:ASP:C	1:N:283:ASP:OD1	2.45	0.54
1:I:189:GLU:OE1	1:I:189:GLU:N	2.39	0.54
1:T:366:SER:O	1:T:367:LYS:HB2	2.07	0.54
1:G:414:THR:HG21	1:H:223:TYR:CD2	2.42	0.54
1:L:152:VAL:HG13	1:L:203:THR:HG22	1.89	0.54
1:A:165:GLN:O	1:A:168:ARG:N	2.40	0.54
1:Q:261:ILE:HG22	1:Q:263:ASN:H	1.72	0.54
1:Q:366:SER:O	1:Q:367:LYS:HB2	2.06	0.54
1:G:35:TYR:CD1	1:G:35:TYR:C	2.79	0.54
1:I:417:ASP:O	1:I:421:VAL:HG23	2.06	0.54
1:S:69:ARG:NH1	1:S:104:SER:O	2.38	0.54
1:S:152:VAL:CG1	1:S:203:THR:HG22	2.37	0.54
1:N:1:MSE:HE2	1:N:4:GLN:HB2	1.89	0.54
1:H:107:GLN:HE22	1:H:170:GLN:HE22	1.53	0.54
1:F:269:LEU:HD11	1:F:350:TYR:CD1	2.41	0.54
1:M:282:ILE:HD12	1:M:288:PHE:CZ	2.43	0.54
1:L:151:TYR:HA	1:L:175:LEU:HD13	1.89	0.54
1:D:261:ILE:HG22	1:D:262:CYS:N	2.22	0.54
1:M:62:PRO:HG2	1:M:64:ASN:ND2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LEU:HD21	1:B:74:ALA:HB1	1.89	0.54
1:D:280:SER:O	1:D:281:MSE:HE2	2.08	0.54
1:T:405:THR:O	1:T:409:ASP:HB2	2.08	0.54
1:P:116:LYS:O	1:P:117:SER:C	2.46	0.54
1:S:47:SER:O	1:S:51:ARG:HG3	2.06	0.54
1:S:293:ALA:O	1:S:294:SER:HB3	2.08	0.54
1:N:379:GLU:HG3	1:P:185:GLN:HA	1.90	0.54
1:E:13:VAL:HG11	1:E:28:LEU:HD22	1.88	0.54
1:A:80:ILE:N	1:A:81:PRO:HD2	2.23	0.54
1:L:247:LEU:HD12	1:L:288:PHE:CE1	2.42	0.54
1:D:231:TYR:CZ	1:D:235:LEU:HD11	2.43	0.54
1:B:99:PHE:C	1:B:99:PHE:CD1	2.80	0.54
1:E:121:TYR:O	1:E:136:ARG:NH2	2.40	0.54
1:S:201:PRO:HB2	1:S:202:PRO:HD3	1.89	0.54
1:F:80:ILE:N	1:F:81:PRO:HD2	2.22	0.54
1:Q:430:ALA:HB3	1:R:391:ARG:O	2.07	0.54
1:G:250:ALA:O	1:G:254:ILE:HG23	2.08	0.54
1:P:121:TYR:O	1:P:136:ARG:NH2	2.41	0.54
1:M:6:LEU:O	1:M:9:ALA:HB3	2.08	0.54
1:N:217:ARG:HG2	1:N:217:ARG:HH11	1.73	0.54
1:N:53:ILE:O	1:N:57:ILE:HG13	2.07	0.54
1:S:208:LEU:O	1:S:209:SER:C	2.46	0.54
1:L:99:PHE:C	1:L:99:PHE:CD1	2.81	0.54
1:M:416:LEU:HG	1:N:420:ALA:HB1	1.90	0.54
1:S:180:VAL:HG12	1:S:181:HIS:N	2.22	0.54
1:D:65:ASN:ND2	1:D:68:ARG:HG3	2.22	0.54
1:J:201:PRO:HB2	1:J:202:PRO:HD3	1.89	0.54
1:P:86:ASP:HB3	1:P:135:LEU:HD22	1.90	0.54
1:K:349:LEU:O	1:K:412:ARG:NH1	2.39	0.54
1:H:208:LEU:O	1:H:211:MSE:N	2.40	0.53
1:G:356:GLU:HG3	1:G:359:ARG:NH2	2.23	0.53
1:B:250:ALA:O	1:B:254:ILE:HG23	2.07	0.53
1:S:129:ASP:O	1:S:131:TRP:N	2.42	0.53
1:M:191:SER:HB2	1:M:228:THR:HG21	1.91	0.53
1:N:80:ILE:N	1:N:81:PRO:HD2	2.21	0.53
1:C:71:LEU:O	1:C:75:VAL:HG23	2.08	0.53
1:S:267:ASP:N	1:S:267:ASP:OD1	2.41	0.53
1:M:85:LEU:O	1:M:135:LEU:HD22	2.07	0.53
1:E:116:LYS:O	1:E:117:SER:C	2.47	0.53
1:O:176:VAL:HG12	1:O:177:ASN:N	2.23	0.53
1:C:215:ILE:HD13	1:C:222:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:262:CYS:HA	1:G:265:LEU:HD12	1.91	0.53
1:I:242:THR:HG22	1:I:301:HIS:HA	1.90	0.53
1:R:28:LEU:O	1:R:32:VAL:HG23	2.07	0.53
1:N:241:ASP:HA	1:N:299:VAL:HG13	1.90	0.53
1:N:254:ILE:HD11	1:N:272:LEU:CD2	2.38	0.53
1:P:237:CYS:SG	1:P:246:LEU:HD21	2.49	0.53
1:F:107:GLN:O	1:F:108:LEU:HD23	2.08	0.53
1:I:349:LEU:O	1:I:412:ARG:NH1	2.38	0.53
1:S:402:THR:OG1	1:S:405:THR:HG23	2.08	0.53
1:L:204:ARG:CZ	1:L:297:TRP:CZ2	2.92	0.53
1:B:3:LEU:O	1:B:7:VAL:HG23	2.08	0.53
1:M:231:TYR:CZ	1:M:235:LEU:HD11	2.44	0.53
1:M:62:PRO:HG2	1:M:64:ASN:CG	2.28	0.53
1:J:89:ALA:O	1:J:93:TRP:CD1	2.61	0.53
1:R:293:ALA:CB	1:R:373:ARG:HE	2.20	0.53
1:C:299:VAL:O	1:C:304:MSE:HE1	2.09	0.53
1:D:32:VAL:HG13	1:D:82:LEU:HD11	1.90	0.53
1:O:1:MSE:HE1	1:O:8:LYS:NZ	2.23	0.53
1:H:47:SER:O	1:H:51:ARG:HG3	2.08	0.53
1:M:251:LEU:O	1:M:254:ILE:N	2.41	0.53
1:L:254:ILE:O	1:L:258:LEU:HB2	2.09	0.53
1:F:366:SER:O	1:F:367:LYS:HB2	2.07	0.53
1:F:115:LEU:HD22	1:F:119:LEU:HD22	1.89	0.53
1:Q:148:VAL:HG21	1:Q:193:CYS:SG	2.49	0.53
1:B:292:THR:HG22	1:D:77:LYS:HD3	1.91	0.53
1:M:401:TYR:CE1	1:M:412:ARG:HG3	2.41	0.53
1:P:404:GLU:O	1:P:408:THR:HG22	2.08	0.53
1:F:386:ASP:O	1:F:388:LEU:N	2.42	0.53
1:N:267:ASP:N	1:N:267:ASP:OD1	2.42	0.53
1:R:401:TYR:CE2	1:R:412:ARG:HG3	2.44	0.52
1:O:99:PHE:CE1	1:O:103:ASN:OD1	2.62	0.52
1:I:204:ARG:HB3	1:I:246:LEU:HD11	1.90	0.52
1:K:142:GLU:HG3	1:K:146:ARG:HD2	1.91	0.52
1:K:10:LEU:O	1:K:14:LEU:HD12	2.09	0.52
1:L:99:PHE:HB3	1:L:100:PRO:HD3	1.91	0.52
1:G:229:GLY:O	1:G:233:LEU:HD13	2.09	0.52
1:G:121:TYR:O	1:G:136:ARG:NH2	2.42	0.52
1:B:255:LEU:HD23	1:B:337:LEU:HB3	1.91	0.52
1:K:393:LEU:HB2	1:L:428:LEU:HD12	1.91	0.52
1:G:1:MSE:HE2	1:G:4:GLN:HB3	1.90	0.52
1:D:242:THR:HB	1:D:301:HIS:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD22	1:A:119:LEU:HD22	1.91	0.52
1:B:2:PRO:HG3	1:B:38:ARG:CD	2.39	0.52
1:A:242:THR:HG21	1:I:110:PRO:HG2	1.91	0.52
1:E:366:SER:O	1:E:367:LYS:CB	2.57	0.52
1:Q:76:LEU:O	1:Q:80:ILE:HG22	2.09	0.52
1:M:208:LEU:HD12	1:M:246:LEU:HD12	1.92	0.52
1:R:35:TYR:CE1	1:R:82:LEU:HG	2.44	0.52
1:H:145:THR:O	1:H:149:ASP:OD1	2.26	0.52
1:K:235:LEU:O	1:K:239:GLU:HG3	2.09	0.52
1:C:99:PHE:CD1	1:C:99:PHE:C	2.83	0.52
1:K:408:THR:O	1:K:409:ASP:CB	2.58	0.52
1:S:282:ILE:HD12	1:S:288:PHE:CE1	2.44	0.52
1:Q:65:ASN:ND2	1:Q:68:ARG:HG3	2.25	0.52
1:H:239:GLU:OE2	1:H:271:ARG:NH2	2.43	0.52
1:L:293:ALA:O	1:L:294:SER:CB	2.58	0.52
1:Q:201:PRO:HB2	1:Q:202:PRO:HD3	1.91	0.52
1:O:420:ALA:HB2	1:P:420:ALA:HB2	1.91	0.52
1:D:154:LYS:HG2	1:D:171:THR:HG21	1.90	0.52
1:L:99:PHE:HB3	1:L:100:PRO:CD	2.40	0.52
1:B:2:PRO:HG3	1:B:38:ARG:HD2	1.91	0.52
1:T:79:VAL:C	1:T:81:PRO:HD2	2.30	0.52
1:K:366:SER:O	1:K:367:LYS:HB2	2.09	0.52
1:E:278:ARG:HD2	1:E:374:TYR:CZ	2.44	0.52
1:Q:241:ASP:OD1	1:Q:297:TRP:NE1	2.32	0.52
1:T:53:ILE:O	1:T:57:ILE:HG13	2.10	0.52
1:L:379:GLU:HG2	1:N:185:GLN:HG2	1.90	0.52
1:K:180:VAL:HG13	1:K:214:VAL:CG2	2.38	0.52
1:Q:171:THR:HG22	1:Q:175:LEU:HD12	1.92	0.52
1:F:354:PHE:CZ	1:F:358:LEU:HD11	2.45	0.52
1:L:380:LEU:HB2	1:N:184:ILE:HD11	1.92	0.52
1:S:241:ASP:HA	1:S:299:VAL:HG13	1.92	0.52
1:Q:217:ARG:HH11	1:Q:217:ARG:HG2	1.74	0.52
1:R:292:THR:HG23	1:R:373:ARG:O	2.09	0.52
1:O:156:ILE:O	1:O:157:GLU:C	2.48	0.52
1:C:396:SER:O	1:C:398:PHE:N	2.43	0.52
1:B:150:LEU:HG	1:B:175:LEU:HD11	1.91	0.52
1:M:360:ASP:CG	1:M:363:LEU:HB2	2.30	0.52
1:J:141:GLU:O	1:J:145:THR:OG1	2.26	0.52
1:K:242:THR:HG21	1:S:110:PRO:HG3	1.91	0.52
1:H:349:LEU:O	1:H:412:ARG:NH1	2.34	0.51
1:C:299:VAL:HG11	1:C:301:HIS:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:409:ASP:OD1	1:Q:409:ASP:C	2.49	0.51
1:Q:345:ILE:HG13	1:Q:345:ILE:O	2.10	0.51
1:P:99:PHE:HB3	1:P:100:PRO:HD3	1.92	0.51
1:T:32:VAL:O	1:T:36:GLN:HG2	2.10	0.51
1:P:102:LEU:O	1:P:171:THR:HG23	2.10	0.51
1:O:47:SER:O	1:O:48:GLN:C	2.48	0.51
1:J:52:HIS:O	1:J:53:ILE:C	2.46	0.51
1:D:292:THR:HG22	1:F:77:LYS:HD3	1.92	0.51
1:A:10:LEU:O	1:A:14:LEU:HD12	2.09	0.51
1:J:83:LEU:HD23	1:J:83:LEU:N	2.24	0.51
1:C:366:SER:O	1:C:367:LYS:CB	2.58	0.51
1:D:277:LEU:O	1:D:277:LEU:HD23	2.10	0.51
1:K:357:PHE:CD2	1:K:358:LEU:HD23	2.45	0.51
1:R:32:VAL:HG13	1:R:82:LEU:HD21	1.91	0.51
1:I:247:LEU:HD12	1:I:288:PHE:CD1	2.45	0.51
1:M:13:VAL:HG13	1:M:14:LEU:HG	1.92	0.51
1:Q:130:GLU:OE1	1:Q:136:ARG:NH1	2.43	0.51
1:O:35:TYR:C	1:O:35:TYR:CD1	2.84	0.51
1:E:151:TYR:HA	1:E:175:LEU:HD13	1.93	0.51
1:R:292:THR:OG1	1:R:293:ALA:N	2.43	0.51
1:R:261:ILE:O	1:R:263:ASN:N	2.39	0.51
1:A:243:SER:O	1:A:244:PRO:C	2.47	0.51
1:C:401:TYR:CZ	1:C:412:ARG:HG3	2.46	0.51
1:A:297:TRP:O	1:A:298:GLU:CB	2.58	0.51
1:C:401:TYR:CE2	1:C:412:ARG:HG3	2.46	0.51
1:Q:43:ASN:HB3	1:Q:46:ASN:HB2	1.92	0.51
1:H:242:THR:CG2	1:H:242:THR:O	2.59	0.51
1:I:121:TYR:O	1:I:136:ARG:NH2	2.44	0.51
1:F:47:SER:O	1:F:51:ARG:HG3	2.11	0.51
1:N:366:SER:O	1:N:367:LYS:HB2	2.10	0.51
1:M:250:ALA:O	1:M:254:ILE:HG23	2.11	0.51
1:H:190:LEU:HD11	1:H:194:PHE:CE2	2.46	0.51
1:M:53:ILE:O	1:M:56:GLU:HB2	2.10	0.51
1:S:402:THR:H	1:S:405:THR:HG1	1.58	0.51
1:M:230:PHE:O	1:M:234:VAL:HG23	2.10	0.51
1:L:46:ASN:O	1:L:50:ILE:HG13	2.11	0.51
1:D:130:GLU:OE1	1:D:136:ARG:NH1	2.43	0.51
1:O:261:ILE:HG21	1:O:264:SER:HB2	1.93	0.51
1:O:291:SER:OG	1:O:292:THR:N	2.43	0.51
1:L:396:SER:C	1:L:398:PHE:N	2.64	0.51
1:I:131:TRP:CE3	1:I:136:ARG:HD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ILE:HB	1:B:206:PRO:HD3	1.93	0.51
1:L:261:ILE:O	1:L:263:ASN:N	2.43	0.51
1:N:406:GLU:O	1:N:412:ARG:NH2	2.42	0.51
1:G:107:GLN:CD	1:G:170:GLN:HE22	2.14	0.51
1:M:366:SER:O	1:M:367:LYS:HB2	2.10	0.51
1:Q:401:TYR:CZ	1:Q:412:ARG:HG3	2.46	0.51
1:J:51:ARG:NH2	1:J:92:GLU:OE2	2.37	0.51
1:S:144:ILE:O	1:S:148:VAL:HG23	2.10	0.51
1:C:401:TYR:OH	1:C:412:ARG:HG3	2.11	0.51
1:F:198:PHE:CE1	1:F:204:ARG:HG2	2.46	0.51
1:J:242:THR:O	1:J:244:PRO:HD3	2.09	0.51
1:F:210:VAL:O	1:F:214:VAL:HG23	2.10	0.51
1:C:297:TRP:O	1:C:298:GLU:HB3	2.11	0.50
1:Q:65:ASN:OD1	1:Q:66:THR:N	2.44	0.50
1:F:27:GLU:O	1:F:30:ALA:HB3	2.11	0.50
1:E:80:ILE:N	1:E:81:PRO:CD	2.74	0.50
1:F:152:VAL:HG13	1:F:203:THR:HG22	1.93	0.50
1:G:80:ILE:N	1:G:81:PRO:CD	2.74	0.50
1:N:203:THR:O	1:N:206:PRO:HD2	2.10	0.50
1:B:63:PHE:CE1	1:B:69:ARG:HA	2.46	0.50
1:M:1:MSE:HE2	1:M:4:GLN:HB2	1.93	0.50
1:S:65:ASN:ND2	1:S:68:ARG:HG3	2.26	0.50
1:P:247:LEU:HD12	1:P:288:PHE:CE1	2.45	0.50
1:R:366:SER:O	1:R:367:LYS:CB	2.58	0.50
1:F:1:MSE:HE2	1:F:4:GLN:HB2	1.92	0.50
1:A:292:THR:HG23	1:A:373:ARG:O	2.11	0.50
1:T:3:LEU:HD23	1:T:3:LEU:O	2.11	0.50
1:F:215:ILE:HD13	1:F:222:LEU:HD22	1.94	0.50
1:E:278:ARG:HD2	1:E:374:TYR:CE1	2.46	0.50
1:G:156:ILE:O	1:G:157:GLU:C	2.50	0.50
1:L:186:ARG:HB3	1:L:189:GLU:OE1	2.12	0.50
1:A:360:ASP:CG	1:A:363:LEU:HB2	2.32	0.50
1:A:396:SER:O	1:A:398:PHE:N	2.44	0.50
1:O:282:ILE:HD12	1:O:288:PHE:CZ	2.47	0.50
1:M:51:ARG:NH2	1:M:92:GLU:OE1	2.44	0.50
1:A:153:SER:O	1:A:157:GLU:HG2	2.12	0.50
1:N:269:LEU:HD22	1:N:273:PHE:CE1	2.47	0.50
1:G:278:ARG:HD2	1:G:374:TYR:CE1	2.47	0.50
1:B:291:SER:OG	1:B:292:THR:N	2.45	0.50
1:G:1:MSE:HE2	1:G:4:GLN:CB	2.41	0.50
1:A:327:GLY:O	1:A:328:SER:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:225:ILE:O	1:O:228:THR:OG1	2.22	0.50
1:F:144:ILE:O	1:F:148:VAL:HG23	2.12	0.50
1:K:80:ILE:N	1:K:81:PRO:HD2	2.27	0.50
1:A:401:TYR:CE2	1:A:412:ARG:HG3	2.47	0.50
1:H:379:GLU:HG3	1:J:185:GLN:HA	1.94	0.50
1:Q:80:ILE:N	1:Q:81:PRO:HD2	2.27	0.50
1:S:109:LYS:N	1:S:110:PRO:CD	2.75	0.50
1:A:243:SER:HB3	1:A:246:LEU:HB3	1.92	0.50
1:J:210:VAL:O	1:J:214:VAL:HG23	2.10	0.50
1:A:35:TYR:CD1	1:A:35:TYR:C	2.85	0.50
1:N:401:TYR:CZ	1:N:412:ARG:HG3	2.47	0.50
1:F:243:SER:HB3	1:F:246:LEU:HB3	1.93	0.50
1:O:215:ILE:CG2	1:O:256:MSE:HB3	2.41	0.50
1:E:205:ILE:HB	1:E:206:PRO:HD3	1.93	0.50
1:C:151:TYR:HB2	1:C:175:LEU:HD13	1.92	0.50
1:M:119:LEU:O	1:M:123:LEU:HD22	2.11	0.50
1:H:176:VAL:HG13	1:H:210:VAL:HG22	1.93	0.50
1:H:80:ILE:N	1:H:81:PRO:HD2	2.27	0.50
1:B:151:TYR:CA	1:B:175:LEU:HD13	2.42	0.50
1:H:300:PHE:CD1	1:H:301:HIS:O	2.64	0.50
1:A:71:LEU:O	1:A:75:VAL:HG23	2.12	0.50
1:Q:348:ALA:O	1:Q:349:LEU:HB2	2.12	0.50
1:A:293:ALA:O	1:A:294:SER:HB3	2.11	0.50
1:B:402:THR:OG1	1:B:404:GLU:HG2	2.11	0.49
1:S:119:LEU:O	1:S:123:LEU:HD22	2.12	0.49
