



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 30, 2025 – 04:23 PM JST

PDB ID : 9IOV / pdb_00009iov
Title : Gossypol bound lactate dehydrogenase A
Authors : Ha, M.S.; Han, C.W.; Jeong, M.S.; Jang, S.B.
Deposited on : 2024-07-09
Resolution : 3.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

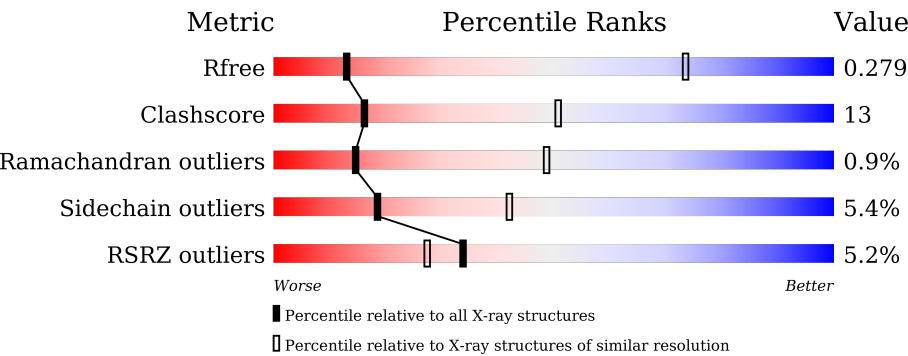
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.98 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}	164625	1059 (4.20-3.76)
Clashscore	180529	1124 (4.20-3.76)
Ramachandran outliers	177936	1073 (4.20-3.76)
Sidechain outliers	177891	1064 (4.20-3.76)
RSRZ outliers	164620	1060 (4.20-3.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	<div><div>2%</div><div>79%</div><div>17%</div><div>..</div></div>
1	B	331	<div><div>2%</div><div>77%</div><div>17%</div><div>5%</div><div>.</div></div>
1	C	331	<div><div>2%</div><div>78%</div><div>18%</div><div>..</div></div>
1	D	331	<div><div>2%</div><div>79%</div><div>17%</div><div>..</div></div>
1	E	331	<div><div>2%</div><div>77%</div><div>19%</div><div>..</div></div>
1	F	331	<div><div>3%</div><div>76%</div><div>20%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	G	331	<div> <div>2%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	H	331	<div> <div>2%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	I	331	<div> <div>2%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	J	331	<div> <div>4%</div> <div>78%</div> <div>18%</div> <div>..</div> </div>
1	K	331	<div> <div>5%</div> <div>75%</div> <div>18%</div> <div>6%</div> <div>.</div> </div>
1	L	331	<div> <div>7%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	M	331	<div> <div>3%</div> <div>77%</div> <div>18%</div> <div>..</div> </div>
1	N	331	<div> <div>6%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	O	331	<div> <div>6%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>
1	P	331	<div> <div>6%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
1	Q	331	<div> <div>8%</div> <div>76%</div> <div>18%</div> <div>5%</div> <div>.</div> </div>
1	R	331	<div> <div>11%</div> <div>76%</div> <div>18%</div> <div>..</div> </div>
1	S	331	<div> <div>8%</div> <div>79%</div> <div>15%</div> <div>..</div> </div>
1	T	331	<div> <div>5%</div> <div>78%</div> <div>18%</div> <div>..</div> </div>
1	U	331	<div> <div>15%</div> <div>76%</div> <div>17%</div> <div>7%</div> </div>
1	V	331	<div> <div>9%</div> <div>82%</div> <div>13%</div> <div>..</div> </div>
1	W	331	<div> <div>4%</div> <div>74%</div> <div>20%</div> <div>5%</div> <div>.</div> </div>
1	X	331	<div> <div>11%</div> <div>79%</div> <div>15%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 61670 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 L-lactate dehydrogenase A chain.

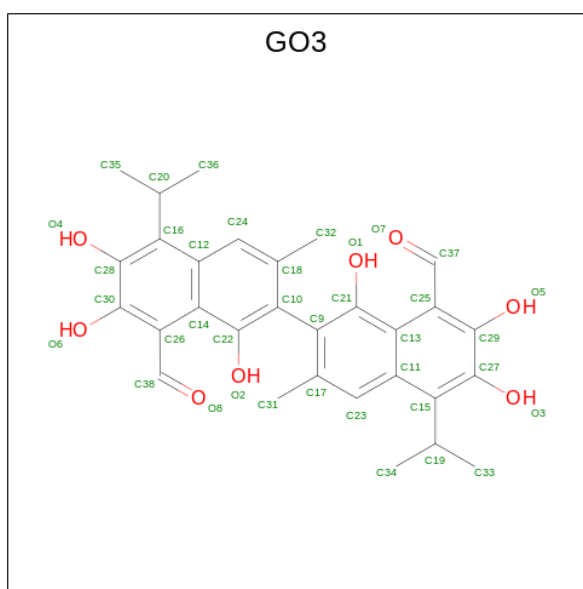
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	B	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	C	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	D	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	E	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	F	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	G	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	H	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	I	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	J	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	K	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	L	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	M	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	N	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	O	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	P	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	R	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	S	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	T	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	U	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	V	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	W	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	X	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			

- Molecule 2 is Gossypol (CCD ID: GO3) (formula: $C_{30}H_{30}O_8$) (labeled as "Ligand of Interest" by depositor).

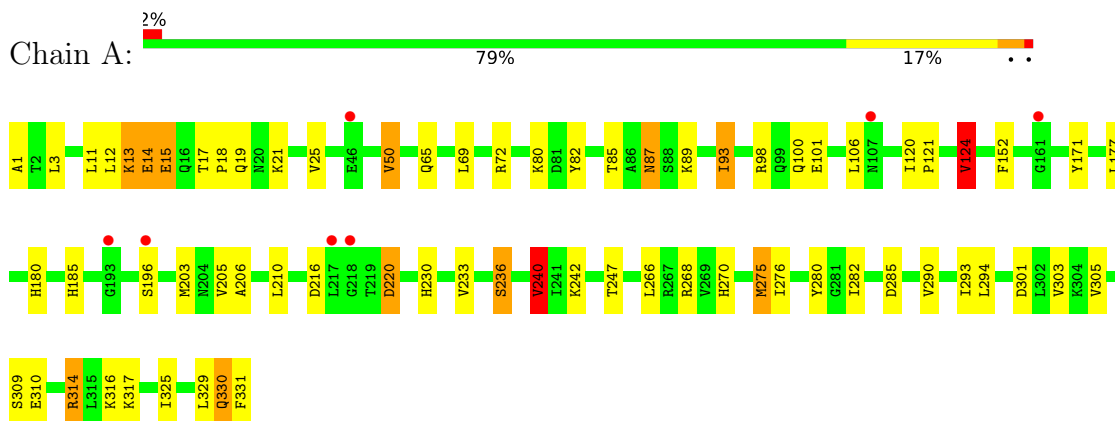


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	Q	1	Total	C	O	0	0
			38	30	8		

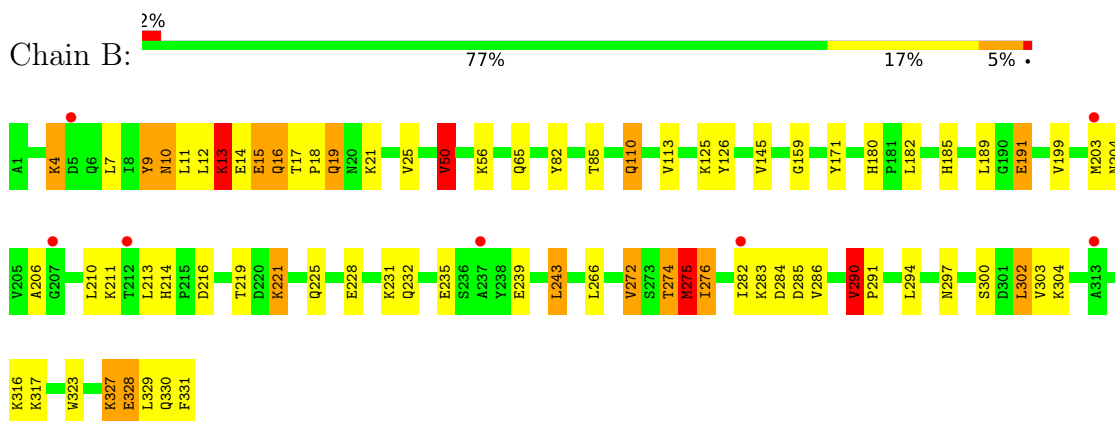
3 Residue-property plots [i](#)

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

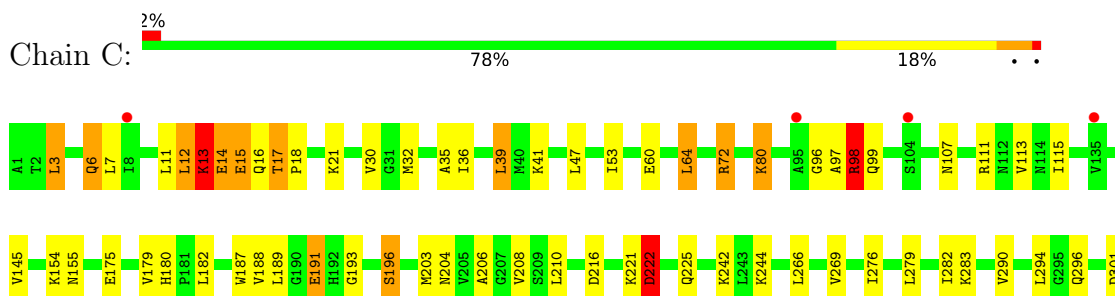
• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain

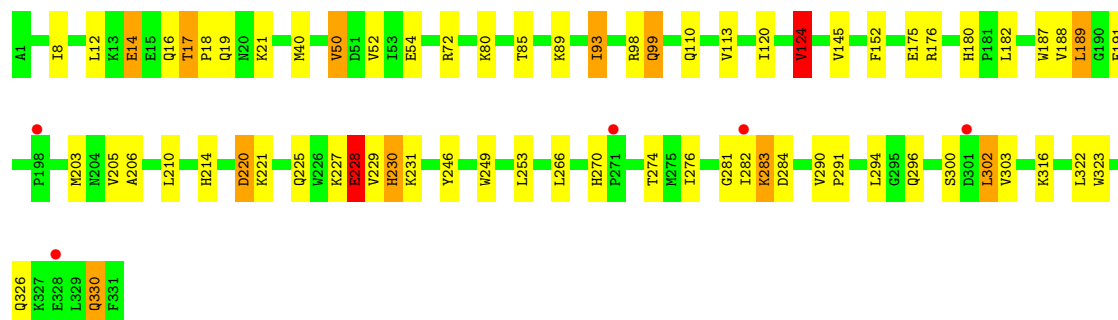
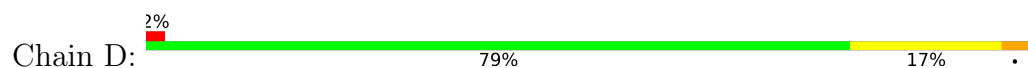


• Molecule 1: L-lactate dehydrogenase A chain

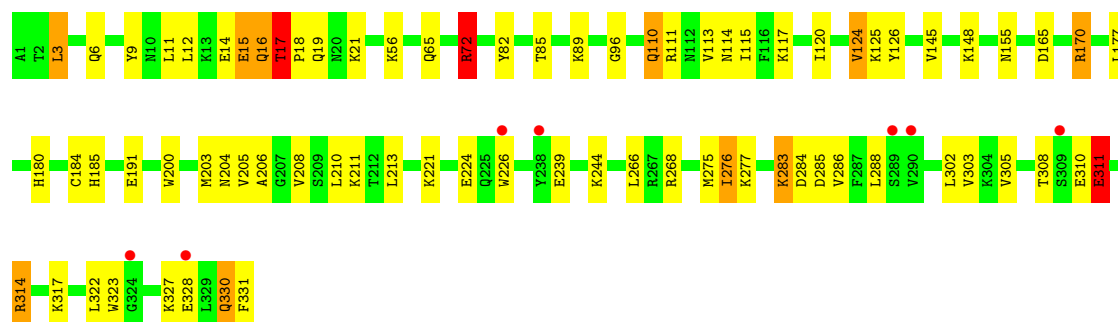
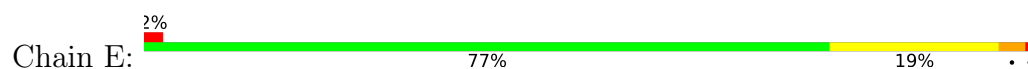




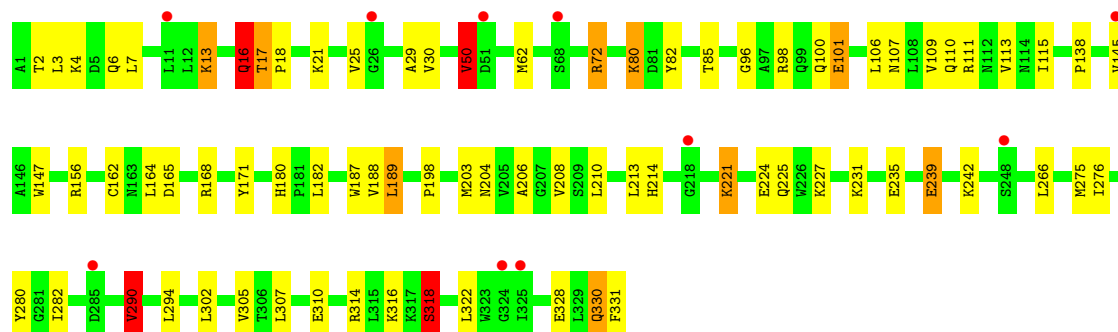
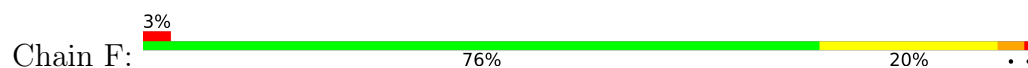
- Molecule 1: L-lactate dehydrogenase A chain



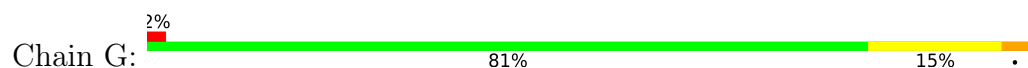
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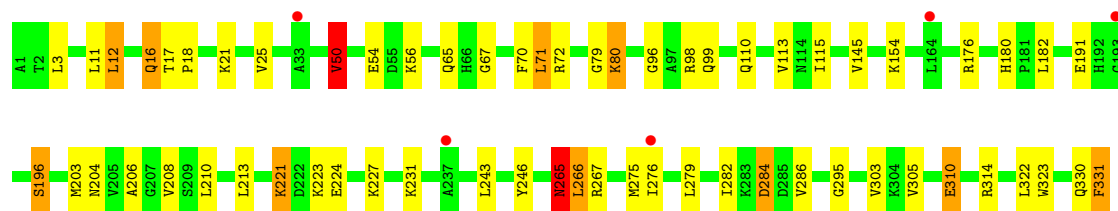


- Molecule 1: L-lactate dehydrogenase A chain

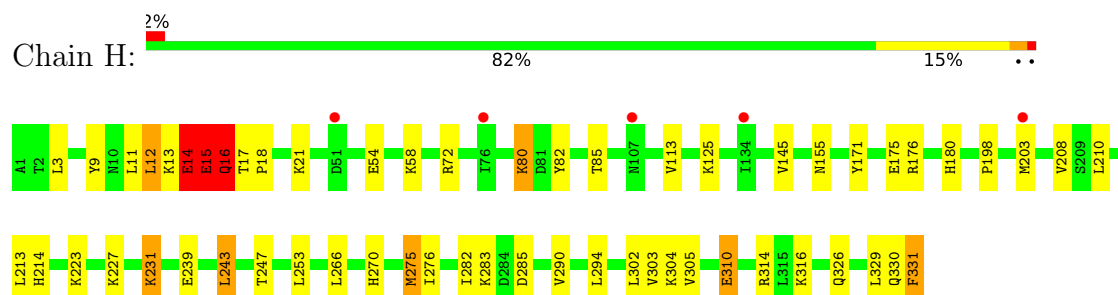


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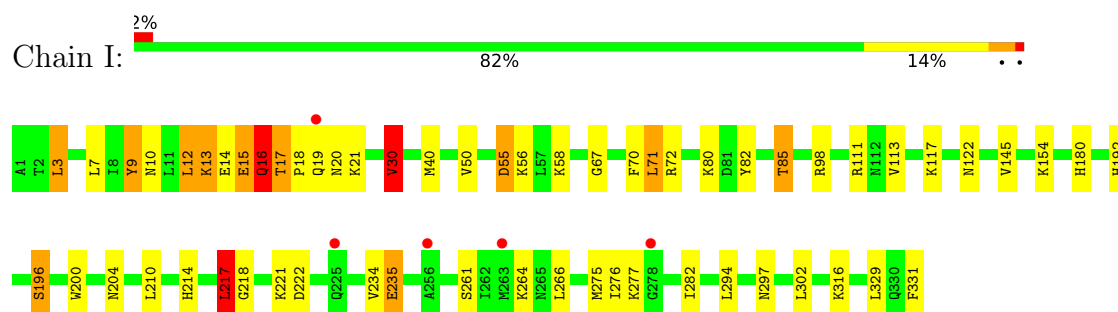




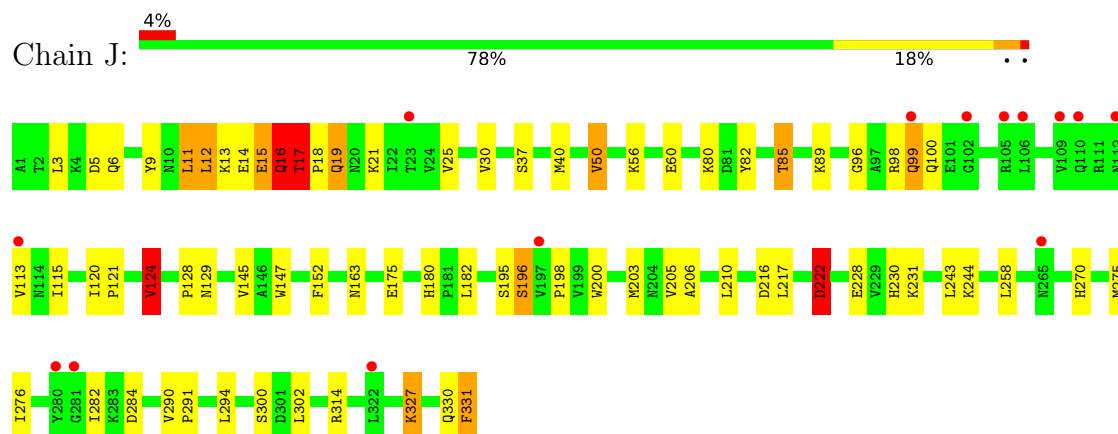
• Molecule 1: L-lactate dehydrogenase A chain



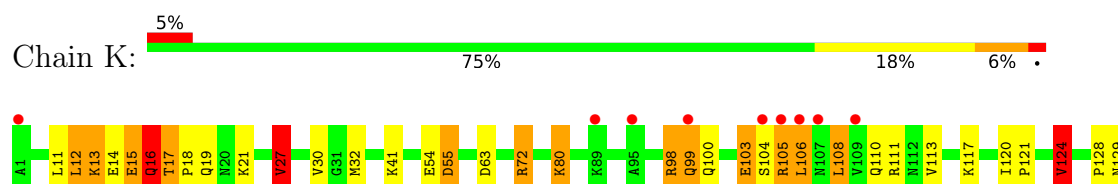
• Molecule 1: L-lactate dehydrogenase A chain

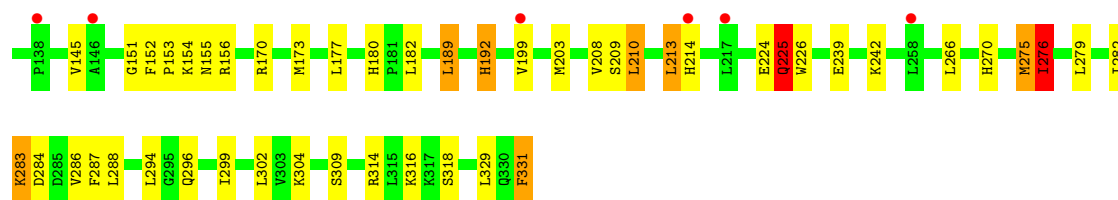


• Molecule 1: L-lactate dehydrogenase A chain

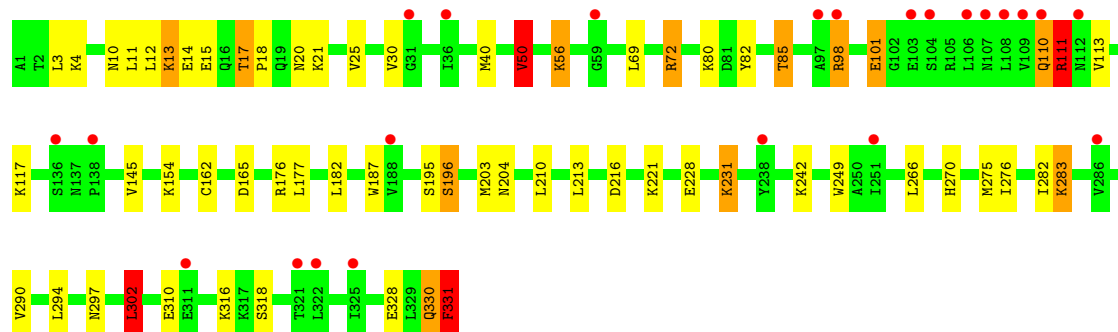
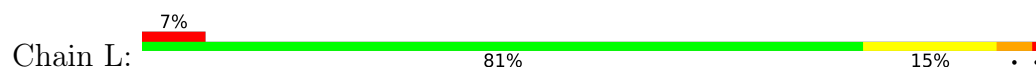


• Molecule 1: L-lactate dehydrogenase A chain

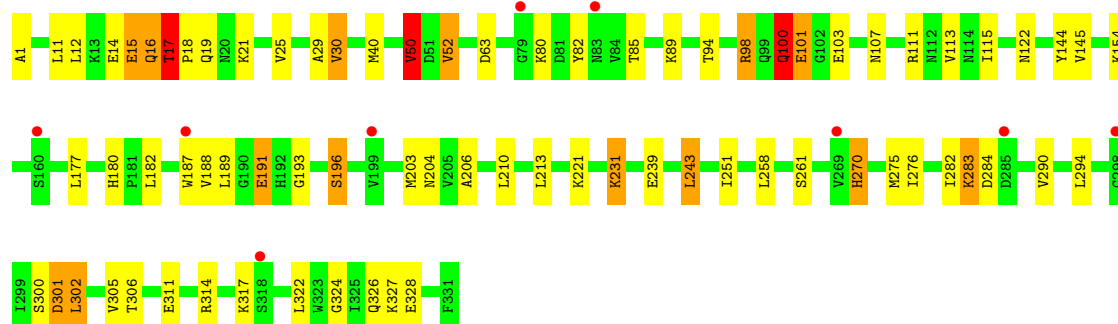
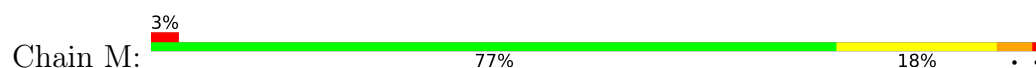




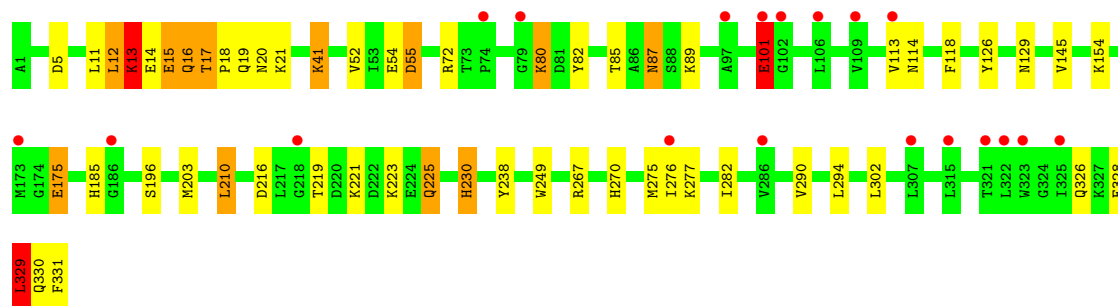
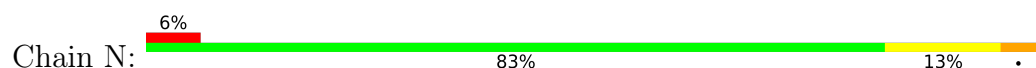
• Molecule 1: L-lactate dehydrogenase A chain



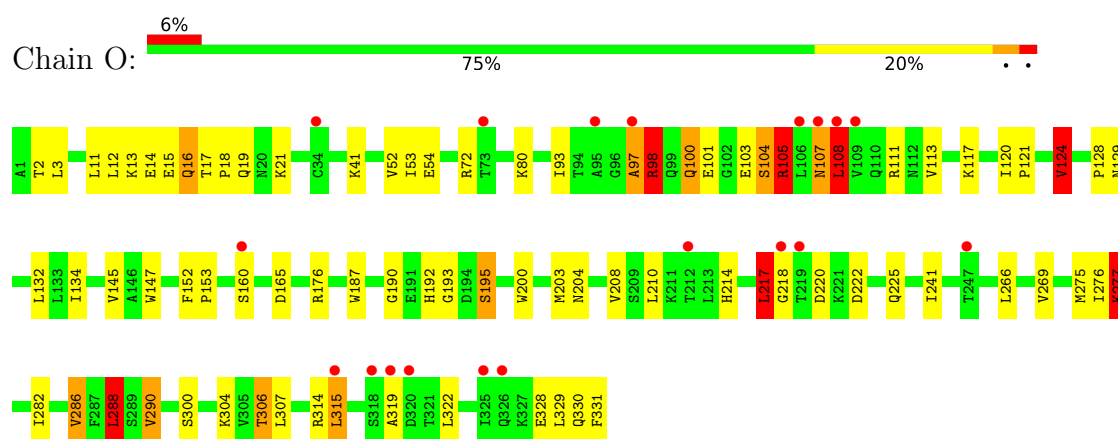
• Molecule 1: L-lactate dehydrogenase A chain



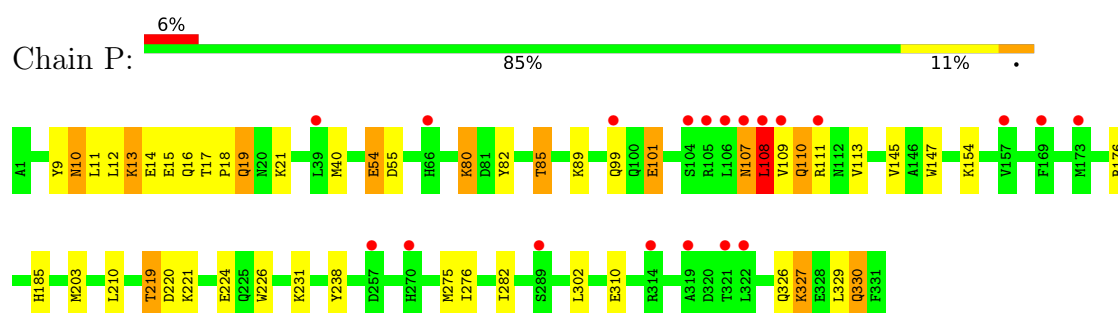
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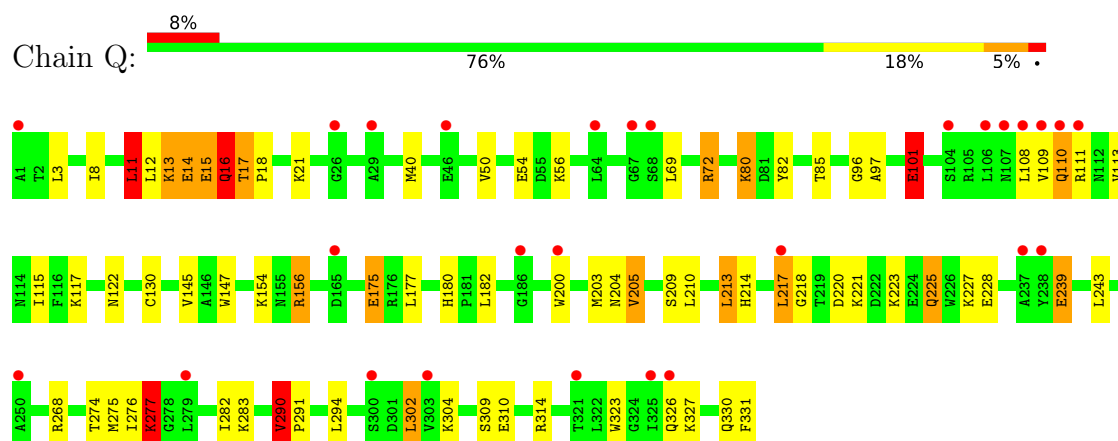
• Molecule 1: L-lactate dehydrogenase A chain



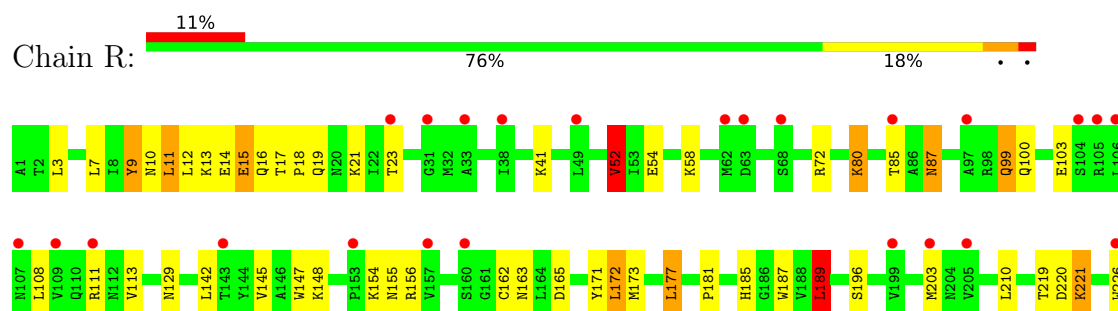
• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain

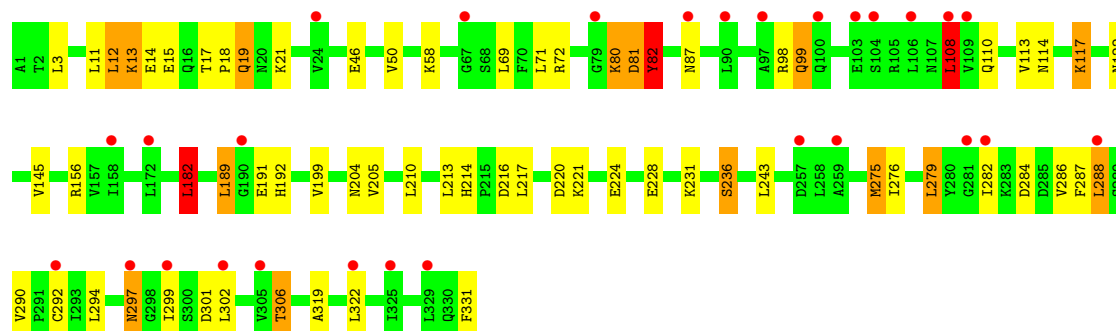
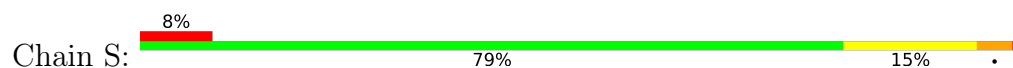


