



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:16 AM UTC

PDB ID : 4RAP / pdb_00004rap
Title : Crystal structure of bacterial iron-containing dodecameric glycosyltransferase TibC from enterotoxigenic E.coli H10407
Authors : Yao, Q.; Lu, Q.; Xu, Y.; Shao, F.
Deposited on : 2014-09-10
Resolution : 2.88 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

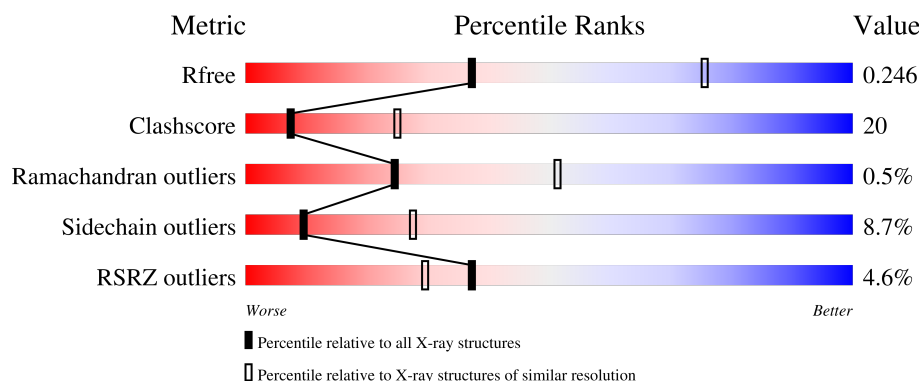
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	406	3% 66% 23% 5% 6%
1	B	406	4% 69% 20% 5% 6%
1	C	406	4% 69% 21% 6% .
1	D	406	4% 67% 20% 6% • 6%
1	E	406	4% 67% 23% 6% .

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Mol	Chain	Length	Quality of chain
1	F	406	10% 60% 26% 8% 6%
1	G	406	6% 68% 23% 5%
1	H	406	2% 71% 19% 5%
1	I	406	3% 71% 21%
1	J	406	2% 75% 16% 5%
1	K	406	2% 70% 20% 5%
1	L	406	7% 58% 27% 6% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 37131 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 Glycosyltransferase TibC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	Se	0	0	0
			3069	1976	536	544	11	2			
1	B	383	Total	C	N	O	S	Se	0	0	0
			3085	1988	538	546	11	2			
1	C	389	Total	C	N	O	S	Se	0	0	0
			3124	2008	545	558	11	2			
1	D	381	Total	C	N	O	S	Se	0	0	0
			3067	1974	536	544	11	2			
1	E	390	Total	C	N	O	S	Se	0	0	0
			3132	2014	546	559	11	2			
1	F	382	Total	C	N	O	S	Se	0	0	0
			3071	1976	537	545	11	2			
1	G	389	Total	C	N	O	S	Se	0	0	0
			3124	2008	545	558	11	2			
1	H	385	Total	C	N	O	S	Se	0	0	0
			3096	1991	541	551	11	2			
1	I	389	Total	C	N	O	S	Se	0	0	0
			3124	2008	545	558	11	2			
1	J	384	Total	C	N	O	S	Se	0	0	0
			3092	1989	540	550	11	2			
1	K	389	Total	C	N	O	S	Se	0	0	0
			3124	2008	545	558	11	2			
1	L	371	Total	C	N	O	S	Se	0	0	0
			2988	1923	522	530	11	2			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	GLU	engineered mutation	UNP Q9S4K6
A	84	ALA	GLU	engineered mutation	UNP Q9S4K6
A	215	ALA	GLN	engineered mutation	UNP Q9S4K6
A	216	ALA	GLU	engineered mutation	UNP Q9S4K6
A	400	ALA	LYS	engineered mutation	UNP Q9S4K6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	401	ALA	LYS	engineered mutation	UNP Q9S4K6
B	83	ALA	GLU	engineered mutation	UNP Q9S4K6
B	84	ALA	GLU	engineered mutation	UNP Q9S4K6
B	215	ALA	GLN	engineered mutation	UNP Q9S4K6
B	216	ALA	GLU	engineered mutation	UNP Q9S4K6
B	400	ALA	LYS	engineered mutation	UNP Q9S4K6
B	401	ALA	LYS	engineered mutation	UNP Q9S4K6
C	83	ALA	GLU	engineered mutation	UNP Q9S4K6
C	84	ALA	GLU	engineered mutation	UNP Q9S4K6
C	215	ALA	GLN	engineered mutation	UNP Q9S4K6
C	216	ALA	GLU	engineered mutation	UNP Q9S4K6
C	400	ALA	LYS	engineered mutation	UNP Q9S4K6
C	401	ALA	LYS	engineered mutation	UNP Q9S4K6
D	83	ALA	GLU	engineered mutation	UNP Q9S4K6
D	84	ALA	GLU	engineered mutation	UNP Q9S4K6
D	215	ALA	GLN	engineered mutation	UNP Q9S4K6
D	216	ALA	GLU	engineered mutation	UNP Q9S4K6
D	400	ALA	LYS	engineered mutation	UNP Q9S4K6
D	401	ALA	LYS	engineered mutation	UNP Q9S4K6
E	83	ALA	GLU	engineered mutation	UNP Q9S4K6
E	84	ALA	GLU	engineered mutation	UNP Q9S4K6
E	215	ALA	GLN	engineered mutation	UNP Q9S4K6
E	216	ALA	GLU	engineered mutation	UNP Q9S4K6
E	400	ALA	LYS	engineered mutation	UNP Q9S4K6
E	401	ALA	LYS	engineered mutation	UNP Q9S4K6
F	83	ALA	GLU	engineered mutation	UNP Q9S4K6
F	84	ALA	GLU	engineered mutation	UNP Q9S4K6
F	215	ALA	GLN	engineered mutation	UNP Q9S4K6
F	216	ALA	GLU	engineered mutation	UNP Q9S4K6
F	400	ALA	LYS	engineered mutation	UNP Q9S4K6
F	401	ALA	LYS	engineered mutation	UNP Q9S4K6
G	83	ALA	GLU	engineered mutation	UNP Q9S4K6
G	84	ALA	GLU	engineered mutation	UNP Q9S4K6
G	215	ALA	GLN	engineered mutation	UNP Q9S4K6
G	216	ALA	GLU	engineered mutation	UNP Q9S4K6
G	400	ALA	LYS	engineered mutation	UNP Q9S4K6
G	401	ALA	LYS	engineered mutation	UNP Q9S4K6
H	83	ALA	GLU	engineered mutation	UNP Q9S4K6
H	84	ALA	GLU	engineered mutation	UNP Q9S4K6
H	215	ALA	GLN	engineered mutation	UNP Q9S4K6
H	216	ALA	GLU	engineered mutation	UNP Q9S4K6
H	400	ALA	LYS	engineered mutation	UNP Q9S4K6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	401	ALA	LYS	engineered mutation	UNP Q9S4K6
I	83	ALA	GLU	engineered mutation	UNP Q9S4K6
I	84	ALA	GLU	engineered mutation	UNP Q9S4K6
I	215	ALA	GLN	engineered mutation	UNP Q9S4K6
I	216	ALA	GLU	engineered mutation	UNP Q9S4K6
I	400	ALA	LYS	engineered mutation	UNP Q9S4K6
I	401	ALA	LYS	engineered mutation	UNP Q9S4K6
J	83	ALA	GLU	engineered mutation	UNP Q9S4K6
J	84	ALA	GLU	engineered mutation	UNP Q9S4K6
J	215	ALA	GLN	engineered mutation	UNP Q9S4K6
J	216	ALA	GLU	engineered mutation	UNP Q9S4K6
J	400	ALA	LYS	engineered mutation	UNP Q9S4K6
J	401	ALA	LYS	engineered mutation	UNP Q9S4K6
K	83	ALA	GLU	engineered mutation	UNP Q9S4K6
K	84	ALA	GLU	engineered mutation	UNP Q9S4K6
K	215	ALA	GLN	engineered mutation	UNP Q9S4K6
K	216	ALA	GLU	engineered mutation	UNP Q9S4K6
K	400	ALA	LYS	engineered mutation	UNP Q9S4K6
K	401	ALA	LYS	engineered mutation	UNP Q9S4K6
L	83	ALA	GLU	engineered mutation	UNP Q9S4K6
L	84	ALA	GLU	engineered mutation	UNP Q9S4K6
L	215	ALA	GLN	engineered mutation	UNP Q9S4K6
L	216	ALA	GLU	engineered mutation	UNP Q9S4K6
L	400	ALA	LYS	engineered mutation	UNP Q9S4K6
L	401	ALA	LYS	engineered mutation	UNP Q9S4K6