1:Q:204:ARG:CZ	1:Q:297:TRP:CZ2	2.94	0.49
1:N:205:ILE:HB	1:N:206:PRO:HD3	1.94	0.49
1:K:151:TYR:HA	1:K:175:LEU:HD13	1.94	0.49
1:E:32:VAL:O	1:E:36:GLN:HG3	2.11	0.49
1:K:201:PRO:HB3	1:K:300:PHE:HB2	1.94	0.49
1:S:54:LEU:HD12	1:S:72:TRP:HZ3	1.76	0.49
1:F:205:ILE:HB	1:F:206:PRO:HD3	1.92	0.49
1:R:349:LEU:O	1:R:412:ARG:NH1	2.43	0.49
1:T:409:ASP:OD1	1:T:411:SER:OG	2.25	0.49
1:N:46:ASN:O	1:N:50:ILE:HG13	2.12	0.49
1:O:80:ILE:N	1:O:81:PRO:CD	2.74	0.49
1:N:131:TRP:O	1:N:135:LEU:HD12	2.11	0.49
1:G:76:LEU:HG	1:G:93:TRP:CH2	2.47	0.49
1:J:80:ILE:N	1:J:81:PRO:HD2	2.27	0.49
1:A:184:ILE:HD11	1:C:380:LEU:HB2	1.94	0.49
1:R:251:LEU:HD22	1:R:255:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:241:ASP:HA	1:K:299:VAL:HG13	1.93	0.49
1:H:14:LEU:HD13	1:H:57:ILE:HG21	1.93	0.49
1:K:71:LEU:O	1:K:75:VAL:HG23	2.12	0.49
1:A:1:MSE:HE2	1:A:4:GLN:HB2	1.93	0.49
1:O:217:ARG:HH11	1:O:217:ARG:HG2	1.75	0.49
1:C:297:TRP:O	1:C:298:GLU:CB	2.59	0.49
1:J:243:SER:HB3	1:J:246:LEU:HB3	1.93	0.49
1:L:273:PHE:HB3	1:L:357:PHE:CZ	2.47	0.49
1:G:243:SER:HB3	1:G:246:LEU:HB3	1.93	0.49
1:I:414:THR:HG21	1:J:223:TYR:CD2	2.47	0.49
1:K:204:ARG:HB3	1:K:246:LEU:HD11	1.94	0.49
1:J:3:LEU:O	1:J:3:LEU:HD23	2.12	0.49
1:T:269:LEU:HD22	1:T:273:PHE:CE1	2.46	0.49
1:B:148:VAL:HG21	1:B:193:CYS:CB	2.42	0.49
1:P:108:LEU:HB3	1:P:111:VAL:HG23	1.93	0.49
1:K:208:LEU:O	1:K:212:VAL:HG13	2.12	0.49
1:N:260:HIS:C	1:N:261:ILE:HG13	2.33	0.49
1:F:175:LEU:O	1:F:179:LEU:HD12	2.13	0.49
1:S:201:PRO:HB2	1:S:202:PRO:CD	2.41	0.49
1:K:366:SER:O	1:K:367:LYS:CB	2.60	0.49
1:C:110:PRO:HG3	1:E:242:THR:HG21	1.94	0.49
1:C:80:ILE:N	1:C:81:PRO:HD2	2.27	0.49
1:D:115:LEU:HD22	1:D:115:LEU:O	2.13	0.49
1:H:65:ASN:ND2	1:H:68:ARG:HG3	2.28	0.49
1:D:409:ASP:OD1	1:D:411:SER:OG	2.27	0.49
1:A:106:THR:HG22	1:A:108:LEU:HB2	1.95	0.49
1:L:1:MSE:HE2	1:L:4:GLN:CB	2.41	0.49
1:P:1:MSE:HG2	1:P:4:GLN:HG3	1.93	0.49
1:H:81:PRO:HA	1:H:121:TYR:CZ	2.47	0.49
1:O:289:PRO:HB3	1:O:374:TYR:HB3	1.94	0.49
1:G:1:MSE:N	1:G:2:PRO:HD3	2.27	0.49
1:E:29:ILE:HG22	1:E:33:GLU:OE2	2.13	0.49
1:T:91:GLY:O	1:T:95:ASP:OD2	2.31	0.49
1:L:235:LEU:O	1:L:239:GLU:HG3	2.13	0.49
1:S:289:PRO:HB2	1:S:374:TYR:HB3	1.94	0.49
1:R:64:ASN:OD1	1:R:68:ARG:NH1	2.44	0.49
1:S:7:VAL:HG13	1:S:53:ILE:HG21	1.94	0.49
1:D:366:SER:O	1:D:367:LYS:HB2	2.12	0.49
1:M:185:GLN:O	1:M:221:ARG:NH2	2.46	0.49
1:F:304:MSE:O	1:F:305:SER:CB	2.61	0.49
1:Q:161:ASP:HA	1:Q:164:SER:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:ALA:O	1:E:431:VAL:HB	2.12	0.49
1:P:99:PHE:CE1	1:P:103:ASN:HB2	2.47	0.49
1:F:299:VAL:O	1:F:304:MSE:HE1	2.13	0.49
1:P:241:ASP:O	1:P:278:ARG:NH2	2.41	0.49
1:T:190:LEU:HD11	1:T:194:PHE:CE2	2.48	0.49
1:C:347:TYR:O	1:C:351:PRO:HB3	2.12	0.49
1:R:225:ILE:HB	1:R:226:PRO:HD3	1.95	0.49
1:T:99:PHE:HB3	1:T:100:PRO:HD3	1.93	0.49
1:E:223:TYR:O	1:E:226:PRO:HD2	2.13	0.49
1:S:201:PRO:HB3	1:S:300:PHE:HB2	1.93	0.49
1:J:267:ASP:N	1:J:267:ASP:OD1	2.45	0.49
1:P:351:PRO:HG3	1:P:395:HIS:CE1	2.48	0.49
1:J:351:PRO:HD2	1:J:406:GLU:OE2	2.12	0.49
1:O:42:GLN:NE2	1:O:81:PRO:O	2.45	0.49
1:J:151:TYR:CE1	1:J:176:VAL:HG23	2.48	0.49
1:O:14:LEU:HA	1:O:71:LEU:HD21	1.94	0.49
1:T:62:PRO:HG2	1:T:64:ASN:ND2	2.28	0.49
1:A:276:TYR:HB2	1:A:342:LEU:HD23	1.95	0.49
1:S:205:ILE:HB	1:S:206:PRO:CD	2.42	0.49
1:M:406:GLU:O	1:M:412:ARG:NH2	2.44	0.48
1:R:408:THR:O	1:R:409:ASP:CB	2.60	0.48
1:J:53:ILE:O	1:J:57:ILE:HG13	2.13	0.48
1:D:343:PHE:CD1	1:D:343:PHE:C	2.87	0.48
1:J:241:ASP:HA	1:J:299:VAL:HG13	1.95	0.48
1:L:38:ARG:HD3	1:L:39:TYR:CZ	2.48	0.48
1:M:217:ARG:O	1:M:218:GLN:C	2.50	0.48
1:E:84:ILE:O	1:E:85:LEU:HD12	2.13	0.48
1:K:401:TYR:CZ	1:K:412:ARG:HG3	2.48	0.48
1:N:203:THR:C	1:N:206:PRO:HD2	2.33	0.48
1:N:297:TRP:O	1:N:298:GLU:CB	2.61	0.48
1:S:205:ILE:HG22	1:S:206:PRO:HD3	1.96	0.48
1:T:121:TYR:O	1:T:136:ARG:NH2	2.45	0.48
1:C:14:LEU:HD13	1:C:57:ILE:HG21	1.94	0.48
1:I:196:HIS:CD2	1:I:197:HIS:CD2	3.00	0.48
1:N:237:CYS:SG	1:N:246:LEU:HD11	2.53	0.48
1:C:158:ASN:O	1:C:159:LEU:CB	2.61	0.48
1:I:255:LEU:HD21	1:I:341:GLN:HB3	1.94	0.48
1:K:414:THR:HG21	1:L:223:TYR:CE2	2.48	0.48
1:T:414:THR:O	1:T:416:LEU:N	2.47	0.48
1:G:35:TYR:CE1	1:G:39:TYR:HB2	2.49	0.48
1:S:293:ALA:O	1:S:294:SER:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:209:SER:HA	1:H:249:TYR:CE1	2.49	0.48
1:J:129:ASP:O	1:J:132:GLY:N	2.43	0.48
1:M:409:ASP:OD1	1:M:411:SER:OG	2.21	0.48
1:S:151:TYR:CA	1:S:175:LEU:HD13	2.41	0.48
1:J:347:TYR:O	1:J:351:PRO:HB3	2.13	0.48
1:B:151:TYR:HA	1:B:175:LEU:HD13	1.96	0.48
1:N:352:ILE:HG21	1:N:403:ALA:HA	1.95	0.48
1:A:211:MSE:O	1:A:215:ILE:HG12	2.14	0.48
1:R:209:SER:HA	1:R:249:TYR:CE1	2.48	0.48
1:I:255:LEU:HD23	1:I:337:LEU:HB3	1.96	0.48
1:F:231:TYR:CZ	1:F:235:LEU:HD11	2.49	0.48
1:B:347:TYR:O	1:B:351:PRO:HB3	2.13	0.48
1:T:52:HIS:O	1:T:56:GLU:HG2	2.12	0.48
1:B:430:ALA:O	1:B:431:VAL:HB	2.13	0.48
1:N:99:PHE:HB3	1:N:100:PRO:CD	2.43	0.48
1:B:349:LEU:O	1:B:412:ARG:NH1	2.46	0.48
1:N:35:TYR:HE2	1:N:46:ASN:HD22	1.62	0.48
1:G:142:GLU:O	1:G:146:ARG:HG3	2.14	0.48
1:Q:410:LYS:C	1:Q:412:ARG:H	2.16	0.48
1:P:241:ASP:HA	1:P:299:VAL:HG13	1.95	0.48
1:O:63:PHE:CE1	1:O:69:ARG:HA	2.48	0.48
1:N:404:GLU:O	1:N:408:THR:HG22	2.14	0.48
1:P:63:PHE:CE2	1:P:69:ARG:HG2	2.49	0.48
1:S:366:SER:O	1:S:367:LYS:CB	2.61	0.48
1:H:269:LEU:HD22	1:H:273:PHE:CE1	2.49	0.48
1:B:293:ALA:HB3	1:B:373:ARG:HE	1.77	0.48
1:P:226:PRO:HG3	1:P:261:ILE:HD11	1.95	0.48
1:G:299:VAL:O	1:G:304:MSE:HE1	2.13	0.48
1:J:366:SER:O	1:J:367:LYS:CB	2.61	0.48
1:T:32:VAL:HG13	1:T:82:LEU:HD21	1.95	0.48
1:S:3:LEU:O	1:S:3:LEU:HD23	2.14	0.48
1:C:267:ASP:OD1	1:C:267:ASP:N	2.47	0.48
1:H:292:THR:HG22	1:J:77:LYS:HE2	1.95	0.48
1:P:80:ILE:N	1:P:81:PRO:CD	2.77	0.48
1:J:353:ASN:HD21	1:J:407:LEU:HG	1.78	0.48
1:F:121:TYR:O	1:F:136:ARG:NH2	2.46	0.48
1:P:430:ALA:O	1:P:431:VAL:CB	2.62	0.48
1:L:396:SER:O	1:L:397:ASN:C	2.52	0.48
1:Q:79:VAL:C	1:Q:81:PRO:HD2	2.34	0.48
1:A:67:ARG:HA	1:A:70:ILE:HD12	1.96	0.48
1:E:113:SER:O	1:E:117:SER:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:99:PHE:N	1:P:100:PRO:CD	2.77	0.48
1:G:79:VAL:C	1:G:81:PRO:HD2	2.34	0.48
1:S:54:LEU:HD12	1:S:72:TRP:CZ3	2.49	0.48
1:L:341:GLN:O	1:L:345:ILE:HG22	2.14	0.48
1:C:121:TYR:O	1:C:136:ARG:NH2	2.45	0.48
1:A:185:GLN:HA	1:C:379:GLU:HG3	1.96	0.48
1:K:243:SER:OG	1:K:302:ASP:CG	2.52	0.48
1:G:115:LEU:HD22	1:G:119:LEU:CD2	2.31	0.48
1:K:152:VAL:CG1	1:K:203:THR:HG22	2.43	0.48
1:S:247:LEU:HD12	1:S:288:PHE:CE1	2.49	0.48
1:A:66:THR:OG1	1:A:67:ARG:N	2.47	0.48
1:T:80:ILE:N	1:T:81:PRO:HD2	2.29	0.48
1:K:62:PRO:HG2	1:K:64:ASN:ND2	2.29	0.48
1:F:231:TYR:O	1:F:234:VAL:N	2.46	0.47
1:E:402:THR:O	1:E:403:ALA:C	2.51	0.47
1:P:251:LEU:HD13	1:P:255:LEU:HD22	1.95	0.47
1:H:223:TYR:O	1:H:226:PRO:HD2	2.14	0.47
1:N:299:VAL:HG11	1:N:301:HIS:CE1	2.49	0.47
1:E:150:LEU:HG	1:E:175:LEU:HD11	1.96	0.47
1:M:77:LYS:HD3	1:O:292:THR:HG22	1.95	0.47
1:T:194:PHE:CD1	1:T:207:ILE:HG12	2.49	0.47
1:H:408:THR:O	1:H:409:ASP:CB	2.61	0.47
1:B:166:GLU:O	1:B:170:GLN:HG3	2.14	0.47
1:M:110:PRO:HG3	1:O:242:THR:HG21	1.95	0.47
1:M:99:PHE:O	1:M:103:ASN:HB2	2.14	0.47
1:H:401:TYR:OH	1:H:412:ARG:HG3	2.14	0.47
1:I:348:ALA:O	1:I:349:LEU:HB2	2.13	0.47
1:B:57:ILE:O	1:B:57:ILE:HG22	2.14	0.47
1:C:64:ASN:OD1	1:C:68:ARG:NH1	2.47	0.47
1:J:66:THR:O	1:J:70:ILE:HD12	2.14	0.47
1:D:84:ILE:HG23	1:D:131:TRP:HB3	1.96	0.47
1:O:3:LEU:O	1:O:3:LEU:HD23	2.13	0.47
1:D:283:ASP:OD1	1:D:284:PRO:N	2.48	0.47
1:O:14:LEU:HD13	1:O:57:ILE:HD13	1.96	0.47
1:A:273:PHE:HE1	1:A:346:LEU:HD22	1.79	0.47
1:L:204:ARG:HB3	1:L:246:LEU:HD11	1.95	0.47
1:P:261:ILE:O	1:P:263:ASN:N	2.47	0.47
1:K:265:LEU:O	1:K:269:LEU:HB2	2.15	0.47
1:P:297:TRP:O	1:P:298:GLU:CB	2.62	0.47
1:M:248:SER:O	1:M:252:SER:OG	2.33	0.47
1:N:72:TRP:O	1:N:76:LEU:HD22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:PHE:O	1:F:234:VAL:HG23	2.14	0.47
1:C:293:ALA:O	1:C:294:SER:HB3	2.15	0.47
1:C:74:ALA:O	1:C:78:THR:HG23	2.14	0.47
1:A:285:THR:HG21	1:I:173:GLU:HG2	1.97	0.47
1:E:90:VAL:HG11	1:E:139:CYS:HB3	1.96	0.47
1:M:35:TYR:CD1	1:M:35:TYR:C	2.87	0.47
1:B:380:LEU:HB2	1:D:184:ILE:HD11	1.96	0.47
1:F:269:LEU:HD22	1:F:273:PHE:CZ	2.49	0.47
1:S:366:SER:O	1:S:367:LYS:HB2	2.14	0.47
1:J:221:ARG:HD2	1:J:224:GLU:OE2	2.14	0.47
1:D:277:LEU:CD2	1:D:277:LEU:C	2.83	0.47
1:L:299:VAL:CG1	1:L:300:PHE:N	2.76	0.47
1:S:148:VAL:HG21	1:S:193:CYS:CB	2.45	0.47
1:M:234:VAL:HG21	1:M:253:PHE:CE1	2.49	0.47
1:M:217:ARG:O	1:M:219:GLY:N	2.47	0.47
1:M:210:VAL:O	1:M:214:VAL:HG23	2.14	0.47
1:A:6:LEU:O	1:A:6:LEU:HD23	2.14	0.47
1:O:96:GLN:O	1:O:97:ILE:HD13	2.15	0.47
1:E:62:PRO:HG2	1:E:64:ASN:OD1	2.15	0.47
1:N:194:PHE:CE1	1:N:207:ILE:HG12	2.50	0.47
1:M:54:LEU:HD12	1:M:72:TRP:CZ3	2.49	0.47
1:M:96:GLN:O	1:M:100:PRO:HG2	2.14	0.47
1:I:262:CYS:HA	1:I:265:LEU:HB2	1.97	0.47
1:S:35:TYR:CD1	1:S:35:TYR:C	2.87	0.47
1:C:3:LEU:HD23	1:C:3:LEU:O	2.15	0.47
1:Q:408:THR:O	1:Q:408:THR:HG23	2.15	0.47
1:H:261:ILE:O	1:H:263:ASN:N	2.47	0.47
1:D:242:THR:HG22	1:D:243:SER:N	2.30	0.47
1:B:150:LEU:O	1:B:154:LYS:HB2	2.14	0.47
1:F:241:ASP:HA	1:F:299:VAL:HG13	1.97	0.47
1:I:99:PHE:CD1	1:I:99:PHE:C	2.87	0.47
1:F:341:GLN:O	1:F:345:ILE:HG22	2.15	0.47
1:R:151:TYR:HA	1:R:175:LEU:HD13	1.96	0.47
1:J:401:TYR:CE2	1:J:412:ARG:HG3	2.50	0.47
1:G:32:VAL:O	1:G:33:GLU:C	2.53	0.47
1:Q:405:THR:O	1:Q:409:ASP:HB3	2.15	0.47
1:G:238:ALA:HA	1:G:247:LEU:CD2	2.44	0.47
1:I:408:THR:O	1:I:409:ASP:HB2	2.15	0.47
1:L:382:SER:O	1:L:383:THR:C	2.53	0.47
1:E:418:SER:OG	1:F:259:SER:HB2	2.15	0.47
1:C:185:GLN:HA	1:E:379:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:GLU:N	1:H:189:GLU:OE1	2.38	0.47
1:A:366:SER:O	1:A:367:LYS:CB	2.62	0.47
1:A:247:LEU:O	1:A:250:ALA:HB3	2.14	0.47
1:Q:297:TRP:O	1:Q:298:GLU:HB3	2.15	0.47
1:M:366:SER:O	1:M:368:HIS:N	2.46	0.47
1:N:204:ARG:CZ	1:N:297:TRP:CZ2	2.98	0.47
1:H:71:LEU:O	1:H:75:VAL:HG23	2.15	0.47
1:K:191:SER:HB3	1:K:211:MSE:HE2	1.97	0.47
1:C:90:VAL:CG2	1:C:142:GLU:HG2	2.45	0.47
1:D:80:ILE:CG2	1:D:81:PRO:HD3	2.45	0.47
1:L:110:PRO:HG3	1:T:242:THR:CG2	2.45	0.47
1:E:144:ILE:O	1:E:148:VAL:HG23	2.15	0.47
1:Q:420:ALA:HB2	1:R:420:ALA:HB2	1.96	0.47
1:Q:366:SER:C	1:Q:368:HIS:H	2.19	0.46
1:N:80:ILE:HG23	1:N:81:PRO:HD3	1.97	0.46
1:R:261:ILE:C	1:R:263:ASN:H	2.18	0.46
1:C:382:SER:O	1:C:383:THR:C	2.52	0.46
1:N:58:TYR:HA	1:N:61:THR:O	2.14	0.46
1:Q:232:ASP:OD1	1:Q:271:ARG:NH2	2.48	0.46
1:D:61:THR:OG1	1:D:61:THR:O	2.31	0.46
1:L:250:ALA:O	1:L:254:ILE:HG23	2.15	0.46
1:Q:14:LEU:HD13	1:Q:57:ILE:HG21	1.96	0.46
1:J:231:TYR:CE2	1:J:235:LEU:HD11	2.50	0.46
1:L:220:PRO:HB2	1:L:221:ARG:HG3	1.97	0.46
1:O:50:ILE:O	1:O:54:LEU:HD22	2.16	0.46
1:G:204:ARG:NH2	1:G:297:TRP:CZ2	2.83	0.46
1:O:99:PHE:CD1	1:O:99:PHE:C	2.89	0.46
1:B:151:TYR:HB2	1:B:175:LEU:HD13	1.97	0.46