• Molecule 1: L-lactate dehydrogenase A chain

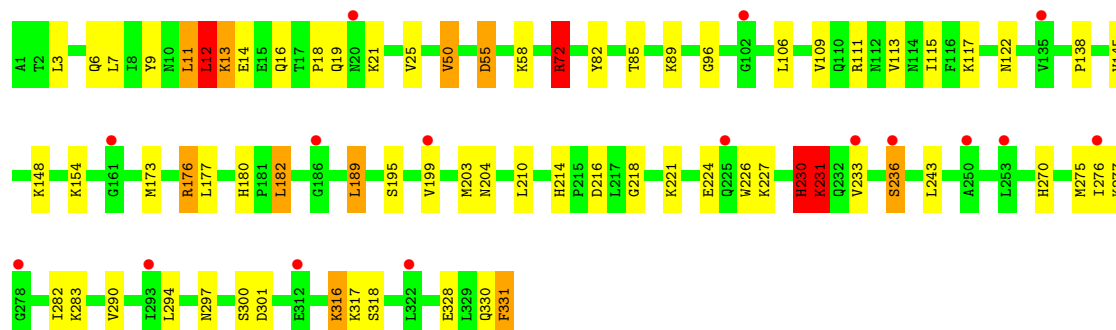
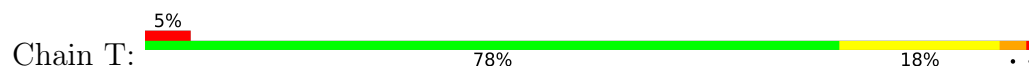




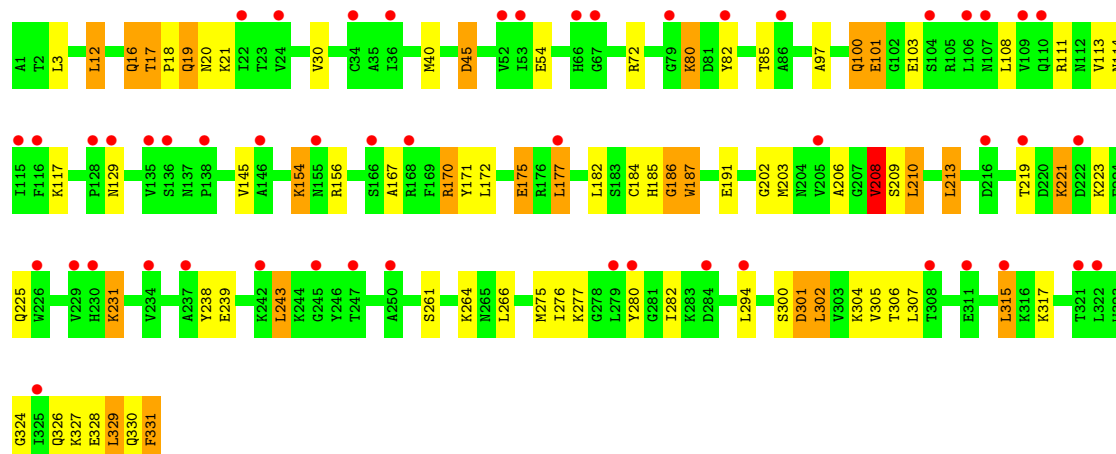
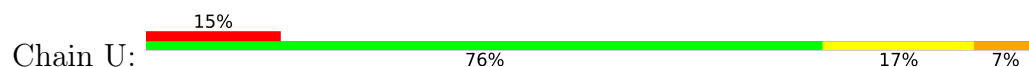
- Molecule 1: L-lactate dehydrogenase A chain



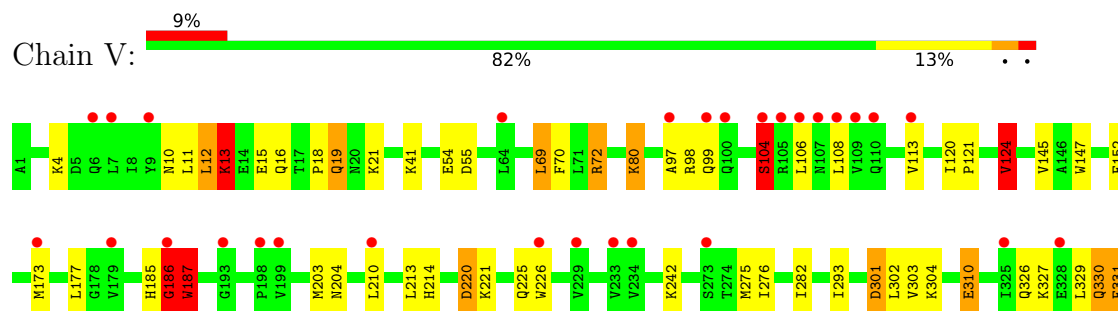
- Molecule 1: L-lactate dehydrogenase A chain



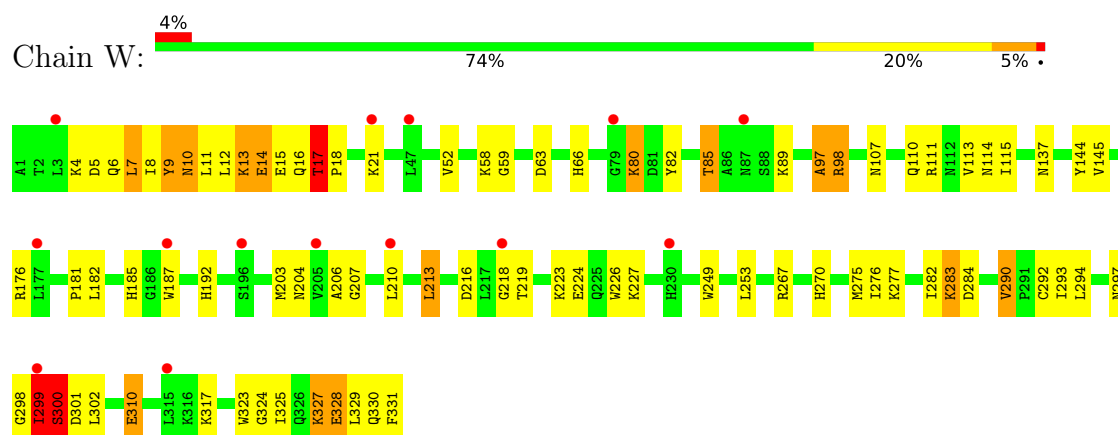
- Molecule 1: L-lactate dehydrogenase A chain



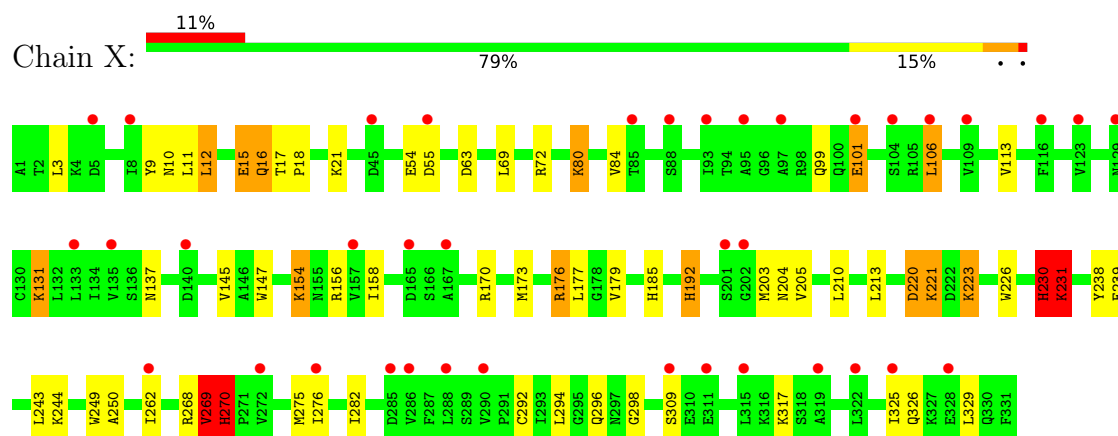
- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.37Å 110.92Å 217.55Å 89.98° 90.04° 88.37°	Depositor
Resolution (Å)	35.56 – 3.98 35.56 – 3.98	Depositor EDS
% Data completeness (in resolution range)	99.1 (35.56-3.98) 99.2 (35.56-3.98)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 3.99Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.238 , 0.273 0.244 , 0.279	Depositor DCC
R_{free} test set	3837 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l 0.056 for -h,k,-l 0.130 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	61670	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GO3

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	0.57	0/2612	1.12	16/3532 (0.5%)
1	B	0.59	1/2612 (0.0%)	1.14	18/3532 (0.5%)
1	C	0.57	0/2612	1.09	11/3532 (0.3%)
1	D	0.58	1/2612 (0.0%)	1.15	17/3532 (0.5%)
1	E	0.59	2/2612 (0.1%)	1.10	9/3532 (0.3%)
1	F	0.54	0/2612	1.10	12/3532 (0.3%)
1	G	0.58	1/2612 (0.0%)	1.10	15/3532 (0.4%)
1	H	0.56	0/2612	1.09	13/3532 (0.4%)
1	I	0.55	0/2612	1.10	13/3532 (0.4%)
1	J	0.59	1/2612 (0.0%)	1.08	13/3532 (0.4%)
1	K	0.67	2/2612 (0.1%)	1.20	18/3532 (0.5%)
1	L	0.55	0/2612	1.06	13/3532 (0.4%)
1	M	0.58	1/2612 (0.0%)	1.10	16/3532 (0.5%)
1	N	0.57	1/2612 (0.0%)	1.07	7/3532 (0.2%)
1	O	0.62	1/2612 (0.0%)	1.25	29/3532 (0.8%)
1	P	0.56	0/2612	1.16	17/3532 (0.5%)
1	Q	0.61	0/2612	1.15	21/3532 (0.6%)
1	R	0.63	1/2612 (0.0%)	1.13	17/3532 (0.5%)
1	S	0.74	5/2612 (0.2%)	1.25	22/3532 (0.6%)
1	T	0.58	0/2612	1.20	10/3532 (0.3%)
1	U	0.59	1/2612 (0.0%)	1.17	18/3532 (0.5%)
1	V	0.60	0/2612	1.10	12/3532 (0.3%)
1	W	0.57	1/2612 (0.0%)	1.11	10/3532 (0.3%)
1	X	0.58	1/2612 (0.0%)	1.19	22/3532 (0.6%)
All	All	0.59	20/62688 (0.0%)	1.14	369/84768 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	K	0	3
1	L	0	2
1	N	0	3
1	O	0	1
1	P	0	2
1	Q	0	1
1	R	0	2
1	S	0	1
1	T	0	3
1	U	0	4
1	V	0	6
1	W	0	3
1	X	0	4
All	All	0	48

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	230	HIS	CE1-NE2	-13.08	1.19	1.32
1	J	230	HIS	CE1-NE2	-10.55	1.22	1.32
1	N	230	HIS	CE1-NE2	-9.01	1.23	1.32
1	G	284	ASP	CG-OD1	-8.15	1.09	1.25
1	U	12	LEU	C-O	-7.40	1.14	1.23
1	S	192	HIS	CG-CD2	6.96	1.43	1.35
1	O	214	HIS	CE1-NE2	-6.62	1.25	1.32
1	E	165	ASP	CG-OD2	-6.58	1.12	1.25
1	S	191	GLU	CD-OE1	6.43	1.37	1.25
1	M	284	ASP	CG-OD2	-5.98	1.14	1.25
1	K	318	SER	CB-OG	-5.75	1.30	1.42
1	X	192	HIS	CE1-NE2	5.61	1.38	1.32
1	W	284	ASP	CG-OD2	-5.60	1.14	1.25
1	E	311	GLU	CD-OE1	-5.59	1.14	1.25
1	K	214	HIS	CD2-NE2	-5.39	1.31	1.37
1	S	108	LEU	C-O	-5.37	1.17	1.24
1	S	287	PHE	C-O	-5.31	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	216	ASP	CG-OD2	5.26	1.35	1.25
1	D	230	HIS	C-O	-5.05	1.17	1.24
1	B	228	GLU	CD-OE2	5.05	1.34	1.25

All (369) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	72	ARG	CB-CG-CD	18.98	154.95	111.30
1	T	230	HIS	O-C-N	-17.09	99.53	122.43
1	X	230	HIS	O-C-N	-16.57	100.23	122.43
1	O	72	ARG	CB-CG-CD	13.99	143.49	111.30
1	A	72	ARG	CB-CG-CD	13.98	143.46	111.30
1	K	103	GLU	CB-CG-CD	13.71	135.90	112.60
1	C	222	ASP	CA-CB-CG	13.27	125.87	112.60
1	E	72	ARG	CB-CG-CD	12.80	140.73	111.30
1	P	107	ASN	CA-C-N	-12.76	105.59	123.20
1	P	107	ASN	C-N-CA	-12.76	105.59	123.20
1	S	81	ASP	CA-C-N	12.46	145.33	121.54
1	S	81	ASP	C-N-CA	12.46	145.33	121.54
1	T	55	ASP	CA-CB-CG	12.37	124.97	112.60
1	U	186	GLY	CA-C-N	12.12	144.70	121.54
1	U	186	GLY	C-N-CA	12.12	144.70	121.54
1	F	72	ARG	CG-CD-NE	12.04	138.48	112.00
1	P	54	GLU	CB-CG-CD	11.91	132.85	112.60
1	K	99	GLN	CB-CG-CD	11.84	132.72	112.60
1	O	98	ARG	CB-CA-C	-11.60	87.34	110.42
1	M	191	GLU	CB-CG-CD	11.20	131.65	112.60
1	E	170	ARG	CB-CG-CD	-11.19	85.56	111.30
1	C	222	ASP	CB-CA-C	-10.87	88.80	110.42
1	V	186	GLY	CA-C-N	10.59	141.78	121.54
1	V	186	GLY	C-N-CA	10.59	141.78	121.54
1	F	156	ARG	NE-CZ-NH1	10.59	132.09	121.50
1	Q	72	ARG	CB-CG-CD	10.19	134.74	111.30
1	D	225	GLN	CB-CG-CD	-10.16	95.32	112.60
1	W	299	ILE	CB-CA-C	9.99	127.67	111.29
1	W	300	SER	N-CA-CB	9.98	127.36	110.49
1	D	230	HIS	O-C-N	-9.89	109.17	122.43
1	B	276	ILE	N-CA-CB	9.87	127.51	111.23
1	D	230	HIS	CA-C-O	9.82	131.46	119.38
1	T	11	LEU	CB-CA-C	-9.73	98.17	112.09
1	V	104	SER	CA-C-O	-9.65	110.57	121.19
1	C	98	ARG	N-CA-CB	9.58	126.68	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	231	LYS	N-CA-C	-9.56	100.37	112.90
1	O	314	ARG	CG-CD-NE	-9.54	91.02	112.00
1	V	124	VAL	CA-CB-CG2	9.51	126.56	110.40
1	J	222	ASP	CB-CA-C	9.46	123.78	110.16
1	S	81	ASP	CB-CA-C	9.41	129.15	110.42
1	O	105	ARG	N-CA-CB	9.36	126.31	110.49
1	O	288	LEU	N-CA-CB	-9.30	95.67	111.21
1	M	101	GLU	CB-CA-C	9.30	128.93	110.42
1	U	114	ASN	CA-CB-CG	9.29	121.89	112.60
1	U	101	GLU	CB-CA-C	9.22	128.78	110.42
1	X	269	VAL	CB-CA-C	9.21	126.40	111.29
1	J	124	VAL	CA-CB-CG2	9.11	125.89	110.40
1	Q	239	GLU	CB-CG-CD	9.00	127.90	112.60
1	X	239	GLU	CB-CG-CD	-9.00	97.30	112.60
1	N	101	GLU	CB-CA-C	8.91	128.14	110.42
1	R	9	TYR	N-CA-C	8.81	120.81	111.03
1	E	17	THR	CA-CB-OG1	8.80	122.81	109.60
1	S	214	HIS	CA-CB-CG	8.76	122.56	113.80
1	K	214	HIS	CA-CB-CG	8.71	122.51	113.80
1	L	101	GLU	CB-CA-C	8.67	127.67	110.42
1	C	314	ARG	CG-CD-NE	8.66	131.06	112.00
1	F	101	GLU	CB-CA-C	8.65	127.64	110.42
1	P	101	GLU	CB-CA-C	8.60	127.53	110.42
1	J	50	VAL	CA-CB-CG2	8.58	124.98	110.40
1	U	19	GLN	CB-CG-CD	-8.48	98.18	112.60
1	U	170	ARG	CB-CG-CD	-8.46	91.84	111.30
1	S	108	LEU	O-C-N	-8.42	111.05	122.33
1	Q	175	GLU	CB-CG-CD	8.37	126.83	112.60
1	X	101	GLU	CB-CA-C	8.34	127.02	110.42
1	I	30	VAL	CA-CB-CG1	8.34	124.58	110.40
1	R	308	THR	CA-CB-OG1	8.33	122.10	109.60
1	V	331	PHE	CA-CB-CG	8.28	122.08	113.80
1	I	55	ASP	CA-CB-CG	8.24	120.84	112.60
1	O	306	THR	CA-CB-OG1	8.22	121.93	109.60
1	X	269	VAL	CA-C-N	8.18	141.76	121.80
1	X	269	VAL	C-N-CA	8.18	141.76	121.80
1	G	265	ASN	CB-CA-C	8.16	126.67	110.42
1	S	306	THR	CA-CB-OG1	8.15	121.83	109.60
1	X	231	LYS	N-CA-C	-8.15	102.23	112.90
1	U	208	VAL	CA-C-O	-8.06	110.91	120.75
1	D	124	VAL	CA-CB-CG2	8.02	124.03	110.40
1	K	111	ARG	CB-CG-CD	8.00	129.70	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	GLU	CB-CA-C	7.93	124.29	110.01
1	J	99	GLN	CB-CG-CD	7.83	125.91	112.60
1	P	176	ARG	CD-NE-CZ	7.72	135.21	124.40
1	O	107	ASN	N-CA-CB	7.71	122.91	110.42
1	F	290	VAL	CA-CB-CG1	7.66	123.42	110.40
1	I	56	LYS	CB-CG-CD	7.64	128.87	111.30
1	O	277	LYS	CB-CA-C	7.64	125.62	110.42
1	B	17	THR	CB-CA-C	7.61	118.45	109.47
1	L	176	ARG	NE-CZ-NH1	-7.59	113.91	121.50
1	H	176	ARG	CD-NE-CZ	7.59	135.02	124.40
1	O	108	LEU	CD1-CG-CD2	-7.59	94.11	110.80
1	P	108	LEU	N-CA-CB	7.58	124.23	110.60
1	X	176	ARG	NE-CZ-NH1	-7.53	113.97	121.50
1	R	87	ASN	CA-CB-CG	7.52	120.12	112.60
1	O	104	SER	CA-C-N	7.52	135.90	121.54
1	O	104	SER	C-N-CA	7.52	135.90	121.54
1	T	176	ARG	CD-NE-CZ	7.50	134.90	124.40
1	M	270	HIS	CB-CG-CD2	7.48	140.92	131.20
1	P	176	ARG	NE-CZ-NH1	-7.48	114.02	121.50
1	D	326	GLN	OE1-CD-NE2	-7.46	115.14	122.60
1	R	290	VAL	CA-CB-CG1	7.45	123.06	110.40
1	H	16	GLN	CA-C-N	7.42	130.75	120.65
1	H	16	GLN	C-N-CA	7.42	130.75	120.65
1	V	186	GLY	O-C-N	-7.40	113.08	122.70
1	A	331	PHE	CB-CA-C	7.37	124.11	110.10
1	D	176	ARG	NE-CZ-NH1	-7.36	114.14	121.50
1	H	176	ARG	NE-CZ-NH1	-7.27	114.23	121.50
1	I	217	LEU	CB-CA-C	7.27	124.89	110.42
1	K	225	GLN	CA-CB-CG	-7.27	99.56	114.10
1	H	72	ARG	CB-CG-CD	7.26	128.01	111.30
1	X	176	ARG	CD-NE-CZ	7.26	134.56	124.40
1	F	318	SER	CA-CB-OG	7.23	125.56	111.10
1	H	275	MET	CG-SD-CE	-7.21	85.04	100.90
1	P	19	GLN	CB-CG-CD	-7.20	100.36	112.60
1	D	228	GLU	CB-CG-CD	-7.20	100.37	112.60
1	L	176	ARG	CD-NE-CZ	7.19	134.47	124.40
1	G	176	ARG	CD-NE-CZ	7.17	134.44	124.40
1	D	176	ARG	CD-NE-CZ	7.15	134.41	124.40
1	O	286	VAL	CA-CB-CG1	7.14	122.53	110.40
1	E	111	ARG	NE-CZ-NH2	7.12	125.61	119.20
1	W	97	ALA	O-C-N	-7.12	114.46	122.86
1	K	192	HIS	CB-CA-C	7.11	124.58	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	288	LEU	N-CA-CB	-7.11	100.33	111.56
1	M	80	LYS	CA-CB-CG	7.08	128.27	114.10
1	A	87	ASN	CA-CB-CG	7.07	119.67	112.60
1	W	330	GLN	N-CA-CB	-7.07	99.55	110.29
1	A	124	VAL	CA-CB-CG2	7.05	122.39	110.40
1	A	329	LEU	CA-C-N	7.02	133.59	122.21
1	A	329	LEU	C-N-CA	7.02	133.59	122.21
1	D	72	ARG	CB-CG-CD	7.02	127.44	111.30
1	K	239	GLU	CB-CG-CD	6.96	124.42	112.60
1	K	214	HIS	CB-CG-CD2	6.95	140.24	131.20
1	O	107	ASN	CB-CA-C	6.95	123.32	110.11
1	Q	205	VAL	CB-CA-C	6.95	122.69	111.29
1	Q	213	LEU	CB-CA-C	6.95	124.01	110.67
1	O	217	LEU	CB-CA-C	6.94	124.23	110.42
1	T	230	HIS	CA-C-O	6.93	127.90	119.38
1	L	331	PHE	CA-CB-CG	6.92	120.72	113.80
1	O	328	GLU	CB-CG-CD	6.92	124.36	112.60
1	O	124	VAL	CA-CB-CG2	6.91	122.14	110.40
1	A	100	GLN	CB-CG-CD	-6.90	100.88	112.60
1	X	156	ARG	NE-CZ-NH1	6.89	128.39	121.50
1	G	176	ARG	NE-CZ-NH1	-6.89	114.61	121.50
1	L	56	LYS	CG-CD-CE	6.87	127.11	111.30
1	X	230	HIS	CA-C-O	6.84	127.80	119.38
1	K	124	VAL	CA-CB-CG2	6.84	122.02	110.40
1	Q	205	VAL	CA-C-O	-6.83	112.25	120.78
1	O	225	GLN	CB-CG-CD	6.79	124.15	112.60
1	O	214	HIS	CB-CG-CD2	6.78	140.01	131.20
1	B	274	THR	O-C-N	6.78	131.47	122.73
1	G	310	GLU	CB-CG-CD	6.77	124.11	112.60
1	S	236	SER	N-CA-CB	6.73	119.77	110.01
1	G	110	GLN	CB-CG-CD	-6.71	101.19	112.60
1	W	310	GLU	CB-CG-CD	-6.71	101.19	112.60
1	S	331	PHE	CB-CA-C	6.67	122.76	110.10
1	C	6	GLN	CB-CG-CD	-6.64	101.32	112.60
1	J	327	LYS	CB-CG-CD	6.60	126.47	111.30
1	E	124	VAL	CA-CB-CG2	6.59	121.60	110.40
1	B	290	VAL	CA-CB-CG1	6.59	121.60	110.40
1	U	231	LYS	CB-CG-CD	6.58	126.44	111.30
1	T	111	ARG	NE-CZ-NH2	6.54	125.08	119.20
1	W	17	THR	CB-CA-C	-6.51	97.34	110.17
1	J	331	PHE	CA-CB-CG	6.50	120.30	113.80
1	U	45	ASP	CB-CA-C	-6.50	100.67	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	176	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	D	330	GLN	CB-CA-C	6.49	121.05	110.22
1	H	15	GLU	N-CA-CB	6.48	121.44	110.49
1	G	56	LYS	CG-CD-CE	6.47	126.18	111.30
1	P	9	TYR	CB-CA-C	6.47	121.68	111.39
1	X	55	ASP	CA-CB-CG	6.47	119.07	112.60
1	F	13	LYS	N-CA-C	-6.46	105.93	113.88
1	B	15	GLU	CB-CG-CD	6.45	123.56	112.60
1	S	236	SER	CB-CA-C	6.43	120.98	110.88
1	M	328	GLU	CB-CG-CD	6.43	123.53	112.60
1	B	9	TYR	CB-CA-C	6.43	123.21	110.42
1	A	314	ARG	CB-CG-CD	6.41	126.05	111.30
1	K	16	GLN	CA-C-N	6.41	129.26	120.67
1	K	16	GLN	C-N-CA	6.41	129.26	120.67
1	G	16	GLN	CA-C-N	6.38	137.37	121.80
1	G	16	GLN	C-N-CA	6.38	137.37	121.80
1	B	185	HIS	CB-CG-CD2	6.37	139.48	131.20
1	Q	314	ARG	CG-CD-NE	6.36	125.99	112.00
1	O	16	GLN	CA-C-N	6.34	137.28	121.80
1	O	16	GLN	C-N-CA	6.34	137.28	121.80
1	Q	277	LYS	CB-CA-C	6.33	123.01	110.42
1	H	310	GLU	CB-CG-CD	6.33	123.36	112.60
1	A	98	ARG	CB-CG-CD	6.31	125.81	111.30
1	V	187	TRP	N-CA-CB	6.29	121.12	110.49
1	R	9	TYR	N-CA-CB	6.28	119.09	109.98
1	X	15	GLU	CB-CA-C	6.26	120.12	111.23
1	K	192	HIS	O-C-N	-6.26	114.27	122.59
1	D	99	GLN	CB-CG-CD	6.25	123.23	112.60
1	J	196	SER	CA-CB-OG	6.25	123.61	111.10
1	X	106	LEU	CD1-CG-CD2	6.25	124.54	110.80
1	W	331	PHE	CA-CB-CG	6.23	120.03	113.80
1	N	290	VAL	CA-CB-CG2	6.21	120.96	110.40
1	Q	56	LYS	CG-CD-CE	6.21	125.58	111.30
1	D	316	LYS	CA-CB-CG	6.21	126.52	114.10
1	O	217	LEU	CA-C-O	-6.21	111.64	120.51
1	Q	290	VAL	CA-CB-CG2	6.20	120.95	110.40
1	D	231	LYS	CA-C-O	6.19	126.99	120.42
1	J	222	ASP	N-CA-CB	6.16	119.24	109.51
1	M	301	ASP	CB-CG-OD2	6.16	132.56	118.40
1	Q	15	GLU	CB-CG-CD	6.15	123.06	112.60
1	X	220	ASP	CA-CB-CG	6.15	118.75	112.60
1	C	191	GLU	CB-CG-CD	6.14	123.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	16	GLN	N-CA-CB	6.14	120.86	110.49
1	B	56	LYS	CG-CD-CE	6.12	125.38	111.30
1	E	185	HIS	CB-CG-CD2	6.11	139.14	131.20
1	J	330	GLN	N-CA-C	6.08	118.68	111.33
1	P	55	ASP	CA-CB-CG	6.08	118.67	112.60
1	J	330	GLN	CB-CA-C	6.05	120.97	110.68
1	I	111	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	V	327	LYS	CB-CA-C	-6.04	99.46	110.63
1	V	72	ARG	CB-CG-CD	6.03	125.16	111.30
1	G	80	LYS	CA-CB-CG	6.03	126.15	114.10
1	T	290	VAL	CA-CB-CG2	6.02	120.63	110.40
1	V	310	GLU	CB-CG-CD	6.01	122.82	112.60
1	I	14	GLU	CB-CG-CD	6.01	122.81	112.60
1	N	87	ASN	CA-CB-CG	6.01	118.61	112.60
1	G	50	VAL	CA-CB-CG2	6.00	120.60	110.40
1	O	104	SER	N-CA-C	6.00	123.57	110.80
1	S	192	HIS	CB-CA-C	5.99	119.47	109.89
1	W	9	TYR	CB-CA-C	5.99	122.33	110.42
1	R	327	LYS	CB-CA-C	-5.98	98.86	110.46
1	D	50	VAL	CA-CB-CG2	5.97	120.54	110.40
1	L	176	ARG	NE-CZ-NH2	5.96	124.57	119.20
1	H	290	VAL	CA-CB-CG2	5.96	120.53	110.40
1	C	331	PHE	CB-CA-C	5.95	121.41	110.10
1	I	9	TYR	CB-CA-C	5.95	122.25	110.42
1	B	275	MET	CA-C-N	5.93	132.64	121.97
1	B	275	MET	C-N-CA	5.93	132.64	121.97
1	S	82	TYR	N-CA-CB	5.93	120.51	110.49
1	L	111	ARG	CG-CD-NE	5.92	125.02	112.00
1	P	176	ARG	NE-CZ-NH2	5.92	124.52	119.20
1	G	196	SER	CA-CB-OG	5.91	122.93	111.10
1	L	50	VAL	CA-CB-CG1	5.90	120.44	110.40
1	M	196	SER	CA-CB-OG	5.89	122.89	111.10
1	Q	156	ARG	CD-NE-CZ	-5.89	116.16	124.40
1	I	192	HIS	CB-CG-CD2	5.88	138.84	131.20
1	S	110	GLN	OE1-CD-NE2	-5.85	116.75	122.60
1	M	231	LYS	CB-CG-CD	5.85	124.75	111.30
1	I	55	ASP	N-CA-CB	5.85	118.49	110.01
1	X	185	HIS	CB-CG-ND1	-5.84	113.93	122.70
1	U	12	LEU	N-CA-CB	-5.82	100.47	111.00
1	U	12	LEU	CA-C-O	5.82	127.35	120.66
1	S	297	ASN	CA-CB-CG	5.79	118.39	112.60
1	B	286	VAL	CA-CB-CG1	5.78	120.22	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	288	LEU	CB-CA-C	-5.77	98.22	111.95
1	R	185	HIS	CB-CG-CD2	5.76	138.69	131.20
1	N	17	THR	CB-CA-C	-5.76	98.83	110.17
1	Q	16	GLN	CA-C-N	5.76	135.85	121.80
1	Q	16	GLN	C-N-CA	5.76	135.85	121.80
1	R	19	GLN	CB-CG-CD	5.74	122.36	112.60
1	B	50	VAL	CA-CB-CG1	5.70	120.09	110.40
1	Q	277	LYS	N-CA-C	5.69	122.93	110.80
1	K	15	GLU	CB-CA-C	5.69	121.74	110.42
1	A	290	VAL	CA-CB-CG2	5.68	120.06	110.40
1	U	156	ARG	NE-CZ-NH1	5.67	127.17	121.50
1	I	196	SER	CA-CB-OG	5.65	122.41	111.10
1	S	15	GLU	CB-CG-CD	5.65	122.21	112.60
1	R	331	PHE	CA-CB-CG	5.64	119.44	113.80
1	A	185	HIS	CB-CG-CD2	5.63	138.52	131.20
1	R	17	THR	OG1-CB-CG2	5.63	120.55	109.30
1	S	182	LEU	CB-CA-C	5.62	121.03	110.63
1	A	12	LEU	N-CA-CB	-5.60	101.11	111.13
1	U	30	VAL	CG1-CB-CG2	-5.60	98.48	110.80
1	C	196	SER	CA-CB-OG	5.59	122.29	111.10
1	V	185	HIS	CB-CG-CD2	5.58	138.46	131.20
1	P	108	LEU	O-C-N	5.58	130.36	122.83
1	V	220	ASP	CA-CB-CG	5.58	118.18	112.60
1	Q	14	GLU	CB-CG-CD	5.58	122.08	112.60
1	P	327	LYS	CA-CB-CG	5.57	125.24	114.10
1	W	290	VAL	CA-CB-CG1	5.56	119.85	110.40
1	L	328	GLU	CB-CG-CD	5.56	122.05	112.60
1	F	290	VAL	CA-CB-CG2	5.54	119.82	110.40
1	G	72	ARG	CG-CD-NE	5.54	124.19	112.00
1	O	72	ARG	CG-CD-NE	-5.52	99.85	112.00
1	R	327	LYS	CA-C-O	5.52	126.39	120.20
1	D	220	ASP	CA-CB-CG	5.52	118.12	112.60
1	X	154	LYS	CG-CD-CE	5.49	123.93	111.30
1	H	176	ARG	NE-CZ-NH2	5.48	124.14	119.20
1	X	185	HIS	CB-CG-CD2	5.48	138.32	131.20
1	A	216	ASP	CA-CB-CG	5.47	118.07	112.60
1	O	290	VAL	CA-CB-CG1	5.46	119.68	110.40
1	B	225	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	L	196	SER	CA-CB-OG	5.46	122.01	111.10
1	F	221	LYS	CG-CD-CE	5.44	123.82	111.30
1	O	195	SER	CA-CB-OG	5.44	121.98	111.10
1	D	227	LYS	CA-CB-CG	5.43	124.96	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	247	THR	CA-CB-OG1	5.42	117.73	109.60
1	F	235	GLU	CB-CG-CD	5.42	121.81	112.60
1	K	27	VAL	CA-CB-CG2	5.41	119.60	110.40
1	R	329	LEU	N-CA-C	5.40	122.31	110.80
1	A	330	GLN	N-CA-C	-5.40	101.08	109.24
1	M	221	LYS	CG-CD-CE	5.39	123.71	111.30
1	I	217	LEU	N-CA-C	5.39	122.28	110.80
1	P	108	LEU	CB-CA-C	5.39	119.67	111.70
1	G	284	ASP	CA-CB-CG	5.38	117.98	112.60
1	S	214	HIS	CB-CG-CD2	5.38	138.19	131.20
1	N	185	HIS	CB-CG-CD2	5.37	138.19	131.20
1	N	20	ASN	CB-CG-OD1	5.36	131.53	120.80
1	D	214	HIS	CB-CG-CD2	5.36	138.16	131.20
1	Q	11	LEU	CA-CB-CG	5.35	135.04	116.30
1	U	175	GLU	CB-CG-CD	-5.35	103.50	112.60
1	M	16	GLN	N-CA-CB	5.35	119.53	110.49
1	B	191	GLU	CB-CG-CD	5.33	121.67	112.60
1	H	326	GLN	CG-CD-NE2	-5.33	108.40	116.40
1	O	214	HIS	CA-CB-CG	5.33	119.12	113.80
1	Q	156	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	X	176	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	275	MET	CG-SD-CE	-5.32	89.21	100.90
1	F	239	GLU	CB-CG-CD	5.31	121.63	112.60
1	A	240	VAL	CA-CB-CG1	5.30	119.42	110.40
1	C	222	ASP	CB-CG-OD2	5.30	130.60	118.40
1	U	72	ARG	CB-CG-CD	5.30	123.50	111.30
1	K	314	ARG	CG-CD-NE	-5.28	100.38	112.00
1	E	314	ARG	CG-CD-NE	5.28	123.62	112.00
1	O	217	LEU	N-CA-C	5.28	122.04	110.80
1	P	15	GLU	CB-CA-C	5.28	124.13	111.83
1	X	270	HIS	N-CA-CB	5.28	119.76	110.37
1	H	175	GLU	CB-CA-C	5.26	119.53	110.79
1	M	17	THR	CB-CA-C	-5.26	99.80	110.17
1	S	275	MET	CG-SD-CE	-5.22	89.41	100.90
1	R	189	LEU	CB-CG-CD1	5.21	126.34	110.70
1	W	176	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	C	244	LYS	CG-CD-CE	5.21	123.28	111.30
1	P	185	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	E	244	LYS	CG-CD-CE	5.19	123.24	111.30
1	R	72	ARG	CB-CG-CD	5.19	123.24	111.30
1	S	288	LEU	CB-CA-C	-5.19	99.31	111.09
1	M	50	VAL	CA-CB-CG1	5.19	119.22	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	244	LYS	CG-CD-CE	5.18	123.22	111.30
1	L	14	GLU	CB-CG-CD	5.18	121.40	112.60
1	Q	101	GLU	CA-CB-CG	5.18	124.46	114.10
1	M	301	ASP	CA-CB-CG	5.18	117.78	112.60
1	S	19	GLN	CB-CG-CD	5.16	121.38	112.60
1	U	331	PHE	CA-CB-CG	5.16	118.96	113.80
1	K	276	ILE	N-CA-CB	-5.14	105.44	112.28
1	R	19	GLN	CA-CB-CG	-5.14	103.81	114.10
1	M	100	GLN	CB-CG-CD	-5.14	103.86	112.60
1	O	176	ARG	NH1-CZ-NH2	5.14	125.98	119.30
1	P	185	HIS	CB-CG-ND1	5.14	130.41	122.70
1	S	117	LYS	CG-CD-CE	5.14	123.12	111.30
1	B	316	LYS	CB-CG-CD	5.14	123.11	111.30
1	N	41	LYS	CD-CE-NZ	5.13	128.33	111.90
1	F	156	ARG	NE-CZ-NH2	-5.13	114.58	119.20
1	F	50	VAL	CA-CB-CG1	5.13	119.12	110.40
1	L	310	GLU	CB-CG-CD	5.12	121.30	112.60
1	J	222	ASP	CB-CG-OD2	5.10	130.14	118.40
1	M	1	ALA	CB-CA-C	5.08	118.13	110.50
1	M	191	GLU	CG-CD-OE2	5.08	130.09	118.40
1	E	15	GLU	CB-CG-CD	5.08	121.24	112.60
1	B	232	GLN	CG-CD-NE2	-5.08	108.78	116.40
1	X	156	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	R	230	HIS	CB-CG-CD2	5.07	137.80	131.20
1	R	52	VAL	CG1-CB-CG2	5.07	121.95	110.80
1	C	242	LYS	CG-CD-CE	5.06	122.94	111.30
1	G	265	ASN	CA-C-N	5.06	131.21	121.54
1	G	265	ASN	C-N-CA	5.06	131.21	121.54
1	X	131	LYS	CB-CG-CD	-5.06	99.67	111.30
1	J	195	SER	N-CA-CB	-5.05	103.18	110.70
1	K	105	ARG	CA-C-O	5.05	127.73	120.51
1	I	16	GLN	CA-C-N	5.05	134.12	121.80
1	I	16	GLN	C-N-CA	5.05	134.12	121.80
1	L	302	LEU	N-CA-CB	5.05	118.92	110.85
1	S	156	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	U	12	LEU	CA-C-N	5.04	131.16	121.54
1	U	12	LEU	C-N-CA	5.04	131.16	121.54
1	B	329	LEU	N-CA-C	5.03	117.72	110.28
1	Q	326	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	K	27	VAL	CA-CB-CG1	5.00	118.90	110.40