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

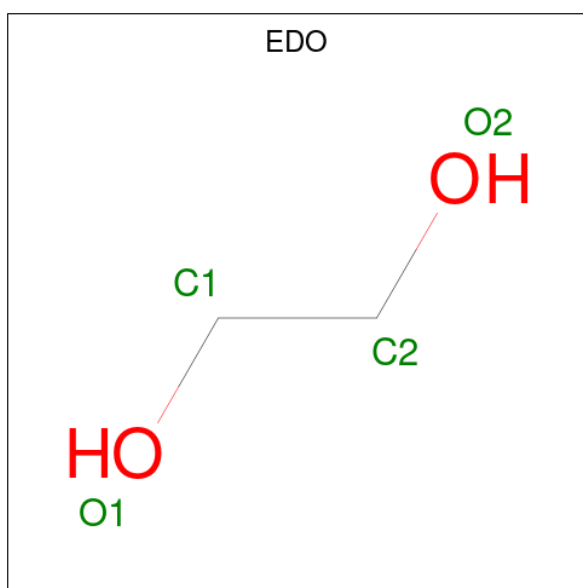
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total	Fe	0	0
			1	1		
2	I	1	Total	Fe	0	0
			1	1		
2	J	1	Total	Fe	0	0
			1	1		
2	K	1	Total	Fe	0	0
			1	1		
2	L	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		

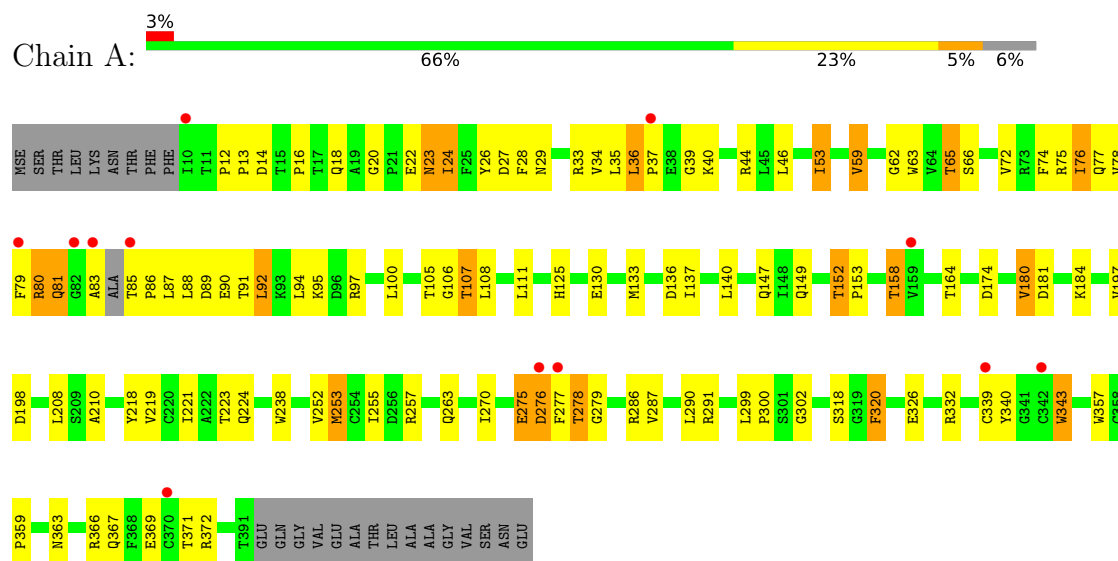
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	O 1	0	0
4	C	1	Total 1	O 1	0	0
4	J	1	Total 1	O 1	0	0