1:L:110:PRO:HG3	1:T:242:THR:HG21	1.98	0.46
1:T:104:SER:OG	1:T:104:SER:O	2.33	0.46
1:L:209:SER:HA	1:L:249:TYR:CE1	2.50	0.46
1:I:70:ILE:HG12	1:I:111:VAL:CG2	2.46	0.46
1:M:76:LEU:HA	1:M:79:VAL:HG22	1.98	0.46
1:R:65:ASN:OD1	1:R:65:ASN:C	2.54	0.46
1:A:130:GLU:OE1	1:A:136:ARG:NH1	2.48	0.46
1:H:235:LEU:O	1:H:239:GLU:HG3	2.15	0.46
1:K:148:VAL:O	1:K:152:VAL:HG23	2.15	0.46
1:F:79:VAL:C	1:F:81:PRO:HD2	2.35	0.46
1:H:408:THR:O	1:H:409:ASP:HB2	2.15	0.46
1:A:54:LEU:HD12	1:A:72:TRP:HZ3	1.80	0.46
1:T:238:ALA:O	1:T:278:ARG:NH1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:PRO:O	1:E:191:SER:OG	2.34	0.46
1:J:251:LEU:HG	1:J:279:PHE:CE2	2.50	0.46
1:D:101:PHE:O	1:D:105:PRO:HA	2.15	0.46
1:D:283:ASP:C	1:D:283:ASP:OD1	2.53	0.46
1:I:366:SER:O	1:I:367:LYS:CB	2.62	0.46
1:S:201:PRO:O	1:S:202:PRO:C	2.52	0.46
1:S:241:ASP:HA	1:S:299:VAL:CG1	2.46	0.46
1:I:84:ILE:O	1:I:85:LEU:HD12	2.15	0.46
1:N:152:VAL:HG21	1:N:197:HIS:ND1	2.30	0.46
1:C:150:LEU:O	1:C:154:LYS:HB2	2.15	0.46
1:T:65:ASN:OD1	1:T:65:ASN:C	2.54	0.46
1:K:163:GLU:O	1:K:164:SER:OG	2.32	0.46
1:A:110:PRO:HG3	1:C:242:THR:HG21	1.97	0.46
1:M:364:TYR:O	1:M:366:SER:O	2.34	0.46
1:L:5:SER:HA	1:L:8:LYS:HE2	1.98	0.46
1:D:225:ILE:HB	1:D:226:PRO:HD3	1.97	0.46
1:J:230:PHE:O	1:J:234:VAL:HG23	2.16	0.46
1:T:6:LEU:O	1:T:9:ALA:HB3	2.16	0.46
1:A:189:GLU:OE1	1:A:189:GLU:N	2.46	0.46
1:S:221:ARG:HB3	1:S:223:TYR:CZ	2.50	0.46
1:H:270:TYR:HB3	1:H:370:PHE:CD2	2.50	0.46
1:A:152:VAL:HG13	1:A:203:THR:HG22	1.96	0.46
1:A:10:LEU:O	1:A:13:VAL:HG12	2.16	0.46
1:K:149:ASP:OD1	1:K:197:HIS:NE2	2.49	0.46
1:M:152:VAL:HG13	1:M:203:THR:HG22	1.98	0.46
1:F:131:TRP:O	1:F:135:LEU:HD12	2.16	0.46
1:T:366:SER:O	1:T:367:LYS:CB	2.63	0.46
1:F:198:PHE:CD1	1:F:204:ARG:HG2	2.50	0.46
1:G:278:ARG:HD2	1:G:374:TYR:CZ	2.50	0.46
1:K:190:LEU:HD23	1:K:211:MSE:SE	2.65	0.46
1:J:99:PHE:C	1:J:99:PHE:CD1	2.89	0.46
1:B:234:VAL:HG11	1:B:253:PHE:CD1	2.51	0.46
1:P:184:ILE:HA	1:P:214:VAL:HG13	1.98	0.46
1:S:297:TRP:O	1:S:298:GLU:HB3	2.15	0.46
1:M:221:ARG:HB3	1:M:223:TYR:CE2	2.51	0.46
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.98	0.46
1:H:300:PHE:CE1	1:H:301:HIS:O	2.69	0.46
1:K:200:ASN:HA	1:K:201:PRO:HD3	1.82	0.46
1:E:140:ALA:O	1:E:144:ILE:HG22	2.16	0.46
1:R:217:ARG:HH11	1:R:217:ARG:HG2	1.81	0.46
1:O:348:ALA:O	1:O:349:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:GLU:OE1	1:G:189:GLU:N	2.49	0.46
1:O:260:HIS:C	1:O:261:ILE:HG13	2.36	0.46
1:K:150:LEU:HG	1:K:175:LEU:HD11	1.99	0.46
1:K:204:ARG:CZ	1:K:297:TRP:CZ2	2.99	0.46
1:H:409:ASP:OD1	1:H:411:SER:OG	2.33	0.46
1:A:77:LYS:HD3	1:C:292:THR:HG22	1.98	0.46
1:I:201:PRO:O	1:I:202:PRO:C	2.54	0.46
1:E:271:ARG:O	1:E:275:ILE:HG13	2.16	0.46
1:B:221:ARG:HB3	1:B:223:TYR:CE2	2.51	0.46
1:G:348:ALA:O	1:G:349:LEU:HB2	2.16	0.46
1:K:294:SER:O	1:K:295:GLY:C	2.55	0.46
1:J:266:ASP:OD2	1:J:410:LYS:NZ	2.49	0.46
1:K:84:ILE:HG23	1:K:131:TRP:HB3	1.98	0.46
1:A:99:PHE:N	1:A:100:PRO:HD2	2.31	0.46
1:P:29:ILE:O	1:P:33:GLU:HG3	2.16	0.46
1:I:1:MSE:HG2	1:I:4:GLN:OE1	2.16	0.45
1:G:215:ILE:O	1:G:216:ARG:C	2.55	0.45
1:J:14:LEU:HD13	1:J:57:ILE:HG21	1.98	0.45
1:Q:348:ALA:O	1:Q:349:LEU:CB	2.64	0.45
1:I:414:THR:O	1:I:416:LEU:N	2.49	0.45
1:I:363:LEU:O	1:I:363:LEU:HD23	2.16	0.45
1:D:107:GLN:O	1:D:108:LEU:HD23	2.16	0.45
1:B:363:LEU:CD2	1:B:367:LYS:HD3	2.46	0.45
1:L:181:HIS:O	1:L:185:GLN:HG3	2.16	0.45
1:O:215:ILE:HG22	1:O:256:MSE:HB3	1.99	0.45
1:K:297:TRP:O	1:K:298:GLU:CB	2.64	0.45
1:D:80:ILE:HG22	1:D:81:PRO:HD3	1.98	0.45
1:G:223:TYR:CD2	1:H:414:THR:HG21	2.51	0.45
1:H:353:ASN:OD1	1:H:407:LEU:HD11	2.17	0.45
1:E:185:GLN:HA	1:G:379:GLU:HG3	1.98	0.45
1:S:268:SER:O	1:S:269:LEU:C	2.55	0.45
1:Q:94:TRP:CD1	1:Q:146:ARG:NE	2.84	0.45
1:J:268:SER:O	1:J:271:ARG:N	2.49	0.45
1:E:132:GLY:O	1:E:135:LEU:HD12	2.17	0.45
1:E:223:TYR:CD2	1:F:414:THR:HG21	2.51	0.45
1:Q:201:PRO:HB3	1:Q:300:PHE:HB2	1.98	0.45
1:I:42:GLN:NE2	1:I:131:TRP:HE1	2.13	0.45
1:L:231:TYR:CZ	1:L:235:LEU:HD11	2.51	0.45
1:E:137:ARG:HB2	1:E:137:ARG:CZ	2.46	0.45
1:Q:351:PRO:O	1:Q:352:ILE:C	2.53	0.45
1:G:220:PRO:HB2	1:G:221:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1:MSE:HG2	1:Q:4:GLN:HB2	1.98	0.45
1:H:297:TRP:O	1:H:298:GLU:CB	2.65	0.45
1:R:401:TYR:CZ	1:R:412:ARG:CG	2.92	0.45
1:E:67:ARG:O	1:E:71:LEU:HB2	2.17	0.45
1:T:401:TYR:OH	1:T:412:ARG:HG3	2.17	0.45
1:B:150:LEU:HD11	1:B:154:LYS:HE3	1.98	0.45
1:G:107:GLN:NE2	1:G:170:GLN:HE22	2.15	0.45
1:S:65:ASN:OD1	1:S:67:ARG:N	2.50	0.45
1:A:176:VAL:O	1:A:180:VAL:HG23	2.17	0.45
1:E:109:LYS:N	1:E:110:PRO:CD	2.80	0.45
1:L:351:PRO:HG3	1:L:395:HIS:CE1	2.52	0.45
1:A:199:LEU:O	1:A:201:PRO:HD3	2.15	0.45
1:O:268:SER:O	1:O:272:LEU:HG	2.16	0.45
1:N:201:PRO:HB2	1:N:202:PRO:HD3	1.99	0.45
1:H:99:PHE:CD1	1:H:99:PHE:C	2.89	0.45
1:I:278:ARG:HD2	1:I:374:TYR:CE1	2.52	0.45
1:C:358:LEU:O	1:C:359:ARG:HB3	2.15	0.45
1:Q:261:ILE:HG21	1:Q:264:SER:HB2	1.99	0.45
1:P:351:PRO:HG3	1:P:395:HIS:ND1	2.32	0.45
1:I:283:ASP:HA	1:I:284:PRO:HD3	1.75	0.45
1:H:354:PHE:CE1	1:H:358:LEU:HD11	2.52	0.45
1:O:352:ILE:HG12	1:O:398:PHE:CE1	2.51	0.45
1:T:266:ASP:N	1:T:266:ASP:OD1	2.49	0.45
1:O:237:CYS:HG	1:O:246:LEU:HD21	1.81	0.45
1:L:281:MSE:HE1	1:L:380:LEU:HG	1.96	0.45
1:E:14:LEU:HD13	1:E:57:ILE:HG21	1.97	0.45
1:N:109:LYS:N	1:N:110:PRO:CD	2.80	0.45
1:O:409:ASP:C	1:O:409:ASP:OD1	2.54	0.45
1:N:366:SER:O	1:N:367:LYS:CB	2.65	0.45
1:N:99:PHE:HB3	1:N:100:PRO:HD3	1.97	0.45
1:B:80:ILE:N	1:B:81:PRO:CD	2.80	0.45
1:D:6:LEU:HD23	1:D:10:LEU:HD13	1.99	0.45
1:D:99:PHE:HB3	1:D:100:PRO:HD3	1.99	0.45
1:J:204:ARG:CZ	1:J:297:TRP:CZ2	3.00	0.45
1:I:404:GLU:O	1:I:407:LEU:N	2.50	0.45
1:D:71:LEU:O	1:D:72:TRP:C	2.55	0.45
1:A:350:TYR:N	1:A:351:PRO:CD	2.79	0.45
1:P:32:VAL:HG13	1:P:82:LEU:HD21	1.98	0.45
1:C:245:ILE:O	1:C:249:TYR:HD2	2.00	0.45
1:Q:141:GLU:O	1:Q:145:THR:OG1	2.29	0.45
1:J:342:LEU:HA	1:J:345:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:343:PHE:C	1:I:343:PHE:CD1	2.90	0.45
1:H:176:VAL:HG12	1:H:180:VAL:HG23	1.98	0.45
1:N:238:ALA:O	1:N:278:ARG:NH1	2.49	0.45
1:B:99:PHE:HB3	1:B:100:PRO:HD3	1.99	0.45
1:C:102:LEU:HD13	1:C:175:LEU:HD21	1.99	0.45
1:I:251:LEU:HD22	1:I:255:LEU:HD22	1.98	0.45
1:B:80:ILE:N	1:B:81:PRO:HD2	2.32	0.45
1:F:268:SER:O	1:F:271:ARG:N	2.49	0.45
1:I:347:TYR:O	1:I:351:PRO:HB3	2.17	0.45
1:L:247:LEU:CD1	1:L:288:PHE:CD1	3.00	0.45
1:R:247:LEU:HD12	1:R:288:PHE:CD1	2.52	0.45
1:E:80:ILE:N	1:E:81:PRO:HD2	2.32	0.45
1:K:151:TYR:CA	1:K:175:LEU:HD13	2.46	0.45
1:K:151:TYR:HA	1:K:175:LEU:CD1	2.47	0.45
1:H:268:SER:O	1:H:269:LEU:C	2.56	0.45
1:L:345:ILE:O	1:L:345:ILE:CG1	2.65	0.45
1:M:263:ASN:C	1:M:265:LEU:H	2.20	0.45
1:B:242:THR:HB	1:B:301:HIS:HA	1.97	0.45
1:H:11:TRP:O	1:H:15:HIS:ND1	2.47	0.45
1:L:210:VAL:O	1:L:211:MSE:C	2.54	0.45
1:I:176:VAL:O	1:I:180:VAL:HG23	2.16	0.45
1:S:213:GLU:OE1	1:S:216:ARG:HD2	2.17	0.45
1:G:177:ASN:C	1:G:177:ASN:OD1	2.54	0.45
1:A:242:THR:HB	1:A:301:HIS:HA	1.99	0.45
1:B:25:LEU:O	1:B:26:THR:C	2.56	0.45
1:A:97:ILE:CA	1:A:100:PRO:HG2	2.47	0.45
1:L:187:PRO:O	1:L:188:LYS:C	2.54	0.45
1:H:286:SER:HB3	1:J:116:LYS:HZ3	1.82	0.45
1:P:84:ILE:C	1:P:85:LEU:HD12	2.36	0.45
1:J:84:ILE:HG23	1:J:131:TRP:HB3	1.99	0.45
1:B:261:ILE:HG21	1:B:264:SER:HB2	1.99	0.45
1:Q:99:PHE:CZ	1:Q:103:ASN:OD1	2.70	0.45
1:L:65:ASN:OD1	1:L:65:ASN:C	2.54	0.45
1:T:76:LEU:HG	1:T:93:TRP:CZ3	2.52	0.45
1:A:205:ILE:O	1:A:209:SER:HB2	2.16	0.44
1:A:293:ALA:O	1:A:294:SER:CB	2.65	0.44
1:L:348:ALA:O	1:L:349:LEU:CB	2.64	0.44
1:P:292:THR:OG1	1:P:293:ALA:N	2.50	0.44
1:H:402:THR:H	1:H:405:THR:HG1	1.63	0.44
1:E:269:LEU:HD22	1:E:273:PHE:CE1	2.51	0.44
1:N:176:VAL:HG12	1:N:177:ASN:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:10:LEU:HD13	1:O:28:LEU:HD13	1.99	0.44
1:L:184:ILE:HD11	1:T:380:LEU:HB2	1.98	0.44
1:Q:266:ASP:OD1	1:Q:266:ASP:N	2.50	0.44
1:E:401:TYR:CE1	1:E:412:ARG:HG3	2.52	0.44
1:O:363:LEU:CD2	1:O:367:LYS:HD2	2.47	0.44
1:N:401:TYR:CE2	1:N:412:ARG:HG3	2.53	0.44
1:B:223:TYR:O	1:B:226:PRO:HD2	2.17	0.44
1:A:176:VAL:O	1:A:177:ASN:C	2.55	0.44
1:K:172:ILE:HG13	1:K:173:GLU:N	2.31	0.44
1:F:251:LEU:HD22	1:F:255:LEU:HD22	1.99	0.44
1:C:236:LYS:O	1:C:237:CYS:C	2.56	0.44
1:P:422:VAL:O	1:P:426:ASN:ND2	2.50	0.44
1:O:377:ASN:HB3	1:O:380:LEU:HB3	1.98	0.44
1:A:278:ARG:HD2	1:A:374:TYR:CZ	2.51	0.44
1:E:243:SER:HB3	1:E:246:LEU:HB3	1.99	0.44
1:E:294:SER:O	1:E:295:GLY:C	2.54	0.44
1:S:140:ALA:O	1:S:144:ILE:HG22	2.16	0.44
1:Q:204:ARG:NH2	1:Q:297:TRP:CZ2	2.85	0.44
1:G:348:ALA:O	1:G:349:LEU:CB	2.65	0.44
1:B:185:GLN:HA	1:J:379:GLU:HG3	1.99	0.44
1:A:261:ILE:O	1:A:263:ASN:N	2.50	0.44
1:T:261:ILE:HG21	1:T:264:SER:HB2	1.99	0.44
1:M:108:LEU:HB2	1:M:111:VAL:HG23	1.98	0.44
1:G:63:PHE:CE1	1:G:69:ARG:HG2	2.53	0.44
1:H:51:ARG:NH2	1:H:92:GLU:OE2	2.50	0.44
1:P:215:ILE:CD1	1:P:222:LEU:HD22	2.46	0.44
1:G:297:TRP:O	1:G:298:GLU:CB	2.64	0.44
1:Q:99:PHE:HB3	1:Q:100:PRO:CD	2.47	0.44
1:R:264:SER:O	1:R:268:SER:OG	2.23	0.44
1:S:251:LEU:HD22	1:S:255:LEU:HD13	1.99	0.44
1:I:47:SER:O	1:I:49:LYS:N	2.50	0.44
1:M:102:LEU:O	1:M:171:THR:HG23	2.17	0.44
1:G:276:TYR:HE2	1:G:358:LEU:HD21	1.82	0.44
1:C:255:LEU:HA	1:C:255:LEU:HD12	1.84	0.44
1:C:27:GLU:O	1:C:30:ALA:HB3	2.18	0.44
1:L:80:ILE:N	1:L:81:PRO:HD2	2.32	0.44
1:O:251:LEU:HD13	1:O:255:LEU:CD2	2.47	0.44
1:Q:366:SER:O	1:Q:367:LYS:CB	2.66	0.44
1:N:251:LEU:O	1:N:254:ILE:N	2.51	0.44
1:S:205:ILE:CB	1:S:206:PRO:CD	2.95	0.44
1:M:217:ARG:HA	1:M:217:ARG:HD3	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:109:LYS:N	1:L:110:PRO:CD	2.81	0.44
1:F:99:PHE:HB3	1:F:100:PRO:CD	2.48	0.44
1:A:357:PHE:CE1	1:A:361:PRO:HB3	2.52	0.44
1:T:171:THR:HG22	1:T:175:LEU:HD12	1.99	0.44
1:O:293:ALA:O	1:O:294:SER:CB	2.65	0.44
1:D:379:GLU:HG3	1:F:185:GLN:HA	1.98	0.44
1:E:152:VAL:HG12	1:E:156:ILE:HD11	2.00	0.44
1:T:181:HIS:O	1:T:185:GLN:HG3	2.18	0.44
1:J:203:THR:O	1:J:206:PRO:HD2	2.17	0.44
1:K:25:LEU:N	1:K:25:LEU:HD12	2.33	0.44
1:A:247:LEU:HD13	1:A:288:PHE:CE2	2.53	0.44
1:D:241:ASP:O	1:D:247:LEU:HD11	2.18	0.44
1:D:135:LEU:O	1:D:136:ARG:C	2.54	0.44
1:T:3:LEU:HD12	1:T:46:ASN:ND2	2.32	0.44
1:A:1:MSE:O	1:A:1:MSE:HG2	2.17	0.44
1:T:261:ILE:CG2	1:T:264:SER:HB2	2.48	0.44
1:O:200:ASN:OD1	1:O:202:PRO:HD2	2.18	0.44
1:S:76:LEU:O	1:S:80:ILE:HG22	2.18	0.44
1:F:294:SER:O	1:F:295:GLY:C	2.56	0.44
1:G:117:SER:OG	1:I:375:SER:HB2	2.18	0.44
1:B:383:THR:HG22	1:B:384:LYS:N	2.32	0.44
1:J:35:TYR:CD1	1:J:35:TYR:C	2.91	0.44
1:R:154:LYS:O	1:R:168:ARG:HD2	2.17	0.44
1:A:87:ARG:NH1	1:A:142:GLU:OE1	2.51	0.44
1:A:209:SER:HA	1:A:249:TYR:CE1	2.53	0.44
1:S:200:ASN:O	1:S:203:THR:OG1	2.11	0.44
1:F:80:ILE:N	1:F:81:PRO:CD	2.81	0.44
1:S:3:LEU:HD23	1:S:7:VAL:CG2	2.48	0.44
1:J:234:VAL:O	1:J:237:CYS:HB3	2.18	0.44
1:E:102:LEU:O	1:E:171:THR:HG23	2.18	0.44
1:D:70:ILE:HG12	1:D:111:VAL:CG2	2.47	0.44