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Mainchain
1	A	330	GLN	Peptide
1	B	13	LYS	Peptide
1	B	191	GLU	Sidechain
1	B	327	LYS	Mainchain
1	B	330	GLN	Peptide
1	B	9	TYR	Mainchain
1	C	329	LEU	Peptide
1	D	230	HIS	Mainchain
1	E	311	GLU	Sidechain
1	F	16	GLN	Peptide
1	G	265	ASN	Mainchain
1	H	16	GLN	Peptide
1	K	108	LEU	Mainchain
1	K	13	LYS	Peptide
1	K	192	HIS	Mainchain
1	L	13	LYS	Peptide
1	L	330	GLN	Peptide
1	N	16	GLN	Peptide
1	N	328	GLU	Peptide
1	N	329	LEU	Mainchain
1	O	12	LEU	Peptide
1	P	16	GLN	Peptide
1	P	326	GLN	Sidechain
1	Q	101	GLU	Sidechain
1	R	13	LYS	Peptide
1	R	301	ASP	Sidechain
1	S	108	LEU	Mainchain
1	T	12	LEU	Mainchain
1	T	230	HIS	Mainchain
1	T	231	LYS	Mainchain
1	U	12	LEU	Peptide
1	U	191	GLU	Sidechain
1	U	208	VAL	Mainchain
1	U	301	ASP	Sidechain
1	V	104	SER	Mainchain
1	V	12	LEU	Peptide
1	V	13	LYS	Peptide
1	V	16	GLN	Peptide
1	V	186	GLY	Mainchain
1	V	301	ASP	Sidechain
1	W	13	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	W	299	ILE	Mainchain
1	W	97	ALA	Mainchain
1	X	230	HIS	Mainchain
1	X	231	LYS	Mainchain
1	X	269	VAL	Mainchain
1	X	326	GLN	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2568	0	2656	63	1
1	B	2568	0	2656	92	1
1	C	2568	0	2656	82	0
1	D	2568	0	2656	54	3
1	E	2568	0	2656	120	0
1	F	2568	0	2656	88	0
1	G	2568	0	2656	63	3
1	H	2568	0	2656	55	0
1	I	2568	0	2656	66	0
1	J	2568	0	2656	110	0
1	K	2568	0	2656	138	0
1	L	2568	0	2656	70	0
1	M	2568	0	2656	75	0
1	N	2568	0	2656	72	0
1	O	2568	0	2656	134	0
1	P	2568	0	2656	65	0
1	Q	2568	0	2656	114	0
1	R	2568	0	2656	101	3
1	S	2568	0	2656	62	0
1	T	2568	0	2656	78	0
1	U	2568	0	2656	111	3
1	V	2568	0	2656	79	0
1	W	2568	0	2656	108	0
1	X	2568	0	2656	112	0
2	Q	38	0	0	18	0
All	All	61670	0	63744	1621	7