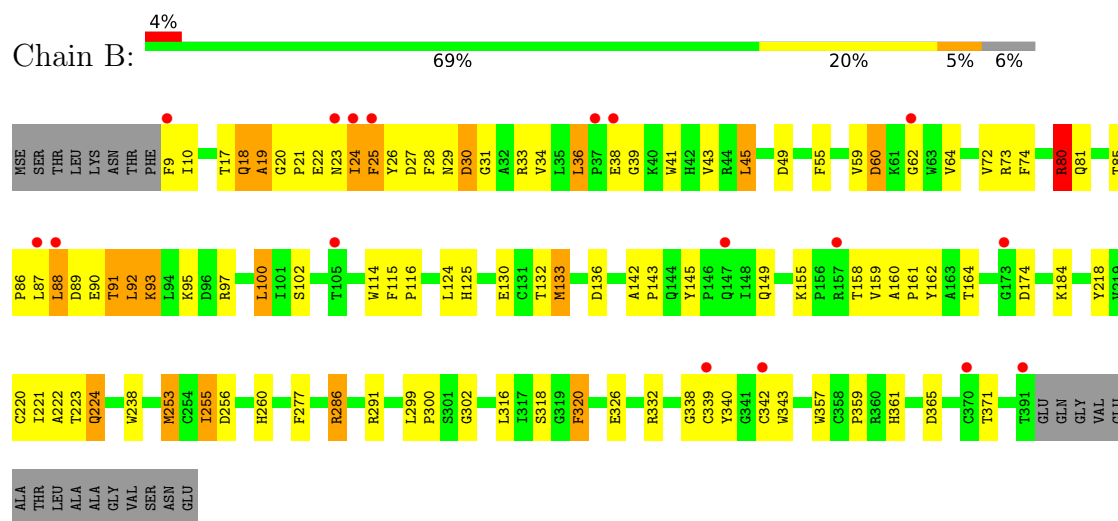
3 Residue-property plots [i](#)