1:P:158:ASN:O	1:P:159:LEU:CB	2.66	0.44
1:H:266:ASP:OD1	1:H:266:ASP:N	2.51	0.44
1:J:32:VAL:CG1	1:J:82:LEU:HD21	2.40	0.44
1:T:414:THR:C	1:T:416:LEU:N	2.71	0.44
1:S:118:ILE:O	1:S:119:LEU:C	2.56	0.44
1:C:396:SER:O	1:C:397:ASN:C	2.57	0.44
1:E:110:PRO:O	1:E:114:ASP:OD1	2.36	0.44
1:P:386:ASP:HB2	1:Q:399:LEU:HD12	1.98	0.44
1:K:368:HIS:O	1:K:369:ASN:CB	2.66	0.44
1:E:198:PHE:CE1	1:E:204:ARG:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:402:THR:HG22	1:T:359:ARG:NH1	2.33	0.44
1:N:14:LEU:CD1	1:N:57:ILE:HG21	2.48	0.44
1:C:299:VAL:HG12	1:C:300:PHE:N	2.33	0.44
1:B:26:THR:HG23	1:J:295:GLY:O	2.18	0.44
1:J:113:SER:O	1:J:116:LYS:HB2	2.18	0.44
1:O:208:LEU:HD21	1:O:234:VAL:HG22	2.00	0.44
1:T:115:LEU:HD22	1:T:119:LEU:CD2	2.48	0.44
1:S:280:SER:O	1:S:281:MSE:HE2	2.18	0.44
1:C:420:ALA:HB2	1:D:420:ALA:HB2	2.00	0.44
1:R:237:CYS:HA	1:R:241:ASP:OD2	2.18	0.44
1:G:99:PHE:C	1:G:99:PHE:CD1	2.92	0.44
1:R:3:LEU:O	1:R:3:LEU:HD22	2.18	0.44
1:M:101:PHE:CD1	1:M:115:LEU:HD12	2.53	0.43
1:N:278:ARG:HD2	1:N:374:TYR:CZ	2.52	0.43
1:R:408:THR:HG23	1:R:408:THR:O	2.17	0.43
1:M:64:ASN:OD1	1:M:64:ASN:N	2.51	0.43
1:A:355:LEU:HD13	1:J:398:PHE:HB3	2.00	0.43
1:F:64:ASN:OD1	1:F:68:ARG:NH1	2.50	0.43
1:B:65:ASN:HD21	1:B:68:ARG:HG3	1.83	0.43
1:G:32:VAL:HG13	1:G:82:LEU:CD2	2.45	0.43
1:B:379:GLU:HG2	1:B:379:GLU:H	1.63	0.43
1:B:25:LEU:O	1:B:28:LEU:N	2.51	0.43
1:H:242:THR:HG21	1:J:110:PRO:CG	2.48	0.43
1:H:10:LEU:O	1:H:14:LEU:HD12	2.18	0.43
1:K:297:TRP:O	1:K:298:GLU:HB3	2.18	0.43
1:R:273:PHE:HB3	1:R:357:PHE:CZ	2.53	0.43
1:P:205:ILE:HB	1:P:206:PRO:HD3	1.99	0.43
1:P:115:LEU:HD22	1:P:119:LEU:HD22	1.99	0.43
1:R:297:TRP:O	1:R:298:GLU:CB	2.67	0.43
1:H:350:TYR:N	1:H:351:PRO:CD	2.81	0.43
1:R:267:ASP:OD1	1:R:267:ASP:N	2.51	0.43
1:H:172:ILE:O	1:H:176:VAL:HG23	2.19	0.43
1:S:221:ARG:HB3	1:S:223:TYR:CE2	2.54	0.43
1:I:62:PRO:HG2	1:I:64:ASN:ND2	2.34	0.43
1:D:242:THR:O	1:D:247:LEU:HD12	2.17	0.43
1:A:204:ARG:CZ	1:A:297:TRP:CZ2	3.01	0.43
1:J:76:LEU:O	1:J:77:LYS:C	2.56	0.43
1:A:185:GLN:HG2	1:C:379:GLU:HG2	2.01	0.43
1:A:285:THR:HG23	1:I:173:GLU:OE2	2.19	0.43
1:M:238:ALA:O	1:M:278:ARG:NH1	2.50	0.43
1:D:151:TYR:HA	1:D:175:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:LEU:O	1:G:14:LEU:HD12	2.18	0.43
1:G:354:PHE:O	1:G:357:PHE:HB3	2.18	0.43
1:M:269:LEU:HD21	1:M:273:PHE:CE1	2.52	0.43
1:E:194:PHE:CG	1:E:207:ILE:HG23	2.54	0.43
1:N:189:GLU:O	1:N:192:SER:N	2.45	0.43
1:D:248:SER:O	1:D:252:SER:OG	2.36	0.43
1:N:46:ASN:HA	1:N:49:LYS:HB2	2.00	0.43
1:R:127:ASP:HB3	1:R:130:GLU:HB2	2.00	0.43
1:J:151:TYR:CA	1:J:175:LEU:HD13	2.48	0.43
1:N:217:ARG:NH1	1:N:217:ARG:HG2	2.33	0.43
1:D:115:LEU:HD22	1:D:119:LEU:HD22	2.00	0.43
1:S:350:TYR:N	1:S:351:PRO:CD	2.81	0.43
1:H:430:ALA:O	1:H:431:VAL:HB	2.19	0.43
1:R:396:SER:HB3	1:S:386:ASP:OD1	2.18	0.43
1:R:119:LEU:O	1:R:123:LEU:HD22	2.18	0.43
1:Q:415:ARG:O	1:Q:419:ILE:HG23	2.18	0.43
1:M:63:PHE:CE2	1:M:69:ARG:HG2	2.53	0.43
1:J:261:ILE:C	1:J:263:ASN:H	2.20	0.43
1:D:25:LEU:HD12	1:D:25:LEU:N	2.33	0.43
1:K:266:ASP:N	1:K:266:ASP:OD1	2.51	0.43
1:E:83:LEU:HD23	1:E:83:LEU:N	2.32	0.43
1:O:222:LEU:O	1:O:223:TYR:C	2.55	0.43
1:B:101:PHE:CD1	1:B:115:LEU:HD12	2.53	0.43
1:I:65:ASN:OD1	1:I:65:ASN:C	2.56	0.43
1:A:163:GLU:O	1:A:164:SER:C	2.56	0.43
1:J:246:LEU:O	1:J:249:TYR:HB2	2.19	0.43
1:N:189:GLU:O	1:N:190:LEU:C	2.56	0.43
1:E:276:TYR:O	1:E:277:LEU:C	2.55	0.43
1:S:352:ILE:HG13	1:S:406:GLU:OE2	2.18	0.43
1:B:378:GLN:O	1:B:381:LEU:HB3	2.17	0.43
1:O:49:LYS:O	1:O:52:HIS:HB2	2.18	0.43
1:M:223:TYR:CD2	1:N:414:THR:HG21	2.54	0.43
1:S:130:GLU:OE1	1:S:136:ARG:NH1	2.52	0.43
1:B:3:LEU:HD12	1:B:46:ASN:ND2	2.33	0.43
1:O:35:TYR:CE1	1:O:39:TYR:HB2	2.53	0.43
1:P:261:ILE:HG22	1:P:262:CYS:N	2.34	0.43
1:J:268:SER:O	1:J:269:LEU:C	2.57	0.43
1:J:116:LYS:O	1:J:117:SER:C	2.57	0.43
1:P:221:ARG:HB3	1:P:223:TYR:CE2	2.54	0.43
1:M:137:ARG:HB2	1:M:137:ARG:CZ	2.49	0.43
1:P:379:GLU:H	1:P:379:GLU:HG2	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:238:ALA:O	1:J:278:ARG:NH1	2.51	0.43
1:R:293:ALA:O	1:R:295:GLY:N	2.52	0.43
1:H:210:VAL:O	1:H:214:VAL:HG23	2.19	0.43
1:R:247:LEU:HD23	1:R:247:LEU:HA	1.87	0.43
1:D:241:ASP:HA	1:D:299:VAL:HG13	2.01	0.43
1:G:107:GLN:OE1	1:G:170:GLN:NE2	2.51	0.43
1:E:53:ILE:O	1:E:57:ILE:HG13	2.18	0.43
1:F:185:GLN:O	1:F:221:ARG:NH2	2.52	0.43
1:M:269:LEU:CD2	1:M:273:PHE:CE1	3.02	0.43
1:H:422:VAL:O	1:H:426:ASN:ND2	2.52	0.43
1:F:43:ASN:HA	1:F:44:PRO:HD2	1.85	0.43
1:D:286:SER:HB3	1:F:116:LYS:HZ2	1.83	0.43
1:D:430:ALA:O	1:D:431:VAL:HB	2.18	0.43
1:H:86:ASP:O	1:H:89:ALA:HB3	2.19	0.43
1:S:408:THR:CG2	1:S:408:THR:O	2.64	0.43
1:O:155:ALA:O	1:O:156:ILE:HG13	2.19	0.43
1:O:79:VAL:O	1:O:82:LEU:HB2	2.19	0.43
1:P:234:VAL:O	1:P:237:CYS:HB3	2.18	0.43
1:J:209:SER:HA	1:J:249:TYR:CE1	2.54	0.43
1:M:259:SER:OG	1:M:260:HIS:CD2	2.71	0.43
1:Q:294:SER:O	1:Q:295:GLY:C	2.57	0.43
1:K:73:LEU:HD12	1:K:111:VAL:HG13	2.01	0.43
1:G:46:ASN:O	1:G:50:ILE:HG13	2.19	0.43
1:Q:277:LEU:HD23	1:Q:277:LEU:O	2.18	0.43
1:H:343:PHE:C	1:H:343:PHE:CD1	2.92	0.43
1:R:348:ALA:O	1:R:349:LEU:HB2	2.18	0.43
1:S:150:LEU:HG	1:S:175:LEU:HD11	2.00	0.43
1:P:35:TYR:HD1	1:P:35:TYR:C	2.20	0.43
1:P:99:PHE:N	1:P:100:PRO:HD2	2.34	0.43
1:H:376:PHE:C	1:H:376:PHE:CD2	2.92	0.43
1:O:198:PHE:CE1	1:O:204:ARG:HG2	2.54	0.43
1:I:194:PHE:CD1	1:I:207:ILE:HG12	2.53	0.43
1:L:270:TYR:OH	1:L:368:HIS:HD2	2.02	0.43
1:T:208:LEU:O	1:T:209:SER:C	2.57	0.43
1:D:271:ARG:HG3	1:D:271:ARG:HH11	1.84	0.43
1:C:217:ARG:HG2	1:C:217:ARG:NH1	2.34	0.43
1:A:185:GLN:O	1:A:186:ARG:HD3	2.18	0.43
1:J:107:GLN:O	1:J:108:LEU:HD23	2.19	0.43
1:T:94:TRP:CH2	1:T:146:ARG:HB3	2.54	0.43
1:K:382:SER:O	1:K:383:THR:C	2.56	0.43
1:G:364:TYR:CE1	1:G:368:HIS:CD2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:282:ILE:HD12	1:N:288:PHE:CZ	2.54	0.43
1:C:242:THR:HB	1:C:301:HIS:HA	2.01	0.42
1:H:81:PRO:HA	1:H:121:TYR:OH	2.19	0.42
1:G:72:TRP:O	1:G:76:LEU:HB2	2.19	0.42
1:G:35:TYR:C	1:G:35:TYR:HD1	2.21	0.42
1:A:118:ILE:O	1:A:119:LEU:C	2.58	0.42
1:Q:297:TRP:O	1:Q:298:GLU:CB	2.65	0.42
1:F:130:GLU:OE1	1:F:136:ARG:NH1	2.52	0.42
1:F:417:ASP:O	1:F:421:VAL:HG23	2.19	0.42
1:P:48:GLN:O	1:P:52:HIS:HB2	2.18	0.42
1:K:247:LEU:HD12	1:K:288:PHE:CD1	2.54	0.42
1:H:230:PHE:O	1:H:234:VAL:HG23	2.18	0.42
1:O:94:TRP:HA	1:O:98:PHE:CD2	2.54	0.42
1:G:25:LEU:O	1:G:26:THR:C	2.56	0.42
1:B:343:PHE:O	1:B:344:SER:C	2.56	0.42
1:Q:221:ARG:HB3	1:Q:223:TYR:CE2	2.54	0.42
1:R:47:SER:O	1:R:51:ARG:HG3	2.19	0.42
1:N:208:LEU:HA	1:N:208:LEU:HD23	1.86	0.42
1:K:271:ARG:H	1:K:271:ARG:HG2	1.62	0.42
1:I:125:PHE:N	1:I:125:PHE:CD2	2.87	0.42
1:A:242:THR:O	1:A:242:THR:CG2	2.67	0.42
1:A:142:GLU:O	1:A:145:THR:N	2.52	0.42
1:K:109:LYS:N	1:K:110:PRO:CD	2.82	0.42
1:N:410:LYS:C	1:N:412:ARG:H	2.22	0.42
1:D:150:LEU:HG	1:D:175:LEU:HD11	2.00	0.42
1:P:3:LEU:O	1:P:7:VAL:HG23	2.19	0.42
1:T:153:SER:OG	1:T:154:LYS:N	2.52	0.42
1:L:194:PHE:CD1	1:L:207:ILE:HG12	2.54	0.42
1:I:140:ALA:O	1:I:141:GLU:C	2.56	0.42
1:B:10:LEU:O	1:B:11:TRP:C	2.57	0.42
1:M:86:ASP:H	1:M:89:ALA:HB3	1.83	0.42
1:I:6:LEU:HD23	1:I:6:LEU:C	2.38	0.42
1:J:136:ARG:HA	1:J:136:ARG:HD2	1.66	0.42
1:O:241:ASP:O	1:O:278:ARG:NH2	2.37	0.42
1:H:261:ILE:HG22	1:H:262:CYS:N	2.34	0.42
1:F:366:SER:O	1:F:367:LYS:CB	2.65	0.42
1:M:217:ARG:HH11	1:M:217:ARG:HG2	1.84	0.42
1:B:430:ALA:O	1:B:431:VAL:CB	2.67	0.42
1:P:152:VAL:HG11	1:P:197:HIS:ND1	2.35	0.42
1:J:50:ILE:O	1:J:54:LEU:HD22	2.19	0.42
1:T:276:TYR:HB2	1:T:342:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:47:SER:O	1:L:51:ARG:HG3	2.20	0.42
1:H:63:PHE:CE2	1:H:69:ARG:HG2	2.54	0.42
1:G:366:SER:O	1:G:367:LYS:HB2	2.18	0.42
1:R:189:GLU:OE1	1:R:189:GLU:N	2.50	0.42
1:S:296:ASN:OD1	1:S:296:ASN:N	2.52	0.42
1:M:62:PRO:CG	1:M:64:ASN:ND2	2.81	0.42
1:O:115:LEU:HD22	1:O:119:LEU:HD22	2.00	0.42
1:D:251:LEU:HD23	1:D:251:LEU:HA	1.87	0.42
1:Q:389:LEU:O	1:Q:392:HIS:N	2.51	0.42
1:H:156:ILE:O	1:H:157:GLU:C	2.57	0.42
1:R:424:LEU:O	1:R:424:LEU:HD23	2.19	0.42
1:F:376:PHE:CD2	1:F:376:PHE:O	2.73	0.42
1:J:152:VAL:CG1	1:J:203:THR:HG22	2.45	0.42
1:G:86:ASP:HB3	1:G:135:LEU:HD21	2.01	0.42
1:I:279:PHE:CD2	1:I:288:PHE:HE2	2.37	0.42
1:P:80:ILE:N	1:P:81:PRO:HD2	2.34	0.42
1:L:191:SER:HB3	1:L:211:MSE:HE2	2.01	0.42
1:Q:220:PRO:HA	1:Q:221:ARG:HA	1.82	0.42
1:D:13:VAL:O	1:D:13:VAL:HG13	2.18	0.42
1:B:299:VAL:HG12	1:B:300:PHE:N	2.33	0.42
1:I:230:PHE:O	1:I:234:VAL:HG23	2.18	0.42
1:H:282:ILE:HD12	1:H:288:PHE:CZ	2.54	0.42
1:F:3:LEU:HD23	1:F:3:LEU:O	2.19	0.42
1:O:430:ALA:O	1:O:431:VAL:CB	2.66	0.42
1:F:98:PHE:CD1	1:F:115:LEU:HD21	2.54	0.42
1:K:80:ILE:N	1:K:81:PRO:CD	2.82	0.42
1:B:79:VAL:C	1:B:81:PRO:HD2	2.40	0.42
1:M:424:LEU:HD22	1:M:428:LEU:CD2	2.49	0.42
1:H:424:LEU:HD22	1:H:428:LEU:CD2	2.50	0.42
1:H:25:LEU:O	1:H:26:THR:C	2.58	0.42
1:H:188:LYS:O	1:H:191:SER:OG	2.28	0.42
1:A:386:ASP:O	1:A:387:GLY:C	2.58	0.42
1:P:348:ALA:O	1:P:349:LEU:HB2	2.19	0.42
1:N:6:LEU:O	1:N:9:ALA:N	2.52	0.42
1:H:217:ARG:HA	1:H:217:ARG:HD3	1.93	0.42
1:T:372:ILE:HA	1:T:372:ILE:HD13	1.72	0.42
1:J:351:PRO:HG2	1:J:406:GLU:OE2	2.19	0.42
1:H:62:PRO:HG2	1:H:64:ASN:HD21	1.84	0.42
1:C:62:PRO:HG2	1:C:64:ASN:ND2	2.35	0.42
1:O:208:LEU:O	1:O:212:VAL:HG13	2.20	0.42
1:I:293:ALA:O	1:I:294:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LYS:N	1:B:110:PRO:CD	2.82	0.42
1:P:49:LYS:O	1:P:53:ILE:HG12	2.19	0.42
1:H:218:GLN:OE1	1:H:260:HIS:NE2	2.42	0.42
1:A:233:LEU:O	1:A:236:LYS:N	2.53	0.42
1:R:262:CYS:HA	1:R:265:LEU:HD12	2.01	0.42
1:C:32:VAL:HG13	1:C:82:LEU:HD21	2.02	0.42
1:A:142:GLU:O	1:A:143:THR:C	2.57	0.42
1:M:404:GLU:O	1:M:408:THR:HG22	2.18	0.42
1:K:110:PRO:HG3	1:M:242:THR:CG2	2.50	0.42
1:M:51:ARG:HH22	1:M:92:GLU:CD	2.23	0.42
1:Q:273:PHE:HB3	1:Q:357:PHE:CZ	2.55	0.42
1:L:150:LEU:HG	1:L:175:LEU:HD11	2.02	0.42
1:E:134:ASP:O	1:E:136:ARG:N	2.53	0.42
1:D:366:SER:O	1:D:367:LYS:CB	2.67	0.42
1:O:65:ASN:O	1:O:69:ARG:HG3	2.19	0.42
1:Q:14:LEU:CD1	1:Q:57:ILE:HG21	2.49	0.42
1:N:187:PRO:O	1:N:191:SER:OG	2.38	0.42
1:B:215:ILE:O	1:B:216:ARG:C	2.57	0.42
1:Q:47:SER:O	1:Q:48:GLN:C	2.58	0.42
1:G:176:VAL:O	1:G:180:VAL:HG23	2.20	0.42
1:T:351:PRO:O	1:T:355:LEU:HG	2.19	0.42
1:R:205:ILE:HB	1:R:206:PRO:CD	2.49	0.42
1:T:291:SER:OG	1:T:292:THR:N	2.52	0.42
1:N:293:ALA:O	1:N:294:SER:CB	2.68	0.42
1:F:42:GLN:HB3	1:F:84:ILE:HD11	2.00	0.42
1:A:343:PHE:CD1	1:A:343:PHE:C	2.92	0.42
1:K:99:PHE:N	1:K:100:PRO:CD	2.83	0.42
1:G:261:ILE:HG22	1:G:262:CYS:N	2.35	0.42
1:S:278:ARG:HD2	1:S:374:TYR:CZ	2.55	0.42
1:K:359:ARG:HG3	1:T:399:LEU:O	2.19	0.42
1:R:430:ALA:O	1:R:431:VAL:HB	2.19	0.42
1:K:33:GLU:O	1:K:36:GLN:HB2	2.20	0.42
1:L:356:GLU:HG3	1:L:359:ARG:HH21	1.83	0.42
1:Q:194:PHE:CD1	1:Q:207:ILE:HG12	2.55	0.42
1:O:418:SER:O	1:O:422:VAL:HG23	2.20	0.42