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 (1621) 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:B:110:GLN:HG3	1:J:129:ASN:ND2	1.26	1.41
1:J:11:LEU:HD21	1:K:302:LEU:CD1	1.52	1.37
1:E:331:PHE:C	1:O:17:THR:HG21	1.51	1.35
1:F:107:ASN:OD1	1:W:115:ILE:HG12	1.23	1.28
1:B:323:TRP:HH2	1:K:129:ASN:OD1	1.10	1.27
1:B:323:TRP:CH2	1:K:129:ASN:OD1	1.88	1.25
1:C:107:ASN:OD1	1:M:115:ILE:HG12	1.23	1.25
1:E:114:ASN:ND2	1:N:129:ASN:OD1	1.70	1.25
2:Q:401:GO3:C34	2:Q:401:GO3:C23	2.06	1.24
1:N:118:PHE:CZ	1:X:223:LYS:HB3	1.71	1.24
1:X:54:GLU:HG3	1:X:80:LYS:CE	1.69	1.21
1:C:111:ARG:NH1	1:M:52:VAL:HG11	1.55	1.20
1:X:54:GLU:CD	1:X:80:LYS:HE3	1.66	1.20
1:R:254:SER:O	1:R:258:LEU:HD23	1.39	1.20
1:I:261:SER:HA	1:I:266:LEU:HD13	1.23	1.19
1:U:261:SER:HA	1:U:266:LEU:HD13	1.23	1.17
1:O:100:GLN:OE1	1:R:111:ARG:NH2	1.77	1.17
1:I:302:LEU:HD13	1:L:11:LEU:HD11	1.17	1.16
1:Q:110:GLN:HB2	2:Q:401:GO3:O6	1.42	1.16
1:J:198:PRO:HD2	1:J:314:ARG:NH1	1.59	1.15
1:B:323:TRP:HH2	1:K:129:ASN:CG	1.54	1.14
1:J:15:GLU:O	1:J:16:GLN:HG2	1.43	1.14
1:E:110:GLN:OE1	1:N:129:ASN:ND2	1.80	1.14
1:O:100:GLN:NE2	1:R:111:ARG:HH12	1.46	1.12
1:Q:210:LEU:HA	1:Q:213:LEU:CD2	1.77	1.11
1:K:16:GLN:HA	1:K:16:GLN:NE2	1.60	1.11
1:P:108:LEU:HB2	1:P:111:ARG:HH21	1.15	1.11
1:X:131:LYS:NZ	1:X:298:GLY:HA2	1.63	1.11
1:K:182:LEU:HD12	1:L:69:LEU:HD12	1.25	1.11
1:I:264:LYS:HB2	1:I:266:LEU:HD11	1.33	1.11
1:Q:277:LYS:O	1:Q:282:ILE:O	1.68	1.11
1:E:302:LEU:HD13	1:H:11:LEU:HD11	1.24	1.10
1:B:283:LYS:HB2	1:K:153:PRO:HD3	1.27	1.10
1:J:11:LEU:CD2	1:K:302:LEU:HD13	1.81	1.10
1:M:11:LEU:HD11	1:P:302:LEU:HD13	1.33	1.10
1:O:93:ILE:HD13	1:O:134:ILE:HD13	1.17	1.09
1:X:54:GLU:HG3	1:X:80:LYS:HE2	1.09	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:12:LEU:CD1	1:K:155:ASN:HB3	1.82	1.09
1:J:198:PRO:HD2	1:J:314:ARG:HH12	0.94	1.09
1:U:264:LYS:HB2	1:U:266:LEU:HD11	1.32	1.09
1:P:219:THR:CG2	1:P:221:LYS:HG2	1.83	1.08
1:C:107:ASN:OD1	1:M:115:ILE:CG1	2.01	1.08
1:E:11:LEU:HD11	1:H:302:LEU:HD13	1.13	1.08
1:N:154:LYS:HD3	1:N:275:MET:HE3	1.29	1.08
1:O:288:LEU:CD1	1:O:322:LEU:HD12	1.83	1.08
1:N:12:LEU:HD11	1:O:300:SER:HB2	1.33	1.07
1:X:131:LYS:HZ2	1:X:298:GLY:HA2	1.00	1.07
1:E:283:LYS:CD	1:O:153:PRO:HB3	1.84	1.07
1:C:111:ARG:NH1	1:M:52:VAL:CG1	2.18	1.07
1:I:302:LEU:HD13	1:L:11:LEU:CD1	1.85	1.06
1:S:114:ASN:HA	1:S:117:LYS:HE3	1.36	1.06
1:T:117:LYS:HZ1	1:T:331:PHE:HA	1.19	1.06
1:T:11:LEU:O	1:T:12:LEU:HB2	1.31	1.06
1:E:283:LYS:HB2	1:O:153:PRO:HD3	1.37	1.06
1:O:111:ARG:NH2	1:R:100:GLN:OE1	1.88	1.06
1:Q:110:GLN:HA	1:Q:110:GLN:HE21	1.12	1.06
1:B:110:GLN:CG	1:J:129:ASN:ND2	2.20	1.04
1:F:110:GLN:HE22	1:F:330:GLN:NE2	1.55	1.04
1:R:54:GLU:CG	1:R:80:LYS:HD2	1.87	1.04
1:W:216:ASP:O	1:W:219:THR:HG22	1.57	1.04
1:E:170:ARG:HD3	1:E:184:CYS:O	1.56	1.04
1:O:100:GLN:CD	1:R:111:ARG:HH12	1.65	1.04
1:E:323:TRP:HH2	1:O:129:ASN:OD1	1.40	1.04
1:F:302:LEU:HD13	1:G:11:LEU:HD11	1.39	1.03
1:Q:268:ARG:HD3	1:S:182:LEU:HD21	1.39	1.03
1:T:106:LEU:O	1:T:109:VAL:HG23	1.58	1.03
1:W:182:LEU:HD11	1:X:72:ARG:HH22	1.19	1.03
1:E:283:LYS:HD2	1:O:153:PRO:CB	1.88	1.03
1:K:103:GLU:OE2	1:K:108:LEU:HD11	1.58	1.03
1:O:93:ILE:HD13	1:O:134:ILE:CD1	1.87	1.03
1:O:52:VAL:O	1:O:80:LYS:HE2	1.57	1.03
1:C:111:ARG:HH12	1:M:52:VAL:HG11	0.90	1.02
1:P:108:LEU:HG	1:P:111:ARG:HE	1.21	1.02
1:E:323:TRP:CH2	1:O:129:ASN:OD1	2.13	1.02
1:F:106:LEU:O	1:F:109:VAL:HG23	1.59	1.02
1:J:11:LEU:CD2	1:K:302:LEU:CD1	2.37	1.02
1:K:225:GLN:OE1	1:K:225:GLN:HA	1.54	1.02
1:J:11:LEU:HD21	1:K:302:LEU:HD13	1.07	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:11:LEU:HD11	1:W:302:LEU:HD13	1.37	1.02
1:C:111:ARG:HH12	1:M:52:VAL:CG1	1.70	1.02
1:W:324:GLY:HA2	1:W:327:LYS:HE3	1.35	1.01
1:X:54:GLU:CG	1:X:80:LYS:CE	2.38	1.01
1:O:105:ARG:O	1:O:108:LEU:HD13	1.57	1.01
1:R:254:SER:O	1:R:258:LEU:CD2	2.07	1.01
1:Q:82:TYR:CD2	1:Q:122:ASN:HB3	1.95	1.01
1:E:11:LEU:CD1	1:H:302:LEU:HD13	1.91	1.01
1:E:323:TRP:HH2	1:O:129:ASN:CG	1.69	1.01
1:B:110:GLN:HG3	1:J:129:ASN:HD22	1.23	1.01
1:H:125:LYS:NZ	1:Q:309:SER:HB2	1.75	1.01
1:Q:3:LEU:HD21	1:R:210:LEU:HD22	1.44	1.00
1:U:16:GLN:O	1:U:17:THR:HG22	1.59	1.00
1:I:9:TYR:HD2	1:L:302:LEU:CD2	1.74	0.99
1:R:163:ASN:ND2	1:R:258:LEU:HD21	1.76	0.99
1:W:98:ARG:HG3	1:W:98:ARG:HH11	1.25	0.99
1:X:131:LYS:HE3	1:X:158:ILE:HD11	1.42	0.99
1:G:67:GLY:O	1:G:71:LEU:HD23	1.63	0.99
1:H:198:PRO:HD2	1:H:314:ARG:HH12	1.21	0.99
1:E:283:LYS:CB	1:O:153:PRO:HD3	1.91	0.99
1:Q:302:LEU:HD23	1:T:11:LEU:HD11	1.41	0.99
1:H:198:PRO:HD2	1:H:314:ARG:NH1	1.75	0.98
1:N:216:ASP:O	1:N:219:THR:HG22	1.61	0.98
1:X:99:GLN:OE1	1:X:238:TYR:HE2	1.47	0.98
1:H:14:GLU:O	1:H:15:GLU:HG2	1.62	0.98
1:I:302:LEU:CD1	1:L:11:LEU:HD11	1.92	0.98
1:M:270:HIS:ND1	1:M:294:LEU:HD22	1.78	0.97
1:E:11:LEU:HD11	1:H:302:LEU:CD1	1.94	0.97
1:L:283:LYS:HE3	1:L:316:LYS:HZ1	1.29	0.97
1:E:275:MET:CE	1:E:285:ASP:HA	1.95	0.97
1:I:9:TYR:CD2	1:L:302:LEU:HD21	2.00	0.97
1:F:107:ASN:OD1	1:W:115:ILE:CG1	2.12	0.97
1:J:300:SER:HB2	1:K:12:LEU:HD11	1.47	0.96
1:K:117:LYS:HE2	1:K:331:PHE:HA	1.45	0.96
1:R:265:ASN:HD22	1:R:296:GLN:H	1.06	0.96
1:T:11:LEU:O	1:T:12:LEU:CB	2.13	0.96
1:Q:109:VAL:CG1	2:Q:401:GO3:O4	2.14	0.96
1:X:131:LYS:HZ3	1:X:262:ILE:HG12	1.31	0.95
1:U:186:GLY:O	1:U:187:TRP:HD1	1.48	0.95
1:F:110:GLN:HE22	1:F:330:GLN:HE21	1.13	0.95
1:E:283:LYS:HD2	1:O:153:PRO:HB3	0.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:324:GLY:HA2	1:M:327:LYS:HE3	1.49	0.95
1:P:219:THR:HG21	1:P:221:LYS:HG2	1.49	0.94
1:I:9:TYR:HD2	1:L:302:LEU:HD21	1.31	0.94
1:T:177:LEU:HD11	1:T:226:TRP:HH2	1.31	0.94
1:X:54:GLU:CG	1:X:80:LYS:HE2	1.98	0.94
1:X:54:GLU:CG	1:X:80:LYS:HE3	1.95	0.94
1:E:275:MET:HE1	1:E:285:ASP:OD1	1.66	0.94
1:J:12:LEU:HD11	1:K:155:ASN:HB3	1.49	0.93
1:N:225:GLN:HE21	1:N:225:GLN:HA	1.29	0.93
1:J:12:LEU:HD11	1:K:155:ASN:CG	1.93	0.93
1:H:125:LYS:HZ1	1:Q:309:SER:HB2	1.32	0.93
1:E:331:PHE:C	1:O:17:THR:CG2	2.42	0.92
1:N:118:PHE:CZ	1:X:223:LYS:CB	2.52	0.92
1:Q:11:LEU:HD22	1:T:300:SER:O	1.69	0.92
1:J:198:PRO:HD3	1:J:314:ARG:HH22	1.35	0.92
1:K:16:GLN:HA	1:K:16:GLN:HE21	1.24	0.92
1:O:288:LEU:CD1	1:O:322:LEU:CD1	2.48	0.92
1:B:297:ASN:OD1	1:C:15:GLU:HB2	1.70	0.92
1:P:108:LEU:HG	1:P:111:ARG:NE	1.84	0.92
1:Q:110:GLN:HB3	2:Q:401:GO3:C38	2.00	0.92
1:I:16:GLN:HG3	1:I:17:THR:H	1.34	0.91
1:J:198:PRO:CD	1:J:314:ARG:HH12	1.84	0.91
1:N:16:GLN:HG2	1:N:17:THR:HG23	1.51	0.91
1:F:280:TYR:CE1	1:F:307:LEU:CD1	2.53	0.91
1:J:198:PRO:CD	1:J:314:ARG:HH22	1.84	0.91
1:E:110:GLN:CD	1:N:129:ASN:ND2	2.27	0.91
1:E:117:LYS:HE3	1:E:331:PHE:HB3	1.49	0.91
1:J:12:LEU:HD11	1:K:155:ASN:CB	2.00	0.91
1:Q:302:LEU:HD23	1:T:11:LEU:CD1	2.00	0.90
1:G:154:LYS:HD2	1:G:275:MET:HE3	1.50	0.90
1:O:145:VAL:HG22	1:O:331:PHE:HZ	1.35	0.90
1:I:12:LEU:HD13	1:I:15:GLU:OE1	1.72	0.90
1:K:100:GLN:CD	1:U:103:GLU:OE2	2.14	0.90
1:X:54:GLU:OE2	1:X:80:LYS:HE3	1.73	0.89
1:E:210:LEU:HG	1:F:3:LEU:HD21	1.54	0.89
1:X:131:LYS:HE3	1:X:158:ILE:CD1	2.02	0.89
1:V:177:LEU:HD11	1:V:226:TRP:HH2	1.37	0.89
1:N:118:PHE:CE1	1:X:223:LYS:CB	2.55	0.89
1:O:93:ILE:CD1	1:O:134:ILE:HD13	2.03	0.88
1:O:111:ARG:HH22	1:R:100:GLN:NE2	1.71	0.88
1:B:283:LYS:CB	1:K:153:PRO:HD3	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:200:TRP:CE3	1:Q:217:LEU:CD1	2.57	0.88
1:B:323:TRP:CH2	1:K:129:ASN:CG	2.47	0.88
1:E:275:MET:HE2	1:E:285:ASP:HA	1.56	0.88
1:N:52:VAL:HG12	1:X:223:LYS:CE	2.04	0.88
1:B:284:ASP:OD1	1:K:156:ARG:NH2	2.05	0.87
1:E:239:GLU:OE1	1:F:62:MET:HE1	1.74	0.87
1:M:191:GLU:OE1	1:M:193:GLY:HA3	1.74	0.87
1:P:108:LEU:CB	1:P:111:ARG:HH21	1.86	0.87
1:K:182:LEU:HD12	1:L:69:LEU:CD1	2.04	0.87
1:X:173:MET:O	1:X:177:LEU:HD13	1.73	0.87
1:P:108:LEU:HB2	1:P:111:ARG:NH2	1.88	0.87
1:Q:200:TRP:CE3	1:Q:217:LEU:HD11	2.10	0.87
1:B:110:GLN:HG3	1:J:129:ASN:HD21	1.33	0.86
1:E:302:LEU:CD1	1:H:11:LEU:HD11	2.05	0.86
1:N:15:GLU:O	1:N:16:GLN:HG2	1.75	0.86
1:T:276:ILE:HD13	1:T:282:ILE:HD13	1.57	0.86
1:M:11:LEU:CD1	1:P:302:LEU:HD13	2.05	0.86
1:U:276:ILE:HD13	1:U:282:ILE:HD13	1.57	0.86
1:L:283:LYS:CE	1:L:316:LYS:HZ1	1.89	0.86
1:S:276:ILE:HD13	1:S:282:ILE:HD13	1.57	0.86
1:V:173:MET:O	1:V:177:LEU:HD13	1.76	0.86
1:K:108:LEU:HD21	1:U:100:GLN:OE1	1.75	0.86
1:O:276:ILE:HD13	1:O:282:ILE:HD13	1.56	0.86
1:R:276:ILE:HD13	1:R:282:ILE:HD13	1.57	0.86
1:P:108:LEU:CG	1:P:111:ARG:HE	1.89	0.86
1:V:11:LEU:CD1	1:W:302:LEU:HD13	2.06	0.86
1:V:69:LEU:HD23	1:V:69:LEU:O	1.73	0.86
1:H:276:ILE:HD13	1:H:282:ILE:HD13	1.58	0.85
1:X:131:LYS:NZ	1:X:262:ILE:HG12	1.90	0.85
1:K:182:LEU:CD1	1:L:69:LEU:HD12	2.06	0.85
1:N:203:MET:HE2	1:N:210:LEU:HD23	1.56	0.85
1:X:276:ILE:HD13	1:X:282:ILE:HD13	1.59	0.85
1:V:186:GLY:O	1:V:187:TRP:HD1	1.58	0.85
1:E:110:GLN:CD	1:N:129:ASN:HD21	1.85	0.85
1:V:276:ILE:HD13	1:V:282:ILE:HD13	1.58	0.85
1:C:276:ILE:HD13	1:C:282:ILE:HD13	1.59	0.85
1:J:276:ILE:HD13	1:J:282:ILE:HD13	1.57	0.85
1:N:276:ILE:HD13	1:N:282:ILE:HD13	1.59	0.85
1:Q:109:VAL:HG11	2:Q:401:GO3:O4	1.76	0.85
1:F:276:ILE:HD13	1:F:282:ILE:HD13	1.58	0.85
1:A:276:ILE:HD13	1:A:282:ILE:HD13	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:54:GLU:HG3	1:R:80:LYS:HD2	1.58	0.85
1:S:189:LEU:CD2	1:S:199:VAL:HG21	2.06	0.84
1:T:177:LEU:HD11	1:T:226:TRP:CH2	2.11	0.84
1:E:117:LYS:CE	1:E:331:PHE:HB3	2.07	0.84
1:E:302:LEU:HD13	1:H:11:LEU:CD1	2.06	0.84
1:V:15:GLU:OE1	1:W:267:ARG:NH1	2.10	0.84
1:Q:117:LYS:HE2	1:Q:331:PHE:O	1.77	0.84
1:Q:276:ILE:HD13	1:Q:282:ILE:HD13	1.58	0.84
1:G:224:GLU:HG3	1:Q:330:GLN:NE2	1.92	0.84
1:I:302:LEU:CD1	1:L:11:LEU:CD1	2.54	0.84
1:B:189:LEU:CD1	1:B:199:VAL:HG21	2.06	0.84
1:N:154:LYS:HD3	1:N:275:MET:CE	2.08	0.84
1:C:39:LEU:HD11	1:C:47:LEU:HD22	1.60	0.84
1:O:105:ARG:C	1:O:108:LEU:HD13	2.01	0.84
1:W:276:ILE:HD13	1:W:282:ILE:HD13	1.58	0.84
1:B:276:ILE:HD13	1:B:282:ILE:HD13	1.58	0.83
1:N:15:GLU:O	1:N:17:THR:HG23	1.77	0.83
1:G:276:ILE:HD13	1:G:282:ILE:HD13	1.61	0.83
1:H:198:PRO:CD	1:H:314:ARG:HH12	1.91	0.83
1:M:276:ILE:HD13	1:M:282:ILE:HD13	1.59	0.83
1:N:12:LEU:HD11	1:O:300:SER:CB	2.09	0.83
1:P:276:ILE:HD13	1:P:282:ILE:HD13	1.58	0.83
1:F:109:VAL:HG22	1:F:138:PRO:HG3	1.60	0.83
1:L:276:ILE:HD13	1:L:282:ILE:HD13	1.59	0.83
1:E:120:ILE:O	1:E:124:VAL:HG23	1.79	0.82
1:U:302:LEU:CD2	1:X:11:LEU:HD11	2.09	0.82
1:J:198:PRO:HD2	1:J:314:ARG:CZ	2.08	0.82
1:O:111:ARG:HH22	1:R:100:GLN:HE22	1.24	0.82
1:H:227:LYS:HE2	1:H:231:LYS:NZ	1.94	0.82
1:J:302:LEU:HD13	1:K:11:LEU:HD11	1.61	0.82
1:D:276:ILE:HD13	1:D:282:ILE:HD13	1.59	0.82
1:J:12:LEU:HD13	1:K:155:ASN:HB3	1.59	0.82
1:B:285:ASP:OD2	1:K:128:PRO:CG	2.26	0.82
1:J:300:SER:CB	1:K:12:LEU:HD11	2.08	0.82
1:K:54:GLU:CD	1:K:80:LYS:HD3	2.04	0.82
1:N:52:VAL:HG12	1:X:223:LYS:HE2	1.62	0.82
1:T:109:VAL:HG22	1:T:138:PRO:HG3	1.59	0.82
1:F:328:GLU:HB3	1:W:107:ASN:O	1.80	0.82
1:X:99:GLN:OE1	1:X:238:TYR:CE2	2.30	0.82
1:I:276:ILE:HD13	1:I:282:ILE:HD13	1.59	0.82
1:U:170:ARG:CD	1:U:184:CYS:O	2.28	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:MET:HE1	1:B:285:ASP:HA	1.60	0.82
1:J:12:LEU:CD1	1:K:155:ASN:CB	2.54	0.82
1:B:189:LEU:CD1	1:B:199:VAL:CG2	2.58	0.81
1:E:110:GLN:CG	1:N:129:ASN:ND2	2.43	0.81
1:Q:210:LEU:HA	1:Q:213:LEU:HD23	1.62	0.81
1:T:177:LEU:CD1	1:T:226:TRP:HH2	1.93	0.81
1:E:3:LEU:HD13	1:E:3:LEU:C	2.06	0.81
1:O:97:ALA:O	1:O:98:ARG:HB2	1.79	0.81
1:U:209:SER:O	1:U:213:LEU:HD22	1.80	0.81
1:D:281:GLY:O	1:D:283:LYS:HD3	1.81	0.81
1:J:15:GLU:O	1:J:16:GLN:CG	2.27	0.81
2:Q:401:GO3:C35	2:Q:401:GO3:C24	2.56	0.81
1:U:208:VAL:HG12	1:U:213:LEU:HD21	1.63	0.81
1:N:118:PHE:CE1	1:X:223:LYS:HB3	2.14	0.81
1:U:170:ARG:HD3	1:U:184:CYS:O	1.80	0.80
1:K:120:ILE:O	1:K:124:VAL:HG22	1.81	0.80
1:T:117:LYS:NZ	1:T:331:PHE:HA	1.96	0.80
1:G:50:VAL:HG12	1:G:79:GLY:O	1.81	0.80
1:P:107:ASN:O	1:P:108:LEU:HD22	1.81	0.80
1:A:120:ILE:O	1:A:124:VAL:HG22	1.82	0.80
1:K:54:GLU:CG	1:K:80:LYS:HD3	2.12	0.80
1:A:240:VAL:HG13	1:A:247:THR:HG22	1.64	0.80
1:D:249:TRP:O	1:D:253:LEU:HD13	1.82	0.80
1:S:276:ILE:HB	1:S:279:LEU:HD12	1.61	0.80
1:G:71:LEU:HD21	1:H:253:LEU:HD13	1.62	0.80
1:F:280:TYR:CE1	1:F:307:LEU:HD12	2.16	0.80
1:C:32:MET:HE1	1:C:64:LEU:HD21	1.63	0.80
1:G:154:LYS:HD2	1:G:275:MET:CE	2.10	0.80
1:X:131:LYS:CE	1:X:158:ILE:CD1	2.60	0.80
1:F:110:GLN:NE2	1:F:330:GLN:HE21	1.79	0.79
1:P:219:THR:HG23	1:P:221:LYS:H	1.47	0.79
1:E:224:GLU:OE1	1:F:2:THR:HA	1.82	0.79
1:P:108:LEU:HD12	1:P:111:ARG:H	1.48	0.79
1:X:131:LYS:HZ1	1:X:262:ILE:CD1	1.94	0.79
1:K:16:GLN:HE21	1:K:16:GLN:CA	1.95	0.79
1:K:276:ILE:HD12	1:K:288:LEU:HD11	1.65	0.79
1:I:297:ASN:OD1	1:L:15:GLU:CB	2.30	0.79
1:B:125:LYS:HE3	1:B:126:TYR:CE2	2.18	0.79
1:K:226:TRP:CZ2	1:L:3:LEU:HD23	2.18	0.79
1:O:120:ILE:O	1:O:124:VAL:HG22	1.81	0.79
1:R:54:GLU:HG2	1:R:80:LYS:HD2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:189:LEU:CD2	1:T:199:VAL:CG2	2.60	0.79
1:X:154:LYS:NZ	1:X:275:MET:HB3	1.96	0.79
1:A:11:LEU:HD11	1:D:302:LEU:HD23	1.61	0.79
1:F:302:LEU:HD13	1:G:11:LEU:CD1	2.13	0.79
1:M:100:GLN:HE21	1:M:103:GLU:HB2	1.48	0.79
1:U:202:GLY:HA2	1:W:207:GLY:O	1.82	0.79
1:M:306:THR:HG22	1:O:208:VAL:HG13	1.65	0.79
1:E:331:PHE:CA	1:O:17:THR:HG21	2.13	0.79
1:K:189:LEU:CD2	1:K:199:VAL:HG21	2.13	0.78
1:O:111:ARG:HH22	1:R:100:GLN:CD	1.90	0.78
1:S:189:LEU:HD23	1:S:199:VAL:HG21	1.66	0.78
1:P:13:LYS:H	1:P:13:LYS:HD3	1.48	0.78
1:U:186:GLY:O	1:U:187:TRP:CD1	2.34	0.78
1:E:331:PHE:OXT	1:O:17:THR:HG21	1.84	0.78
1:A:69:LEU:HD12	1:B:182:LEU:HD12	1.66	0.78
1:K:27:VAL:HG22	1:K:32:MET:SD	2.24	0.78
1:J:290:VAL:HG12	1:J:291:PRO:HD2	1.66	0.78
1:O:111:ARG:CZ	1:R:100:GLN:OE1	2.30	0.77
1:U:182:LEU:HD11	1:V:72:ARG:NH2	1.98	0.77
1:O:100:GLN:NE2	1:R:111:ARG:NH1	2.29	0.77
1:B:285:ASP:OD2	1:K:128:PRO:CB	2.33	0.77
1:W:182:LEU:HD11	1:X:72:ARG:NH2	1.96	0.77
1:X:177:LEU:HD11	1:X:226:TRP:HH2	1.48	0.77
1:W:7:LEU:HD11	1:X:205:VAL:HB	1.67	0.77
1:X:269:VAL:O	1:X:292:CYS:O	2.02	0.77
1:Q:82:TYR:CD2	1:Q:122:ASN:CB	2.68	0.77
1:O:100:GLN:HG3	1:R:103:GLU:CD	2.10	0.77
1:C:328:GLU:HG3	1:M:111:ARG:NE	2.00	0.76
1:E:3:LEU:HD13	1:E:3:LEU:O	1.85	0.76
1:E:170:ARG:CD	1:E:184:CYS:O	2.32	0.76
1:A:124:VAL:HG12	1:A:152:PHE:CE1	2.21	0.76
1:K:182:LEU:HD21	1:L:72:ARG:NH1	2.00	0.76
1:A:240:VAL:CG1	1:A:247:THR:HG22	2.15	0.76
1:V:186:GLY:O	1:V:187:TRP:CD1	2.38	0.76
1:F:328:GLU:HB3	1:W:111:ARG:HH21	1.50	0.76
1:O:100:GLN:CD	1:R:111:ARG:NH1	2.43	0.76
1:O:100:GLN:HG3	1:R:103:GLU:OE1	1.85	0.76
1:X:131:LYS:HZ2	1:X:298:GLY:CA	1.91	0.76
1:C:14:GLU:HG2	1:C:16:GLN:CG	2.16	0.76
1:D:124:VAL:HG13	1:D:152:PHE:CE1	2.21	0.76
1:L:283:LYS:HE3	1:L:316:LYS:NZ	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:172:LEU:HD23	1:U:175:GLU:OE1	1.86	0.76
1:W:144:TYR:CE2	1:W:329:LEU:HD23	2.21	0.76
1:F:198:PRO:HD2	1:F:314:ARG:NH1	2.01	0.75
1:K:100:GLN:HE22	1:U:108:LEU:CD2	1.98	0.75
1:F:110:GLN:NE2	1:F:330:GLN:NE2	2.33	0.75
1:G:276:ILE:HD11	1:G:286:VAL:HG13	1.66	0.75
1:K:124:VAL:HG12	1:K:152:PHE:CE1	2.22	0.75
1:U:261:SER:CA	1:U:266:LEU:HD13	2.13	0.75
1:K:208:VAL:HG12	1:K:213:LEU:HD21	1.68	0.75
1:E:327:LYS:HE3	1:N:17:THR:HG21	1.67	0.75
1:K:189:LEU:HD23	1:K:199:VAL:HG21	1.67	0.75
1:R:258:LEU:N	1:R:258:LEU:HD22	2.02	0.75
1:U:315:LEU:O	1:U:315:LEU:HD23	1.86	0.75
1:O:288:LEU:HD11	1:O:322:LEU:HD12	1.66	0.75
1:S:189:LEU:CD2	1:S:199:VAL:CG2	2.64	0.75
1:U:266:LEU:N	1:U:266:LEU:HD12	2.01	0.75
1:O:93:ILE:HD11	1:O:132:LEU:HD22	1.69	0.74
1:O:277:LYS:O	1:O:282:ILE:O	2.05	0.74
1:I:266:LEU:N	1:I:266:LEU:HD12	2.01	0.74
1:R:290:VAL:HG22	1:R:291:PRO:HD2	1.67	0.74
1:R:187:TRP:HB3	1:R:189:LEU:HD11	1.67	0.74
1:S:276:ILE:HG22	1:S:279:LEU:HD11	1.69	0.74
1:O:108:LEU:N	1:O:108:LEU:HD12	2.02	0.74
1:Q:213:LEU:HG	1:R:3:LEU:CD1	2.18	0.74
1:F:239:GLU:OE1	1:F:242:LYS:HE2	1.86	0.74
1:B:13:LYS:HD3	1:B:13:LYS:H	1.53	0.74
1:E:72:ARG:NH1	1:F:182:LEU:HD11	2.03	0.74
1:J:300:SER:HA	1:K:12:LEU:HD21	1.70	0.74
1:U:154:LYS:HE2	1:X:11:LEU:CD2	2.18	0.74
1:B:189:LEU:HD12	1:B:199:VAL:HG23	1.70	0.74
1:V:98:ARG:C	1:V:108:LEU:HD11	2.12	0.74
1:J:163:ASN:ND2	1:J:258:LEU:HD21	2.03	0.74
1:O:124:VAL:HG12	1:O:152:PHE:CE1	2.22	0.74
1:U:280:TYR:CE1	1:U:307:LEU:HD13	2.23	0.73
1:W:182:LEU:CD1	1:X:72:ARG:HH22	2.00	0.73
1:W:293:ILE:O	1:W:299:ILE:O	2.06	0.73
1:K:14:GLU:HG3	1:K:16:GLN:HG2	1.70	0.73
1:Q:110:GLN:HA	1:Q:110:GLN:NE2	1.91	0.73
1:F:302:LEU:CD1	1:G:11:LEU:HD11	2.18	0.73
1:Q:117:LYS:NZ	1:Q:330:GLN:O	2.18	0.73
1:L:30:VAL:HG23	1:L:98:ARG:NH1	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:301:ASP:OD2	1:P:10:ASN:ND2	2.20	0.73
1:R:173:MET:O	1:R:177:LEU:HD22	1.88	0.73
1:N:326:GLN:O	1:N:329:LEU:HG	1.88	0.73
1:K:209:SER:O	1:K:213:LEU:HD22	1.88	0.73
1:O:100:GLN:OE1	1:R:111:ARG:CZ	2.37	0.73
1:U:264:LYS:HB2	1:U:266:LEU:CD1	2.16	0.73
1:B:274:THR:HG23	1:B:275:MET:O	1.88	0.73
1:K:100:GLN:CG	1:U:103:GLU:OE2	2.37	0.72
1:K:103:GLU:OE2	1:U:100:GLN:CG	2.37	0.72
1:M:180:HIS:HB2	1:O:266:LEU:O	1.89	0.72
1:O:124:VAL:HG12	1:O:152:PHE:CZ	2.24	0.72
1:V:121:PRO:HA	1:V:124:VAL:HG23	1.71	0.72
1:I:261:SER:CA	1:I:266:LEU:HD13	2.13	0.72
1:P:108:LEU:HG	1:P:111:ARG:HB2	1.71	0.72
1:R:11:LEU:CD2	1:S:302:LEU:HD13	2.19	0.72
1:G:67:GLY:O	1:G:71:LEU:CD2	2.37	0.72
1:F:280:TYR:HE1	1:F:307:LEU:HD12	1.53	0.72
1:G:70:PHE:C	1:G:71:LEU:HD22	2.14	0.72
1:I:58:LYS:HE2	1:J:243:LEU:HD11	1.71	0.72
1:I:297:ASN:OD1	1:L:15:GLU:HB2	1.89	0.72
1:K:124:VAL:HG12	1:K:152:PHE:CZ	2.25	0.72
1:O:276:ILE:HD11	1:O:286:VAL:HG13	1.71	0.72
1:H:125:LYS:NZ	1:Q:309:SER:CB	2.53	0.72
1:K:189:LEU:CD2	1:K:199:VAL:CG2	2.68	0.72
1:E:285:ASP:OD2	1:O:128:PRO:CG	2.38	0.72
1:P:108:LEU:CG	1:P:111:ARG:NE	2.49	0.72
1:I:13:LYS:H	1:I:13:LYS:HD3	1.55	0.72
1:C:328:GLU:HB2	1:M:111:ARG:HH21	1.54	0.71
1:I:72:ARG:NH2	1:J:182:LEU:HD11	2.04	0.71
1:O:288:LEU:HD13	1:O:322:LEU:HD12	1.71	0.71
1:E:110:GLN:CG	1:N:129:ASN:HD21	2.03	0.71
1:M:290:VAL:CG2	1:M:302:LEU:HD13	2.20	0.71
1:V:69:LEU:HD23	1:V:69:LEU:C	2.15	0.71
1:N:302:LEU:HD13	1:O:11:LEU:HD11	1.72	0.71
1:S:71:LEU:O	1:S:72:ARG:NH1	2.23	0.71
1:F:13:LYS:H	1:F:13:LYS:HD3	1.54	0.71
1:O:288:LEU:HD12	1:O:322:LEU:CD1	2.18	0.71
1:Q:323:TRP:HZ2	1:Q:327:LYS:HE2	1.56	0.71
1:J:121:PRO:HA	1:J:124:VAL:HG23	1.72	0.71
1:F:82:TYR:O	1:F:85:THR:HB	1.91	0.71
1:H:227:LYS:HE2	1:H:231:LYS:HZ3	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:300:SER:HA	1:K:12:LEU:CD2	2.20	0.71
1:E:331:PHE:OXT	1:O:17:THR:CG2	2.39	0.71
1:H:82:TYR:O	1:H:85:THR:HB	1.91	0.71
1:M:82:TYR:O	1:M:85:THR:HB	1.91	0.71
1:N:82:TYR:O	1:N:85:THR:HB	1.91	0.71
1:C:111:ARG:NH1	1:M:52:VAL:HG12	2.06	0.70
1:E:308:THR:HG23	1:E:311:GLU:OE2	1.91	0.70
1:I:82:TYR:O	1:I:85:THR:HB	1.91	0.70
1:T:189:LEU:HD21	1:T:199:VAL:HG21	1.71	0.70
1:U:82:TYR:O	1:U:85:THR:HB	1.91	0.70
1:A:124:VAL:HG12	1:A:152:PHE:CZ	2.26	0.70
1:D:93:ILE:HD12	1:D:120:ILE:CD1	2.20	0.70
1:T:82:TYR:O	1:T:85:THR:HB	1.91	0.70
1:A:82:TYR:O	1:A:85:THR:HB	1.91	0.70
1:A:93:ILE:HD12	1:A:120:ILE:CD1	2.21	0.70
1:H:125:LYS:HZ2	1:Q:309:SER:HB2	1.55	0.70
1:E:82:TYR:O	1:E:85:THR:HB	1.91	0.70
1:R:203:MET:HE2	1:R:210:LEU:HD13	1.73	0.70
1:R:308:THR:HG23	1:R:311:GLU:H	1.56	0.70
1:H:275:MET:HE2	1:H:285:ASP:HA	1.73	0.70
1:O:111:ARG:NH2	1:R:100:GLN:CD	2.49	0.70
1:R:320:ASP:C	1:R:320:ASP:OD1	2.32	0.70
1:W:82:TYR:O	1:W:85:THR:HB	1.92	0.70
1:B:189:LEU:HD13	1:B:199:VAL:HG21	1.73	0.70
1:B:19:GLN:HE22	1:C:296:GLN:CD	1.99	0.70
1:T:189:LEU:CD2	1:T:199:VAL:HG23	2.20	0.70
1:Q:130:CYS:O	1:Q:156:ARG:NH2	2.25	0.70
1:U:203:MET:HE2	1:U:210:LEU:HD23	1.73	0.70
1:A:180:HIS:HB2	1:C:266:LEU:O	1.92	0.70
1:B:82:TYR:O	1:B:85:THR:HB	1.91	0.70
1:H:310:GLU:CD	1:H:314:ARG:HD2	2.17	0.70
1:I:15:GLU:HG3	1:L:297:ASN:CG	2.17	0.70
1:G:221:LYS:H	1:G:221:LYS:HD2	1.57	0.69
1:K:72:ARG:NH1	1:L:182:LEU:HD11	2.06	0.69
1:S:189:LEU:HD22	1:S:199:VAL:HG23	1.72	0.69
1:U:145:VAL:HG22	1:U:329:LEU:HD21	1.72	0.69
1:D:203:MET:HE2	1:D:210:LEU:HD12	1.73	0.69
1:Q:225:GLN:HE21	1:Q:225:GLN:HA	1.57	0.69
1:B:19:GLN:NE2	1:C:296:GLN:OE1	2.25	0.69
1:N:118:PHE:CE1	1:X:223:LYS:HB2	2.26	0.69
1:W:98:ARG:HH11	1:W:98:ARG:CG	2.01	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:82:TYR:HD2	1:Q:122:ASN:HB3	1.53	0.69
1:S:82:TYR:CD2	1:S:122:ASN:HB3	2.27	0.69
1:E:283:LYS:HB3	1:O:153:PRO:HD3	1.74	0.69
1:Q:82:TYR:O	1:Q:85:THR:HB	1.91	0.69
1:J:82:TYR:O	1:J:85:THR:HB	1.92	0.69
1:L:82:TYR:O	1:L:85:THR:HB	1.91	0.69
1:T:189:LEU:CD2	1:T:199:VAL:HG21	2.23	0.69
1:X:173:MET:O	1:X:177:LEU:CD1	2.41	0.69
1:V:113:VAL:HG21	1:V:329:LEU:HD22	1.74	0.69
1:J:124:VAL:HG13	1:J:152:PHE:CE1	2.27	0.69
1:V:173:MET:O	1:V:177:LEU:CD1	2.40	0.69
1:E:323:TRP:CH2	1:O:129:ASN:CG	2.61	0.68
1:L:283:LYS:H	1:L:283:LYS:HD2	1.58	0.68
1:T:173:MET:O	1:T:177:LEU:HD13	1.93	0.68
1:U:276:ILE:CD1	1:U:282:ILE:HD13	2.24	0.68
1:X:131:LYS:NZ	1:X:262:ILE:CD1	2.56	0.68
1:D:120:ILE:O	1:D:124:VAL:HG23	1.93	0.68
1:I:266:LEU:HD12	1:I:266:LEU:H	1.57	0.68
1:O:100:GLN:HE22	1:R:111:ARG:HH12	1.36	0.68
1:A:203:MET:HE2	1:A:210:LEU:HD12	1.75	0.68
1:X:131:LYS:CE	1:X:298:GLY:HA2	2.23	0.68
1:J:198:PRO:HD2	1:J:314:ARG:NH2	2.08	0.68
1:U:266:LEU:HD12	1:U:266:LEU:H	1.57	0.68
1:T:12:LEU:HD13	1:T:13:LYS:N	2.07	0.68
1:B:189:LEU:HD23	1:B:290:VAL:HA	1.74	0.68
1:K:103:GLU:OE2	1:U:100:GLN:CD	2.37	0.68
1:L:110:GLN:HG2	1:L:111:ARG:N	2.03	0.68
1:M:182:LEU:HD11	1:N:72:ARG:NH1	2.09	0.68
1:Q:11:LEU:CD2	1:T:300:SER:O	2.42	0.68
1:E:205:VAL:HB	1:F:7:LEU:HD21	1.75	0.68
1:E:3:LEU:HD23	1:F:214:HIS:CB	2.24	0.68
1:K:180:HIS:HE1	1:K:182:LEU:HD13	1.59	0.68
1:O:307:LEU:HD11	1:O:315:LEU:HD23	1.76	0.68
1:K:110:GLN:HE21	1:K:110:GLN:HA	1.59	0.68
1:P:203:MET:HE2	1:P:210:LEU:HD12	1.76	0.68
1:S:182:LEU:HD21	1:T:72:ARG:HH11	1.59	0.68
1:A:236:SER:O	1:A:240:VAL:HG12	1.94	0.67
1:B:110:GLN:HB3	1:J:128:PRO:HG2	1.75	0.67
1:D:93:ILE:HD12	1:D:120:ILE:HD11	1.76	0.67
1:O:276:ILE:CD1	1:O:282:ILE:HD13	2.24	0.67
1:A:13:LYS:H	1:A:13:LYS:HD3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LEU:HD21	1:B:291:PRO:HD3	1.76	0.67
1:J:198:PRO:CD	1:J:314:ARG:NH2	2.56	0.67
1:B:285:ASP:OD2	1:K:128:PRO:HG3	1.94	0.67
1:E:210:LEU:CG	1:F:3:LEU:HD21	2.23	0.67
1:I:82:TYR:CD2	1:I:122:ASN:HB3	2.29	0.67
1:X:154:LYS:HZ3	1:X:275:MET:HB3	1.58	0.67
1:A:276:ILE:CD1	1:A:282:ILE:HD13	2.24	0.67
1:B:331:PHE:OXT	1:K:17:THR:HB	1.94	0.67
1:Q:276:ILE:CD1	1:Q:282:ILE:HD13	2.24	0.67
1:W:6:GLN:NE2	1:X:213:LEU:HD22	2.09	0.67
1:W:276:ILE:CD1	1:W:282:ILE:HD13	2.24	0.67
1:E:275:MET:HE1	1:E:285:ASP:CG	2.19	0.67
1:N:276:ILE:CD1	1:N:282:ILE:HD13	2.25	0.67
1:R:276:ILE:CD1	1:R:282:ILE:HD13	2.24	0.67
1:T:276:ILE:CD1	1:T:282:ILE:HD13	2.24	0.67
1:X:177:LEU:HD11	1:X:226:TRP:CH2	2.30	0.67
1:B:276:ILE:HD13	1:B:282:ILE:CD1	2.25	0.67
2:Q:401:GO3:O4	2:Q:401:GO3:C36	2.43	0.67
1:V:302:LEU:HD13	1:W:11:LEU:HD11	1.76	0.67
1:B:328:GLU:OE2	1:J:19:GLN:NE2	2.27	0.67
1:C:276:ILE:CD1	1:C:282:ILE:HD13	2.25	0.67
1:J:300:SER:HB2	1:K:12:LEU:CD1	2.22	0.67
1:Q:3:LEU:HD21	1:R:210:LEU:CD2	2.22	0.67
1:Q:200:TRP:HE3	1:Q:217:LEU:HD11	1.60	0.67
1:S:276:ILE:HD13	1:S:282:ILE:CD1	2.24	0.67
1:U:276:ILE:HD13	1:U:282:ILE:CD1	2.25	0.67
1:C:14:GLU:O	1:C:16:GLN:HG2	1.95	0.67
1:P:276:ILE:HD13	1:P:282:ILE:CD1	2.25	0.67
1:Q:110:GLN:CB	2:Q:401:GO3:C38	2.72	0.67
1:S:182:LEU:CD2	1:T:72:ARG:HH11	2.07	0.67
1:U:302:LEU:HD23	1:X:11:LEU:CD1	2.25	0.67
1:F:276:ILE:CD1	1:F:282:ILE:HD13	2.24	0.67
1:U:3:LEU:HD22	1:V:214:HIS:HB3	1.77	0.67
1:G:276:ILE:HD13	1:G:282:ILE:CD1	2.25	0.66
1:M:276:ILE:CD1	1:M:282:ILE:HD13	2.25	0.66
1:P:82:TYR:O	1:P:85:THR:HB	1.95	0.66
1:P:108:LEU:CD1	1:P:111:ARG:H	2.08	0.66
1:X:276:ILE:HD13	1:X:282:ILE:CD1	2.25	0.66
1:H:276:ILE:CD1	1:H:282:ILE:HD13	2.24	0.66
1:K:189:LEU:HD22	1:K:199:VAL:HG23	1.77	0.66
1:L:10:ASN:ND2	1:L:13:LYS:HE3	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:108:LEU:HD23	1:P:111:ARG:CZ	2.25	0.66
1:R:187:TRP:HB3	1:R:189:LEU:CD1	2.23	0.66
1:B:180:HIS:HE1	1:B:182:LEU:HD13	1.60	0.66
1:I:264:LYS:HB2	1:I:266:LEU:CD1	2.17	0.66
1:N:12:LEU:O	1:N:13:LYS:HB3	1.94	0.66
1:S:114:ASN:HA	1:S:117:LYS:CE	2.20	0.66
1:L:276:ILE:CD1	1:L:282:ILE:HD13	2.24	0.66
1:O:276:ILE:HD13	1:O:282:ILE:CD1	2.25	0.66
1:Q:276:ILE:HD13	1:Q:282:ILE:CD1	2.25	0.66
1:V:177:LEU:HD11	1:V:226:TRP:CH2	2.28	0.66
1:W:8:ILE:HD13	1:X:177:LEU:O	1.96	0.66
1:X:131:LYS:NZ	1:X:262:ILE:CG1	2.58	0.66
1:C:39:LEU:CD1	1:C:47:LEU:HD22	2.25	0.66
1:D:276:ILE:CD1	1:D:282:ILE:HD13	2.25	0.66
1:I:276:ILE:HD13	1:I:282:ILE:CD1	2.25	0.66
1:O:53:ILE:HG23	1:R:52:VAL:CG1	2.26	0.66
1:R:266:LEU:O	1:T:180:HIS:HB2	1.94	0.66
1:V:12:LEU:HB2	1:W:300:SER:HA	1.76	0.66
1:G:224:GLU:HG3	1:Q:330:GLN:HE22	1.60	0.66
1:O:145:VAL:HG22	1:O:331:PHE:CZ	2.26	0.66
1:T:276:ILE:HD13	1:T:282:ILE:CD1	2.25	0.66
1:V:276:ILE:HD13	1:V:282:ILE:CD1	2.25	0.66
1:X:276:ILE:CD1	1:X:282:ILE:HD13	2.25	0.66
1:P:276:ILE:CD1	1:P:282:ILE:HD13	2.25	0.66
1:A:93:ILE:HD12	1:A:120:ILE:HD11	1.76	0.66
1:V:276:ILE:CD1	1:V:282:ILE:HD13	2.25	0.66
1:H:203:MET:HE2	1:H:210:LEU:HD12	1.78	0.66
1:Q:50:VAL:HG11	1:Q:82:TYR:CE1	2.31	0.66
1:U:154:LYS:HE2	1:X:11:LEU:HD21	1.78	0.66
1:U:307:LEU:HD12	1:U:307:LEU:N	2.10	0.66
1:L:276:ILE:HD13	1:L:282:ILE:CD1	2.26	0.66
1:S:189:LEU:HD22	1:S:199:VAL:CG2	2.26	0.66
1:U:324:GLY:O	1:U:328:GLU:OE1	2.14	0.66
1:C:14:GLU:HG2	1:C:16:GLN:HG3	1.77	0.65
1:D:276:ILE:HD13	1:D:282:ILE:CD1	2.26	0.65
1:N:114:ASN:HD22	1:W:5:ASP:CG	2.04	0.65
1:U:221:LYS:H	1:U:221:LYS:HD2	1.61	0.65
1:C:276:ILE:HD13	1:C:282:ILE:CD1	2.25	0.65
1:G:331:PHE:C	1:G:331:PHE:CD2	2.75	0.65
1:I:3:LEU:HD11	1:J:210:LEU:HG	1.78	0.65
1:J:163:ASN:HD22	1:J:258:LEU:HD21	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:ILE:HD13	1:F:282:ILE:CD1	2.25	0.65
1:G:276:ILE:CD1	1:G:282:ILE:HD13	2.26	0.65
1:I:9:TYR:CD2	1:L:302:LEU:CD2	2.62	0.65
1:M:82:TYR:CD2	1:M:122:ASN:HB3	2.31	0.65
1:O:105:ARG:CA	1:O:108:LEU:HD13	2.26	0.65
1:R:276:ILE:HD13	1:R:282:ILE:CD1	2.25	0.65
1:X:269:VAL:C	1:X:292:CYS:O	2.39	0.65
1:I:50:VAL:HG11	1:I:82:TYR:CE1	2.31	0.65
1:J:276:ILE:HD13	1:J:282:ILE:CD1	2.25	0.65
1:J:290:VAL:CG1	1:J:291:PRO:HD2	2.25	0.65
1:W:276:ILE:HD13	1:W:282:ILE:CD1	2.25	0.65
1:B:180:HIS:CE1	1:B:182:LEU:HD13	2.32	0.65
1:J:276:ILE:CD1	1:J:282:ILE:HD13	2.24	0.65
1:P:109:VAL:CG1	1:P:110:GLN:HE21	2.10	0.65
1:L:10:ASN:HD21	1:L:13:LYS:HG3	1.62	0.65
1:M:191:GLU:OE1	1:M:193:GLY:CA	2.43	0.65
1:V:124:VAL:CG1	1:V:152:PHE:CE1	2.80	0.65
1:E:11:LEU:CD1	1:H:302:LEU:CD1	2.65	0.65
1:E:266:LEU:O	1:G:180:HIS:HB2	1.96	0.65
1:M:290:VAL:HG21	1:M:302:LEU:HD13	1.79	0.65
1:I:276:ILE:CD1	1:I:282:ILE:HD13	2.25	0.65
1:K:180:HIS:CE1	1:K:182:LEU:HD13	2.32	0.65
1:N:12:LEU:CD1	1:O:300:SER:HB2	2.21	0.65
1:B:276:ILE:CD1	1:B:282:ILE:HD13	2.26	0.65
1:U:170:ARG:HD2	1:U:184:CYS:O	1.96	0.65
1:C:30:VAL:HG23	1:C:98:ARG:HH12	1.60	0.65
1:F:328:GLU:OE1	1:W:111:ARG:HG3	1.96	0.65
1:H:276:ILE:HD13	1:H:282:ILE:CD1	2.26	0.65
1:P:113:VAL:HG21	1:P:329:LEU:HD22	1.78	0.65
1:A:240:VAL:HG13	1:A:247:THR:CG2	2.27	0.64
1:E:110:GLN:HG3	1:N:129:ASN:ND2	2.12	0.64
1:I:16:GLN:CG	1:I:17:THR:H	2.02	0.64
1:M:276:ILE:HD13	1:M:282:ILE:CD1	2.25	0.64
1:N:276:ILE:HD13	1:N:282:ILE:CD1	2.26	0.64
1:Q:109:VAL:CG1	2:Q:401:GO3:C28	2.76	0.64
1:R:258:LEU:CD2	1:R:258:LEU:N	2.60	0.64
1:U:117:LYS:NZ	1:U:330:GLN:O	2.22	0.64
1:X:113:VAL:HG21	1:X:329:LEU:CD2	2.26	0.64
1:H:125:LYS:HZ2	1:Q:309:SER:CB	2.08	0.64
1:M:261:SER:HB2	1:M:270:HIS:HE1	1.63	0.64
1:O:100:GLN:CG	1:R:103:GLU:OE2	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:14:GLU:CG	1:K:16:GLN:HG2	2.27	0.64
1:L:330:GLN:O	1:L:330:GLN:HG2	1.98	0.64
1:F:100:GLN:HG3	1:W:80:LYS:HE3	1.78	0.64
1:X:131:LYS:CE	1:X:158:ILE:HD11	2.22	0.64
1:F:30:VAL:HG23	1:F:98:ARG:HH12	1.62	0.64
1:L:216:ASP:OD1	1:L:221:LYS:HD2	1.97	0.64
1:N:52:VAL:HG12	1:X:223:LYS:NZ	2.13	0.64
1:X:16:GLN:HG3	1:X:17:THR:H	1.62	0.64
1:Q:15:GLU:C	1:Q:16:GLN:HG2	2.23	0.64
1:V:113:VAL:HG21	1:V:329:LEU:CD2	2.28	0.64
1:X:131:LYS:CE	1:X:158:ILE:HD13	2.26	0.64
1:O:105:ARG:O	1:O:108:LEU:CD1	2.39	0.64
1:E:15:GLU:O	1:E:16:GLN:HB2	1.98	0.64
1:G:331:PHE:C	1:G:331:PHE:HD2	2.05	0.64
1:U:185:HIS:CE1	1:W:185:HIS:CE1	2.86	0.63
1:A:11:LEU:CD1	1:D:302:LEU:HD23	2.28	0.63
1:A:276:ILE:HD13	1:A:282:ILE:CD1	2.27	0.63
1:K:55:ASP:CG	1:U:80:LYS:HE2	2.22	0.63
1:K:100:GLN:HG2	1:U:111:ARG:HH22	1.61	0.63
1:T:275:MET:HE3	1:T:277:LYS:HB3	1.79	0.63
1:D:188:VAL:C	1:D:189:LEU:HD23	2.24	0.63
1:B:159:GLY:O	1:B:272:VAL:HG12	1.99	0.63
1:G:276:ILE:HD11	1:G:286:VAL:CG1	2.29	0.63
1:I:297:ASN:OD1	1:L:15:GLU:HB3	1.98	0.63
1:M:144:TYR:CG	1:M:326:GLN:NE2	2.66	0.63
1:Q:110:GLN:CB	2:Q:401:GO3:O6	2.33	0.63
1:B:328:GLU:OE1	1:J:17:THR:HB	1.97	0.63
1:E:3:LEU:C	1:E:3:LEU:CD1	2.72	0.63
1:F:188:VAL:C	1:F:189:LEU:HD23	2.24	0.63
1:M:188:VAL:C	1:M:189:LEU:HD23	2.23	0.63
1:Q:117:LYS:HE2	1:Q:331:PHE:C	2.23	0.63
1:A:310:GLU:CD	1:A:314:ARG:HD2	2.24	0.63
1:T:109:VAL:HG22	1:T:138:PRO:CG	2.29	0.63
1:W:224:GLU:OE1	1:X:3:LEU:HB3	1.98	0.63
1:C:328:GLU:HG3	1:M:111:ARG:HE	1.62	0.62
1:F:266:LEU:O	1:H:180:HIS:HB2	1.99	0.62
1:C:188:VAL:C	1:C:189:LEU:HD23	2.24	0.62
1:Q:210:LEU:HA	1:Q:213:LEU:HD21	1.76	0.62
1:R:54:GLU:CG	1:R:80:LYS:CD	2.72	0.62
1:S:276:ILE:CD1	1:S:282:ILE:HD13	2.26	0.62
1:V:10:ASN:ND2	1:W:301:ASP:OD2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:131:LYS:HZ1	1:X:262:ILE:HD11	1.64	0.62
1:J:12:LEU:HD13	1:K:155:ASN:CB	2.27	0.62
1:J:11:LEU:HD23	1:K:299:ILE:HG22	1.81	0.62
1:J:25:VAL:HG22	1:J:50:VAL:HG22	1.80	0.62
1:T:189:LEU:HD21	1:T:199:VAL:CG2	2.29	0.62
1:B:13:LYS:O	1:B:15:GLU:HG3	1.99	0.62
1:H:310:GLU:OE1	1:H:314:ARG:HD2	1.98	0.62
1:U:186:GLY:C	1:U:187:TRP:CD1	2.78	0.62
1:O:100:GLN:CB	1:R:103:GLU:OE2	2.48	0.62
1:W:6:GLN:HE21	1:X:213:LEU:HD22	1.63	0.62
1:V:13:LYS:H	1:V:13:LYS:HD2	1.64	0.62
1:K:55:ASP:OD1	1:U:80:LYS:HE2	2.00	0.61
1:P:109:VAL:HG12	1:P:110:GLN:HE21	1.65	0.61
1:P:110:GLN:CD	1:P:110:GLN:H	2.08	0.61
1:Q:109:VAL:HG12	2:Q:401:GO3:C28	2.30	0.61
1:U:280:TYR:HE1	1:U:307:LEU:HD13	1.65	0.61
1:G:310:GLU:OE1	1:G:314:ARG:HG3	2.00	0.61
1:J:290:VAL:HG12	1:J:291:PRO:CD	2.31	0.61
1:O:307:LEU:CD1	1:O:315:LEU:HD23	2.29	0.61
1:E:3:LEU:HD23	1:F:214:HIS:HB3	1.82	0.61
1:F:100:GLN:HG3	1:W:80:LYS:CE	2.31	0.61
1:J:200:TRP:HB3	1:J:217:LEU:HD23	1.80	0.61
1:B:189:LEU:HD13	1:B:199:VAL:CG2	2.29	0.61
1:N:302:LEU:HD13	1:O:11:LEU:CD1	2.30	0.61
1:V:15:GLU:HB3	1:W:297:ASN:ND2	2.15	0.61
1:B:303:VAL:HG11	1:D:206:ALA:HB3	1.83	0.61
1:F:16:GLN:HG3	1:F:17:THR:N	2.14	0.61
1:G:3:LEU:HD13	1:H:214:HIS:HB2	1.82	0.61
1:G:25:VAL:HG22	1:G:50:VAL:HG23	1.82	0.61
1:S:50:VAL:HG11	1:S:82:TYR:CE1	2.35	0.61
1:F:280:TYR:CE1	1:F:307:LEU:HD13	2.36	0.61
1:F:109:VAL:HG22	1:F:138:PRO:CG	2.31	0.61
1:C:7:LEU:HD21	1:D:205:VAL:HB	1.83	0.61
1:Q:210:LEU:HA	1:Q:213:LEU:HD22	1.77	0.61
1:S:213:LEU:O	1:T:6:GLN:NE2	2.31	0.61
1:C:13:LYS:O	1:C:15:GLU:HG3	2.01	0.60
1:J:216:ASP:O	1:J:222:ASP:HB3	2.00	0.60
1:J:216:ASP:HB3	1:J:222:ASP:CB	2.31	0.60
1:N:5:ASP:O	1:O:304:LYS:NZ	2.31	0.60
1:P:108:LEU:CB	1:P:111:ARG:HE	2.13	0.60
1:Q:225:GLN:O	1:Q:228:GLU:HG3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:114:ASN:ND2	1:W:5:ASP:OD2	2.29	0.60
1:Q:210:LEU:O	1:Q:213:LEU:HD23	2.01	0.60
1:U:19:GLN:O	1:U:20:ASN:ND2	2.33	0.60
1:X:16:GLN:CG	1:X:17:THR:H	2.13	0.60
1:G:71:LEU:HD22	1:G:71:LEU:N	2.17	0.60
1:J:12:LEU:HD21	1:K:155:ASN:ND2	2.16	0.60
1:V:97:ALA:O	1:V:108:LEU:HD13	2.01	0.60
1:W:298:GLY:O	1:W:299:ILE:O	2.18	0.60
1:T:195:SER:O	1:T:318:SER:OG	2.19	0.60
1:D:124:VAL:HG13	1:D:152:PHE:CZ	2.37	0.60
1:P:108:LEU:HG	1:P:111:ARG:CG	2.31	0.60
1:E:213:LEU:O	1:F:6:GLN:NE2	2.34	0.60
1:J:11:LEU:HD21	1:K:302:LEU:HD12	1.74	0.60
1:U:302:LEU:HD21	1:X:11:LEU:HD11	1.82	0.60
1:A:280:TYR:O	1:A:316:LYS:NZ	2.34	0.60
1:J:25:VAL:HG22	1:J:50:VAL:CG2	2.31	0.60
1:K:110:GLN:HA	1:K:110:GLN:NE2	2.14	0.60
1:Q:323:TRP:CZ2	1:Q:327:LYS:HE2	2.36	0.60
1:V:204:ASN:HA	1:V:210:LEU:HD13	1.83	0.60
1:J:11:LEU:HD21	1:K:302:LEU:HD11	1.71	0.60
1:R:308:THR:HG22	1:R:311:GLU:CG	2.32	0.60
1:B:283:LYS:HB2	1:K:153:PRO:CD	2.16	0.59
1:C:36:ILE:HD11	1:D:253:LEU:HD11	1.84	0.59
1:R:258:LEU:CD2	1:R:258:LEU:H	2.15	0.59
1:U:302:LEU:CD2	1:X:11:LEU:CD1	2.80	0.59
1:J:124:VAL:CG1	1:J:152:PHE:CE1	2.85	0.59
1:K:189:LEU:HD23	1:K:199:VAL:CG2	2.32	0.59
1:L:283:LYS:NZ	1:L:316:LYS:HZ1	2.00	0.59
1:M:29:ALA:HB3	1:M:98:ARG:HH22	1.68	0.59
1:F:164:LEU:HD21	1:F:168:ARG:NH2	2.18	0.59
1:O:108:LEU:HD12	1:O:108:LEU:H	1.66	0.59
1:R:52:VAL:O	1:R:80:LYS:NZ	2.34	0.59
1:B:285:ASP:OD2	1:K:128:PRO:HB2	2.03	0.59
1:H:239:GLU:O	1:H:243:LEU:HD13	2.03	0.59
1:O:2:THR:HA	1:P:224:GLU:OE1	2.02	0.59
1:V:302:LEU:HD13	1:W:11:LEU:CD1	2.32	0.59
1:W:66:HIS:HB2	1:X:250:ALA:HB2	1.84	0.59
1:C:328:GLU:CG	1:M:111:ARG:HE	2.15	0.59
1:K:103:GLU:OE1	1:U:100:GLN:HB2	2.03	0.59
1:L:30:VAL:HG23	1:L:98:ARG:HH11	1.67	0.59
1:O:105:ARG:C	1:O:108:LEU:CD1	2.74	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:300:SER:HB2	1:X:15:GLU:OE1	2.03	0.59
1:A:205:VAL:HB	1:B:7:LEU:HD21	1.84	0.59
1:C:72:ARG:CZ	1:D:182:LEU:HD11	2.32	0.59
1:H:275:MET:HE2	1:H:285:ASP:CA	2.33	0.59
1:R:11:LEU:HD21	1:S:302:LEU:HD13	1.85	0.59
1:F:318:SER:O	1:F:322:LEU:HD12	2.03	0.58
1:J:30:VAL:HG23	1:J:98:ARG:HH12	1.66	0.58
1:K:203:MET:HE2	1:K:210:LEU:HD23	1.86	0.58
1:A:301:ASP:HB3	1:D:8:ILE:CG2	2.33	0.58
1:Q:214:HIS:HB2	1:R:3:LEU:HD13	1.84	0.58
1:Q:268:ARG:HD3	1:S:182:LEU:CD2	2.25	0.58
1:T:82:TYR:CD2	1:T:122:ASN:HB3	2.38	0.58
1:A:301:ASP:HB3	1:D:8:ILE:HG23	1.84	0.58
1:E:328:GLU:OE2	1:N:19:GLN:NE2	2.36	0.58
1:V:120:ILE:O	1:V:124:VAL:HG22	2.03	0.58
1:A:121:PRO:HA	1:A:124:VAL:CG2	2.34	0.58
1:C:39:LEU:HD11	1:C:47:LEU:CD2	2.31	0.58
1:O:121:PRO:HA	1:O:124:VAL:CG2	2.34	0.58
1:U:219:THR:HB	1:U:221:LYS:HZ2	1.67	0.58
1:E:6:GLN:NE2	1:F:213:LEU:O	2.34	0.58
1:Q:210:LEU:CA	1:Q:213:LEU:HD23	2.31	0.58
1:U:3:LEU:CD1	1:V:213:LEU:HB3	2.34	0.58
1:D:290:VAL:CG1	1:D:291:PRO:HD2	2.34	0.58
1:E:3:LEU:HD23	1:F:214:HIS:HB2	1.86	0.58
1:O:3:LEU:HB2	1:P:224:GLU:OE2	2.03	0.58
1:M:30:VAL:HG22	1:M:251:ILE:HG21	1.85	0.58
1:O:100:GLN:OE1	1:R:111:ARG:NH1	2.36	0.58
1:T:96:GLY:HA2	1:T:115:ILE:HD13	1.85	0.58
1:N:267:ARG:HD2	1:O:15:GLU:OE2	2.03	0.58
1:C:35:ALA:O	1:C:39:LEU:HD22	2.03	0.58
1:C:191:GLU:OE1	1:C:193:GLY:HA3	2.03	0.58
1:C:328:GLU:CD	1:M:111:ARG:HE	2.11	0.58
1:K:54:GLU:OE2	1:U:54:GLU:HB2	2.03	0.57
1:K:121:PRO:HA	1:K:124:VAL:CG2	2.34	0.57
1:A:19:GLN:HE22	1:D:296:GLN:CD	2.12	0.57
1:D:290:VAL:HG12	1:D:291:PRO:HD2	1.86	0.57
1:E:275:MET:CE	1:E:285:ASP:OD1	2.47	0.57
1:I:275:MET:HE3	1:I:277:LYS:HB3	1.85	0.57
1:W:323:TRP:O	1:W:327:LYS:CG	2.51	0.57
1:N:225:GLN:HE21	1:N:225:GLN:CA	2.10	0.57
1:Q:304:LYS:HD3	1:T:9:TYR:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:190:GLY:HA2	1:O:288:LEU:HG	1.86	0.57
1:P:54:GLU:HG2	1:P:80:LYS:HD3	1.87	0.57
1:R:163:ASN:HD22	1:R:258:LEU:HD21	1.62	0.57
1:T:13:LYS:H	1:T:13:LYS:HZ2	1.50	0.57
1:U:239:GLU:O	1:U:243:LEU:HD13	2.02	0.57
1:V:55:ASP:C	1:V:55:ASP:OD1	2.47	0.57
1:J:290:VAL:CG1	1:J:291:PRO:CD	2.83	0.57
1:K:224:GLU:OE2	1:L:3:LEU:HB2	2.04	0.57
1:Q:210:LEU:CA	1:Q:213:LEU:CD2	2.69	0.57
1:R:173:MET:HG2	1:R:177:LEU:CD2	2.34	0.57
1:V:15:GLU:HB3	1:W:297:ASN:HD21	1.69	0.57
1:F:111:ARG:CZ	1:W:52:VAL:HG21	2.35	0.57
1:G:265:ASN:O	1:G:295:GLY:HA2	2.05	0.57
1:K:189:LEU:HD22	1:K:199:VAL:CG2	2.33	0.57
1:A:93:ILE:CD1	1:A:120:ILE:CD1	2.83	0.57
1:S:189:LEU:HD23	1:S:199:VAL:CG2	2.33	0.57
1:B:25:VAL:HG22	1:B:50:VAL:HG13	1.86	0.57
1:X:203:MET:HE2	1:X:210:LEU:HD23	1.86	0.57
1:J:124:VAL:HG13	1:J:152:PHE:CZ	2.39	0.57
1:M:324:GLY:CA	1:M:327:LYS:HE3	2.31	0.57
1:F:96:GLY:HA2	1:F:115:ILE:HD13	1.87	0.57
1:Q:96:GLY:HA2	1:Q:115:ILE:HD13	1.87	0.57
1:W:275:MET:HE3	1:W:277:LYS:HB3	1.86	0.57
1:J:89:LYS:NZ	1:K:19:GLN:HG3	2.19	0.56
1:J:120:ILE:O	1:J:124:VAL:HG22	2.05	0.56
1:L:195:SER:O	1:L:318:SER:OG	2.24	0.56
1:Q:69:LEU:HD13	1:R:181:PRO:HB2	1.88	0.56
1:R:11:LEU:HD23	1:S:302:LEU:HD13	1.86	0.56
1:B:189:LEU:CD2	1:B:291:PRO:HD3	2.35	0.56
1:G:330:GLN:O	1:G:331:PHE:HB3	2.04	0.56
1:N:225:GLN:HA	1:N:225:GLN:NE2	2.09	0.56
1:W:63:ASP:HB3	1:X:249:TRP:HD1	1.70	0.56
1:W:144:TYR:HE2	1:W:329:LEU:HD23	1.70	0.56
1:G:50:VAL:CG1	1:G:79:GLY:O	2.52	0.56
1:H:9:TYR:CD1	2:Q:401:GO3:C34	2.88	0.56
1:J:11:LEU:CD2	1:K:302:LEU:HD12	2.32	0.56
1:P:108:LEU:HD23	1:P:111:ARG:NE	2.20	0.56
1:R:163:ASN:ND2	1:R:258:LEU:CD2	2.62	0.56
1:U:154:LYS:HE2	1:X:11:LEU:HD23	1.86	0.56
1:E:303:VAL:HG11	1:G:206:ALA:HB3	1.87	0.56
1:R:15:GLU:CD	1:R:15:GLU:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:290:VAL:HG21	1:M:302:LEU:CD1	2.35	0.56
1:O:111:ARG:NH2	1:R:100:GLN:HE22	2.00	0.56
1:P:219:THR:CG2	1:P:221:LYS:CG	2.74	0.56
1:S:18:PRO:HG3	1:S:46:GLU:OE1	2.06	0.56
1:A:240:VAL:CG1	1:A:247:THR:CG2	2.84	0.56
1:E:110:GLN:HG3	1:N:129:ASN:HD22	1.70	0.56
1:Q:243:LEU:HD11	1:R:58:LYS:HD3	1.88	0.56