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

• Molecule 1: Glycosyltransferase TibC

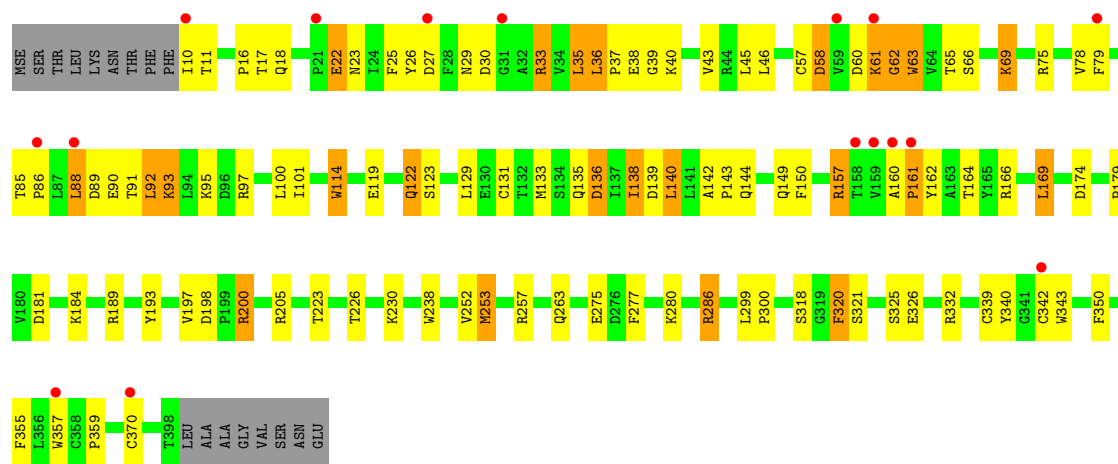


• Molecule 1: Glycosyltransferase TibC

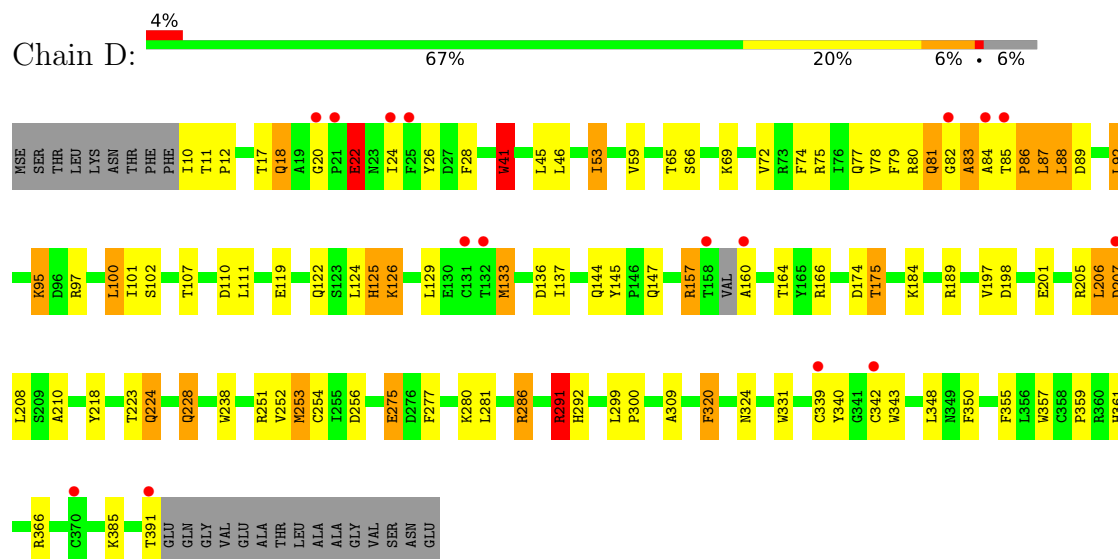


• Molecule 1: Glycosyltransferase TibC

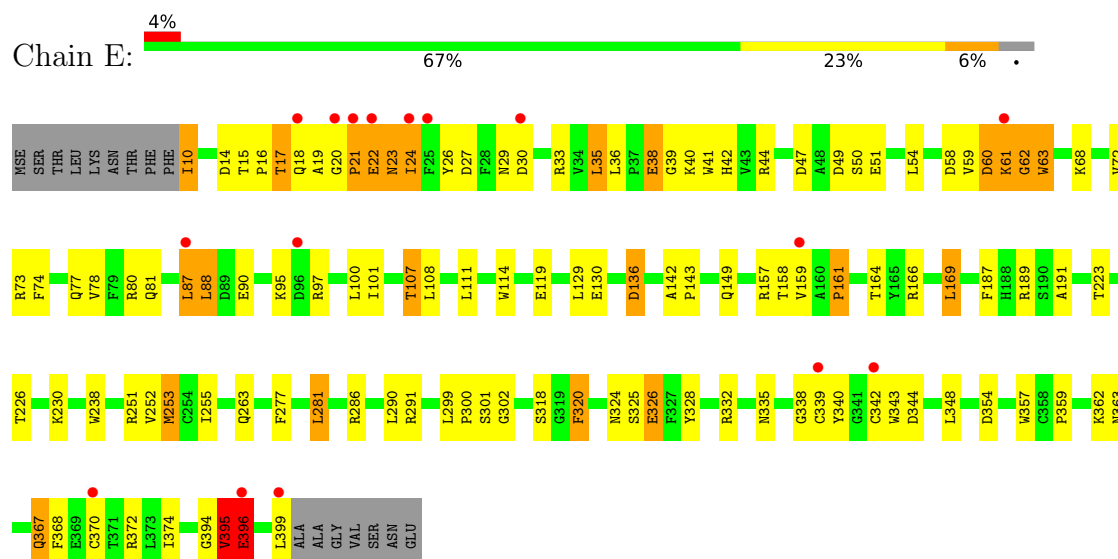




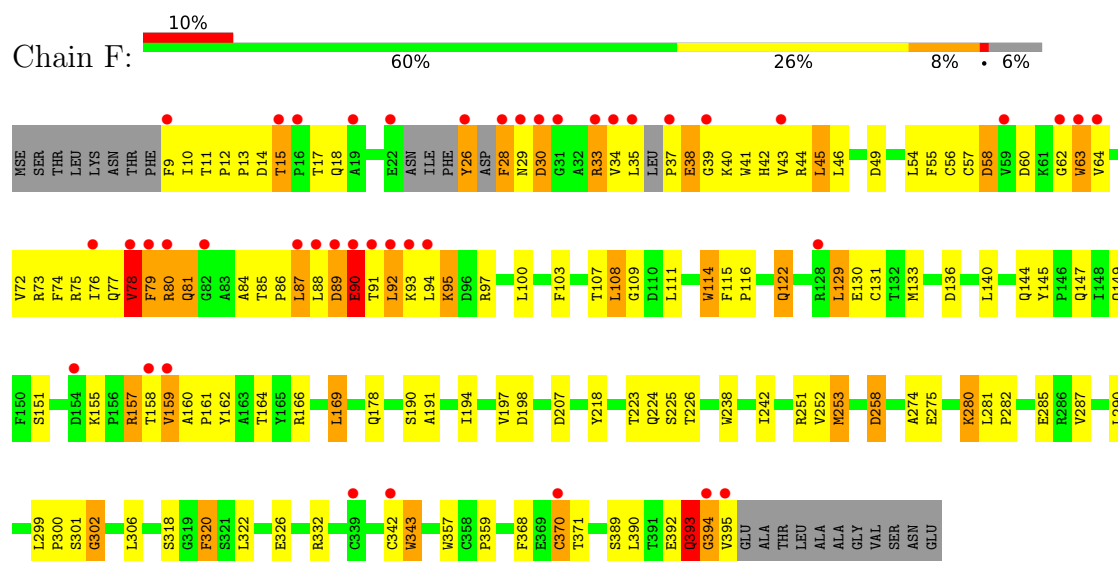
- Molecule 1: Glycosyltransferase TibC



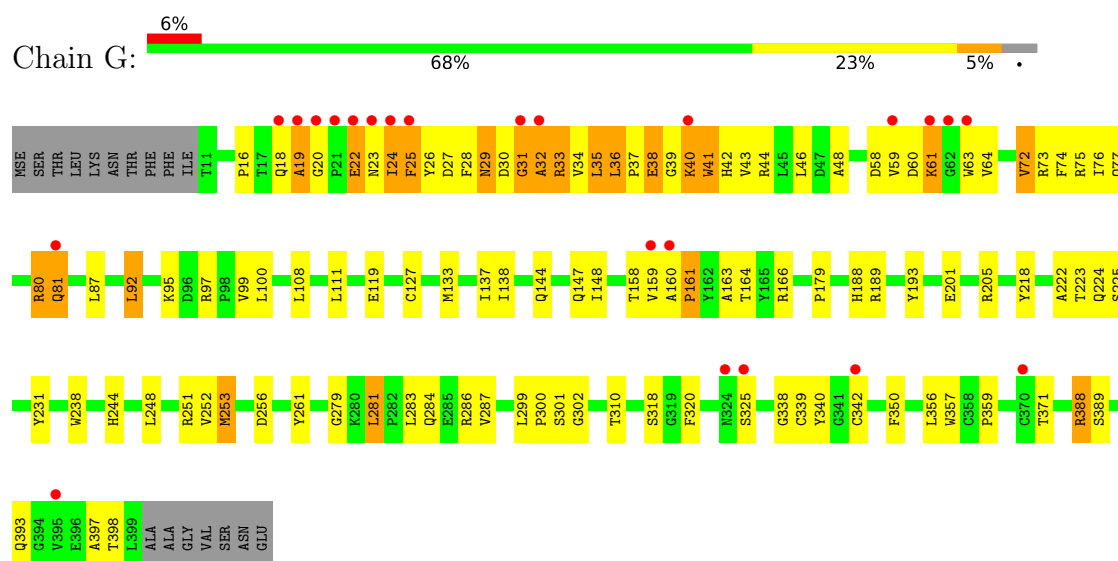
- Molecule 1: Glycosyltransferase TibC



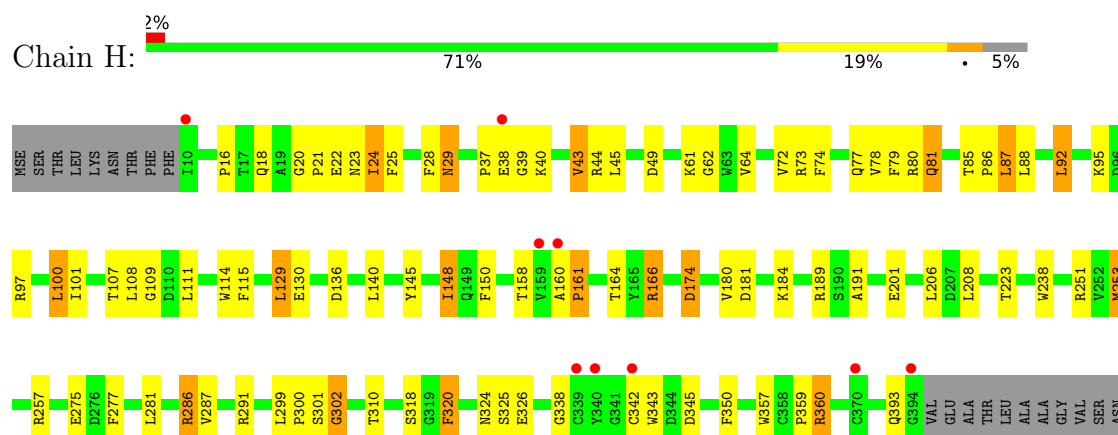
- Molecule 1: Glycosyltransferase TibC



- Molecule 1: Glycosyltransferase TibC

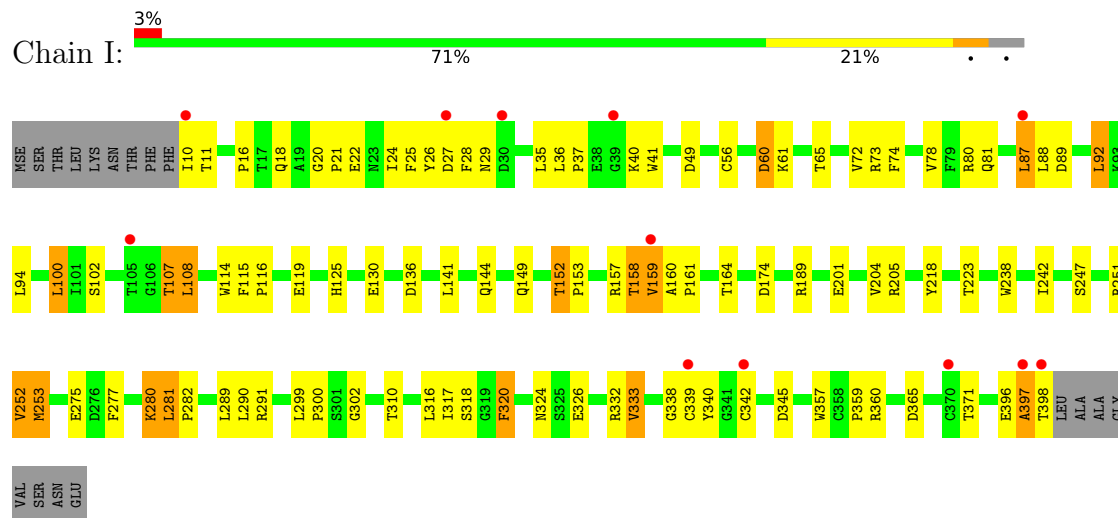


- Molecule 1: Glycosyltransferase TibC

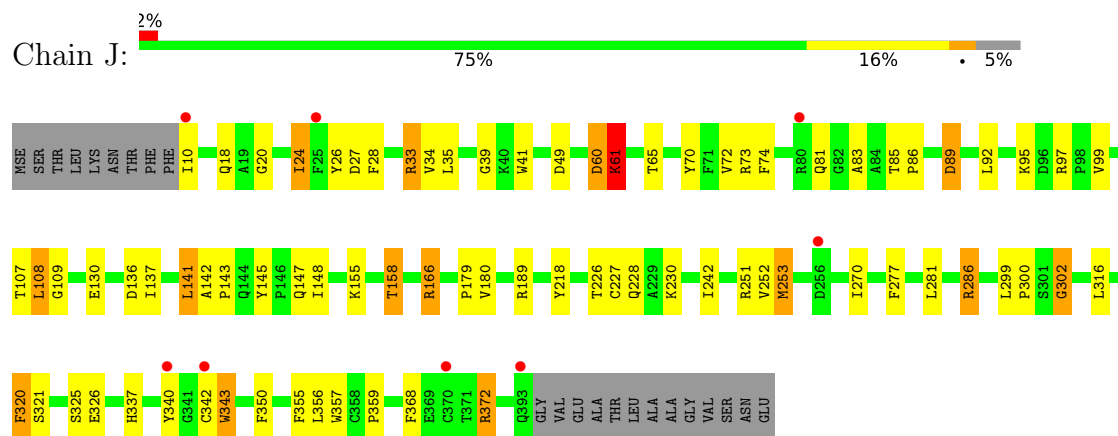


GLU

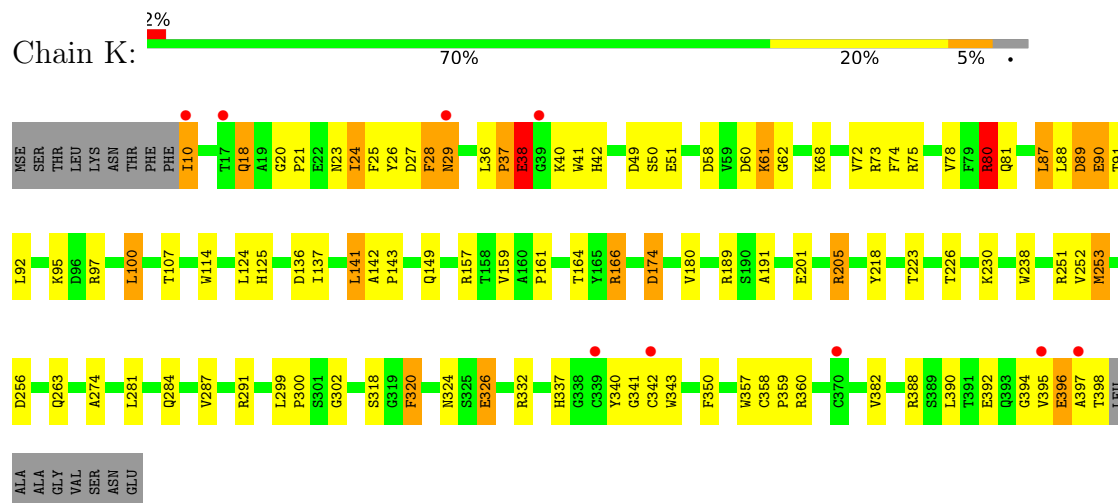
- Molecule 1: Glycosyltransferase TibC



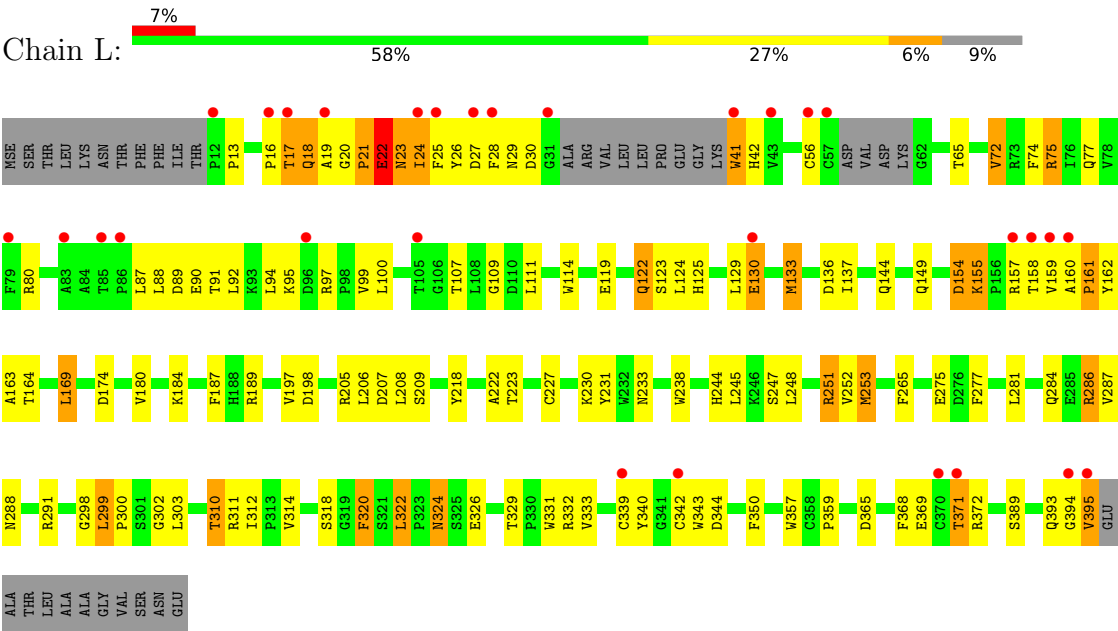
- Molecule 1: Glycosyltransferase TibC



- Molecule 1: Glycosyltransferase TibC