1:J:120:PHE:HE2	1:J:178:VAL:HG13	1.84	0.42
1:F:297:TRP:O	1:F:298:GLU:HB3	2.20	0.42
1:I:273:PHE:HB3	1:I:357:PHE:CZ	2.55	0.42
1:O:410:LYS:HA	1:O:410:LYS:HD3	1.95	0.42
1:M:184:ILE:HD13	1:M:184:ILE:HG21	1.66	0.42
1:L:205:ILE:HB	1:L:206:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:THR:O	1:A:408:THR:HG23	2.20	0.42
1:E:221:ARG:HB3	1:E:223:TYR:CE2	2.55	0.42
1:B:99:PHE:C	1:B:99:PHE:HD1	2.24	0.42
1:Q:65:ASN:O	1:Q:69:ARG:HG3	2.19	0.42
1:P:99:PHE:C	1:P:99:PHE:CD1	2.94	0.42
1:R:251:LEU:HD23	1:R:251:LEU:HA	1.94	0.42
1:A:1:MSE:CE	1:A:4:GLN:HB2	2.49	0.42
1:M:99:PHE:CE1	1:M:103:ASN:ND2	2.88	0.42
1:J:269:LEU:HD22	1:J:273:PHE:CE1	2.55	0.42
1:D:350:TYR:N	1:D:351:PRO:CD	2.83	0.42
1:R:375:SER:CB	1:T:117:SER:HA	2.49	0.42
1:T:169:ASN:HA	1:T:172:ILE:HG12	2.02	0.42
1:K:184:ILE:HD11	1:M:377:ASN:ND2	2.35	0.42
1:Q:283:ASP:C	1:Q:283:ASP:OD1	2.58	0.42
1:M:267:ASP:N	1:M:267:ASP:OD1	2.51	0.42
1:L:61:THR:O	1:L:61:THR:OG1	2.37	0.42
1:B:144:ILE:O	1:B:148:VAL:HG23	2.20	0.41
1:T:401:TYR:CE2	1:T:412:ARG:HG3	2.55	0.41
1:I:99:PHE:HB3	1:I:100:PRO:HD3	2.02	0.41
1:I:180:VAL:O	1:I:184:ILE:HG23	2.20	0.41
1:D:350:TYR:O	1:D:351:PRO:C	2.56	0.41
1:B:114:ASP:OD1	1:J:290:SER:OG	2.34	0.41
1:S:107:GLN:NE2	1:S:170:GLN:NE2	2.67	0.41
1:I:268:SER:O	1:I:269:LEU:C	2.59	0.41
1:G:109:LYS:N	1:G:110:PRO:CD	2.83	0.41
1:J:61:THR:O	1:J:61:THR:OG1	2.34	0.41
1:Q:3:LEU:O	1:Q:3:LEU:HD23	2.20	0.41
1:L:278:ARG:HB2	1:L:374:TYR:CE2	2.55	0.41
1:H:176:VAL:O	1:H:177:ASN:C	2.59	0.41
1:O:79:VAL:C	1:O:81:PRO:HD2	2.39	0.41
1:K:278:ARG:HD2	1:K:374:TYR:CZ	2.55	0.41
1:M:208:LEU:HD23	1:M:208:LEU:HA	1.92	0.41
1:S:208:LEU:HA	1:S:208:LEU:HD23	1.93	0.41
1:P:86:ASP:CB	1:P:135:LEU:HD22	2.51	0.41
1:J:231:TYR:CZ	1:J:235:LEU:HD11	2.56	0.41
1:Q:140:ALA:O	1:Q:141:GLU:C	2.59	0.41
1:E:68:ARG:O	1:E:72:TRP:N	2.43	0.41
1:L:424:LEU:O	1:L:424:LEU:HD23	2.20	0.41
1:F:343:PHE:CD1	1:F:343:PHE:C	2.94	0.41
1:C:137:ARG:CZ	1:C:137:ARG:HB2	2.50	0.41
1:K:136:ARG:HA	1:K:136:ARG:HD2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:408:THR:OG1	1:E:408:THR:O	2.30	0.41
1:M:401:TYR:OH	1:M:412:ARG:HG2	2.21	0.41
1:M:254:ILE:O	1:M:255:LEU:C	2.56	0.41
1:N:14:LEU:HD13	1:N:57:ILE:HG21	2.03	0.41
1:L:396:SER:C	1:L:398:PHE:H	2.24	0.41
1:O:278:ARG:HD2	1:O:374:TYR:CZ	2.55	0.41
1:F:269:LEU:HD11	1:F:350:TYR:CG	2.55	0.41
1:C:421:VAL:HG21	1:D:262:CYS:SG	2.60	0.41
1:D:136:ARG:HA	1:D:136:ARG:HD2	1.88	0.41
1:F:376:PHE:CD2	1:F:376:PHE:C	2.94	0.41
1:D:255:LEU:HA	1:D:255:LEU:HD12	1.98	0.41
1:E:2:PRO:HB3	1:E:38:ARG:CD	2.50	0.41
1:R:39:TYR:N	1:R:40:PRO:CD	2.83	0.41
1:C:414:THR:O	1:C:415:ARG:C	2.58	0.41
1:T:86:ASP:OD1	1:T:86:ASP:N	2.53	0.41
1:Q:35:TYR:CD1	1:Q:35:TYR:C	2.93	0.41
1:J:147:LEU:HA	1:J:147:LEU:HD23	1.92	0.41
1:H:251:LEU:HD22	1:H:255:LEU:CD2	2.44	0.41
1:G:198:PHE:CD1	1:G:204:ARG:HG2	2.54	0.41
1:C:410:LYS:O	1:C:412:ARG:N	2.53	0.41
1:A:99:PHE:CD1	1:A:99:PHE:C	2.93	0.41
1:C:251:LEU:HD22	1:C:255:LEU:HD22	2.02	0.41
1:D:286:SER:HB3	1:F:116:LYS:NZ	2.34	0.41
1:K:342:LEU:HA	1:K:345:ILE:HG22	2.01	0.41
1:E:6:LEU:O	1:E:9:ALA:HB3	2.20	0.41
1:C:152:VAL:HG12	1:C:153:SER:N	2.34	0.41
1:Q:90:VAL:CG2	1:Q:142:GLU:HG2	2.51	0.41
1:L:266:ASP:N	1:L:266:ASP:OD1	2.53	0.41
1:J:408:THR:O	1:J:408:THR:HG23	2.19	0.41
1:F:296:ASN:OD1	1:F:296:ASN:N	2.53	0.41
1:A:136:ARG:HD2	1:A:136:ARG:HA	1.87	0.41
1:G:154:LYS:O	1:G:168:ARG:NH1	2.54	0.41
1:M:208:LEU:HD12	1:M:246:LEU:HD11	2.03	0.41
1:A:203:THR:O	1:A:206:PRO:HD2	2.20	0.41
1:B:25:LEU:CD2	1:B:74:ALA:HB1	2.50	0.41
1:E:10:LEU:HA	1:E:13:VAL:HG12	2.02	0.41
1:A:80:ILE:O	1:A:81:PRO:C	2.57	0.41
1:N:80:ILE:HG23	1:N:81:PRO:CD	2.50	0.41
1:P:350:TYR:N	1:P:351:PRO:CD	2.83	0.41
1:I:209:SER:HA	1:I:249:TYR:CE1	2.56	0.41
1:N:47:SER:O	1:N:48:GLN:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:HA	1:B:208:LEU:HD23	1.91	0.41
1:O:32:VAL:O	1:O:33:GLU:C	2.59	0.41
1:N:130:GLU:O	1:N:130:GLU:HG2	2.19	0.41
1:A:152:VAL:CG1	1:A:203:THR:HG22	2.51	0.41
1:O:282:ILE:HG23	1:O:282:ILE:O	2.19	0.41
1:A:285:THR:CG2	1:I:173:GLU:HG2	2.51	0.41
1:B:260:HIS:C	1:B:261:ILE:HG13	2.40	0.41
1:N:215:ILE:O	1:N:216:ARG:C	2.58	0.41
1:Q:180:VAL:HG12	1:Q:181:HIS:N	2.34	0.41
1:S:254:ILE:O	1:S:257:ILE:HG22	2.20	0.41
1:S:190:LEU:HG	1:S:194:PHE:CE2	2.55	0.41
1:G:281:MSE:SE	1:G:376:PHE:HB2	2.71	0.41
1:A:65:ASN:HD21	1:A:68:ARG:HG3	1.86	0.41
1:B:401:TYR:HB3	1:B:405:THR:OG1	2.21	0.41
1:G:181:HIS:O	1:G:185:GLN:HG3	2.20	0.41
1:H:194:PHE:CE1	1:H:207:ILE:HG23	2.55	0.41
1:I:348:ALA:O	1:I:349:LEU:CB	2.68	0.41
1:N:348:ALA:O	1:N:349:LEU:CB	2.65	0.41
1:D:235:LEU:O	1:D:239:GLU:CG	2.68	0.41
1:C:299:VAL:CG1	1:C:300:PHE:N	2.83	0.41
1:P:201:PRO:HB3	1:P:300:PHE:HB2	2.02	0.41
1:B:73:LEU:O	1:B:74:ALA:C	2.59	0.41
1:N:254:ILE:HD11	1:N:272:LEU:HD21	2.02	0.41
1:J:243:SER:O	1:J:244:PRO:C	2.59	0.41
1:D:70:ILE:HG12	1:D:111:VAL:HG21	2.03	0.41
1:Q:293:ALA:C	1:Q:295:GLY:N	2.74	0.41
1:I:192:SER:O	1:I:195:CYS:HB2	2.20	0.41
1:Q:108:LEU:HD21	1:S:303:PHE:HB2	2.03	0.41
1:F:66:THR:O	1:F:69:ARG:N	2.53	0.41
1:F:201:PRO:HB2	1:F:202:PRO:HD3	2.02	0.41
1:E:97:ILE:O	1:E:100:PRO:HG2	2.21	0.41
1:F:225:ILE:HB	1:F:226:PRO:HD3	2.03	0.41
1:I:190:LEU:HD12	1:I:190:LEU:HA	1.81	0.41
1:L:282:ILE:CD1	1:L:288:PHE:CZ	2.96	0.41
1:H:62:PRO:HG2	1:H:64:ASN:ND2	2.36	0.41
1:P:217:ARG:HG2	1:P:217:ARG:NH1	2.35	0.41
1:R:51:ARG:HG2	1:R:83:LEU:HD13	2.02	0.41
1:T:342:LEU:HA	1:T:345:ILE:HG22	2.01	0.41
1:H:25:LEU:O	1:H:27:GLU:N	2.53	0.41
1:G:413:TRP:O	1:G:416:LEU:HB2	2.21	0.41
1:B:35:TYR:CE1	1:B:82:LEU:HG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:380:LEU:HB2	1:R:184:ILE:HD11	2.01	0.41
1:T:429:ASN:C	1:T:431:VAL:H	2.24	0.41
1:K:65:ASN:HD21	1:K:68:ARG:HG3	1.86	0.41
1:R:220:PRO:HB2	1:R:221:ARG:HG2	2.03	0.41
1:M:90:VAL:HG23	1:M:90:VAL:O	2.20	0.41
1:N:86:ASP:HB3	1:N:135:LEU:CD2	2.51	0.41
1:H:3:LEU:O	1:H:7:VAL:HG23	2.21	0.41
1:J:182:TYR:O	1:J:185:GLN:N	2.52	0.41
1:H:131:TRP:HZ3	1:H:139:CYS:SG	2.44	0.41
1:F:175:LEU:HD23	1:F:175:LEU:HA	1.85	0.41
1:Q:254:ILE:HG21	1:Q:254:ILE:HD13	1.78	0.41
1:N:76:LEU:O	1:N:80:ILE:HG22	2.21	0.41
1:G:1:MSE:HE1	1:G:8:LYS:HE2	2.03	0.41
1:T:49:LYS:O	1:T:53:ILE:HG12	2.21	0.41
1:E:242:THR:O	1:E:242:THR:CG2	2.68	0.41
1:C:53:ILE:O	1:C:57:ILE:HG13	2.20	0.41
1:P:225:ILE:HB	1:P:226:PRO:HD3	2.03	0.41
1:P:297:TRP:O	1:P:298:GLU:HB3	2.21	0.41
1:E:154:LYS:HG2	1:E:171:THR:HG21	2.03	0.41
1:F:65:ASN:ND2	1:F:68:ARG:HG3	2.35	0.41
1:F:376:PHE:O	1:F:376:PHE:CG	2.72	0.41
1:N:191:SER:HB3	1:N:211:MSE:HE2	2.02	0.41
1:L:251:LEU:HG	1:L:279:PHE:CE2	2.56	0.41
1:N:33:GLU:O	1:N:36:GLN:N	2.54	0.41
1:N:394:ALA:HB3	1:O:389:LEU:HG	2.03	0.41
1:E:8:LYS:O	1:E:12:ASN:OD1	2.38	0.41
1:I:233:LEU:HD12	1:I:233:LEU:HA	1.78	0.41
1:F:32:VAL:O	1:F:35:TYR:HB3	2.20	0.41
1:T:251:LEU:HG	1:T:279:PHE:CE2	2.56	0.41
1:K:123:LEU:O	1:K:124:ILE:HD13	2.21	0.41
1:D:208:LEU:HA	1:D:208:LEU:HD23	1.85	0.41
1:H:32:VAL:O	1:H:36:GLN:HG3	2.21	0.41
1:M:204:ARG:CZ	1:M:297:TRP:CZ2	3.04	0.41
1:F:136:ARG:HA	1:F:136:ARG:HD2	1.86	0.41
1:I:363:LEU:CD2	1:I:363:LEU:O	2.68	0.41
1:F:99:PHE:HE1	1:F:103:ASN:HD22	1.69	0.41
1:O:98:PHE:HD1	1:O:115:LEU:HD21	1.85	0.41
1:S:107:GLN:O	1:S:108:LEU:HD23	2.21	0.41
1:Q:262:CYS:SG	1:R:421:VAL:HG21	2.60	0.41
1:N:139:CYS:O	1:N:143:THR:OG1	2.38	0.41
1:D:3:LEU:HD23	1:D:7:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:415:ARG:O	1:F:419:ILE:HG23	2.21	0.41
1:F:399:LEU:HD21	1:G:355:LEU:HD22	2.02	0.41
1:H:345:ILE:O	1:H:348:ALA:O	2.39	0.41
1:J:153:SER:OG	1:J:154:LYS:N	2.54	0.41
1:M:201:PRO:HB3	1:M:300:PHE:HB2	2.03	0.41
1:N:1:MSE:HE2	1:N:4:GLN:CB	2.50	0.40
1:L:281:MSE:SE	1:L:377:ASN:H	2.54	0.40
1:O:65:ASN:ND2	1:O:68:ARG:HG3	2.35	0.40
1:A:200:ASN:HA	1:A:201:PRO:HD2	1.90	0.40
1:L:244:PRO:O	1:L:245:ILE:C	2.59	0.40
1:J:194:PHE:CD1	1:J:207:ILE:HG23	2.56	0.40
1:R:139:CYS:O	1:R:140:ALA:C	2.60	0.40
1:Q:245:ILE:O	1:Q:249:TYR:HD2	2.03	0.40
1:H:50:ILE:O	1:H:54:LEU:HD22	2.21	0.40
1:F:277:LEU:HD23	1:F:277:LEU:O	2.21	0.40
1:K:101:PHE:CD1	1:K:101:PHE:C	2.94	0.40
1:C:235:LEU:O	1:C:239:GLU:HG2	2.20	0.40
1:J:119:LEU:O	1:J:123:LEU:HD22	2.22	0.40
1:T:273:PHE:HB3	1:T:357:PHE:CD2	2.56	0.40
1:N:145:THR:O	1:N:146:ARG:C	2.59	0.40
1:N:89:ALA:O	1:N:93:TRP:HD1	2.04	0.40
1:J:430:ALA:O	1:J:431:VAL:CB	2.69	0.40
1:B:28:LEU:O	1:B:32:VAL:HG23	2.22	0.40
1:D:65:ASN:ND2	1:D:68:ARG:CG	2.84	0.40
1:O:107:GLN:HE22	1:O:170:GLN:NE2	2.18	0.40
1:N:137:ARG:HG2	1:N:141:GLU:OE1	2.21	0.40
1:H:237:CYS:SG	1:H:246:LEU:HD21	2.61	0.40
1:K:51:ARG:HG2	1:K:83:LEU:HD13	2.03	0.40
1:Q:109:LYS:N	1:Q:110:PRO:CD	2.84	0.40
1:M:271:ARG:O	1:M:275:ILE:HG13	2.22	0.40
1:D:352:ILE:HB	1:D:406:GLU:OE1	2.21	0.40
1:R:208:LEU:O	1:R:212:VAL:HG13	2.22	0.40
1:M:342:LEU:HA	1:M:342:LEU:HD12	1.85	0.40
1:Q:208:LEU:HA	1:Q:208:LEU:HD23	1.95	0.40
1:N:49:LYS:O	1:N:53:ILE:HG12	2.20	0.40
1:J:80:ILE:HA	1:J:83:LEU:HG	2.03	0.40
1:N:204:ARG:O	1:N:205:ILE:C	2.60	0.40
1:G:238:ALA:O	1:G:278:ARG:NH1	2.49	0.40
1:S:3:LEU:O	1:S:7:VAL:HG23	2.22	0.40
1:T:63:PHE:CE1	1:T:69:ARG:HA	2.56	0.40
1:G:144:ILE:HG23	1:G:145:THR:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:84:ILE:O	1:S:85:LEU:HD12	2.21	0.40
1:A:299:VAL:HG12	1:A:300:PHE:N	2.36	0.40
1:E:254:ILE:CG1	1:E:255:LEU:N	2.82	0.40
1:C:275:ILE:O	1:C:276:TYR:C	2.60	0.40
1:G:299:VAL:CG1	1:G:301:HIS:CE1	2.96	0.40
1:N:94:TRP:CG	1:N:146:ARG:HD3	2.57	0.40
1:I:156:ILE:HD11	1:I:203:THR:HG22	2.02	0.40
1:A:164:SER:O	1:A:165:GLN:C	2.60	0.40
1:S:209:SER:HA	1:S:249:TYR:CE1	2.57	0.40
1:A:106:THR:O	1:A:108:LEU:N	2.53	0.40
1:Q:57:ILE:O	1:Q:57:ILE:HG22	2.20	0.40
1:H:414:THR:C	1:H:416:LEU:H	2.25	0.40
1:D:208:LEU:HD21	1:D:234:VAL:HG22	2.03	0.40
1:M:347:TYR:O	1:M:351:PRO:HB3	2.20	0.40
1:F:270:TYR:HB3	1:F:370:PHE:CE2	2.56	0.40
1:F:283:ASP:HA	1:F:284:PRO:HD3	1.96	0.40
1:K:396:SER:O	1:K:398:PHE:N	2.55	0.40
1:H:248:SER:O	1:H:252:SER:OG	2.38	0.40
1:E:215:ILE:CG2	1:E:256:MSE:HB3	2.52	0.40
1:E:341:GLN:O	1:E:345:ILE:HG22	2.22	0.40
1:A:283:ASP:CG	1:A:284:PRO:HD2	2.42	0.40
1:N:118:ILE:O	1:N:122:ILE:HG13	2.22	0.40
1:A:104:SER:HA	1:A:105:PRO:HD3	1.90	0.40
1:G:389:LEU:C	1:G:391:ARG:H	2.25	0.40
1:P:265:LEU:O	1:P:269:LEU:HB2	2.22	0.40
1:J:354:PHE:CZ	1:J:358:LEU:HD11	2.56	0.40
1:H:247:LEU:HA	1:H:247:LEU:HD23	1.95	0.40
1:A:247:LEU:CD1	1:A:288:PHE:CD1	3.03	0.40
1:H:80:ILE:HD12	1:H:93:TRP:CH2	2.57	0.40
1:P:62:PRO:HG2	1:P:64:ASN:ND2	2.36	0.40
1:N:297:TRP:O	1:N:298:GLU:HB3	2.20	0.40
1:J:99:PHE:O	1:J:103:ASN:HB2	2.20	0.40
1:S:230:PHE:O	1:S:234:VAL:HG23	2.22	0.40
1:T:244:PRO:HD2	1:T:302:ASP:OD2	2.22	0.40
1:E:237:CYS:O	1:E:241:ASP:HB2	2.21	0.40
1:Q:343:PHE:C	1:Q:343:PHE:CD1	2.94	0.40
1:P:282:ILE:HG23	1:P:282:ILE:O	2.21	0.40
1:P:208:LEU:HD23	1:P:208:LEU:HA	1.87	0.40
1:G:380:LEU:HD12	1:G:380:LEU:HA	1.83	0.40