1:V:11:LEU:HB2	1:W:300:SER:O	2.05	0.56
1:V:12:LEU:HA	1:V:13:LYS:HE3	1.86	0.56
1:B:11:LEU:HD11	1:C:302:LEU:HD13	1.88	0.56
1:D:93:ILE:CD1	1:D:120:ILE:CD1	2.82	0.56
1:E:328:GLU:HA	1:N:19:GLN:HE22	1.71	0.56
1:K:276:ILE:HD13	1:K:282:ILE:CD1	2.36	0.56
1:O:105:ARG:CA	1:O:108:LEU:CD1	2.83	0.56
1:V:304:LYS:CE	1:W:5:ASP:O	2.54	0.56
1:E:96:GLY:HA2	1:E:115:ILE:HD13	1.86	0.55
1:I:329:LEU:HB3	1:I:331:PHE:CE2	2.40	0.55
1:J:96:GLY:HA2	1:J:115:ILE:HD13	1.88	0.55
1:P:219:THR:HG23	1:P:221:LYS:HG2	1.80	0.55
1:M:154:LYS:HD3	1:M:275:MET:HE3	1.89	0.55
1:N:55:ASP:OD1	1:N:55:ASP:N	2.39	0.55
1:P:109:VAL:HG12	1:P:110:GLN:NE2	2.21	0.55
1:S:13:LYS:H	1:S:13:LYS:HD2	1.71	0.55
1:X:131:LYS:HZ3	1:X:262:ILE:CG1	2.09	0.55
1:A:305:VAL:HA	1:C:208:VAL:CG2	2.36	0.55
1:U:208:VAL:CG1	1:U:213:LEU:HD21	2.34	0.55
1:H:13:LYS:HG3	1:H:14:GLU:H	1.71	0.55
1:J:30:VAL:HG23	1:J:98:ARG:NH1	2.21	0.55
1:L:117:LYS:NZ	1:L:331:PHE:HA	2.20	0.55
1:B:285:ASP:CG	1:K:128:PRO:HB2	2.32	0.55
1:J:13:LYS:HG3	1:J:14:GLU:N	2.21	0.55
1:K:108:LEU:HD21	1:U:100:GLN:CD	2.30	0.55
1:M:206:ALA:HA	1:O:187:TRP:CZ2	2.41	0.55
1:N:12:LEU:HD21	1:O:300:SER:HA	1.89	0.55
1:O:52:VAL:O	1:O:80:LYS:CE	2.46	0.55
1:R:54:GLU:HG2	1:R:80:LYS:CD	2.36	0.55
1:W:7:LEU:HD12	1:X:177:LEU:HD23	1.87	0.55
1:E:308:THR:CG2	1:E:311:GLU:OE2	2.55	0.55
1:L:283:LYS:CE	1:L:316:LYS:NZ	2.65	0.55
1:R:147:TRP:CH2	1:R:275:MET:HE1	2.42	0.55
1:K:54:GLU:CD	1:K:80:LYS:CD	2.78	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:100:GLN:CB	1:U:103:GLU:OE2	2.54	0.55
1:V:13:LYS:HD2	1:V:13:LYS:N	2.22	0.55
1:B:13:LYS:HG2	1:B:14:GLU:N	2.21	0.55
1:G:224:GLU:CG	1:Q:330:GLN:NE2	2.67	0.55
1:E:200:TRP:HE1	1:E:314:ARG:HH12	1.55	0.55
1:P:147:TRP:CH2	1:P:275:MET:HE1	2.41	0.55
1:W:15:GLU:O	1:W:16:GLN:HG3	2.07	0.55
1:C:311:GLU:HA	1:C:314:ARG:NH1	2.22	0.55
1:S:276:ILE:HG22	1:S:279:LEU:CD1	2.37	0.55
1:U:239:GLU:O	1:U:243:LEU:HD22	2.07	0.55
1:J:300:SER:HA	1:K:12:LEU:HG	1.90	0.54
1:E:285:ASP:OD2	1:O:128:PRO:HG3	2.07	0.54
1:P:108:LEU:HG	1:P:111:ARG:CB	2.36	0.54
1:U:187:TRP:NE1	1:W:206:ALA:HA	2.21	0.54
1:X:154:LYS:HZ2	1:X:275:MET:HB3	1.69	0.54
1:K:276:ILE:HD13	1:K:282:ILE:HD12	1.89	0.54
1:V:147:TRP:CH2	1:V:275:MET:HE1	2.42	0.54
1:A:266:LEU:O	1:C:180:HIS:HB2	2.08	0.54
1:F:100:GLN:HB3	1:W:80:LYS:NZ	2.23	0.54
1:I:117:LYS:HZ3	1:I:331:PHE:HB3	1.72	0.54
1:I:329:LEU:HB3	1:I:331:PHE:HE2	1.72	0.54
1:M:30:VAL:HG12	1:M:94:THR:HB	1.89	0.54
1:O:117:LYS:NZ	1:O:330:GLN:O	2.39	0.54
1:Q:147:TRP:CH2	1:Q:275:MET:HE1	2.42	0.54
1:I:180:HIS:HB2	1:K:266:LEU:O	2.07	0.54
1:K:208:VAL:CG1	1:K:213:LEU:HD21	2.38	0.54
1:K:283:LYS:HE3	1:K:316:LYS:NZ	2.23	0.54
1:T:330:GLN:CD	1:T:330:GLN:N	2.66	0.54
1:W:7:LEU:HD11	1:X:205:VAL:CB	2.35	0.54
1:W:249:TRP:HD1	1:X:63:ASP:HB3	1.71	0.54
1:B:300:SER:O	1:C:11:LEU:HB2	2.07	0.54
1:E:285:ASP:OD2	1:O:128:PRO:CB	2.56	0.54
1:E:330:GLN:HB2	1:O:19:GLN:HE22	1.72	0.54
1:C:32:MET:HE1	1:C:64:LEU:CD2	2.37	0.54
1:F:25:VAL:HG22	1:F:50:VAL:HG13	1.90	0.54
1:C:328:GLU:HB2	1:M:111:ARG:NH2	2.23	0.54
1:K:54:GLU:CG	1:K:80:LYS:CD	2.86	0.54
1:U:45:ASP:OD1	1:U:45:ASP:C	2.50	0.54
1:U:301:ASP:OD2	1:X:10:ASN:ND2	2.35	0.54
1:W:323:TRP:O	1:W:327:LYS:HG2	2.07	0.54
1:C:328:GLU:HB2	1:M:107:ASN:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:MET:CE	1:E:285:ASP:CA	2.77	0.54
1:K:27:VAL:HG13	1:K:27:VAL:O	2.08	0.54
1:P:330:GLN:O	1:P:330:GLN:HG2	2.06	0.54
1:Q:8:ILE:HG23	1:T:301:ASP:HB3	1.90	0.54
1:T:25:VAL:HG22	1:T:50:VAL:CG1	2.38	0.54
1:T:25:VAL:HG22	1:T:50:VAL:HG13	1.90	0.54
1:U:280:TYR:CE1	1:U:307:LEU:CD1	2.89	0.54
1:X:204:ASN:HA	1:X:210:LEU:HD13	1.89	0.54
1:E:155:ASN:ND2	1:H:12:LEU:HD11	2.22	0.54
1:E:221:LYS:H	1:E:221:LYS:HD2	1.73	0.54
1:J:147:TRP:CH2	1:J:275:MET:HE1	2.42	0.54
1:Q:213:LEU:HD11	1:R:7:LEU:HB2	1.89	0.54
1:S:69:LEU:HD12	1:T:182:LEU:HD12	1.89	0.54
1:W:137:ASN:HD21	1:W:192:HIS:HD2	1.54	0.54
1:U:225:GLN:HE21	1:U:225:GLN:CA	2.21	0.53
1:F:111:ARG:NH1	1:W:52:VAL:CG2	2.71	0.53
1:J:16:GLN:O	1:K:296:GLN:NE2	2.41	0.53
1:M:25:VAL:HG22	1:M:50:VAL:HG13	1.88	0.53
1:Q:204:ASN:HA	1:Q:210:LEU:HD13	1.91	0.53
1:R:290:VAL:HG22	1:R:291:PRO:CD	2.39	0.53
1:U:304:LYS:HD2	1:X:9:TYR:HB2	1.91	0.53
1:W:58:LYS:HG2	1:X:243:LEU:HD13	1.89	0.53
1:W:327:LYS:O	1:W:328:GLU:HG3	2.07	0.53
1:T:331:PHE:HD1	1:T:331:PHE:O	1.92	0.53
1:C:12:LEU:O	1:C:13:LYS:HB2	2.08	0.53
1:E:14:GLU:HG3	1:E:15:GLU:H	1.74	0.53
1:I:15:GLU:CG	1:L:297:ASN:OD1	2.56	0.53
1:U:16:GLN:O	1:U:17:THR:CG2	2.47	0.53
1:D:52:VAL:HA	1:D:80:LYS:HE3	1.90	0.53
1:A:13:LYS:HG2	1:A:14:GLU:H	1.74	0.53
1:C:64:LEU:CD1	1:D:249:TRP:CD1	2.92	0.53
1:P:108:LEU:CD2	1:P:111:ARG:NE	2.71	0.53
1:V:124:VAL:CG1	1:V:152:PHE:CZ	2.91	0.53
1:X:268:ARG:O	1:X:269:VAL:O	2.27	0.53
1:E:276:ILE:HD12	1:E:288:LEU:HG	1.90	0.53
1:L:204:ASN:HA	1:L:210:LEU:HD13	1.90	0.53
1:F:147:TRP:CH2	1:F:275:MET:HE1	2.44	0.53
1:O:54:GLU:OE2	1:R:54:GLU:HB2	2.08	0.53
1:T:12:LEU:HD13	1:T:13:LYS:H	1.72	0.53
1:V:302:LEU:CD1	1:W:11:LEU:HD11	2.40	0.53
1:B:204:ASN:HA	1:B:210:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:VAL:CG1	1:D:152:PHE:CE1	2.92	0.52
1:I:234:VAL:HG12	1:I:235:GLU:OE1	2.07	0.52
1:K:16:GLN:NE2	1:K:16:GLN:CA	2.44	0.52
1:O:93:ILE:HD11	1:O:132:LEU:CD2	2.38	0.52
1:V:69:LEU:C	1:V:69:LEU:CD2	2.81	0.52
1:V:124:VAL:HG12	1:V:152:PHE:CE1	2.44	0.52
1:M:25:VAL:HG22	1:M:50:VAL:CG1	2.39	0.52
1:R:10:ASN:ND2	1:S:301:ASP:OD2	2.21	0.52
1:E:268:ARG:HD3	1:G:182:LEU:HD13	1.92	0.52
1:O:108:LEU:N	1:O:108:LEU:CD1	2.72	0.52
1:R:15:GLU:CD	1:R:15:GLU:N	2.68	0.52
1:U:225:GLN:HA	1:U:225:GLN:NE2	2.24	0.52
1:A:124:VAL:CG1	1:A:152:PHE:CE1	2.91	0.52
1:U:19:GLN:NE2	1:X:296:GLN:OE1	2.42	0.52
1:A:25:VAL:HG22	1:A:50:VAL:HG13	1.90	0.52
1:J:216:ASP:HB3	1:J:222:ASP:HB2	1.91	0.52
1:O:105:ARG:HA	1:O:108:LEU:CD1	2.38	0.52
1:A:13:LYS:HD3	1:A:13:LYS:N	2.24	0.52
1:Q:200:TRP:CE3	1:Q:217:LEU:HD12	2.44	0.52
1:V:12:LEU:HD12	1:W:300:SER:HA	1.92	0.52
1:F:25:VAL:HG22	1:F:50:VAL:CG1	2.40	0.52
1:O:100:GLN:HE22	1:R:111:ARG:NH1	2.02	0.52
1:O:204:ASN:HA	1:O:210:LEU:HD13	1.91	0.52
1:U:225:GLN:HE21	1:U:225:GLN:HA	1.75	0.52
1:U:275:MET:HE3	1:U:277:LYS:HB3	1.91	0.52
1:X:177:LEU:HD12	1:X:177:LEU:N	2.25	0.52
1:A:25:VAL:HG22	1:A:50:VAL:CG1	2.39	0.52
1:G:330:GLN:O	1:G:331:PHE:CB	2.58	0.52
1:J:300:SER:HA	1:K:12:LEU:CG	2.39	0.52
1:L:25:VAL:HG22	1:L:50:VAL:HG13	1.90	0.52
1:B:283:LYS:CB	1:K:153:PRO:CD	2.83	0.52
1:C:325:ILE:O	1:C:328:GLU:HG2	2.10	0.52
1:G:223:LYS:HB3	1:Q:330:GLN:HE21	1.73	0.52
1:I:217:LEU:O	1:I:222:ASP:OD2	2.28	0.52
1:O:111:ARG:NH2	1:R:100:GLN:NE2	2.50	0.52
1:A:69:LEU:O	1:B:182:LEU:HD11	2.10	0.52
1:C:328:GLU:OE1	1:M:111:ARG:HG3	2.10	0.52
1:Q:213:LEU:CD2	1:R:3:LEU:HD11	2.39	0.52
1:T:189:LEU:HD23	1:T:199:VAL:CG2	2.39	0.52
1:U:305:VAL:O	1:U:307:LEU:CD1	2.58	0.52
1:E:125:LYS:HE2	1:E:126:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:GLU:HG3	1:H:80:LYS:HD3	1.92	0.51
1:J:120:ILE:O	1:J:124:VAL:CG2	2.58	0.51
1:K:100:GLN:HE22	1:U:108:LEU:HD23	1.74	0.51
1:K:108:LEU:CD2	1:U:100:GLN:OE1	2.55	0.51
1:M:239:GLU:O	1:M:243:LEU:HD22	2.09	0.51
1:O:286:VAL:HG11	1:O:319:ALA:HB1	1.91	0.51
2:Q:401:GO3:C32	2:Q:401:GO3:C17	2.88	0.51
1:X:147:TRP:CH2	1:X:275:MET:HE1	2.43	0.51
1:E:204:ASN:HA	1:E:210:LEU:HD13	1.91	0.51
1:J:200:TRP:HB3	1:J:217:LEU:CD2	2.41	0.51
1:L:25:VAL:HG22	1:L:50:VAL:CG1	2.40	0.51
1:T:214:HIS:CE1	1:T:216:ASP:HB2	2.45	0.51
1:U:306:THR:HG21	1:W:213:LEU:HD11	1.92	0.51
1:A:101:GLU:OE2	1:A:242:LYS:HE2	2.10	0.51
1:G:65:GLN:HB3	1:H:171:TYR:CZ	2.46	0.51
1:L:228:GLU:HA	1:L:231:LYS:HD3	1.93	0.51
1:C:14:GLU:OE2	1:C:15:GLU:N	2.42	0.51
1:F:30:VAL:HG23	1:F:98:ARG:NH1	2.26	0.51
1:B:110:GLN:CG	1:J:129:ASN:HD21	2.05	0.51
1:K:54:GLU:HG3	1:K:80:LYS:CD	2.41	0.51
1:X:137:ASN:HD21	1:X:192:HIS:HD2	1.57	0.51
1:E:275:MET:HE3	1:E:285:ASP:HA	1.86	0.51
1:I:15:GLU:HG3	1:L:297:ASN:OD1	2.10	0.51
1:I:15:GLU:HG3	1:L:297:ASN:ND2	2.25	0.51
1:J:15:GLU:C	1:J:16:GLN:HG2	2.30	0.51
1:T:330:GLN:CD	1:T:330:GLN:H	2.18	0.51
1:X:131:LYS:HD2	1:X:298:GLY:N	2.25	0.51
1:D:187:TRP:HB3	1:D:189:LEU:HD21	1.93	0.51
1:Q:180:HIS:CE1	1:Q:182:LEU:HD12	2.46	0.51
1:B:10:ASN:HA	1:C:301:ASP:OD2	2.11	0.51
1:C:328:GLU:OE2	1:M:107:ASN:O	2.28	0.51
1:E:283:LYS:CB	1:O:153:PRO:CD	2.80	0.51
1:I:117:LYS:NZ	1:I:331:PHE:HB3	2.26	0.51
1:J:12:LEU:HD11	1:K:155:ASN:OD1	2.09	0.51
1:M:40:MET:HE1	1:N:41:LYS:HG3	1.93	0.51
1:V:69:LEU:HD22	1:V:70:PHE:CD1	2.45	0.51
1:A:121:PRO:HA	1:A:124:VAL:HG23	1.93	0.51
1:B:13:LYS:HD3	1:B:13:LYS:N	2.25	0.51
1:G:96:GLY:HA2	1:G:115:ILE:HD13	1.92	0.51
1:N:154:LYS:HE3	1:O:11:LEU:HD23	1.92	0.51
1:N:80:LYS:NZ	1:X:221:LYS:HB2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:14:GLU:HG2	1:Q:15:GLU:N	2.26	0.50
1:Q:225:GLN:HA	1:Q:225:GLN:NE2	2.25	0.50
1:S:243:LEU:HD13	1:T:58:LYS:HG2	1.93	0.50
1:E:65:GLN:HB3	1:F:171:TYR:CZ	2.46	0.50
1:P:219:THR:CG2	1:P:221:LYS:H	2.20	0.50
1:A:171:TYR:CZ	1:B:65:GLN:HB3	2.46	0.50
1:K:124:VAL:CG1	1:K:152:PHE:CE1	2.93	0.50
1:L:283:LYS:NZ	1:L:316:LYS:NZ	2.59	0.50
1:V:120:ILE:O	1:V:124:VAL:CG2	2.60	0.50
1:E:180:HIS:HB2	1:G:266:LEU:O	2.10	0.50
1:J:12:LEU:CD1	1:K:155:ASN:CG	2.77	0.50
1:J:163:ASN:HD22	1:J:270:HIS:HB3	1.77	0.50
1:Q:210:LEU:C	1:Q:213:LEU:HD23	2.37	0.50
1:D:290:VAL:CG1	1:D:291:PRO:CD	2.90	0.50
1:A:305:VAL:HA	1:C:208:VAL:HG21	1.94	0.50
1:B:189:LEU:CD1	1:B:199:VAL:HG23	2.31	0.50
1:E:208:VAL:CG2	1:G:305:VAL:HA	2.42	0.50
1:P:219:THR:HG21	1:P:221:LYS:CG	2.31	0.50
1:Q:110:GLN:HE21	1:Q:110:GLN:CA	2.04	0.50
2:Q:401:GO3:C38	2:Q:401:GO3:O2	2.59	0.50
1:X:113:VAL:HG21	1:X:329:LEU:HD22	1.94	0.50
1:E:239:GLU:OE2	1:F:62:MET:SD	2.70	0.50
1:J:6:GLN:O	1:K:304:LYS:HE3	2.12	0.50
1:K:104:SER:O	1:K:106:LEU:N	2.45	0.50
1:N:11:LEU:HB2	1:O:300:SER:O	2.11	0.50
1:O:100:GLN:CG	1:R:103:GLU:CD	2.82	0.50
1:S:210:LEU:HD23	1:T:3:LEU:HD21	1.93	0.50
1:U:167:ALA:HB2	1:V:70:PHE:HZ	1.77	0.50
1:V:177:LEU:N	1:V:177:LEU:HD12	2.26	0.50
1:E:117:LYS:HE2	1:E:331:PHE:HB3	1.91	0.50
1:L:10:ASN:HD21	1:L:13:LYS:HE3	1.74	0.50
1:O:3:LEU:HD23	1:P:226:TRP:CZ2	2.47	0.50
1:P:107:ASN:O	1:P:108:LEU:CD2	2.57	0.50
1:V:12:LEU:HB2	1:W:300:SER:CA	2.41	0.50
1:C:310:GLU:HG2	1:C:314:ARG:HH11	1.75	0.49
1:E:177:LEU:HD21	1:E:226:TRP:CH2	2.46	0.49
1:I:204:ASN:HA	1:I:210:LEU:HD13	1.94	0.49
1:M:11:LEU:HD23	1:P:154:LYS:HE3	1.94	0.49
1:Q:15:GLU:HA	1:T:297:ASN:HD21	1.76	0.49
1:V:104:SER:OG	1:V:106:LEU:HD12	2.12	0.49
1:W:327:LYS:C	1:W:328:GLU:HG3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:HIS:HB2	1:D:266:LEU:O	2.12	0.49
1:N:13:LYS:HG2	1:N:14:GLU:N	2.26	0.49
1:N:118:PHE:HZ	1:X:223:LYS:HB3	1.55	0.49
1:U:306:THR:C	1:U:307:LEU:HD12	2.37	0.49
1:O:3:LEU:N	1:P:224:GLU:OE1	2.46	0.49
1:R:171:TYR:HD2	1:R:172:LEU:CD1	2.25	0.49
1:W:204:ASN:HA	1:W:210:LEU:HD13	1.94	0.49
1:X:131:LYS:HD3	1:X:262:ILE:CG2	2.42	0.49
1:F:180:HIS:HB2	1:H:266:LEU:O	2.13	0.49
1:F:328:GLU:CB	1:W:107:ASN:O	2.57	0.49
1:K:121:PRO:HA	1:K:124:VAL:HG23	1.94	0.49
1:O:147:TRP:CH2	1:O:275:MET:HE1	2.47	0.49
1:Q:15:GLU:HG3	1:T:297:ASN:HD22	1.78	0.49
1:R:308:THR:CG2	1:R:311:GLU:H	2.24	0.49
1:F:111:ARG:NH1	1:W:52:VAL:HG23	2.27	0.49
1:F:164:LEU:HD21	1:F:168:ARG:CZ	2.42	0.49
1:R:18:PRO:HB2	1:R:21:LYS:HB2	1.95	0.49
1:T:204:ASN:HA	1:T:210:LEU:HD13	1.94	0.49
1:C:187:TRP:HB3	1:C:189:LEU:HD21	1.94	0.49
1:H:9:TYR:CE1	2:Q:401:GO3:C19	2.96	0.49
1:I:19:GLN:O	1:I:20:ASN:ND2	2.45	0.49
1:L:290:VAL:HG21	1:L:302:LEU:HD12	1.94	0.49
1:U:315:LEU:HD23	1:U:315:LEU:C	2.37	0.49
1:V:69:LEU:HD22	1:V:70:PHE:CE1	2.47	0.49
1:X:54:GLU:CD	1:X:80:LYS:CE	2.56	0.49
1:X:170:ARG:HA	1:X:173:MET:HE3	1.95	0.49
1:B:214:HIS:CE1	1:B:216:ASP:HB2	2.47	0.49
1:E:12:LEU:HD11	1:H:155:ASN:ND2	2.27	0.49
1:M:50:VAL:HG11	1:M:82:TYR:CE1	2.48	0.49
1:P:108:LEU:CB	1:P:111:ARG:NH2	2.61	0.49
1:S:276:ILE:CB	1:S:279:LEU:HD12	2.37	0.49
1:C:204:ASN:HA	1:C:210:LEU:HD13	1.94	0.49
1:O:121:PRO:HA	1:O:124:VAL:HG23	1.95	0.49
1:Q:302:LEU:HD23	1:T:11:LEU:HD13	1.89	0.49
1:E:177:LEU:HD21	1:E:226:TRP:HH2	1.78	0.49
1:N:82:TYR:O	1:N:126:TYR:CD1	2.66	0.49
1:P:19:GLN:O	1:P:89:LYS:HE3	2.13	0.49
1:S:288:LEU:HD23	1:S:322:LEU:CD1	2.43	0.49
1:U:302:LEU:HD23	1:X:11:LEU:HD13	1.95	0.49
1:E:82:TYR:O	1:E:126:TYR:CD1	2.66	0.49
1:F:100:GLN:CD	1:W:80:LYS:HD2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:LYS:HE2	1:G:231:LYS:NZ	2.28	0.49
1:W:181:PRO:HB2	1:X:69:LEU:HD13	1.95	0.49
1:W:182:LEU:CD1	1:X:72:ARG:NH2	2.66	0.49
1:E:19:GLN:O	1:E:89:LYS:HE3	2.13	0.48
1:M:19:GLN:O	1:M:89:LYS:HE2	2.12	0.48
1:W:59:GLY:HA3	1:X:244:LYS:HB3	1.95	0.48
1:A:19:GLN:O	1:A:89:LYS:HE3	2.13	0.48
1:B:110:GLN:CG	1:J:129:ASN:HD22	2.06	0.48
1:C:16:GLN:O	1:C:17:THR:HG22	2.13	0.48
1:E:275:MET:CE	1:E:285:ASP:CG	2.85	0.48
1:E:305:VAL:HA	1:G:208:VAL:CG2	2.43	0.48
1:M:63:ASP:HB3	1:N:249:TRP:HD1	1.77	0.48
1:P:330:GLN:O	1:P:330:GLN:CG	2.60	0.48
1:R:171:TYR:CD2	1:R:172:LEU:HD12	2.48	0.48
1:K:283:LYS:HE3	1:K:316:LYS:HZ1	1.77	0.48
1:S:18:PRO:HG2	1:S:21:LYS:HD2	1.94	0.48
1:W:224:GLU:OE1	1:X:3:LEU:CB	2.60	0.48
1:W:323:TRP:O	1:W:327:LYS:HG3	2.11	0.48
1:E:275:MET:HE3	1:E:285:ASP:CA	2.43	0.48
1:F:187:TRP:HB3	1:F:189:LEU:HD21	1.95	0.48
1:M:100:GLN:NE2	1:M:103:GLU:HB2	2.22	0.48
1:Q:268:ARG:CD	1:S:182:LEU:HD11	2.43	0.48
1:E:15:GLU:O	1:E:16:GLN:CB	2.60	0.48
1:G:204:ASN:HA	1:G:210:LEU:HD13	1.95	0.48
1:K:103:GLU:CD	1:U:100:GLN:HB2	2.37	0.48
1:M:182:LEU:HD11	1:N:72:ARG:HH11	1.74	0.48
1:R:99:GLN:OE1	1:R:238:TYR:HE2	1.96	0.48
1:J:16:GLN:CG	1:J:17:THR:H	2.25	0.48
1:M:187:TRP:HB3	1:M:189:LEU:HD21	1.96	0.48
1:N:19:GLN:O	1:N:89:LYS:HE3	2.13	0.48
1:K:30:VAL:HB	1:K:98:ARG:HH21	1.78	0.48
1:N:18:PRO:HB2	1:N:21:LYS:HB2	1.96	0.48
1:P:108:LEU:HD11	1:P:110:GLN:OE1	2.13	0.48
1:V:10:ASN:HA	1:W:301:ASP:OD2	2.14	0.48
1:I:329:LEU:CB	1:I:331:PHE:HE2	2.26	0.48
1:P:13:LYS:HG2	1:P:14:GLU:N	2.29	0.48
1:R:196:SER:OG	1:R:230:HIS:CE1	2.66	0.48
1:S:72:ARG:CZ	1:T:182:LEU:HD21	2.43	0.48
1:T:18:PRO:HB2	1:T:21:LYS:HB2	1.95	0.48
1:U:40:MET:HE1	1:V:41:LYS:HG3	1.95	0.48
1:F:203:MET:HE2	1:F:210:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:302:LEU:CD1	1:K:11:LEU:HD11	2.40	0.48
1:Q:110:GLN:HB3	2:Q:401:GO3:O8	2.13	0.48
1:Q:209:SER:O	1:Q:213:LEU:HD22	2.14	0.48
1:U:186:GLY:C	1:U:187:TRP:HD1	2.14	0.48
1:K:103:GLU:OE2	1:U:100:GLN:HG3	2.12	0.48
1:U:45:ASP:O	1:U:45:ASP:CG	2.53	0.48
1:E:221:LYS:HD2	1:E:221:LYS:N	2.29	0.47
1:I:214:HIS:HB2	1:J:3:LEU:HD13	1.96	0.47
1:M:18:PRO:HB2	1:M:21:LYS:HB2	1.96	0.47
1:M:204:ASN:HA	1:M:210:LEU:HD13	1.95	0.47
1:M:270:HIS:CE1	1:M:294:LEU:HD22	2.46	0.47
1:S:18:PRO:HB2	1:S:21:LYS:HB2	1.96	0.47
1:U:3:LEU:HD22	1:V:214:HIS:CB	2.44	0.47
1:U:177:LEU:O	1:V:4:LYS:HE3	2.13	0.47
1:A:3:LEU:HD22	1:B:214:HIS:HD2	1.79	0.47
1:A:124:VAL:CG1	1:A:152:PHE:CZ	2.95	0.47
1:F:305:VAL:HA	1:H:208:VAL:HG21	1.96	0.47
1:I:302:LEU:CD1	1:L:11:LEU:HD13	2.42	0.47
1:J:56:LYS:HE2	1:J:60:GLU:OE2	2.13	0.47
1:R:148:LYS:HG3	1:R:331:PHE:CZ	2.49	0.47
1:V:203:MET:HE2	1:V:210:LEU:HD22	1.95	0.47
1:X:18:PRO:HB2	1:X:21:LYS:HB2	1.96	0.47
1:A:18:PRO:HB2	1:A:21:LYS:HB2	1.96	0.47
1:B:239:GLU:O	1:B:243:LEU:HD22	2.14	0.47
1:G:276:ILE:CD1	1:G:286:VAL:HG13	2.39	0.47
1:J:11:LEU:HD12	1:K:154:LYS:HE3	1.97	0.47
1:J:300:SER:CA	1:K:12:LEU:HD21	2.43	0.47
1:M:261:SER:CB	1:M:270:HIS:HE1	2.25	0.47
1:R:171:TYR:CD2	1:R:172:LEU:CD1	2.97	0.47
1:U:3:LEU:CD1	1:V:213:LEU:CB	2.92	0.47
1:B:290:VAL:HG21	1:B:302:LEU:HD13	1.96	0.47
1:F:227:LYS:HG2	1:F:231:LYS:HZ2	1.79	0.47
1:G:71:LEU:CD2	1:G:71:LEU:N	2.77	0.47
1:G:203:MET:HE2	1:G:210:LEU:HD22	1.97	0.47
1:K:182:LEU:HD11	1:L:69:LEU:O	2.15	0.47
1:N:114:ASN:ND2	1:W:5:ASP:CG	2.70	0.47
1:O:217:LEU:O	1:O:222:ASP:OD2	2.32	0.47
1:C:216:ASP:HB3	1:C:222:ASP:HA	1.96	0.47
1:V:18:PRO:HB2	1:V:21:LYS:HB2	1.97	0.47
1:V:304:LYS:NZ	1:W:5:ASP:O	2.47	0.47
1:C:14:GLU:CG	1:C:16:GLN:HG3	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:PRO:HB2	1:C:21:LYS:HB2	1.96	0.47
1:C:30:VAL:HG23	1:C:98:ARG:NH1	2.28	0.47
1:K:100:GLN:NE2	1:U:108:LEU:CD2	2.74	0.47
1:Q:82:TYR:HD2	1:Q:122:ASN:CB	2.15	0.47
1:V:19:GLN:HG2	1:W:89:LYS:NZ	2.29	0.47
1:X:131:LYS:HE2	1:X:262:ILE:HD13	1.96	0.47
1:A:106:LEU:HD22	1:A:325:ILE:CD1	2.44	0.47
1:A:177:LEU:HA	1:B:4:LYS:HG3	1.97	0.47
1:D:19:GLN:O	1:D:89:LYS:HE2	2.13	0.47
1:E:302:LEU:CD1	1:H:11:LEU:CD1	2.81	0.47
1:K:18:PRO:HB2	1:K:21:LYS:HB2	1.97	0.47
1:K:41:LYS:HG3	1:L:40:MET:HE1	1.96	0.47
1:K:124:VAL:CG1	1:K:152:PHE:CZ	2.96	0.47
1:L:117:LYS:HZ2	1:L:331:PHE:HA	1.78	0.47
1:W:18:PRO:HB2	1:W:21:LYS:HB2	1.96	0.47
1:D:93:ILE:CD1	1:D:120:ILE:HD13	2.44	0.47
1:E:206:ALA:HB3	1:G:303:VAL:HG11	1.97	0.47
1:E:331:PHE:OXT	1:O:17:THR:HB	2.14	0.47
1:F:305:VAL:HA	1:H:208:VAL:CG2	2.45	0.47
1:G:282:ILE:HG21	1:G:286:VAL:CG1	2.45	0.47
1:N:54:GLU:HG2	1:N:80:LYS:HD3	1.97	0.47
1:A:93:ILE:CD1	1:A:120:ILE:HD13	2.44	0.47
1:B:331:PHE:OXT	1:K:17:THR:CB	2.61	0.47
1:C:3:LEU:HD11	1:D:210:LEU:HD13	1.96	0.47
1:F:204:ASN:HA	1:F:210:LEU:HD13	1.96	0.47
1:G:221:LYS:HD2	1:G:221:LYS:N	2.27	0.47
1:O:18:PRO:HB2	1:O:21:LYS:HB2	1.97	0.47
1:Q:109:VAL:HG13	2:Q:401:GO3:O6	2.15	0.47
1:U:18:PRO:HB2	1:U:21:LYS:HB2	1.97	0.47
1:U:305:VAL:O	1:U:307:LEU:HD12	2.14	0.47
1:W:4:LYS:NZ	1:X:176:ARG:O	2.36	0.47
1:F:18:PRO:HB2	1:F:21:LYS:HB2	1.96	0.47
1:L:18:PRO:HB2	1:L:21:LYS:HB2	1.96	0.47
1:M:191:GLU:HG3	1:M:322:LEU:HD21	1.97	0.47
1:O:124:VAL:CG1	1:O:152:PHE:CE1	2.95	0.47
1:E:177:LEU:O	1:F:4:LYS:HE3	2.15	0.46
1:O:101:GLU:HG2	1:O:241:ILE:HG22	1.97	0.46
1:R:308:THR:HG22	1:R:311:GLU:CD	2.40	0.46
1:T:19:GLN:O	1:T:89:LYS:HE3	2.13	0.46
1:W:325:ILE:O	1:W:328:GLU:HG3	2.15	0.46
1:B:274:THR:OG1	1:B:275:MET:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:PRO:HB2	1:D:21:LYS:HB2	1.96	0.46
1:F:100:GLN:HB3	1:W:80:LYS:HZ2	1.80	0.46
1:J:228:GLU:OE1	1:J:231:LYS:HD2	2.16	0.46
1:N:175:GLU:OE2	1:N:175:GLU:HA	2.15	0.46
1:O:165:ASP:OD1	1:O:192:HIS:ND1	2.47	0.46
1:Q:97:ALA:HB3	1:Q:108:LEU:HD22	1.97	0.46
1:S:217:LEU:HD13	1:T:3:LEU:HD22	1.96	0.46
1:B:13:LYS:HG2	1:B:14:GLU:H	1.81	0.46
1:C:12:LEU:HD13	1:C:15:GLU:HB3	1.97	0.46
1:F:16:GLN:HE21	1:F:17:THR:HA	1.79	0.46
1:H:18:PRO:HB2	1:H:21:LYS:HB2	1.96	0.46
1:K:113:VAL:HG21	1:K:329:LEU:HD22	1.97	0.46
1:S:286:VAL:HG11	1:S:319:ALA:HA	1.97	0.46
1:E:285:ASP:CG	1:O:128:PRO:HB2	2.40	0.46
1:J:18:PRO:HB2	1:J:21:LYS:HB2	1.98	0.46
1:A:106:LEU:HD22	1:A:325:ILE:HD12	1.98	0.46
1:B:12:LEU:CD1	1:C:155:ASN:ND2	2.79	0.46
1:B:110:GLN:HE21	1:J:129:ASN:ND2	2.14	0.46
1:C:328:GLU:CB	1:M:107:ASN:O	2.63	0.46
1:F:328:GLU:HB3	1:W:111:ARG:NH2	2.26	0.46
1:K:54:GLU:CD	1:U:54:GLU:OE2	2.59	0.46
1:M:203:MET:HE2	1:M:210:LEU:HD22	1.97	0.46
1:P:108:LEU:HG	1:P:111:ARG:CD	2.44	0.46
1:B:18:PRO:HB2	1:B:21:LYS:HB2	1.98	0.46
1:Q:97:ALA:CB	1:Q:108:LEU:HD22	2.46	0.46
1:S:82:TYR:CD2	1:S:122:ASN:CB	2.97	0.46
1:S:204:ASN:HA	1:S:210:LEU:HD13	1.97	0.46
1:S:217:LEU:HD13	1:T:3:LEU:CD2	2.46	0.46
1:X:106:LEU:HB3	1:X:325:ILE:HD13	1.98	0.46
1:A:293:ILE:CD1	1:C:179:VAL:HG22	2.45	0.46
1:I:7:LEU:HD21	1:J:205:VAL:HB	1.98	0.46
1:S:58:LYS:HG2	1:T:243:LEU:HD13	1.98	0.46
1:B:266:LEU:O	1:D:180:HIS:HB2	2.16	0.46
1:D:54:GLU:HG2	1:D:80:LYS:HG3	1.97	0.46
1:I:18:PRO:HB2	1:I:21:LYS:HB2	1.96	0.46
1:Q:290:VAL:HG23	1:Q:302:LEU:HD13	1.97	0.46
1:U:221:LYS:H	1:U:221:LYS:CD	2.28	0.46
1:W:327:LYS:O	1:W:328:GLU:CB	2.62	0.46
1:K:284:ASP:HB2	1:K:286:VAL:HG23	1.96	0.46
1:Q:18:PRO:HB2	1:Q:21:LYS:HB2	1.97	0.46
1:R:302:LEU:CD2	1:S:11:LEU:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:PRO:HB2	1:E:21:LYS:HB2	1.97	0.46
1:A:206:ALA:HB2	1:C:269:VAL:HG11	1.96	0.45
1:L:154:LYS:NZ	1:L:275:MET:HE2	2.31	0.45
1:Q:290:VAL:CG2	1:Q:302:LEU:HD13	2.47	0.45
1:I:13:LYS:HD3	1:I:13:LYS:N	2.26	0.45
1:J:9:TYR:CE2	1:J:11:LEU:HD13	2.51	0.45
1:O:108:LEU:CD1	1:O:108:LEU:H	2.27	0.45
1:R:99:GLN:OE1	1:R:238:TYR:CE2	2.69	0.45
1:U:19:GLN:C	1:U:20:ASN:HD22	2.24	0.45
1:V:124:VAL:HG13	1:V:152:PHE:CZ	2.51	0.45
1:V:302:LEU:HB2	1:W:9:TYR:HB3	1.98	0.45
1:B:214:HIS:HE1	1:B:216:ASP:HB2	1.80	0.45
1:D:16:GLN:O	1:D:17:THR:HG22	2.16	0.45
1:H:329:LEU:O	1:H:331:PHE:CE1	2.69	0.45
1:K:103:GLU:OE2	1:U:100:GLN:CB	2.63	0.45
1:Q:323:TRP:CE2	1:Q:327:LYS:HG2	2.51	0.45
1:S:224:GLU:CD	1:T:3:LEU:H	2.25	0.45
1:E:82:TYR:C	1:E:126:TYR:CD1	2.95	0.45
1:F:206:ALA:HB3	1:H:303:VAL:HG11	1.98	0.45
1:Q:15:GLU:HA	1:T:297:ASN:ND2	2.31	0.45
1:Q:109:VAL:HG12	2:Q:401:GO3:O4	2.09	0.45
1:Q:290:VAL:CG2	1:Q:302:LEU:CD1	2.95	0.45
1:O:276:ILE:O	1:O:277:LYS:C	2.59	0.45
1:R:171:TYR:HD2	1:R:172:LEU:HD13	1.81	0.45
1:S:205:VAL:HB	1:T:7:LEU:HD21	1.99	0.45
1:W:218:GLY:O	1:W:227:LYS:HD3	2.16	0.45
1:G:18:PRO:HB2	1:G:21:LYS:HB2	1.97	0.45
1:I:154:LYS:HE2	1:L:11:LEU:HD23	1.97	0.45
1:O:100:GLN:HG3	1:R:103:GLU:OE2	2.14	0.45
1:R:203:MET:HB3	1:R:210:LEU:HD12	1.99	0.45
1:E:328:GLU:OE2	1:N:18:PRO:O	2.35	0.45
1:E:9:TYR:HB2	1:H:304:LYS:HD2	1.98	0.45
1:E:110:GLN:CB	1:N:129:ASN:HD21	2.28	0.45
1:F:208:VAL:CG2	1:H:305:VAL:HA	2.47	0.45
1:O:113:VAL:HG21	1:O:329:LEU:HD22	1.99	0.45
1:P:18:PRO:HB2	1:P:21:LYS:HB2	1.97	0.45
1:S:113:VAL:HG22	1:S:145:VAL:HG21	1.99	0.45
1:H:239:GLU:O	1:H:243:LEU:HD22	2.17	0.45
1:O:124:VAL:CG1	1:O:152:PHE:CZ	2.98	0.45
1:S:210:LEU:HG	1:T:3:LEU:HD11	1.99	0.45
1:U:3:LEU:HD13	1:V:213:LEU:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LYS:HG3	1:B:328:GLU:OE2	2.17	0.45
1:C:80:LYS:HB3	1:C:80:LYS:HE3	1.71	0.45
1:F:29:ALA:HB3	1:F:98:ARG:HH22	1.82	0.45
1:S:99:GLN:HE21	1:S:108:LEU:HD11	1.81	0.45
1:T:189:LEU:HD22	1:T:199:VAL:HG23	1.97	0.45
1:X:131:LYS:NZ	1:X:262:ILE:HD13	2.30	0.45
1:B:203:MET:HE2	1:B:210:LEU:CD2	2.48	0.44
1:G:227:LYS:HE2	1:G:231:LYS:HZ3	1.83	0.44
1:G:243:LEU:HD21	1:H:58:LYS:HD3	2.00	0.44
1:K:170:ARG:HA	1:K:173:MET:HE3	2.00	0.44
1:N:82:TYR:C	1:N:126:TYR:CD1	2.95	0.44
1:V:97:ALA:C	1:V:108:LEU:HD13	2.42	0.44
1:X:113:VAL:HG22	1:X:145:VAL:HG21	1.98	0.44
1:B:110:GLN:CB	1:J:128:PRO:HG2	2.44	0.44
1:O:203:MET:HE2	1:O:210:LEU:CD2	2.47	0.44
1:P:13:LYS:HG2	1:P:14:GLU:H	1.80	0.44
1:W:283:LYS:HE3	1:W:283:LYS:HB2	1.74	0.44
1:A:268:ARG:HD3	1:C:182:LEU:HD13	1.99	0.44
1:D:228:GLU:HG3	1:D:229:VAL:N	2.29	0.44
1:W:98:ARG:HG3	1:W:98:ARG:NH1	2.06	0.44
1:W:110:GLN:HE21	1:W:114:ASN:ND2	2.15	0.44
1:X:131:LYS:CE	1:X:298:GLY:CA	2.94	0.44
1:I:30:VAL:HG12	1:I:98:ARG:NH1	2.33	0.44
1:K:276:ILE:HD12	1:K:276:ILE:HG21	1.55	0.44
1:Q:304:LYS:CD	1:T:9:TYR:HB2	2.48	0.44
1:T:148:LYS:HG3	1:T:331:PHE:HE2	1.83	0.44
1:V:11:LEU:CD1	1:W:302:LEU:CD1	2.89	0.44
1:W:325:ILE:O	1:W:328:GLU:CG	2.65	0.44
1:E:330:GLN:NE2	1:N:89:LYS:HE2	2.32	0.44
1:F:302:LEU:CD1	1:G:11:LEU:CD1	2.88	0.44
1:R:113:VAL:HG22	1:R:145:VAL:HG21	1.99	0.44
1:R:177:LEU:HD11	1:R:226:TRP:CH2	2.53	0.44
1:R:290:VAL:CG2	1:R:291:PRO:HD2	2.42	0.44
1:T:230:HIS:O	1:T:230:HIS:CG	2.71	0.44
1:X:131:LYS:CE	1:X:262:ILE:HD13	2.47	0.44
1:E:305:VAL:HA	1:G:208:VAL:HG22	2.00	0.44
1:R:23:THR:OG1	1:R:85:THR:HG23	2.18	0.44
1:S:80:LYS:HB3	1:S:80:LYS:HE3	1.79	0.44
1:A:280:TYR:O	1:A:316:LYS:HE2	2.18	0.44
1:D:290:VAL:HG12	1:D:291:PRO:CD	2.47	0.44
1:E:3:LEU:HB3	1:F:224:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:CYS:HA	1:F:165:ASP:OD2	2.18	0.44
1:M:258:LEU:HD23	1:M:270:HIS:ND1	2.32	0.44
1:N:113:VAL:HG22	1:N:145:VAL:HG21	2.00	0.44
1:R:296:GLN:NE2	1:S:19:GLN:HG2	2.32	0.44
1:V:330:GLN:OE1	1:V:330:GLN:N	2.44	0.44
1:C:189:LEU:HD13	1:C:290:VAL:HA	2.00	0.44
1:E:208:VAL:HG21	1:G:305:VAL:HA	1.99	0.44
1:G:12:LEU:C	1:G:12:LEU:HD13	2.43	0.44
1:I:16:GLN:CG	1:I:17:THR:N	2.75	0.44
1:K:113:VAL:HG22	1:K:145:VAL:HG21	1.99	0.44
1:O:41:LYS:HG3	1:P:40:MET:HE1	2.00	0.44
1:U:307:LEU:N	1:U:307:LEU:CD1	2.80	0.44
1:B:110:GLN:HE21	1:J:129:ASN:HD22	1.65	0.44
1:B:283:LYS:HB3	1:K:151:GLY:O	2.17	0.44
1:F:13:LYS:H	1:F:13:LYS:CD	2.27	0.44
1:L:203:MET:HE2	1:L:210:LEU:CD2	2.48	0.44
1:V:301:ASP:OD1	1:W:10:ASN:HA	2.18	0.44
1:X:203:MET:HE2	1:X:210:LEU:CD2	2.46	0.44
1:A:210:LEU:HD21	1:B:7:LEU:HD22	2.00	0.43
1:L:302:LEU:H	1:L:302:LEU:HD23	1.84	0.43
1:P:108:LEU:HA	1:P:108:LEU:HD13	1.48	0.43
1:Q:217:LEU:HD13	1:Q:218:GLY:N	2.33	0.43
1:A:19:GLN:NE2	1:D:296:GLN:OE1	2.50	0.43
1:I:72:ARG:HH22	1:J:182:LEU:HD11	1.77	0.43
1:N:114:ASN:ND2	1:W:5:ASP:OD1	2.51	0.43
1:O:105:ARG:HA	1:O:108:LEU:HD13	1.98	0.43
1:P:80:LYS:H	1:P:80:LYS:HG3	1.44	0.43
1:T:270:HIS:HB2	1:T:294:LEU:HD13	2.00	0.43
1:W:203:MET:HE2	1:W:210:LEU:HD22	2.01	0.43
1:X:230:HIS:CG	1:X:230:HIS:O	2.71	0.43
1:B:113:VAL:HG22	1:B:145:VAL:HG21	2.00	0.43
1:D:283:LYS:CE	1:D:283:LYS:H	2.31	0.43
1:J:19:GLN:O	1:J:89:LYS:HE3	2.17	0.43
1:L:154:LYS:HZ2	1:L:275:MET:HE2	1.83	0.43
1:M:189:LEU:HD13	1:M:290:VAL:HA	2.00	0.43
1:M:306:THR:CG2	1:O:208:VAL:HG13	2.43	0.43
1:V:113:VAL:HG22	1:V:145:VAL:HG21	1.98	0.43
1:W:292:CYS:HB3	1:W:299:ILE:HG23	1.99	0.43
1:E:210:LEU:CD2	1:F:3:LEU:HD21	2.49	0.43
1:F:328:GLU:OE2	1:W:110:GLN:N	2.40	0.43
1:I:266:LEU:N	1:I:266:LEU:CD1	2.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:100:GLN:OE1	1:R:108:LEU:HD23	2.18	0.43
1:Q:15:GLU:O	1:Q:16:GLN:HG2	2.17	0.43
1:T:176:ARG:NH1	1:T:224:GLU:O	2.50	0.43
1:D:98:ARG:NH1	1:D:246:TYR:HB3	2.34	0.43
1:I:82:TYR:CD2	1:I:122:ASN:CB	3.00	0.43
1:M:300:SER:O	1:M:301:ASP:OD2	2.36	0.43
1:S:276:ILE:HB	1:S:279:LEU:CD1	2.41	0.43
1:T:117:LYS:HZ1	1:T:331:PHE:CA	2.08	0.43
1:U:113:VAL:HG22	1:U:145:VAL:HG21	2.01	0.43
1:G:223:LYS:HB3	1:Q:330:GLN:NE2	2.33	0.43
1:U:206:ALA:HA	1:W:187:TRP:CZ2	2.53	0.43
1:G:265:ASN:O	1:G:267:ARG:N	2.50	0.43
1:J:216:ASP:CB	1:J:222:ASP:HB2	2.49	0.43
1:Q:11:LEU:CD2	1:T:300:SER:C	2.92	0.43
1:Q:217:LEU:CD1	1:Q:217:LEU:C	2.92	0.43
1:Q:274:THR:CG2	1:Q:302:LEU:HD11	2.49	0.43
1:R:113:VAL:HG21	1:R:329:LEU:CD2	2.48	0.43
1:V:326:GLN:HA	1:V:329:LEU:HD12	2.00	0.43
1:W:110:GLN:HE21	1:W:114:ASN:HD21	1.66	0.43
1:W:328:GLU:CD	1:W:328:GLU:C	2.87	0.43
1:D:189:LEU:HD13	1:D:290:VAL:HA	2.01	0.43
1:F:113:VAL:HG22	1:F:145:VAL:HG21	2.01	0.43
1:G:54:GLU:OE1	1:G:80:LYS:HD3	2.19	0.43
1:H:113:VAL:HG22	1:H:145:VAL:HG21	2.01	0.43
1:I:40:MET:HE1	1:J:37:SER:HA	2.01	0.43
1:J:25:VAL:HG13	1:J:50:VAL:HG23	1.99	0.43
1:J:206:ALA:HA	1:L:187:TRP:CZ2	2.54	0.43
1:M:261:SER:CB	1:M:270:HIS:CE1	3.01	0.43
1:R:54:GLU:CD	1:R:80:LYS:CD	2.92	0.43
1:R:162:CYS:HA	1:R:165:ASP:OD2	2.18	0.43
1:W:15:GLU:C	1:W:16:GLN:HG3	2.44	0.43
1:A:15:GLU:OE1	1:D:300:SER:CB	2.67	0.43
1:A:65:GLN:HB3	1:B:171:TYR:CE2	2.54	0.43
1:A:220:ASP:OD1	1:A:220:ASP:N	2.52	0.43
1:B:203:MET:HE2	1:B:210:LEU:HD23	2.00	0.43
1:C:113:VAL:HG22	1:C:145:VAL:HG21	2.00	0.43
1:M:113:VAL:HG22	1:M:145:VAL:HG21	2.00	0.43
1:Q:268:ARG:HD2	1:S:182:LEU:HD11	2.00	0.43
1:Q:276:ILE:CG2	1:Q:290:VAL:CG2	2.97	0.43
1:U:208:VAL:HG12	1:U:213:LEU:CD2	2.42	0.43
1:A:303:VAL:HG11	1:C:206:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:VAL:HG22	1:B:50:VAL:CG1	2.48	0.43
1:C:203:MET:HE2	1:C:210:LEU:HD22	2.00	0.43
1:U:167:ALA:CB	1:V:70:PHE:CZ	3.02	0.43
1:U:326:GLN:O	1:U:329:LEU:HB2	2.18	0.43
1:W:98:ARG:CG	1:W:98:ARG:NH1	2.70	0.43
1:B:206:ALA:HB3	1:D:303:VAL:HG11	2.01	0.42
1:B:327:LYS:HG3	1:B:328:GLU:CD	2.43	0.42
1:G:282:ILE:HG21	1:G:286:VAL:HG12	2.01	0.42
1:A:233:VAL:O	1:A:236:SER:OG	2.37	0.42
1:A:275:MET:HE2	1:A:285:ASP:HA	2.00	0.42
1:D:283:LYS:N	1:D:283:LYS:CD	2.83	0.42
1:E:148:LYS:HB3	1:E:331:PHE:HE2	1.84	0.42
1:I:113:VAL:HG22	1:I:145:VAL:HG21	2.01	0.42
1:J:113:VAL:HG22	1:J:145:VAL:HG21	2.00	0.42
1:N:80:LYS:HB3	1:N:80:LYS:HE2	1.83	0.42
1:O:97:ALA:O	1:O:98:ARG:CB	2.56	0.42
1:O:105:ARG:NH2	1:O:193:GLY:HA2	2.34	0.42
1:Q:213:LEU:HG	1:R:3:LEU:HD12	1.98	0.42
1:U:315:LEU:C	1:U:315:LEU:CD2	2.92	0.42
1:D:113:VAL:HG22	1:D:145:VAL:HG21	2.01	0.42
1:I:9:TYR:HB3	1:L:302:LEU:CD2	2.50	0.42
1:I:200:TRP:CE2	1:I:218:GLY:HA3	2.54	0.42
1:N:101:GLU:O	1:N:238:TYR:HD1	2.02	0.42
1:T:216:ASP:OD1	1:T:221:LYS:HD2	2.19	0.42
1:X:18:PRO:HG3	1:X:21:LYS:HD2	2.01	0.42
1:X:131:LYS:HD3	1:X:262:ILE:HG21	2.00	0.42
1:C:99:GLN:H	1:C:99:GLN:HG2	1.62	0.42
1:C:311:GLU:HG2	1:C:314:ARG:HH22	1.84	0.42
1:D:50:VAL:CG2	1:D:85:THR:CG2	2.97	0.42
1:E:113:VAL:HG22	1:E:145:VAL:HG21	2.01	0.42
1:H:80:LYS:HE2	1:H:80:LYS:HB3	1.83	0.42
1:I:40:MET:CE	1:J:40:MET:HB2	2.50	0.42
1:I:67:GLY:O	1:I:71:LEU:HD13	2.19	0.42
1:K:63:ASP:HB3	1:L:249:TRP:HD1	1.85	0.42
1:P:99:GLN:OE1	1:P:238:TYR:CE1	2.73	0.42
1:S:284:ASP:HB2	1:S:286:VAL:HG23	2.02	0.42
1:T:117:LYS:NZ	1:T:331:PHE:CA	2.75	0.42
1:W:226:TRP:CE2	1:X:3:LEU:HD23	2.54	0.42
1:F:225:GLN:HA	1:F:225:GLN:NE2	2.34	0.42
1:J:18:PRO:HG3	1:J:21:LYS:HD2	2.01	0.42
1:L:162:CYS:HA	1:L:165:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:283:LYS:HD2	1:L:283:LYS:N	2.29	0.42
1:N:196:SER:OG	1:N:230:HIS:CE1	2.72	0.42
1:O:105:ARG:HA	1:O:108:LEU:HD11	2.00	0.42
1:S:276:ILE:CD1	1:S:288:LEU:HD12	2.50	0.42
1:S:288:LEU:CD2	1:S:322:LEU:HD12	2.50	0.42
1:T:113:VAL:HG22	1:T:145:VAL:HG21	2.02	0.42
1:E:203:MET:HE2	1:E:210:LEU:CD2	2.50	0.42
1:F:16:GLN:HG3	1:F:17:THR:CA	2.49	0.42
1:H:227:LYS:HE2	1:H:231:LYS:CE	2.49	0.42
1:J:203:MET:HE2	1:J:210:LEU:HD23	2.01	0.42
1:K:177:LEU:O	1:L:4:LYS:HE3	2.20	0.42
1:M:30:VAL:HG22	1:M:251:ILE:CG2	2.50	0.42
1:O:100:GLN:HB2	1:R:103:GLU:OE2	2.18	0.42
1:O:113:VAL:HG22	1:O:145:VAL:HG21	2.00	0.42
1:Q:274:THR:HG21	1:Q:302:LEU:HD11	2.02	0.42
1:S:12:LEU:HD12	1:S:12:LEU:HA	1.76	0.42
1:U:19:GLN:C	1:U:20:ASN:ND2	2.77	0.42
1:V:99:GLN:N	1:V:108:LEU:HD11	2.34	0.42
1:X:177:LEU:CD1	1:X:226:TRP:HH2	2.24	0.42
1:D:50:VAL:HG21	1:D:85:THR:CG2	2.50	0.42
1:E:276:ILE:O	1:E:277:LYS:C	2.62	0.42
1:L:30:VAL:CG2	1:L:98:ARG:HH11	2.30	0.42
1:N:118:PHE:CE1	1:X:223:LYS:CA	3.03	0.42
1:P:54:GLU:HG3	1:P:80:LYS:HG2	2.01	0.42
1:P:113:VAL:HG22	1:P:145:VAL:HG21	2.01	0.42
1:Q:156:ARG:HH21	1:Q:156:ARG:HD2	1.42	0.42
1:R:219:THR:OG1	1:R:221:LYS:HG2	2.19	0.42
1:S:72:ARG:HH12	1:T:182:LEU:HD11	1.84	0.42
1:W:80:LYS:HB3	1:W:80:LYS:HE2	1.62	0.42
1:X:131:LYS:HE2	1:X:131:LYS:HB3	1.67	0.42
1:C:222:ASP:HB3	1:C:225:GLN:H	1.83	0.42
1:H:54:GLU:CG	1:H:80:LYS:HD3	2.50	0.42
1:K:226:TRP:CE2	1:L:3:LEU:HD23	2.54	0.42
1:M:283:LYS:HE3	1:M:283:LYS:HB2	1.85	0.42
1:M:311:GLU:HG2	1:M:314:ARG:HH12	1.85	0.42
1:P:19:GLN:HE21	1:P:19:GLN:HB3	1.63	0.42
1:T:316:LYS:HE3	1:T:316:LYS:HB3	1.61	0.42
1:U:167:ALA:HB2	1:V:70:PHE:CZ	2.55	0.42
1:V:330:GLN:O	1:V:330:GLN:CD	2.63	0.42
1:B:304:LYS:HE3	1:C:6:GLN:O	2.20	0.42
1:E:148:LYS:HB2	1:E:331:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:LEU:HD13	1:F:290:VAL:HA	2.01	0.42
1:M:82:TYR:CD2	1:M:122:ASN:CB	3.02	0.42
1:M:290:VAL:HG23	1:M:302:LEU:HD13	2.00	0.42
1:E:276:ILE:HG21	1:E:288:LEU:HD12	2.01	0.42
1:G:98:ARG:HH12	1:G:246:TYR:HB2	1.84	0.42
1:G:99:GLN:H	1:G:99:GLN:HG2	1.65	0.42
1:I:72:ARG:NH2	1:J:182:LEU:CD1	2.78	0.42
1:Q:203:MET:HE2	1:Q:210:LEU:CD2	2.50	0.42
1:Q:243:LEU:CD1	1:R:58:LYS:HD3	2.49	0.42
1:A:280:TYR:O	1:A:316:LYS:CE	2.67	0.41
1:C:53:ILE:HG23	1:C:53:ILE:O	2.20	0.41
1:C:96:GLY:HA2	1:C:115:ILE:HD13	2.02	0.41
1:K:275:MET:CG	1:K:287:PHE:CE1	3.03	0.41
1:O:200:TRP:CE2	1:O:218:GLY:HA3	2.55	0.41
1:P:13:LYS:HD3	1:P:13:LYS:N	2.26	0.41
1:V:293:ILE:HD11	1:X:179:VAL:HG22	2.02	0.41
1:W:145:VAL:HG22	1:W:329:LEU:HD22	2.02	0.41
1:F:213:LEU:HD23	1:F:213:LEU:HA	1.92	0.41
1:L:113:VAL:HG22	1:L:145:VAL:HG21	2.00	0.41
1:Q:12:LEU:C	1:Q:13:LYS:HG2	2.45	0.41
1:Q:108:LEU:HD23	1:Q:111:ARG:CZ	2.50	0.41
1:B:290:VAL:CG2	1:B:302:LEU:HD13	2.50	0.41
1:F:198:PRO:CD	1:F:314:ARG:NH1	2.78	0.41
1:J:300:SER:O	1:K:11:LEU:HB2	2.21	0.41
1:O:15:GLU:HG3	1:O:16:GLN:H	1.86	0.41
1:O:108:LEU:HA	1:O:111:ARG:HH21	1.84	0.41
1:T:203:MET:HE2	1:T:210:LEU:HD22	2.02	0.41
1:T:233:VAL:O	1:T:236:SER:OG	2.38	0.41
1:W:270:HIS:CD2	1:W:294:LEU:HD22	2.56	0.41
1:A:196:SER:OG	1:A:230:HIS:CE1	2.73	0.41
1:B:12:LEU:HD11	1:C:155:ASN:ND2	2.35	0.41
1:E:276:ILE:HD13	1:E:286:VAL:O	2.20	0.41
1:Q:12:LEU:HD23	1:Q:12:LEU:HA	1.87	0.41
1:Q:113:VAL:HG22	1:Q:145:VAL:HG21	2.01	0.41
1:V:303:VAL:HA	1:W:7:LEU:O	2.20	0.41
1:W:113:VAL:HG22	1:W:145:VAL:HG21	2.03	0.41
1:B:219:THR:OG1	1:B:221:LYS:HG2	2.21	0.41
1:B:231:LYS:O	1:B:235:GLU:CD	2.63	0.41
1:C:35:ALA:C	1:C:39:LEU:HD22	2.46	0.41
1:I:70:PHE:C	1:I:71:LEU:CD1	2.93	0.41
1:J:5:ASP:O	1:K:304:LYS:NZ	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:13:LYS:O	1:J:15:GLU:HG3	2.20	0.41
1:Q:54:GLU:CG	1:Q:80:LYS:HD3	2.50	0.41
1:E:275:MET:HE2	1:E:277:LYS:HB2	2.03	0.41
1:F:80:LYS:HE2	1:F:80:LYS:HB3	1.57	0.41
1:G:113:VAL:HG22	1:G:145:VAL:HG21	2.02	0.41
1:H:14:GLU:HB2	1:H:15:GLU:H	1.69	0.41
1:K:108:LEU:HD21	1:U:100:GLN:NE2	2.36	0.41
1:O:3:LEU:HD21	1:P:210:LEU:HD13	2.03	0.41
1:Q:276:ILE:HG21	1:Q:290:VAL:HG22	2.03	0.41
1:S:276:ILE:CB	1:S:279:LEU:CD1	2.98	0.41
1:V:186:GLY:C	1:V:187:TRP:CD1	2.97	0.41
1:B:171:TYR:CD1	1:B:171:TYR:C	2.98	0.41
1:D:191:GLU:HG3	1:D:322:LEU:HD21	2.02	0.41
1:H:270:HIS:CD2	1:H:294:LEU:HD22	2.56	0.41
1:Q:40:MET:HE1	1:R:41:LYS:HG3	2.01	0.41
1:R:155:ASN:CG	1:S:12:LEU:CD2	2.94	0.41
1:V:18:PRO:HG3	1:V:21:LYS:HD2	2.03	0.41
1:W:8:ILE:CD1	1:X:177:LEU:O	2.65	0.41
1:J:180:HIS:HB2	1:L:266:LEU:O	2.20	0.41
1:Q:290:VAL:HG23	1:Q:302:LEU:CD1	2.50	0.41
1:R:142:LEU:HD23	1:R:142:LEU:HA	1.96	0.41
1:T:218:GLY:O	1:T:227:LYS:HG3	2.21	0.41
1:C:41:LYS:HG3	1:D:40:MET:HE1	2.03	0.41
1:D:14:GLU:O	1:D:14:GLU:HG2	2.21	0.41
1:G:223:LYS:HD3	1:G:223:LYS:HA	1.68	0.41
1:K:270:HIS:CD2	1:K:294:LEU:HD22	2.56	0.41
1:M:305:VAL:HA	1:O:208:VAL:HG21	2.03	0.41
1:Q:290:VAL:HG12	1:Q:291:PRO:HD2	2.01	0.41
1:U:54:GLU:HG3	1:U:80:LYS:HD2	2.03	0.41
1:V:54:GLU:HG3	1:V:80:LYS:HD2	2.03	0.41
1:X:12:LEU:HD23	1:X:12:LEU:HA	1.90	0.41
1:A:270:HIS:CD2	1:A:294:LEU:HD22	2.56	0.41
1:L:270:HIS:CD2	1:L:294:LEU:HD22	2.56	0.41
1:P:109:VAL:CG1	1:P:110:GLN:NE2	2.80	0.41
1:Q:108:LEU:HD23	1:Q:111:ARG:NH2	2.36	0.41
1:R:270:HIS:CD2	1:R:294:LEU:HD22	2.56	0.41
1:V:177:LEU:CD1	1:V:226:TRP:HH2	2.20	0.41
1:D:270:HIS:CD2	1:D:294:LEU:HD22	2.56	0.40
1:E:285:ASP:OD2	1:O:128:PRO:HB2	2.21	0.40
1:F:328:GLU:CG	1:W:107:ASN:O	2.69	0.40
1:G:191:GLU:HG3	1:G:322:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:70:PHE:C	1:I:71:LEU:HD12	2.46	0.40
1:O:329:LEU:HD23	1:O:329:LEU:HA	1.95	0.40
1:U:171:TYR:CE2	1:U:175:GLU:OE1	2.74	0.40
1:U:301:ASP:OD2	1:X:10:ASN:HA	2.21	0.40
1:C:18:PRO:HG3	1:C:21:LYS:HD2	2.03	0.40
1:E:191:GLU:HG3	1:E:322:LEU:HD21	2.03	0.40
1:M:206:ALA:HB2	1:O:269:VAL:HG11	2.01	0.40
1:T:270:HIS:CD2	1:T:294:LEU:HD13	2.56	0.40
1:W:13:LYS:HG3	1:W:14:GLU:N	2.36	0.40
1:X:270:HIS:CD2	1:X:294:LEU:HD22	2.57	0.40
1:E:331:PHE:OXT	1:O:17:THR:CB	2.69	0.40
1:G:331:PHE:CD2	1:G:331:PHE:N	2.87	0.40
1:I:20:ASN:ND2	1:L:20:ASN:HD21	2.19	0.40
1:J:99:GLN:H	1:J:99:GLN:HG2	1.57	0.40
1:Q:145:VAL:HG13	1:Q:331:PHE:HE1	1.86	0.40
1:R:155:ASN:CG	1:S:12:LEU:HD22	2.46	0.40
1:R:290:VAL:CG2	1:R:291:PRO:CD	2.99	0.40
1:U:97:ALA:CB	1:U:111:ARG:HH11	2.34	0.40
1:V:11:LEU:O	1:V:13:LYS:HE3	2.21	0.40
1:C:14:GLU:O	1:C:15:GLU:OE2	2.38	0.40
1:D:274:THR:CG2	1:D:302:LEU:HD11	2.52	0.40
1:K:103:GLU:CD	1:U:100:GLN:HG3	2.47	0.40
1:N:270:HIS:CD2	1:N:294:LEU:HD22	2.56	0.40
1:U:18:PRO:HG3	1:U:21:LYS:HD2	2.03	0.40
1:C:60:GLU:HA	1:C:60:GLU:OE1	2.22	0.40
1:S:292:CYS:HB3	1:S:299:ILE:HG23	2.04	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:323:TRP:CH2	1:R:129:ASN:OD1[1_565]	1.36	0.84
1:D:323:TRP:CH2	1:U:129:ASN:OD1[1_545]	1.41	0.79
1:D:323:TRP:CZ2	1:U:129:ASN:OD1[1_545]	1.83	0.37
1:A:309:SER:CB	1:B:216:ASP:OD1[1_655]	1.85	0.35
1:D:323:TRP:CH2	1:U:129:ASN:CG[1_545]	1.89	0.31
1:G:323:TRP:CZ2	1:R:129:ASN:OD1[1_565]	2.08	0.12
1:G:284:ASP:OD1	1:R:156:ARG:NH2[1_565]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/331 (99%)	319 (97%)	9 (3%)	1 (0%)	37	70
1	B	329/331 (99%)	316 (96%)	11 (3%)	2 (1%)	22	58
1	C	329/331 (99%)	314 (95%)	11 (3%)	4 (1%)	11	42
1	D	329/331 (99%)	320 (97%)	7 (2%)	2 (1%)	22	58
1	E	329/331 (99%)	318 (97%)	9 (3%)	2 (1%)	22	58
1	F	329/331 (99%)	321 (98%)	6 (2%)	2 (1%)	22	58
1	G	329/331 (99%)	318 (97%)	8 (2%)	3 (1%)	14	49
1	H	329/331 (99%)	318 (97%)	8 (2%)	3 (1%)	14	49
1	I	329/331 (99%)	317 (96%)	8 (2%)	4 (1%)	11	42
1	J	329/331 (99%)	320 (97%)	7 (2%)	2 (1%)	22	58
1	K	329/331 (99%)	315 (96%)	11 (3%)	3 (1%)	14	49
1	L	329/331 (99%)	318 (97%)	9 (3%)	2 (1%)	22	58
1	M	329/331 (99%)	316 (96%)	8 (2%)	5 (2%)	8	39
1	N	329/331 (99%)	315 (96%)	10 (3%)	4 (1%)	11	42
1	O	329/331 (99%)	316 (96%)	7 (2%)	6 (2%)	7	35
1	P	329/331 (99%)	316 (96%)	10 (3%)	3 (1%)	14	49
1	Q	329/331 (99%)	314 (95%)	11 (3%)	4 (1%)	11	42
1	R	329/331 (99%)	315 (96%)	11 (3%)	3 (1%)	14	49
1	S	329/331 (99%)	318 (97%)	8 (2%)	3 (1%)	14	49
1	T	329/331 (99%)	318 (97%)	9 (3%)	2 (1%)	22	58
1	U	329/331 (99%)	315 (96%)	11 (3%)	3 (1%)	14	49
1	V	329/331 (99%)	318 (97%)	10 (3%)	1 (0%)	37	70
1	W	329/331 (99%)	316 (96%)	8 (2%)	5 (2%)	8	39
1	X	329/331 (99%)	317 (96%)	8 (2%)	4 (1%)	11	42
All	All	7896/7944 (99%)	7608 (96%)	215 (3%)	73 (1%)	14	49