● Molecule 1: Glycosyltransferase TibC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.79Å 314.37Å 164.53Å 90.00° 101.44° 90.00°	Depositor
Resolution (Å)	19.92 – 2.88 19.92 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.92-2.88) 99.0 (19.92-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.208 , 0.245 0.212 , 0.246	Depositor DCC
R_{free} test set	9781 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	37131	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: EDO, FE

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	0.83	0/3164	0.90	5/4310 (0.1%)
1	B	0.87	3/3182 (0.1%)	0.91	6/4336 (0.1%)
1	C	0.90	2/3220 (0.1%)	0.93	5/4388 (0.1%)
1	D	0.83	2/3162 (0.1%)	0.90	5/4307 (0.1%)
1	E	0.90	3/3228 (0.1%)	0.94	4/4399 (0.1%)
1	F	0.84	2/3164 (0.1%)	0.96	12/4305 (0.3%)
1	G	0.83	2/3220 (0.1%)	0.91	2/4388 (0.0%)
1	H	0.83	2/3192 (0.1%)	0.88	2/4349 (0.0%)
1	I	0.84	2/3220 (0.1%)	0.88	4/4388 (0.1%)
1	J	0.89	1/3188 (0.0%)	0.91	5/4344 (0.1%)
1	K	0.96	4/3220 (0.1%)	1.06	16/4388 (0.4%)
1	L	0.88	3/3081 (0.1%)	0.89	2/4195 (0.0%)