There are no symmetry-related clashes.

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	395/434 (91%)	331 (84%)	45 (11%)	19 (5%)	3	20
1	B	383/434 (88%)	333 (87%)	33 (9%)	17 (4%)	3	22
1	C	383/434 (88%)	335 (88%)	36 (9%)	12 (3%)	5	32
1	D	383/434 (88%)	333 (87%)	41 (11%)	9 (2%)	8	39
1	E	383/434 (88%)	336 (88%)	35 (9%)	12 (3%)	5	32
1	F	383/434 (88%)	347 (91%)	29 (8%)	7 (2%)	11	46
1	G	383/434 (88%)	325 (85%)	48 (12%)	10 (3%)	7	36
1	H	383/434 (88%)	320 (84%)	46 (12%)	17 (4%)	3	22
1	I	383/434 (88%)	328 (86%)	39 (10%)	16 (4%)	3	23
1	J	383/434 (88%)	314 (82%)	55 (14%)	14 (4%)	4	27
1	K	395/434 (91%)	346 (88%)	36 (9%)	13 (3%)	5	30
1	L	383/434 (88%)	327 (85%)	47 (12%)	9 (2%)	8	39
1	M	383/434 (88%)	327 (85%)	46 (12%)	10 (3%)	7	36
1	N	383/434 (88%)	323 (84%)	50 (13%)	10 (3%)	7	36
1	O	383/434 (88%)	331 (86%)	42 (11%)	10 (3%)	7	36
1	P	383/434 (88%)	342 (89%)	31 (8%)	10 (3%)	7	36
1	Q	383/434 (88%)	308 (80%)	63 (16%)	12 (3%)	5	32
1	R	383/434 (88%)	334 (87%)	41 (11%)	8 (2%)	9	42
1	S	383/434 (88%)	315 (82%)	58 (15%)	10 (3%)	7	36
1	T	383/434 (88%)	343 (90%)	35 (9%)	5 (1%)	15	52
All	All	7684/8680 (88%)	6598 (86%)	856 (11%)	230 (3%)	5	33