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	C	13	LYS
1	C	97	ALA
1	C	98	ARG
1	E	16	GLN
1	F	101	GLU
1	G	17	THR
1	G	266	LEU
1	I	217	LEU
1	J	17	THR
1	K	15	GLU
1	L	17	THR
1	L	101	GLU
1	M	16	GLN
1	M	17	THR
1	M	101	GLU
1	N	101	GLU
1	N	329	LEU
1	O	97	ALA
1	O	98	ARG
1	O	217	LEU
1	O	277	LYS
1	P	101	GLU
1	Q	16	GLN
1	Q	277	LYS
1	S	81	ASP
1	S	82	TYR
1	T	12	LEU
1	U	17	THR
1	U	101	GLU
1	U	187	TRP
1	V	187	TRP
1	W	299	ILE
1	W	300	SER
1	X	101	GLU
1	X	269	VAL
1	B	10	ASN
1	E	17	THR
1	F	16	GLN
1	I	16	GLN
1	J	16	GLN
1	K	105	ARG

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Mol	Chain	Res	Type
1	M	14	GLU
1	N	13	LYS
1	N	330	GLN
1	O	105	ARG
1	R	329	LEU
1	W	328	GLU
1	B	16	GLN
1	G	16	GLN
1	H	15	GLU
1	M	15	GLU
1	O	104	SER
1	P	10	ASN
1	S	17	THR
1	W	10	ASN
1	X	16	GLN
1	C	17	THR
1	D	17	THR
1	I	10	ASN
1	I	17	THR
1	K	13	LYS
1	R	16	GLN
1	R	330	GLN
1	X	270	HIS
1	D	14	GLU
1	H	16	GLN
1	P	17	THR
1	Q	17	THR
1	W	17	THR
1	H	14	GLU
1	T	16	GLN
1	Q	205	VAL