All	All	0.87	26/38241 (0.1%)	0.93	68/52097 (0.1%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	29	ASN	C-O	-19.64	1.01	1.24
1	K	29	ASN	C-N	9.57	1.51	1.34
1	J	342	CYS	CA-CB	7.34	1.65	1.53
1	I	342	CYS	CA-CB	7.24	1.65	1.53
1	K	342	CYS	CA-CB	6.87	1.64	1.53
1	E	338	GLY	N-CA	6.87	1.50	1.44
1	E	342	CYS	CA-CB	6.83	1.64	1.53
1	B	342	CYS	CA-CB	6.82	1.64	1.53
1	G	342	CYS	CA-CB	6.81	1.64	1.53
1	L	342	CYS	CA-CB	6.77	1.64	1.53
1	D	342	CYS	CA-CB	6.62	1.64	1.53
1	C	342	CYS	CA-CB	6.61	1.64	1.53
1	K	28	PHE	C-N	6.45	1.42	1.33
1	F	342	CYS	CA-CB	6.27	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	370	CYS	CA-CB	5.83	1.62	1.53
1	H	342	CYS	CA-CB	5.57	1.62	1.53
1	F	370	CYS	CA-CB	5.42	1.62	1.53
1	H	338	GLY	N-CA	5.39	1.49	1.44
1	B	338	GLY	N-CA	5.37	1.49	1.44
1	C	370	CYS	CA-CB	5.28	1.61	1.53
1	D	86	PRO	N-CD	5.17	1.54	1.47
1	I	338	GLY	N-CA	5.17	1.49	1.44
1	L	13	PRO	N-CD	5.12	1.54	1.47
1	L	244	HIS	CG-CD2	5.05	1.41	1.35
1	G	338	GLY	N-CA	5.04	1.49	1.44
1	B	260	HIS	CG-CD2	5.00	1.41	1.35