All (230) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	MSE

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Mol	Chain	Res	Type
1	A	64	ASN
1	A	164	SER
1	A	165	GLN
1	A	262	CYS
1	A	298	GLU
1	A	328	SER
1	A	397	ASN
1	A	409	ASP
1	B	165	GLN
1	B	261	ILE
1	B	359	ARG
1	B	397	ASN
1	C	293	ALA
1	C	359	ARG
1	E	135	LEU
1	E	293	ALA
1	G	2	PRO
1	H	130	GLU
1	H	262	CYS
1	H	282	ILE
1	H	293	ALA
1	H	409	ASP
1	I	2	PRO
1	I	293	ALA
1	I	409	ASP
1	K	295	GLY
1	K	409	ASP
1	K	415	ARG
1	L	26	THR
1	L	262	CYS
1	L	349	LEU
1	L	397	ASN
1	M	135	LEU
1	N	293	ALA
1	O	156	ILE
1	O	157	GLU
1	O	223	TYR
1	P	157	GLU
1	P	159	LEU
1	P	262	CYS
1	Q	48	GLN
1	Q	159	LEU

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Mol	Chain	Res	Type
1	Q	298	GLU
1	R	262	CYS
1	R	349	LEU
1	R	409	ASP
1	S	130	GLU
1	S	241	ASP
1	A	294	SER
1	B	10	LEU
1	B	26	THR
1	B	349	LEU
1	C	262	CYS
1	C	295	GLY
1	C	397	ASN
1	D	2	PRO
1	D	133	GLY
1	D	157	GLU
1	E	261	ILE
1	E	295	GLY
1	F	92	GLU
1	F	295	GLY
1	F	369	ASN
1	F	387	GLY
1	G	26	THR
1	G	266	ASP
1	G	295	GLY
1	G	298	GLU
1	H	26	THR
1	H	62	PRO
1	H	415	ARG
1	I	62	PRO
1	I	157	GLU
1	I	159	LEU
1	I	349	LEU
1	I	415	ARG
1	J	60	LYS
1	J	181	HIS
1	J	294	SER
1	J	367	LYS
1	J	397	ASN
1	K	2	PRO
1	K	165	GLN
1	K	298	GLU

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Mol	Chain	Res	Type
1	L	130	GLU
1	M	62	PRO
1	M	218	GLN
1	M	261	ILE
1	M	298	GLU
1	N	159	LEU
1	O	2	PRO
1	O	261	ILE
1	O	298	GLU
1	O	349	LEU
1	P	62	PRO
1	P	295	GLY
1	P	396	SER
1	Q	47	SER
1	Q	295	GLY
1	Q	382	SER
1	Q	409	ASP
1	R	62	PRO
1	S	261	ILE
1	S	294	SER
1	T	261	ILE
1	T	397	ASN
1	T	415	ARG
1	A	74	ALA
1	A	367	LYS
1	B	2	PRO
1	B	40	PRO
1	B	103	ASN
1	B	383	THR
1	C	159	LEU
1	C	369	ASN
1	C	411	SER
1	D	64	ASN
1	D	261	ILE
1	D	415	ARG
1	E	62	PRO
1	E	119	LEU
1	E	130	GLU
1	G	397	ASN
1	H	2	PRO
1	H	107	GLN
1	H	294	SER

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Mol	Chain	Res	Type
1	H	367	LYS
1	H	413	TRP
1	I	262	CYS
1	I	302	ASP
1	I	383	THR
1	J	92	GLU
1	J	159	LEU
1	J	256	MSE
1	J	262	CYS
1	J	383	THR
1	J	409	ASP
1	K	128	GLU
1	K	154	LYS
1	K	369	ASN
1	L	159	LEU
1	M	107	GLN
1	M	130	GLU
1	M	159	LEU
1	M	409	ASP
1	N	62	PRO
1	N	135	LEU
1	N	261	ILE
1	N	298	GLU
1	O	26	THR
1	O	130	GLU
1	P	298	GLU
1	P	367	LYS
1	P	415	ARG
1	Q	2	PRO
1	Q	383	THR
1	R	2	PRO
1	S	409	ASP
1	T	295	GLY
1	A	2	PRO
1	A	358	LEU
1	B	62	PRO
1	B	157	GLU
1	B	348	ALA
1	C	62	PRO
1	C	367	LYS
1	D	293	ALA
1	E	101	PHE

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Mol	Chain	Res	Type
1	E	409	ASP
1	G	62	PRO
1	H	77	LYS
1	H	195	CYS
1	I	47	SER
1	I	107	GLN
1	J	382	SER
1	K	329	SER
1	K	397	ASN
1	L	409	ASP
1	L	411	SER
1	M	302	ASP
1	N	181	HIS
1	N	241	ASP
1	O	293	ALA
1	P	2	PRO
1	Q	62	PRO
1	S	107	GLN
1	S	189	GLU
1	S	258	LEU
1	A	62	PRO
1	A	166	GLU
1	B	70	ILE
1	B	298	GLU
1	C	219	GLY
1	D	243	SER
1	F	367	LYS
1	G	157	GLU
1	I	154	LYS
1	J	349	LEU
1	K	62	PRO
1	L	359	ARG
1	N	11	TRP
1	R	298	GLU
1	S	119	LEU
1	A	293	ALA
1	B	159	LEU
1	D	62	PRO
1	E	165	GLN
1	H	261	ILE
1	I	158	ASN
1	I	295	GLY

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Mol	Chain	Res	Type
1	J	2	PRO
1	K	331	PRO
1	N	40	PRO
1	S	202	PRO
1	E	118	ILE
1	F	62	PRO
1	G	152	VAL
1	C	261	ILE
1	E	2	PRO
1	F	261	ILE
1	G	148	VAL
1	Q	299	VAL
1	R	295	GLY
1	T	2	PRO
1	A	118	ILE
1	A	176	VAL
1	H	160	GLY
1	Q	261	ILE
1	R	282	ILE

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	361/398 (91%)	311 (86%)	50 (14%)	4 20
1	B	352/398 (88%)	310 (88%)	42 (12%)	6 27
1	C	352/398 (88%)	306 (87%)	46 (13%)	5 22
1	D	352/398 (88%)	307 (87%)	45 (13%)	5 23
1	E	352/398 (88%)	300 (85%)	52 (15%)	4 17
1	F	352/398 (88%)	312 (89%)	40 (11%)	7 29
1	G	352/398 (88%)	310 (88%)	42 (12%)	6 27
1	H	352/398 (88%)	309 (88%)	43 (12%)	6 26
1	I	352/398 (88%)	298 (85%)	54 (15%)	3 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	352/398 (88%)	306 (87%)	46 (13%)	5	22
1	K	361/398 (91%)	313 (87%)	48 (13%)	5	21
1	L	352/398 (88%)	309 (88%)	43 (12%)	6	26
1	M	352/398 (88%)	311 (88%)	41 (12%)	7	29
1	N	352/398 (88%)	306 (87%)	46 (13%)	5	22
1	O	352/398 (88%)	300 (85%)	52 (15%)	4	17
1	P	352/398 (88%)	304 (86%)	48 (14%)	5	21
1	Q	352/398 (88%)	303 (86%)	49 (14%)	4	20
1	R	352/398 (88%)	313 (89%)	39 (11%)	8	31
1	S	352/398 (88%)	313 (89%)	39 (11%)	8	31
1	T	352/398 (88%)	309 (88%)	43 (12%)	6	26
All	All	7058/7960 (89%)	6150 (87%)	908 (13%)	5	23

All (908) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	26	THR
1	A	35	TYR
1	A	36	GLN
1	A	52	HIS
1	A	55	ASP
1	A	61	THR
1	A	63	PHE
1	A	64	ASN
1	A	66	THR
1	A	76	LEU
1	A	78	THR
1	A	82	LEU
1	A	86	ASP
1	A	90	VAL
1	A	108	LEU
1	A	113	SER
1	A	115	LEU
1	A	119	LEU
1	A	123	LEU
1	A	129	ASP
1	A	134	ASP

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Mol	Chain	Res	Type
1	A	143	THR
1	A	157	GLU
1	A	165	GLN
1	A	196	HIS
1	A	205	ILE
1	A	209	SER
1	A	221	ARG
1	A	251	LEU
1	A	254	ILE
1	A	255	LEU
1	A	258	LEU
1	A	264	SER
1	A	265	LEU
1	A	266	ASP
1	A	268	SER
1	A	269	LEU
1	A	277	LEU
1	A	284	PRO
1	A	285	THR
1	A	286	SER
1	A	340	SER
1	A	363	LEU
1	A	375	SER
1	A	396	SER
1	A	405	THR
1	A	416	LEU
1	A	424	LEU
1	A	428	LEU
1	B	1	MSE
1	B	4	GLN
1	B	6	LEU
1	B	10	LEU
1	B	13	VAL
1	B	26	THR
1	B	27	GLU
1	B	45	THR
1	B	52	HIS
1	B	54	LEU
1	B	60	LYS
1	B	61	THR
1	B	63	PHE
1	B	76	LEU

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Mol	Chain	Res	Type
1	B	78	THR
1	B	82	LEU
1	B	85	LEU
1	B	99	PHE
1	B	108	LEU
1	B	115	LEU
1	B	119	LEU
1	B	123	LEU
1	B	177	ASN
1	B	196	HIS
1	B	205	ILE
1	B	221	ARG
1	B	233	LEU
1	B	251	LEU
1	B	255	LEU
1	B	265	LEU
1	B	267	ASP
1	B	269	LEU
1	B	277	LEU
1	B	285	THR
1	B	304	MSE
1	B	338	ASP
1	B	375	SER
1	B	379	GLU
1	B	404	GLU
1	B	418	SER
1	B	424	LEU
1	B	428	LEU
1	C	1	MSE
1	C	3	LEU
1	C	26	THR
1	C	29	ILE
1	C	34	SER
1	C	36	GLN
1	C	38	ARG
1	C	43	ASN
1	C	45	THR
1	C	52	HIS
1	C	54	LEU
1	C	60	LYS
1	C	61	THR
1	C	64	ASN

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Mol	Chain	Res	Type
1	C	66	THR
1	C	76	LEU
1	C	82	LEU
1	C	85	LEU
1	C	107	GLN
1	C	115	LEU
1	C	119	LEU
1	C	123	LEU
1	C	191	SER
1	C	196	HIS
1	C	221	ARG
1	C	226	PRO
1	C	239	GLU
1	C	251	LEU
1	C	254	ILE
1	C	255	LEU
1	C	258	LEU
1	C	265	LEU
1	C	267	ASP
1	C	269	LEU
1	C	285	THR
1	C	302	ASP
1	C	304	MSE
1	C	337	LEU
1	C	371	GLN
1	C	382	SER
1	C	391	ARG
1	C	396	SER
1	C	400	LYS
1	C	404	GLU
1	C	424	LEU
1	C	428	LEU
1	D	1	MSE
1	D	13	VAL
1	D	26	THR
1	D	34	SER
1	D	45	THR
1	D	52	HIS
1	D	54	LEU
1	D	60	LYS
1	D	61	THR
1	D	64	ASN

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Mol	Chain	Res	Type
1	D	66	THR
1	D	76	LEU
1	D	82	LEU
1	D	85	LEU
1	D	115	LEU
1	D	119	LEU
1	D	123	LEU
1	D	128	GLU
1	D	153	SER
1	D	191	SER
1	D	196	HIS
1	D	205	ILE
1	D	221	ARG
1	D	232	ASP
1	D	251	LEU
1	D	252	SER
1	D	254	ILE
1	D	255	LEU
1	D	257	ILE
1	D	259	SER
1	D	264	SER
1	D	265	LEU
1	D	268	SER
1	D	269	LEU
1	D	271	ARG
1	D	290	SER
1	D	304	MSE
1	D	340	SER
1	D	363	LEU
1	D	375	SER
1	D	382	SER
1	D	391	ARG
1	D	412	ARG
1	D	424	LEU
1	D	428	LEU
1	E	1	MSE
1	E	3	LEU
1	E	10	LEU
1	E	13	VAL
1	E	26	THR
1	E	34	SER
1	E	37	GLN

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Mol	Chain	Res	Type
1	E	45	THR
1	E	54	LEU
1	E	60	LYS
1	E	64	ASN
1	E	66	THR
1	E	71	LEU
1	E	76	LEU
1	E	78	THR
1	E	82	LEU
1	E	108	LEU
1	E	110	PRO
1	E	115	LEU
1	E	119	LEU
1	E	123	LEU
1	E	126	HIS
1	E	128	GLU
1	E	136	ARG
1	E	154	LYS
1	E	191	SER
1	E	196	HIS
1	E	221	ARG
1	E	233	LEU
1	E	251	LEU
1	E	252	SER
1	E	254	ILE
1	E	255	LEU
1	E	264	SER
1	E	265	LEU
1	E	266	ASP
1	E	267	ASP
1	E	269	LEU
1	E	277	LEU
1	E	292	THR
1	E	302	ASP
1	E	304	MSE
1	E	345	ILE
1	E	363	LEU
1	E	375	SER
1	E	379	GLU
1	E	396	SER
1	E	404	GLU
1	E	408	THR

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Mol	Chain	Res	Type
1	E	417	ASP
1	E	424	LEU
1	E	428	LEU
1	F	1	MSE
1	F	10	LEU
1	F	26	THR
1	F	36	GLN
1	F	45	THR
1	F	52	HIS
1	F	54	LEU
1	F	60	LYS
1	F	63	PHE
1	F	76	LEU
1	F	77	LYS
1	F	82	LEU
1	F	108	LEU
1	F	115	LEU
1	F	119	LEU
1	F	123	LEU
1	F	126	HIS
1	F	136	ARG
1	F	184	ILE
1	F	192	SER
1	F	221	ARG
1	F	232	ASP
1	F	245	ILE
1	F	251	LEU
1	F	252	SER
1	F	254	ILE
1	F	255	LEU
1	F	257	ILE
1	F	258	LEU
1	F	259	SER
1	F	264	SER
1	F	267	ASP
1	F	268	SER
1	F	269	LEU
1	F	285	THR
1	F	291	SER
1	F	302	ASP
1	F	304	MSE
1	F	337	LEU

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Mol	Chain	Res	Type
1	F	404	GLU
1	G	1	MSE
1	G	5	SER
1	G	26	THR
1	G	35	TYR
1	G	45	THR
1	G	54	LEU
1	G	55	ASP
1	G	57	ILE
1	G	76	LEU
1	G	82	LEU
1	G	90	VAL
1	G	95	ASP
1	G	108	LEU
1	G	115	LEU
1	G	119	LEU
1	G	123	LEU
1	G	126	HIS
1	G	134	ASP
1	G	136	ARG
1	G	184	ILE
1	G	232	ASP
1	G	251	LEU
1	G	254	ILE
1	G	255	LEU
1	G	258	LEU
1	G	259	SER
1	G	264	SER
1	G	266	ASP
1	G	269	LEU
1	G	285	THR
1	G	290	SER
1	G	302	ASP
1	G	304	MSE
1	G	345	ILE
1	G	363	LEU
1	G	375	SER
1	G	382	SER
1	G	383	THR
1	G	396	SER
1	G	408	THR
1	G	417	ASP

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Mol	Chain	Res	Type
1	G	424	LEU
1	H	12	ASN
1	H	26	THR
1	H	35	TYR
1	H	45	THR
1	H	48	GLN
1	H	52	HIS
1	H	60	LYS
1	H	64	ASN
1	H	66	THR
1	H	72	TRP
1	H	76	LEU
1	H	78	THR
1	H	82	LEU
1	H	85	LEU
1	H	90	VAL
1	H	108	LEU
1	H	115	LEU
1	H	119	LEU
1	H	123	LEU
1	H	149	ASP
1	H	201	PRO
1	H	209	SER
1	H	221	ARG
1	H	233	LEU
1	H	251	LEU
1	H	252	SER
1	H	254	ILE
1	H	255	LEU
1	H	258	LEU
1	H	265	LEU
1	H	266	ASP
1	H	269	LEU
1	H	277	LEU
1	H	280	SER
1	H	290	SER
1	H	304	MSE
1	H	341	GLN
1	H	391	ARG
1	H	405	THR
1	H	408	THR
1	H	411	SER

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Mol	Chain	Res	Type
1	H	424	LEU
1	H	428	LEU
1	I	1	MSE
1	I	3	LEU
1	I	26	THR
1	I	45	THR
1	I	48	GLN
1	I	54	LEU
1	I	55	ASP
1	I	57	ILE
1	I	60	LYS
1	I	61	THR
1	I	67	ARG
1	I	76	LEU
1	I	78	THR
1	I	82	LEU
1	I	87	ARG
1	I	88	GLN
1	I	109	LYS
1	I	115	LEU
1	I	119	LEU
1	I	123	LEU
1	I	126	HIS
1	I	129	ASP
1	I	134	ASP
1	I	136	ARG
1	I	154	LYS
1	I	184	ILE
1	I	191	SER
1	I	195	CYS
1	I	200	ASN
1	I	209	SER
1	I	221	ARG
1	I	232	ASP
1	I	233	LEU
1	I	242	THR
1	I	251	LEU
1	I	254	ILE
1	I	257	ILE
1	I	265	LEU
1	I	268	SER
1	I	269	LEU