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/287 (100%)	275 (96%)	12 (4%)	25	48
1	B	287/287 (100%)	271 (94%)	16 (6%)	17	41
1	C	287/287 (100%)	269 (94%)	18 (6%)	15	38
1	D	287/287 (100%)	273 (95%)	14 (5%)	21	44
1	E	287/287 (100%)	275 (96%)	12 (4%)	25	48
1	F	287/287 (100%)	273 (95%)	14 (5%)	21	44
1	G	287/287 (100%)	279 (97%)	8 (3%)	38	59
1	H	287/287 (100%)	273 (95%)	14 (5%)	21	44
1	I	287/287 (100%)	273 (95%)	14 (5%)	21	44
1	J	287/287 (100%)	270 (94%)	17 (6%)	16	39
1	K	287/287 (100%)	265 (92%)	22 (8%)	10	33
1	L	287/287 (100%)	269 (94%)	18 (6%)	15	38
1	M	287/287 (100%)	271 (94%)	16 (6%)	17	41
1	N	287/287 (100%)	274 (96%)	13 (4%)	23	46
1	O	287/287 (100%)	272 (95%)	15 (5%)	19	43
1	P	287/287 (100%)	274 (96%)	13 (4%)	23	46
1	Q	287/287 (100%)	265 (92%)	22 (8%)	10	33
1	R	287/287 (100%)	264 (92%)	23 (8%)	10	32
1	S	287/287 (100%)	266 (93%)	21 (7%)	11	34
1	T	287/287 (100%)	271 (94%)	16 (6%)	17	41
1	U	287/287 (100%)	268 (93%)	19 (7%)	14	37
1	V	287/287 (100%)	275 (96%)	12 (4%)	25	48
1	W	287/287 (100%)	272 (95%)	15 (5%)	19	43
1	X	287/287 (100%)	278 (97%)	9 (3%)	35	56
All	All	6888/6888 (100%)	6515 (95%)	373 (5%)	18	42

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	14	GLU
1	A	15	GLU

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Mol	Chain	Res	Type
1	A	50	VAL
1	A	80	LYS
1	A	87	ASN
1	A	93	ILE
1	A	124	VAL
1	A	220	ASP
1	A	236	SER
1	A	240	VAL
1	A	317	LYS
1	B	4	LYS
1	B	13	LYS
1	B	16	GLN
1	B	19	GLN
1	B	50	VAL
1	B	110	GLN
1	B	211	LYS
1	B	213	LEU
1	B	221	LYS
1	B	243	LEU
1	B	272	VAL
1	B	275	MET
1	B	290	VAL
1	B	294	LEU
1	B	302	LEU
1	B	317	LYS
1	C	3	LEU
1	C	12	LEU
1	C	13	LYS
1	C	14	GLU
1	C	15	GLU
1	C	39	LEU
1	C	64	LEU
1	C	72	ARG
1	C	80	LYS
1	C	98	ARG
1	C	154	LYS
1	C	175	GLU
1	C	196	SER
1	C	221	LYS
1	C	222	ASP
1	C	279	LEU
1	C	283	LYS

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Mol	Chain	Res	Type
1	C	294	LEU
1	D	12	LEU
1	D	93	ILE
1	D	99	GLN
1	D	110	GLN
1	D	124	VAL
1	D	175	GLU
1	D	189	LEU
1	D	220	ASP
1	D	221	LYS
1	D	228	GLU
1	D	283	LYS
1	D	284	ASP
1	D	302	LEU
1	D	330	GLN
1	E	3	LEU
1	E	17	THR
1	E	56	LYS
1	E	72	ARG
1	E	110	GLN
1	E	211	LYS
1	E	276	ILE
1	E	283	LYS
1	E	284	ASP
1	E	310	GLU
1	E	317	LYS
1	E	330	GLN
1	F	16	GLN
1	F	17	THR
1	F	50	VAL
1	F	72	ARG
1	F	80	LYS
1	F	189	LEU
1	F	221	LYS
1	F	290	VAL
1	F	294	LEU
1	F	310	GLU
1	F	316	LYS
1	F	318	SER
1	F	330	GLN
1	F	331	PHE
1	G	12	LEU

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Mol	Chain	Res	Type
1	G	50	VAL
1	G	71	LEU
1	G	196	SER
1	G	213	LEU
1	G	221	LYS
1	G	279	LEU
1	G	331	PHE
1	H	3	LEU
1	H	12	LEU
1	H	14	GLU
1	H	15	GLU
1	H	17	THR
1	H	80	LYS
1	H	213	LEU
1	H	223	LYS
1	H	231	LYS
1	H	243	LEU
1	H	283	LYS
1	H	316	LYS
1	H	330	GLN
1	H	331	PHE
1	I	3	LEU
1	I	12	LEU
1	I	13	LYS
1	I	15	GLU
1	I	30	VAL
1	I	55	ASP
1	I	71	LEU
1	I	80	LYS
1	I	85	THR
1	I	196	SER
1	I	221	LYS
1	I	235	GLU
1	I	294	LEU
1	I	316	LYS
1	J	11	LEU
1	J	12	LEU
1	J	15	GLU
1	J	16	GLN
1	J	17	THR
1	J	19	GLN
1	J	80	LYS

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Mol	Chain	Res	Type
1	J	85	THR
1	J	100	GLN
1	J	124	VAL
1	J	175	GLU
1	J	196	SER
1	J	222	ASP
1	J	284	ASP
1	J	294	LEU
1	J	327	LYS
1	J	331	PHE
1	K	12	LEU
1	K	16	GLN
1	K	17	THR
1	K	27	VAL
1	K	55	ASP
1	K	72	ARG
1	K	80	LYS
1	K	98	ARG
1	K	99	GLN
1	K	106	LEU
1	K	124	VAL
1	K	189	LEU
1	K	210	LEU
1	K	213	LEU
1	K	225	GLN
1	K	242	LYS
1	K	275	MET
1	K	276	ILE
1	K	279	LEU
1	K	283	LYS
1	K	309	SER
1	K	331	PHE
1	L	12	LEU
1	L	17	THR
1	L	50	VAL
1	L	56	LYS
1	L	72	ARG
1	L	80	LYS
1	L	85	THR
1	L	98	ARG
1	L	110	GLN
1	L	111	ARG

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Mol	Chain	Res	Type
1	L	177	LEU
1	L	196	SER
1	L	213	LEU
1	L	231	LYS
1	L	242	LYS
1	L	283	LYS
1	L	302	LEU
1	L	331	PHE
1	M	12	LEU
1	M	15	GLU
1	M	17	THR
1	M	30	VAL
1	M	50	VAL
1	M	52	VAL
1	M	98	ARG
1	M	100	GLN
1	M	177	LEU
1	M	196	SER
1	M	213	LEU
1	M	231	LYS
1	M	243	LEU
1	M	283	LYS
1	M	302	LEU
1	M	317	LYS
1	N	12	LEU
1	N	13	LYS
1	N	15	GLU
1	N	55	ASP
1	N	80	LYS
1	N	87	ASN
1	N	175	GLU
1	N	210	LEU
1	N	221	LYS
1	N	223	LYS
1	N	225	GLN
1	N	277	LYS
1	N	331	PHE
1	O	13	LYS
1	O	14	GLU
1	O	98	ARG
1	O	100	GLN
1	O	103	GLU

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Mol	Chain	Res	Type
1	O	107	ASN
1	O	108	LEU
1	O	124	VAL
1	O	160	SER
1	O	195	SER
1	O	220	ASP
1	O	288	LEU
1	O	290	VAL
1	O	306	THR
1	O	315	LEU
1	P	11	LEU
1	P	12	LEU
1	P	13	LYS
1	P	80	LYS
1	P	85	THR
1	P	108	LEU
1	P	110	GLN
1	P	219	THR
1	P	220	ASP
1	P	231	LYS
1	P	310	GLU
1	P	327	LYS
1	P	330	GLN
1	Q	11	LEU
1	Q	13	LYS
1	Q	17	THR
1	Q	72	ARG
1	Q	80	LYS
1	Q	101	GLU
1	Q	110	GLN
1	Q	154	LYS
1	Q	175	GLU
1	Q	177	LEU
1	Q	217	LEU
1	Q	220	ASP
1	Q	221	LYS
1	Q	223	LYS
1	Q	225	GLN
1	Q	227	LYS
1	Q	239	GLU
1	Q	283	LYS
1	Q	290	VAL

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Mol	Chain	Res	Type
1	Q	294	LEU
1	Q	302	LEU
1	Q	310	GLU
1	R	9	TYR
1	R	11	LEU
1	R	12	LEU
1	R	14	GLU
1	R	15	GLU
1	R	52	VAL
1	R	80	LYS
1	R	87	ASN
1	R	99	GLN
1	R	154	LYS
1	R	172	LEU
1	R	177	LEU
1	R	189	LEU
1	R	220	ASP
1	R	221	LYS
1	R	258	LEU
1	R	284	ASP
1	R	290	VAL
1	R	302	LEU
1	R	308	THR
1	R	317	LYS
1	R	320	ASP
1	R	331	PHE
1	S	3	LEU
1	S	12	LEU
1	S	13	LYS
1	S	14	GLU
1	S	80	LYS
1	S	87	ASN
1	S	98	ARG
1	S	99	GLN
1	S	182	LEU
1	S	189	LEU
1	S	220	ASP
1	S	221	LYS
1	S	228	GLU
1	S	231	LYS
1	S	236	SER
1	S	275	MET