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	29	ASN	CA-C-O	23.34	145.29	120.55
1	K	29	ASN	O-C-N	-12.66	108.70	122.12
1	E	396	GLU	N-CA-C	-11.82	98.86	113.28
1	K	28	PHE	CA-C-N	11.53	135.73	120.28
1	K	28	PHE	C-N-CA	11.53	135.73	120.28
1	C	62	GLY	N-CA-C	10.84	125.73	112.73
1	F	394	GLY	N-CA-C	10.24	124.38	112.50
1	K	28	PHE	O-C-N	-10.06	109.89	122.26
1	A	39	GLY	N-CA-C	-9.15	98.52	110.69
1	A	80	ARG	N-CA-C	-8.97	99.07	110.19
1	K	29	ASN	CA-C-N	-8.55	111.57	123.03
1	K	29	ASN	C-N-CA	-8.55	111.57	123.03
1	I	302	GLY	N-CA-C	8.40	122.81	112.64
1	J	302	GLY	N-CA-C	8.34	122.73	112.64
1	A	302	GLY	N-CA-C	7.83	122.11	112.64
1	F	393	GLN	N-CA-C	7.52	121.43	111.28
1	K	302	GLY	N-CA-C	7.26	121.43	112.64
1	D	41	TRP	N-CA-C	7.22	119.90	109.14
1	L	80	ARG	N-CA-C	-7.22	98.28	109.76
1	F	302	GLY	N-CA-C	7.18	121.33	112.64
1	B	19	ALA	N-CA-C	7.09	120.05	111.40
1	H	302	GLY	N-CA-C	7.06	121.44	112.83
1	D	125	HIS	N-CA-C	6.76	121.70	113.38
1	E	62	GLY	N-CA-C	6.70	120.27	112.50
1	F	159	VAL	N-CA-C	-6.69	98.55	108.99
1	G	302	GLY	N-CA-C	6.69	120.99	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	360	ARG	N-CA-C	6.62	118.57	111.36
1	A	210	ALA	N-CA-C	6.54	117.12	109.60
1	E	63	TRP	N-CA-C	6.42	119.40	109.07
1	B	114	TRP	N-CA-C	6.29	118.22	111.36
1	G	29	ASN	N-CA-C	6.28	117.92	111.14
1	I	41	TRP	N-CA-C	6.27	118.94	109.23
1	J	83	ALA	N-CA-C	6.26	118.80	110.53
1	F	343	TRP	N-CA-C	6.19	118.83	111.71
1	F	114	TRP	N-CA-C	6.19	118.11	111.36
1	K	358	CYS	O-C-N	6.11	124.94	121.27
1	B	39	GLY	N-CA-C	6.08	119.99	112.64
1	E	302	GLY	N-CA-C	6.08	120.24	112.83
1	K	358	CYS	CA-C-N	-6.06	112.32	119.05
1	K	358	CYS	C-N-CA	-6.06	112.32	119.05
1	D	291	ARG	N-CA-C	-5.97	101.57	110.23
1	J	343	TRP	N-CA-C	5.79	118.37	111.71
1	F	90	GLU	N-CA-C	5.79	118.66	110.14
1	L	133	MSE	CB-CA-C	-5.77	99.87	111.17
1	F	15	THR	CA-C-N	5.69	126.02	119.93
1	F	15	THR	C-N-CA	5.69	126.02	119.93
1	K	337	HIS	N-CA-C	5.56	119.79	112.89
1	I	114	TRP	N-CA-C	5.55	117.41	111.36
1	J	337	HIS	N-CA-C	5.52	119.86	113.18
1	B	302	GLY	N-CA-C	5.49	119.52	112.83
1	K	80	ARG	N-CA-C	-5.47	102.79	110.50
1	K	341	GLY	N-CA-C	5.43	122.30	114.10
1	A	343	TRP	N-CA-C	5.37	118.05	111.82
1	I	80	ARG	N-CA-C	-5.34	101.96	109.96
1	C	63	TRP	N-CA-C	5.32	117.92	109.24
1	J	61	LYS	N-CA-C	5.30	118.71	111.39
1	D	22	GLU	CB-CA-C	-5.27	104.46	111.63
1	C	61	LYS	N-CA-C	5.25	117.30	110.53
1	H	29	ASN	N-CA-C	5.20	119.62	113.28
1	K	38	GLU	N-CA-C	5.19	117.51	111.02
1	C	343	TRP	N-CA-C	5.16	117.64	111.71
1	F	78	VAL	N-CA-C	5.13	115.24	107.75
1	C	114	TRP	N-CA-C	5.11	116.93	111.36
1	F	79	PHE	CA-C-N	-5.10	114.33	121.72
1	F	79	PHE	C-N-CA	-5.10	114.33	121.72
1	D	157	ARG	N-CA-C	5.06	116.48	111.07
1	B	80	ARG	N-CA-C	-5.04	103.39	110.50
1	B	361	HIS	N-CA-C	5.00	120.47	113.02

There are no chirality outliers.

There are no planarity outliers.