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Mol	Chain	Res	Type
1	I	277	LEU
1	I	286	SER
1	I	289	PRO
1	I	291	SER
1	I	304	MSE
1	I	341	GLN
1	I	363	LEU
1	I	375	SER
1	I	396	SER
1	I	408	THR
1	I	416	LEU
1	I	418	SER
1	I	424	LEU
1	I	428	LEU
1	J	13	VAL
1	J	14	LEU
1	J	26	THR
1	J	35	TYR
1	J	36	GLN
1	J	47	SER
1	J	54	LEU
1	J	60	LYS
1	J	61	THR
1	J	63	PHE
1	J	66	THR
1	J	76	LEU
1	J	78	THR
1	J	82	LEU
1	J	115	LEU
1	J	119	LEU
1	J	123	LEU
1	J	145	THR
1	J	156	ILE
1	J	176	VAL
1	J	199	LEU
1	J	221	ARG
1	J	233	LEU
1	J	242	THR
1	J	248	SER
1	J	251	LEU
1	J	252	SER
1	J	254	ILE

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Mol	Chain	Res	Type
1	J	255	LEU
1	J	265	LEU
1	J	267	ASP
1	J	268	SER
1	J	269	LEU
1	J	277	LEU
1	J	286	SER
1	J	302	ASP
1	J	304	MSE
1	J	337	LEU
1	J	341	GLN
1	J	363	LEU
1	J	375	SER
1	J	391	ARG
1	J	396	SER
1	J	417	ASP
1	J	424	LEU
1	J	427	SER
1	K	1	MSE
1	K	3	LEU
1	K	4	GLN
1	K	13	VAL
1	K	14	LEU
1	K	26	THR
1	K	29	ILE
1	K	36	GLN
1	K	45	THR
1	K	54	LEU
1	K	60	LYS
1	K	61	THR
1	K	77	LYS
1	K	78	THR
1	K	82	LEU
1	K	85	LEU
1	K	92	GLU
1	K	108	LEU
1	K	115	LEU
1	K	119	LEU
1	K	134	ASP
1	K	154	LYS
1	K	157	GLU
1	K	158	ASN

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Mol	Chain	Res	Type
1	K	159	LEU
1	K	165	GLN
1	K	174	CYS
1	K	196	HIS
1	K	209	SER
1	K	221	ARG
1	K	227	GLN
1	K	233	LEU
1	K	251	LEU
1	K	254	ILE
1	K	255	LEU
1	K	265	LEU
1	K	266	ASP
1	K	269	LEU
1	K	271	ARG
1	K	285	THR
1	K	286	SER
1	K	302	ASP
1	K	304	MSE
1	K	305	SER
1	K	337	LEU
1	K	340	SER
1	K	363	LEU
1	K	428	LEU
1	L	1	MSE
1	L	13	VAL
1	L	26	THR
1	L	34	SER
1	L	37	GLN
1	L	45	THR
1	L	52	HIS
1	L	54	LEU
1	L	55	ASP
1	L	57	ILE
1	L	60	LYS
1	L	61	THR
1	L	66	THR
1	L	76	LEU
1	L	77	LYS
1	L	82	LEU
1	L	108	LEU
1	L	115	LEU

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Mol	Chain	Res	Type
1	L	119	LEU
1	L	123	LEU
1	L	126	HIS
1	L	176	VAL
1	L	184	ILE
1	L	221	ARG
1	L	233	LEU
1	L	248	SER
1	L	251	LEU
1	L	254	ILE
1	L	255	LEU
1	L	257	ILE
1	L	265	LEU
1	L	266	ASP
1	L	267	ASP
1	L	268	SER
1	L	269	LEU
1	L	290	SER
1	L	304	MSE
1	L	363	LEU
1	L	375	SER
1	L	383	THR
1	L	424	LEU
1	L	426	ASN
1	L	428	LEU
1	M	1	MSE
1	M	26	THR
1	M	36	GLN
1	M	49	LYS
1	M	52	HIS
1	M	54	LEU
1	M	57	ILE
1	M	66	THR
1	M	76	LEU
1	M	82	LEU
1	M	90	VAL
1	M	106	THR
1	M	115	LEU
1	M	117	SER
1	M	119	LEU
1	M	123	LEU
1	M	134	ASP

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Mol	Chain	Res	Type
1	M	136	ARG
1	M	196	HIS
1	M	217	ARG
1	M	221	ARG
1	M	233	LEU
1	M	248	SER
1	M	251	LEU
1	M	252	SER
1	M	254	ILE
1	M	255	LEU
1	M	258	LEU
1	M	265	LEU
1	M	266	ASP
1	M	267	ASP
1	M	269	LEU
1	M	277	LEU
1	M	286	SER
1	M	291	SER
1	M	304	MSE
1	M	363	LEU
1	M	396	SER
1	M	408	THR
1	M	424	LEU
1	M	428	LEU
1	N	1	MSE
1	N	6	LEU
1	N	10	LEU
1	N	26	THR
1	N	34	SER
1	N	36	GLN
1	N	45	THR
1	N	52	HIS
1	N	76	LEU
1	N	79	VAL
1	N	82	LEU
1	N	85	LEU
1	N	115	LEU
1	N	119	LEU
1	N	123	LEU
1	N	136	ARG
1	N	143	THR
1	N	184	ILE

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Mol	Chain	Res	Type
1	N	191	SER
1	N	201	PRO
1	N	221	ARG
1	N	233	LEU
1	N	242	THR
1	N	248	SER
1	N	251	LEU
1	N	254	ILE
1	N	255	LEU
1	N	258	LEU
1	N	259	SER
1	N	265	LEU
1	N	267	ASP
1	N	268	SER
1	N	269	LEU
1	N	286	SER
1	N	290	SER
1	N	291	SER
1	N	304	MSE
1	N	337	LEU
1	N	363	LEU
1	N	380	LEU
1	N	391	ARG
1	N	404	GLU
1	N	417	ASP
1	N	419	ILE
1	N	424	LEU
1	N	428	LEU
1	O	1	MSE
1	O	6	LEU
1	O	10	LEU
1	O	27	GLU
1	O	45	THR
1	O	54	LEU
1	O	60	LYS
1	O	64	ASN
1	O	66	THR
1	O	68	ARG
1	O	76	LEU
1	O	78	THR
1	O	82	LEU
1	O	85	LEU

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Mol	Chain	Res	Type
1	O	99	PHE
1	O	115	LEU
1	O	117	SER
1	O	119	LEU
1	O	123	LEU
1	O	129	ASP
1	O	134	ASP
1	O	154	LYS
1	O	184	ILE
1	O	192	SER
1	O	196	HIS
1	O	215	ILE
1	O	221	ARG
1	O	251	LEU
1	O	252	SER
1	O	254	ILE
1	O	255	LEU
1	O	265	LEU
1	O	269	LEU
1	O	291	SER
1	O	304	MSE
1	O	337	LEU
1	O	340	SER
1	O	341	GLN
1	O	357	PHE
1	O	375	SER
1	O	379	GLU
1	O	382	SER
1	O	391	ARG
1	O	396	SER
1	O	404	GLU
1	O	408	THR
1	O	414	THR
1	O	416	LEU
1	O	417	ASP
1	O	418	SER
1	O	424	LEU
1	O	428	LEU
1	P	1	MSE
1	P	26	THR
1	P	35	TYR
1	P	36	GLN

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Mol	Chain	Res	Type
1	P	37	GLN
1	P	46	ASN
1	P	48	GLN
1	P	52	HIS
1	P	54	LEU
1	P	57	ILE
1	P	60	LYS
1	P	64	ASN
1	P	66	THR
1	P	76	LEU
1	P	82	LEU
1	P	83	LEU
1	P	107	GLN
1	P	108	LEU
1	P	113	SER
1	P	115	LEU
1	P	117	SER
1	P	119	LEU
1	P	123	LEU
1	P	134	ASP
1	P	154	LYS
1	P	184	ILE
1	P	191	SER
1	P	192	SER
1	P	196	HIS
1	P	221	ARG
1	P	233	LEU
1	P	242	THR
1	P	251	LEU
1	P	254	ILE
1	P	255	LEU
1	P	259	SER
1	P	269	LEU
1	P	282	ILE
1	P	292	THR
1	P	302	ASP
1	P	304	MSE
1	P	341	GLN
1	P	363	LEU
1	P	375	SER
1	P	379	GLU
1	P	386	ASP

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Mol	Chain	Res	Type
1	P	416	LEU
1	P	424	LEU
1	Q	4	GLN
1	Q	10	LEU
1	Q	26	THR
1	Q	35	TYR
1	Q	48	GLN
1	Q	52	HIS
1	Q	54	LEU
1	Q	60	LYS
1	Q	61	THR
1	Q	63	PHE
1	Q	65	ASN
1	Q	79	VAL
1	Q	108	LEU
1	Q	115	LEU
1	Q	123	LEU
1	Q	126	HIS
1	Q	128	GLU
1	Q	192	SER
1	Q	196	HIS
1	Q	216	ARG
1	Q	221	ARG
1	Q	232	ASP
1	Q	233	LEU
1	Q	242	THR
1	Q	245	ILE
1	Q	248	SER
1	Q	251	LEU
1	Q	254	ILE
1	Q	255	LEU
1	Q	257	ILE
1	Q	259	SER
1	Q	265	LEU
1	Q	266	ASP
1	Q	268	SER
1	Q	269	LEU
1	Q	277	LEU
1	Q	291	SER
1	Q	302	ASP
1	Q	304	MSE
1	Q	337	LEU

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Mol	Chain	Res	Type
1	Q	341	GLN
1	Q	379	GLU
1	Q	391	ARG
1	Q	396	SER
1	Q	414	THR
1	Q	417	ASP
1	Q	419	ILE
1	Q	424	LEU
1	Q	427	SER
1	R	1	MSE
1	R	3	LEU
1	R	13	VAL
1	R	26	THR
1	R	45	THR
1	R	54	LEU
1	R	60	LYS
1	R	61	THR
1	R	66	THR
1	R	76	LEU
1	R	82	LEU
1	R	115	LEU
1	R	117	SER
1	R	119	LEU
1	R	123	LEU
1	R	126	HIS
1	R	129	ASP
1	R	149	ASP
1	R	154	LYS
1	R	191	SER
1	R	192	SER
1	R	196	HIS
1	R	221	ARG
1	R	251	LEU
1	R	254	ILE
1	R	264	SER
1	R	266	ASP
1	R	267	ASP
1	R	269	LEU
1	R	277	LEU
1	R	280	SER
1	R	304	MSE
1	R	340	SER

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Mol	Chain	Res	Type
1	R	363	LEU
1	R	391	ARG
1	R	396	SER
1	R	404	GLU
1	R	416	LEU
1	R	428	LEU
1	S	26	THR
1	S	45	THR
1	S	52	HIS
1	S	54	LEU
1	S	55	ASP
1	S	57	ILE
1	S	60	LYS
1	S	65	ASN
1	S	66	THR
1	S	76	LEU
1	S	77	LYS
1	S	82	LEU
1	S	87	ARG
1	S	115	LEU
1	S	119	LEU
1	S	123	LEU
1	S	149	ASP
1	S	156	ILE
1	S	180	VAL
1	S	196	HIS
1	S	221	ARG
1	S	233	LEU
1	S	242	THR
1	S	251	LEU
1	S	254	ILE
1	S	255	LEU
1	S	258	LEU
1	S	265	LEU
1	S	267	ASP
1	S	268	SER
1	S	269	LEU
1	S	277	LEU
1	S	304	MSE
1	S	337	LEU
1	S	375	SER
1	S	404	GLU

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Mol	Chain	Res	Type
1	S	414	THR
1	S	424	LEU
1	S	428	LEU
1	T	36	GLN
1	T	45	THR
1	T	55	ASP
1	T	57	ILE
1	T	61	THR
1	T	69	ARG
1	T	76	LEU
1	T	78	THR
1	T	82	LEU
1	T	85	LEU
1	T	90	VAL
1	T	104	SER
1	T	108	LEU
1	T	113	SER
1	T	115	LEU
1	T	126	HIS
1	T	134	ASP
1	T	143	THR
1	T	149	ASP
1	T	153	SER
1	T	191	SER
1	T	196	HIS
1	T	221	ARG
1	T	251	LEU
1	T	255	LEU
1	T	258	LEU
1	T	259	SER
1	T	265	LEU
1	T	266	ASP
1	T	269	LEU
1	T	286	SER
1	T	291	SER
1	T	304	MSE
1	T	337	LEU
1	T	340	SER
1	T	341	GLN
1	T	362	LYS
1	T	363	LEU
1	T	396	SER

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Mol	Chain	Res	Type
1	T	400	LYS
1	T	415	ARG
1	T	424	LEU
1	T	428	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	B	12	ASN
1	B	65	ASN
1	C	36	GLN
1	C	368	HIS
1	F	218	GLN
1	G	42	GLN
1	G	96	GLN
1	G	170	GLN
1	G	196	HIS
1	G	200	ASN
1	G	218	GLN
1	H	107	GLN
1	I	196	HIS
1	I	197	HIS
1	J	36	GLN
1	K	165	GLN
1	L	36	GLN
1	L	185	GLN
1	L	368	HIS
1	M	260	HIS
1	M	368	HIS
1	N	36	GLN
1	N	96	GLN
1	N	107	GLN
1	N	185	GLN
1	O	65	ASN
1	O	170	GLN
1	P	107	GLN
1	P	426	ASN
1	Q	36	GLN
1	R	301	HIS
1	R	368	HIS
1	S	36	GLN

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Mol	Chain	Res	Type
1	S	107	GLN
1	S	197	HIS
1	S	353	ASN
1	T	36	GLN
1	T	107	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	397/434 (91%)	-0.39	6 (1%) 76 71	56, 93, 146, 184	0
1	B	386/434 (88%)	-0.52	0 100 100	55, 89, 133, 176	0
1	C	386/434 (88%)	-0.61	3 (0%) 87 84	56, 80, 125, 155	0
1	D	386/434 (88%)	-0.50	4 (1%) 84 80	56, 86, 126, 166	0
1	E	386/434 (88%)	-0.48	2 (0%) 91 90	55, 86, 144, 192	0
1	F	386/434 (88%)	-0.55	1 (0%) 94 94	57, 93, 130, 164	0
1	G	386/434 (88%)	-0.56	0 100 100	53, 84, 123, 149	0
1	H	386/434 (88%)	-0.35	4 (1%) 84 80	56, 102, 155, 199	0
1	I	386/434 (88%)	-0.49	2 (0%) 91 90	51, 85, 124, 171	0
1	J	386/434 (88%)	-0.49	1 (0%) 94 94	52, 93, 137, 179	0
1	K	397/434 (91%)	-0.36	10 (2%) 61 54	58, 89, 139, 212	0
1	L	386/434 (88%)	-0.51	1 (0%) 94 94	51, 84, 126, 168	0
1	M	386/434 (88%)	-0.49	6 (1%) 74 69	48, 85, 144, 176	0
1	N	386/434 (88%)	-0.49	2 (0%) 91 90	50, 85, 133, 177	0
1	O	386/434 (88%)	-0.53	0 100 100	47, 77, 117, 162	0
1	P	386/434 (88%)	-0.44	4 (1%) 84 80	53, 85, 142, 188	0
1	Q	386/434 (88%)	-0.24	12 (3%) 52 46	51, 101, 154, 201	0
1	R	386/434 (88%)	-0.55	1 (0%) 94 94	54, 85, 129, 164	0
1	S	386/434 (88%)	-0.33	6 (1%) 74 69	69, 106, 155, 189	0
1	T	386/434 (88%)	-0.41	4 (1%) 84 80	62, 94, 151, 193	0
All	All	7742/8680 (89%)	-0.46	69 (0%) 85 82	47, 89, 141, 212	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	328	SER	7.4
1	K	329	SER	6.9
1	K	327	GLY	6.2
1	H	161	ASP	5.5
1	I	161	ASP	4.9
1	L	305	SER	4.6
1	A	328	SER	4.6
1	K	330	GLN	4.0
1	A	329	SER	3.9
1	P	161	ASP	3.7
1	A	431	VAL	3.7
1	K	305	SER	3.6
1	K	306	THR	3.3
1	Q	11	TRP	3.3
1	S	40	PRO	3.3
1	Q	40	PRO	3.2
1	H	38	ARG	3.2
1	S	88	GLN	3.2
1	N	2	PRO	3.1
1	T	160	GLY	3.0
1	S	2	PRO	3.0
1	A	327	GLY	2.9
1	Q	3	LEU	2.9
1	M	3	LEU	2.8
1	M	159	LEU	2.7
1	P	159	LEU	2.7
1	A	131	TRP	2.7
1	P	160	GLY	2.7
1	M	160	GLY	2.7
1	M	336	SER	2.6
1	H	160	GLY	2.6
1	Q	27	GLU	2.6
1	F	415	ARG	2.6
1	R	431	VAL	2.5
1	D	160	GLY	2.5
1	P	4	GLN	2.5
1	T	161	ASP	2.5
1	K	431	VAL	2.5
1	Q	12	ASN	2.5
1	D	431	VAL	2.4
1	H	159	LEU	2.4
1	E	431	VAL	2.4
1	C	161	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	160	GLY	2.4
1	T	60	LYS	2.4
1	N	27	GLU	2.3
1	C	160	GLY	2.3
1	K	2	PRO	2.3
1	Q	50	ILE	2.3
1	S	160	GLY	2.3
1	Q	4	GLN	2.3
1	Q	161	ASP	2.3
1	Q	6	LEU	2.3
1	E	2	PRO	2.2
1	T	431	VAL	2.2
1	S	41	LYS	2.1
1	Q	56	GLU	2.1
1	K	4	GLN	2.1
1	C	431	VAL	2.1
1	M	158	ASN	2.1
1	A	60	LYS	2.1
1	Q	117	SER	2.1
1	S	375	SER	2.1
1	J	126	HIS	2.0
1	K	38	ARG	2.0
1	M	161	ASP	2.0
1	Q	37	GLN	2.0
1	D	161	ASP	2.0
1	D	158	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.