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Mol	Chain	Res	Type
1	S	279	LEU
1	S	290	VAL
1	S	294	LEU
1	S	297	ASN
1	S	306	THR
1	T	12	LEU
1	T	13	LYS
1	T	14	GLU
1	T	50	VAL
1	T	55	ASP
1	T	72	ARG
1	T	154	LYS
1	T	182	LEU
1	T	189	LEU
1	T	231	LYS
1	T	236	SER
1	T	283	LYS
1	T	316	LYS
1	T	317	LYS
1	T	328	GLU
1	T	331	PHE
1	U	16	GLN
1	U	80	LYS
1	U	100	GLN
1	U	154	LYS
1	U	177	LEU
1	U	210	LEU
1	U	213	LEU
1	U	221	LYS
1	U	223	LYS
1	U	231	LYS
1	U	238	TYR
1	U	243	LEU
1	U	294	LEU
1	U	302	LEU
1	U	315	LEU
1	U	317	LYS
1	U	327	LYS
1	U	329	LEU
1	U	331	PHE
1	V	13	LYS
1	V	19	GLN

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Mol	Chain	Res	Type
1	V	69	LEU
1	V	80	LYS
1	V	124	VAL
1	V	220	ASP
1	V	221	LYS
1	V	225	GLN
1	V	242	LYS
1	V	310	GLU
1	V	330	GLN
1	V	331	PHE
1	W	7	LEU
1	W	12	LEU
1	W	14	GLU
1	W	17	THR
1	W	80	LYS
1	W	85	THR
1	W	98	ARG
1	W	213	LEU
1	W	223	LYS
1	W	253	LEU
1	W	283	LYS
1	W	290	VAL
1	W	310	GLU
1	W	317	LYS
1	W	327	LYS
1	X	12	LEU
1	X	80	LYS
1	X	84	VAL
1	X	220	ASP
1	X	221	LYS
1	X	223	LYS
1	X	231	LYS
1	X	309	SER
1	X	317	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (146) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	19	GLN
1	A	66	HIS
1	A	100	GLN

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Mol	Chain	Res	Type
1	A	230	HIS
1	A	232	GLN
1	A	297	ASN
1	B	10	ASN
1	B	20	ASN
1	B	66	HIS
1	B	110	GLN
1	B	214	HIS
1	B	232	GLN
1	B	330	GLN
1	C	16	GLN
1	C	20	ASN
1	C	100	GLN
1	C	232	GLN
1	C	297	ASN
1	D	66	HIS
1	D	122	ASN
1	D	297	ASN
1	E	20	ASN
1	E	114	ASN
1	E	192	HIS
1	E	232	GLN
1	E	297	ASN
1	F	16	GLN
1	F	20	ASN
1	F	66	HIS
1	F	100	GLN
1	F	110	GLN
1	F	114	ASN
1	F	122	ASN
1	F	225	GLN
1	F	232	GLN
1	F	297	ASN
1	G	10	ASN
1	G	20	ASN
1	G	225	GLN
1	H	6	GLN
1	H	16	GLN
1	H	19	GLN
1	H	20	ASN
1	H	100	GLN
1	H	110	GLN

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Mol	Chain	Res	Type
1	I	20	ASN
1	I	110	GLN
1	I	232	GLN
1	I	296	GLN
1	J	10	ASN
1	J	16	GLN
1	J	19	GLN
1	J	20	ASN
1	J	163	ASN
1	J	326	GLN
1	K	16	GLN
1	K	20	ASN
1	K	100	GLN
1	K	110	GLN
1	K	122	ASN
1	L	6	GLN
1	L	10	ASN
1	L	107	ASN
1	L	232	GLN
1	M	10	ASN
1	M	20	ASN
1	M	110	GLN
1	M	232	GLN
1	N	10	ASN
1	N	19	GLN
1	N	87	ASN
1	N	100	GLN
1	N	122	ASN
1	N	129	ASN
1	N	225	GLN
1	N	230	HIS
1	N	232	GLN
1	O	6	GLN
1	O	10	ASN
1	O	16	GLN
1	O	232	GLN
1	O	326	GLN
1	P	6	GLN
1	P	19	GLN
1	P	20	ASN
1	P	66	HIS
1	P	110	GLN

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Mol	Chain	Res	Type
1	P	296	GLN
1	P	297	ASN
1	P	330	GLN
1	Q	6	GLN
1	Q	10	ASN
1	Q	99	GLN
1	Q	110	GLN
1	Q	225	GLN
1	Q	232	GLN
1	Q	330	GLN
1	R	20	ASN
1	R	122	ASN
1	R	230	HIS
1	R	232	GLN
1	R	265	ASN
1	R	296	GLN
1	S	10	ASN
1	S	19	GLN
1	S	20	ASN
1	S	66	HIS
1	S	99	GLN
1	S	107	ASN
1	S	297	ASN
1	S	326	GLN
1	T	10	ASN
1	T	110	GLN
1	T	232	GLN
1	T	297	ASN
1	U	6	GLN
1	U	10	ASN
1	U	19	GLN
1	U	20	ASN
1	U	185	HIS
1	U	225	GLN
1	U	232	GLN
1	V	6	GLN
1	V	10	ASN
1	V	20	ASN
1	V	110	GLN
1	V	122	ASN
1	W	6	GLN
1	W	10	ASN

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Mol	Chain	Res	Type
1	W	20	ASN
1	W	66	HIS
1	W	110	GLN
1	W	114	ASN
1	W	137	ASN
1	W	185	HIS
1	W	214	HIS
1	W	232	GLN
1	W	297	ASN
1	W	330	GLN
1	X	6	GLN
1	X	16	GLN
1	X	19	GLN
1	X	99	GLN
1	X	137	ASN
1	X	297	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GO3	Q	401	-	41,41,41	2.06	7 (17%)	64,64,64	3.17	34 (53%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GO3	Q	401	-	-	8/16/16/16	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	401	GO3	O7-C37	6.30	1.43	1.21
2	Q	401	GO3	C25-C37	6.07	1.58	1.45
2	Q	401	GO3	O8-C38	5.21	1.39	1.21
2	Q	401	GO3	C26-C38	4.04	1.54	1.45
2	Q	401	GO3	C11-C13	-2.79	1.37	1.42
2	Q	401	GO3	C15-C19	-2.20	1.48	1.52
2	Q	401	GO3	C15-C11	-2.06	1.39	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	401	GO3	C9-C10-C18	-10.76	104.41	120.26
2	Q	401	GO3	C10-C9-C21	-7.65	106.82	119.67
2	Q	401	GO3	C9-C10-C22	6.92	131.30	119.67
2	Q	401	GO3	C33-C19-C15	-6.80	97.61	112.94
2	Q	401	GO3	O8-C38-C26	-6.53	103.90	124.11
2	Q	401	GO3	C30-C26-C38	6.10	122.89	116.45
2	Q	401	GO3	C10-C9-C17	5.53	128.41	120.26
2	Q	401	GO3	C10-C22-C14	-5.04	114.53	122.82
2	Q	401	GO3	C29-C25-C37	4.40	121.11	116.45
2	Q	401	GO3	C27-C15-C11	3.99	123.00	117.95
2	Q	401	GO3	C14-C26-C38	-3.76	121.24	125.55
2	Q	401	GO3	C25-C13-C11	3.76	123.07	119.23
2	Q	401	GO3	C23-C17-C9	-3.34	115.07	119.12
2	Q	401	GO3	C18-C24-C12	-3.27	116.93	122.66
2	Q	401	GO3	C23-C11-C13	3.18	124.25	119.03
2	Q	401	GO3	O3-C27-C15	-2.89	116.63	121.01
2	Q	401	GO3	C24-C12-C16	-2.86	113.87	121.10
2	Q	401	GO3	C21-C9-C17	2.84	123.64	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	401	GO3	C26-C14-C22	-2.73	120.25	123.86
2	Q	401	GO3	C21-C13-C11	-2.64	113.92	117.30
2	Q	401	GO3	O5-C29-C25	-2.64	118.99	122.70
2	Q	401	GO3	C24-C18-C10	2.59	122.26	119.12
2	Q	401	GO3	O6-C30-C26	-2.53	119.15	122.70
2	Q	401	GO3	C22-C10-C18	2.40	122.95	119.30
2	Q	401	GO3	C32-C18-C24	-2.37	114.67	120.34
2	Q	401	GO3	C24-C12-C14	2.36	122.90	119.03
2	Q	401	GO3	O4-C28-C16	-2.29	117.54	121.01
2	Q	401	GO3	C13-C25-C37	-2.29	122.93	125.55
2	Q	401	GO3	C19-C15-C11	-2.26	116.36	121.74
2	Q	401	GO3	C22-C14-C12	2.22	120.14	117.30
2	Q	401	GO3	C15-C11-C13	-2.21	117.28	120.52
2	Q	401	GO3	O2-C22-C10	2.11	124.30	120.18
2	Q	401	GO3	C36-C20-C35	-2.09	105.44	110.31
2	Q	401	GO3	C34-C19-C15	-2.04	108.33	112.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	401	GO3	C11-C15-C19-C34
2	Q	401	GO3	C27-C15-C19-C34
2	Q	401	GO3	C14-C26-C38-O8
2	Q	401	GO3	C30-C26-C38-O8
2	Q	401	GO3	C12-C16-C20-C36
2	Q	401	GO3	C28-C16-C20-C36
2	Q	401	GO3	C28-C16-C20-C35
2	Q	401	GO3	C12-C16-C20-C35

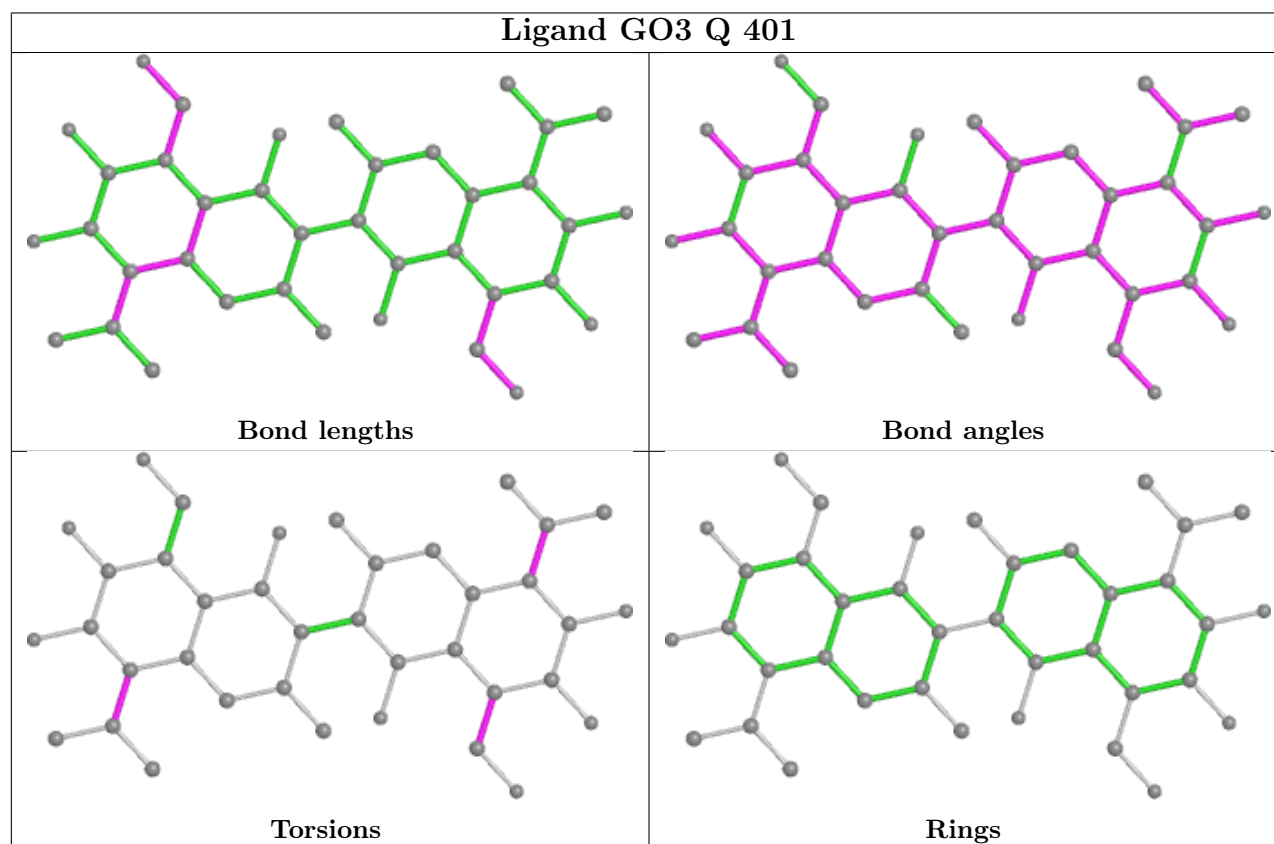
There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	401	GO3	18	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	331/331 (100%)	0.37	7 (2%) 63 47	0, 31, 61, 99	0
1	B	331/331 (100%)	0.38	7 (2%) 63 47	15, 36, 61, 98	0
1	C	331/331 (100%)	0.39	5 (1%) 71 55	13, 38, 74, 116	0
1	D	331/331 (100%)	0.30	5 (1%) 71 55	0, 26, 61, 91	0
1	E	331/331 (100%)	0.40	7 (2%) 63 47	14, 34, 69, 119	0
1	F	331/331 (100%)	0.42	10 (3%) 52 39	16, 39, 69, 89	0
1	G	331/331 (100%)	0.34	5 (1%) 71 55	17, 38, 68, 91	0
1	H	331/331 (100%)	0.34	5 (1%) 71 55	7, 26, 45, 61	0
1	I	331/331 (100%)	0.29	5 (1%) 71 55	16, 31, 60, 77	0
1	J	331/331 (100%)	0.48	14 (4%) 41 32	10, 33, 88, 185	0
1	K	331/331 (100%)	0.49	15 (4%) 39 30	12, 38, 77, 167	0
1	L	331/331 (100%)	0.56	23 (6%) 24 21	13, 42, 110, 191	0
1	M	331/331 (100%)	0.45	9 (2%) 56 42	15, 43, 77, 102	0
1	N	331/331 (100%)	0.62	19 (5%) 30 25	21, 60, 136, 279	0
1	O	331/331 (100%)	0.70	19 (5%) 30 25	12, 55, 115, 187	0
1	P	331/331 (100%)	0.63	20 (6%) 29 24	22, 54, 108, 245	0
1	Q	331/331 (100%)	0.74	27 (8%) 19 17	20, 59, 118, 219	0
1	R	331/331 (100%)	1.01	36 (10%) 12 12	32, 78, 142, 242	0
1	S	331/331 (100%)	0.87	28 (8%) 18 17	26, 69, 116, 145	0
1	T	331/331 (100%)	0.63	16 (4%) 36 29	15, 56, 98, 123	0
1	U	331/331 (100%)	1.12	51 (15%) 6 9	33, 92, 165, 238	0
1	V	331/331 (100%)	0.71	29 (8%) 17 15	20, 54, 122, 250	0
1	W	331/331 (100%)	0.60	14 (4%) 41 32	16, 53, 109, 148	0
1	X	331/331 (100%)	1.02	38 (11%) 11 12	34, 85, 153, 330	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7944/7944 (100%)	0.58	414 (5%) 34 27	0, 46, 115, 330	0

All (414) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	276	ILE	7.0
1	V	106	LEU	5.9
1	R	106	LEU	5.7
1	J	106	LEU	5.5
1	K	105	ARG	5.1
1	W	79	GLY	5.1
1	Q	67	GLY	5.0
1	U	34	CYS	4.9
1	X	135	VAL	4.7
1	S	302	LEU	4.7
1	O	106	LEU	4.6
1	Q	104	SER	4.5
1	P	106	LEU	4.4
1	Q	107	ASN	4.4
1	S	281	GLY	4.4
1	X	290	VAL	4.4
1	A	161	GLY	4.3
1	Q	109	VAL	4.3
1	R	234	VAL	4.3
1	Q	108	LEU	4.2
1	W	299	ILE	4.2
1	G	193	GLY	4.1
1	R	293	ILE	4.1
1	V	9	TYR	4.1
1	X	157	VAL	4.0
1	S	106	LEU	4.0
1	P	108	LEU	4.0
1	Q	300	SER	4.0
1	X	286	VAL	3.9
1	O	108	LEU	3.9
1	M	318	SER	3.9
1	O	95	ALA	3.9
1	U	106	LEU	3.9
1	V	105	ARG	3.9
1	X	116	PHE	3.9
1	V	107	ASN	3.9
1	U	109	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	Q	111	ARG	3.8
1	K	214	HIS	3.8
1	Q	238	TYR	3.8
1	V	179	VAL	3.8
1	B	207	GLY	3.8
1	R	157	VAL	3.8
1	Q	321	THR	3.7
1	M	160	SER	3.7
1	R	322	LEU	3.7
1	U	116	PHE	3.7
1	F	11	LEU	3.7
1	L	31	GLY	3.7
1	J	109	VAL	3.7
1	R	143	THR	3.7
1	Q	237	ALA	3.6
1	U	216	ASP	3.6
1	L	107	ASN	3.6
1	N	106	LEU	3.6
1	G	237	ALA	3.5
1	I	256	ALA	3.5
1	U	146	ALA	3.5
1	L	104	SER	3.5
1	S	67	GLY	3.5
1	Q	106	LEU	3.5
1	U	237	ALA	3.5
1	R	205	VAL	3.5
1	V	108	LEU	3.4
1	X	97	ALA	3.4
1	U	226	TRP	3.4
1	L	325	ILE	3.4
1	S	292	CYS	3.4
1	S	322	LEU	3.4
1	S	109	VAL	3.4
1	X	106	LEU	3.3
1	E	289	SER	3.3
1	U	177	LEU	3.3
1	X	165	ASP	3.3
1	K	104	SER	3.2
1	K	99	GLN	3.2
1	V	97	ALA	3.2
1	X	95	ALA	3.2
1	U	136	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	97	ALA	3.2
1	K	106	LEU	3.2
1	D	301	ASP	3.2
1	R	63	ASP	3.2
1	R	315	LEU	3.2
1	V	99	GLN	3.1
1	X	325	ILE	3.1
1	P	105	ARG	3.1
1	O	97	ALA	3.1
1	N	79	GLY	3.1
1	N	218	GLY	3.1
1	W	210	LEU	3.1
1	O	107	ASN	3.1
1	U	155	ASN	3.1
1	O	109	VAL	3.1
1	X	123	VAL	3.1
1	X	272	VAL	3.1
1	Q	279	LEU	3.1
1	U	315	LEU	3.1
1	K	146	ALA	3.1
1	D	328	GLU	3.0
1	B	203	MET	3.0
1	R	109	VAL	3.0
1	X	309	SER	3.0
1	T	225	GLN	3.0
1	V	233	VAL	3.0
1	U	230	HIS	3.0
1	M	187	TRP	3.0
1	R	31	GLY	3.0
1	V	226	TRP	3.0
1	O	315	LEU	3.0
1	O	318	SER	3.0
1	V	273	SER	3.0
1	R	97	ALA	3.0
1	W	47	LEU	2.9
1	X	45	ASP	2.9
1	F	218	GLY	2.9
1	S	108	LEU	2.9
1	J	112	ASN	2.9
1	P	107	ASN	2.9
1	R	269	VAL	2.9
1	L	238	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	138	PRO	2.9
1	L	106	LEU	2.9
1	X	315	LEU	2.9
1	U	166	SER	2.9
1	R	23	THR	2.9
1	S	24	VAL	2.8
1	A	107	ASN	2.8
1	P	321	THR	2.8
1	W	21	LYS	2.8
1	X	311	GLU	2.8
1	O	218	GLY	2.8
1	I	225	GLN	2.8
1	P	109	VAL	2.8
1	P	104	SER	2.8
1	V	173	MET	2.8
1	H	76	ILE	2.8
1	S	158	ILE	2.8
1	O	247	THR	2.8
1	Q	29	ALA	2.8
1	U	205	VAL	2.7
1	F	324	GLY	2.7
1	D	282	ILE	2.7
1	F	51	ASP	2.7
1	Q	217	LEU	2.7
1	R	203	MET	2.7
1	R	226	TRP	2.7
1	S	97	ALA	2.7
1	R	111	ARG	2.7
1	Q	110	GLN	2.7
1	U	219	THR	2.7
1	J	102	GLY	2.7
1	W	196	SER	2.7
1	K	217	LEU	2.7
1	V	7	LEU	2.7
1	U	52	VAL	2.7
1	T	322	LEU	2.7
1	X	109	VAL	2.6
1	U	66	HIS	2.6
1	V	110	GLN	2.6
1	U	325	ILE	2.6
1	T	20	ASN	2.6
1	L	251	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	S	282	ILE	2.6
1	O	73	THR	2.6
1	C	104	SER	2.6
1	V	109	VAL	2.6
1	P	319	ALA	2.6
1	P	39	LEU	2.6
1	P	270	HIS	2.6
1	L	138	PRO	2.6
1	H	51	ASP	2.6
1	L	98	ARG	2.6
1	N	186	GLY	2.6
1	V	328	GLU	2.6
1	J	322	LEU	2.6
1	S	288	LEU	2.6
1	L	36	ILE	2.6
1	U	36	ILE	2.6
1	N	101	GLU	2.5
1	J	113	VAL	2.5
1	N	286	VAL	2.5
1	V	229	VAL	2.5
1	L	108	LEU	2.5
1	N	322	LEU	2.5
1	W	3	LEU	2.5
1	F	248	SER	2.5
1	N	173	MET	2.5
1	S	104	SER	2.5
1	R	252	GLY	2.5
1	S	297	ASN	2.5
1	E	290	VAL	2.5
1	L	110	GLN	2.5
1	U	79	GLY	2.5
1	U	104	SER	2.5
1	W	218	GLY	2.5
1	D	271	PRO	2.5
1	R	49	LEU	2.5
1	W	315	LEU	2.5
1	S	190	GLY	2.5
1	N	315	LEU	2.5
1	K	199	VAL	2.5
1	S	100	GLN	2.5
1	R	250	ALA	2.5
1	N	102	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	74	PRO	2.5
1	V	198	PRO	2.5
1	Q	325	ILE	2.5
1	I	19	GLN	2.5
1	X	285	ASP	2.4
1	G	33	ALA	2.4
1	X	319	ALA	2.4
1	R	105	ARG	2.4
1	P	173	MET	2.4
1	R	62	MET	2.4
1	U	24	VAL	2.4
1	R	104	SER	2.4
1	J	110	GLN	2.4
1	L	112	ASN	2.4
1	O	326	GLN	2.4
1	A	193	GLY	2.4
1	L	59	GLY	2.4
1	O	34	CYS	2.4
1	N	109	VAL	2.4
1	Q	186	GLY	2.4
1	C	95	ALA	2.4
1	O	319	ALA	2.4
1	U	86	ALA	2.4
1	X	5	ASP	2.4
1	S	90	LEU	2.4
1	T	186	GLY	2.4
1	U	234	VAL	2.4
1	V	193	GLY	2.4
1	X	93	ILE	2.4
1	F	285	ASP	2.4
1	R	68	SER	2.4
1	X	140	ASP	2.4
1	J	105	ARG	2.4
1	J	265	ASN	2.4
1	T	253	LEU	2.4
1	A	218	GLY	2.4
1	M	199	VAL	2.4
1	S	325	ILE	2.4
1	T	199	VAL	2.4
1	L	136	SER	2.4
1	H	107	ASN	2.4
1	F	325	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	157	VAL	2.3
1	J	281	GLY	2.3
1	V	186	GLY	2.3
1	G	164	LEU	2.3
1	W	230	HIS	2.3
1	A	196	SER	2.3
1	B	5	ASP	2.3
1	R	160	SER	2.3
1	V	104	SER	2.3
1	L	286	VAL	2.3
1	V	234	VAL	2.3
1	X	104	SER	2.3
1	T	102	GLY	2.3
1	T	278	GLY	2.3
1	U	245	GLY	2.3
1	N	97	ALA	2.3
1	P	322	LEU	2.3
1	X	101	GLU	2.3
1	F	145	VAL	2.3
1	L	109	VAL	2.3
1	S	305	VAL	2.3
1	U	242	LYS	2.3
1	F	26	GLY	2.3
1	R	301	ASP	2.3
1	T	236	SER	2.3
1	U	107	ASN	2.3
1	X	202	GLY	2.3
1	E	226	TRP	2.3
1	E	328	GLU	2.3
1	Q	303	VAL	2.3
1	P	169	PHE	2.3
1	E	324	GLY	2.3
1	M	79	GLY	2.3
1	X	133	LEU	2.3
1	N	323	TRP	2.3
1	H	203	MET	2.3
1	I	263	MET	2.3
1	U	311	GLU	2.3
1	W	205	VAL	2.3
1	V	6	GLN	2.3
1	U	168	ARG	2.3
1	I	278	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	U	279	LEU	2.3
1	P	289	SER	2.3
1	C	8	ILE	2.2
1	Q	46	GLU	2.2
1	R	199	VAL	2.2
1	V	113	VAL	2.2
1	Q	64	LEU	2.2
1	X	322	LEU	2.2
1	Q	1	ALA	2.2
1	U	222	ASP	2.2
1	X	201	SER	2.2
1	R	38	ILE	2.2
1	J	197	VAL	2.2
1	V	100	GLN	2.2
1	F	68	SER	2.2
1	Q	165	ASP	2.2
1	R	107	ASN	2.2
1	S	87	ASN	2.2
1	U	115	ILE	2.2
1	U	284	ASP	2.2
1	U	138	PRO	2.2
1	U	229	VAL	2.2
1	P	111	ARG	2.2
1	S	103	GLU	2.2
1	P	66	HIS	2.2
1	Q	326	GLN	2.2
1	S	79	GLY	2.2
1	T	161	GLY	2.2
1	U	110	GLN	2.2
1	R	259	ALA	2.2
1	O	325	ILE	2.2
1	U	247	THR	2.2
1	D	198	PRO	2.2
1	K	109	VAL	2.2
1	X	88	SER	2.2
1	W	177	LEU	2.2
1	X	167	ALA	2.2
1	U	22	ILE	2.2
1	C	135	VAL	2.2
1	J	23	THR	2.2
1	P	314	ARG	2.2
1	U	308	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	321	THR	2.2
1	X	55	ASP	2.2
1	U	67	GLY	2.2
1	X	262	ILE	2.2
1	S	329	LEU	2.2
1	V	64	LEU	2.2
1	X	85	THR	2.2
1	W	87	ASN	2.2
1	X	328	GLU	2.1
1	J	99	GLN	2.1
1	T	276	ILE	2.1
1	U	53	ILE	2.1
1	L	188	VAL	2.1
1	M	269	VAL	2.1
1	N	113	VAL	2.1
1	T	135	VAL	2.1
1	K	258	LEU	2.1
1	U	294	LEU	2.1
1	L	321	THR	2.1
1	O	320	ASP	2.1
1	U	129	ASN	2.1
1	E	238	TYR	2.1
1	H	134	ILE	2.1
1	N	325	ILE	2.1
1	R	230	HIS	2.1
1	T	250	ALA	2.1
1	U	322	LEU	2.1
1	X	288	LEU	2.1
1	B	212	THR	2.1
1	O	212	THR	2.1
1	N	276	ILE	2.1
1	U	250	ALA	2.1
1	U	128	PRO	2.1
1	N	321	THR	2.1
1	E	309	SER	2.1
1	M	83	ASN	2.1
1	M	285	ASP	2.1
1	M	298	GLY	2.1
1	V	325	ILE	2.1
1	P	257	ASP	2.1
1	S	259	ALA	2.1
1	N	307	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	T	233	VAL	2.1
1	U	135	VAL	2.1
1	O	219	THR	2.1
1	S	299	ILE	2.1
1	J	280	TYR	2.1
1	U	82	TYR	2.1
1	K	1	ALA	2.1
1	A	217	LEU	2.1
1	L	322	LEU	2.1
1	S	172	LEU	2.1
1	P	99	GLN	2.1
1	R	153	PRO	2.1
1	W	187	TRP	2.1
1	A	46	GLU	2.1
1	L	103	GLU	2.1
1	Q	26	GLY	2.1
1	B	237	ALA	2.1
1	B	313	ALA	2.1
1	K	89	LYS	2.1
1	K	95	ALA	2.1
1	R	33	ALA	2.1
1	S	257	ASP	2.0
1	T	293	ILE	2.0
1	X	8	ILE	2.0
1	C	306	THR	2.0
1	R	278	GLY	2.0
1	V	210	LEU	2.0
1	L	311	GLU	2.0
1	Q	250	ALA	2.0
1	K	107	ASN	2.0
1	O	160	SER	2.0
1	Q	68	SER	2.0
1	X	129	ASN	2.0
1	G	276	ILE	2.0
1	Q	200	TRP	2.0
1	R	85	THR	2.0
1	R	258	LEU	2.0
1	U	280	TYR	2.0
1	T	312	GLU	2.0
1	V	199	VAL	2.0
1	B	282	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

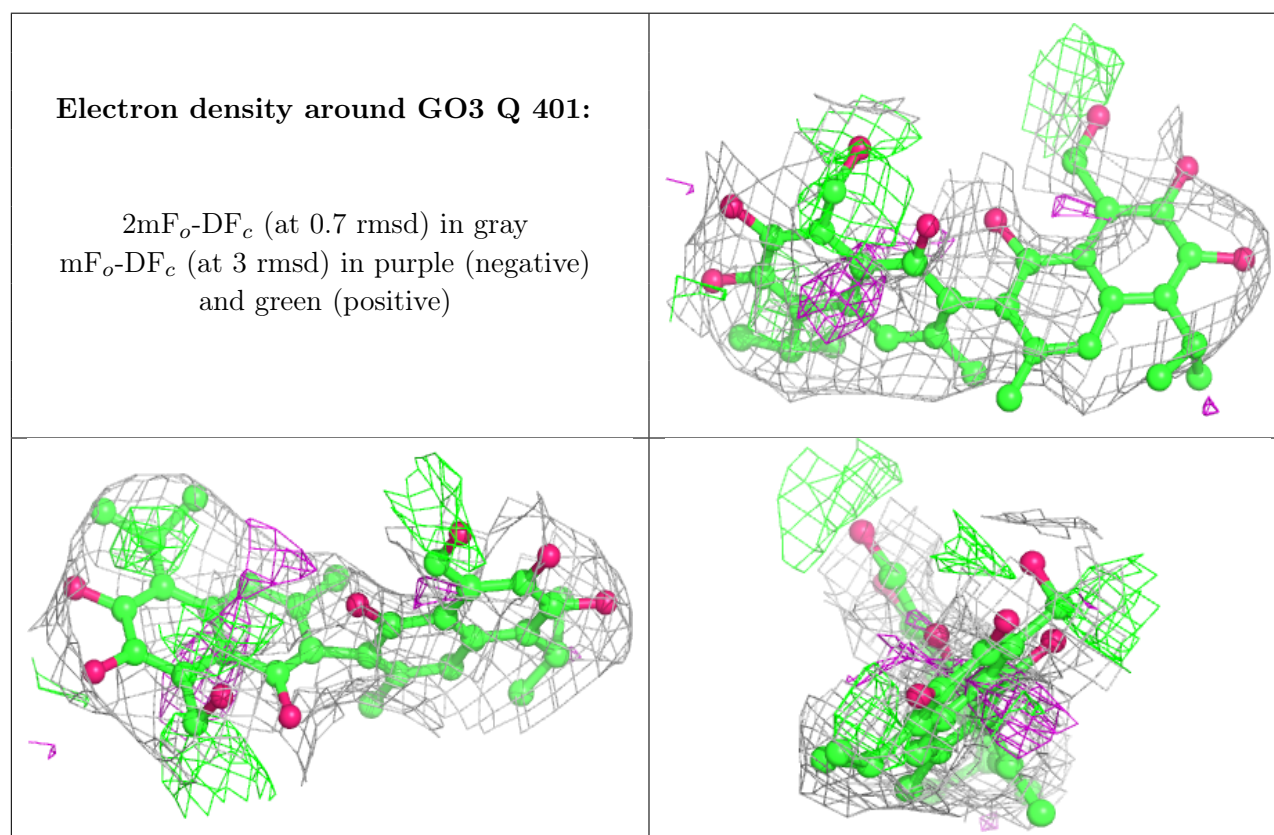
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GO3	Q	401	38/38	0.80	0.18	18,23,27,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.