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	3069	0	2975	125	0
1	B	3085	0	2990	126	0
1	C	3124	0	3025	127	0
1	D	3067	0	2971	120	0
1	E	3132	0	3037	117	0
1	F	3071	0	2972	170	0
1	G	3124	0	3026	173	0
1	H	3096	0	2998	81	0
1	I	3124	0	3026	95	0
1	J	3092	0	2996	76	0
1	K	3124	0	3025	100	0
1	L	2988	0	2880	188	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	C	4	0	6	2	0
3	I	8	0	12	0	0
3	J	4	0	6	1	0
3	L	4	0	6	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	J	1	0	0	0	0
All	All	37131	0	35951	1494	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1494) 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:A:253:MSE:HG2	1:A:277:PHE:CE2	1.42	1.53
1:J:108:LEU:HD21	1:J:302:GLY:C	1.33	1.52
1:C:138:ILE:CD1	1:C:150:PHE:HB3	1.45	1.47
1:G:24:ILE:CG2	1:G:37:PRO:HD3	1.42	1.47
1:A:253:MSE:CG	1:A:277:PHE:CE2	2.03	1.40
1:A:276:ASP:HB2	1:A:278:THR:CG2	1.48	1.39
1:L:21:PRO:CG	1:L:87:LEU:CD2	2.03	1.37
1:J:108:LEU:HD21	1:J:302:GLY:CA	1.54	1.34
1:C:138:ILE:HD11	1:C:150:PHE:CB	1.55	1.34
1:A:276:ASP:CB	1:A:278:THR:HG23	1.58	1.33
1:C:35:LEU:HD22	1:C:63:TRP:CZ3	1.62	1.32
1:G:18:GLN:HA	1:G:19:ALA:CB	1.59	1.30
1:C:85:THR:HG22	1:C:86:PRO:CD	1.60	1.30
1:H:130:GLU:OE1	1:H:158:THR:HG23	1.30	1.30
1:G:24:ILE:CG2	1:G:37:PRO:CD	2.11	1.27
1:D:206:LEU:O	1:D:208:LEU:CD1	1.81	1.27
1:L:21:PRO:CB	1:L:87:LEU:HD21	1.63	1.25
1:C:35:LEU:HA	1:C:62:GLY:O	1.37	1.24
1:F:130:GLU:OE2	1:F:157:ARG:HB2	1.32	1.24
1:L:16:PRO:HB2	1:L:25:PHE:O	1.34	1.24
1:D:83:ALA:HB1	1:D:84:ALA:CA	1.68	1.23
1:G:24:ILE:HG22	1:G:37:PRO:CD	1.69	1.23
1:J:108:LEU:CD1	1:J:302:GLY:HA3	1.65	1.23
1:F:78:VAL:HG23	1:F:88:LEU:CD1	1.68	1.21
1:B:92:LEU:HD23	1:B:92:LEU:O	1.36	1.21
1:L:133:MSE:CE	1:L:137:ILE:HB	1.72	1.20
1:F:282:PRO:HD2	1:F:285:GLU:OE2	1.43	1.19
1:G:18:GLN:O	1:G:25:PHE:HB3	1.40	1.17
1:G:32:ALA:O	1:G:33:ARG:HD3	1.43	1.17
1:K:394:GLY:HA2	1:K:395:VAL:HG22	1.27	1.16
1:L:21:PRO:HG2	1:L:87:LEU:CD2	1.70	1.16
1:J:108:LEU:CD2	1:J:302:GLY:CA	2.23	1.15
1:F:87:LEU:N	1:F:87:LEU:HD12	1.62	1.14
1:I:317:ILE:HA	1:I:333:VAL:HG23	1.16	1.14
1:G:133:MSE:HE3	1:G:137:ILE:HB	1.19	1.14
1:L:21:PRO:CG	1:L:87:LEU:HD21	1.71	1.14
1:A:76:ILE:HD12	1:A:90:GLU:O	1.44	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:VAL:CG2	1:F:88:LEU:CD1	2.25	1.13
1:F:108:LEU:HD21	1:F:302:GLY:HA3	1.20	1.13
1:I:24:ILE:HD12	1:I:37:PRO:HD3	1.29	1.13
1:A:276:ASP:HA	1:A:277:PHE:HB2	1.14	1.12
1:C:75:ARG:HG3	1:C:91:THR:HG22	1.23	1.13
1:D:83:ALA:CB	1:D:84:ALA:HA	1.64	1.12
1:J:108:LEU:HD11	1:J:302:GLY:HA3	1.19	1.12
1:L:21:PRO:HB2	1:L:87:LEU:HD21	1.18	1.12
1:A:253:MSE:CG	1:A:277:PHE:CD2	2.32	1.11
1:D:206:LEU:O	1:D:208:LEU:HD12	1.45	1.11
1:C:17:THR:CG2	1:C:160:ALA:HB1	1.81	1.10
1:K:78:VAL:HG22	1:K:88:LEU:HB2	1.19	1.10
1:L:251:ARG:HG2	1:L:253:MSE:HE1	1.18	1.10
1:F:122:GLN:HB2	1:F:129:LEU:HD23	1.34	1.09
1:J:108:LEU:CD2	1:J:302:GLY:HA3	1.80	1.09
1:C:17:THR:HG21	1:C:160:ALA:HB1	1.25	1.08
1:G:22:GLU:HG2	1:G:24:ILE:HD12	1.35	1.07
1:G:24:ILE:HB	1:G:35:LEU:O	1.53	1.07
1:F:281:LEU:HB3	1:F:285:GLU:OE2	1.54	1.07
1:G:32:ALA:O	1:G:33:ARG:CD	2.02	1.07
1:J:108:LEU:CD2	1:J:302:GLY:C	2.27	1.07
1:G:32:ALA:O	1:G:33:ARG:CG	2.02	1.06
1:F:26:TYR:HA	1:F:34:VAL:HA	1.11	1.06
1:L:322:LEU:HD23	1:L:344:ASP:OD2	1.54	1.06
1:A:78:VAL:HG22	1:A:88:LEU:HB3	1.36	1.06
1:A:276:ASP:CG	1:A:278:THR:HG23	1.79	1.06
1:J:108:LEU:HD13	1:J:109:GLY:H	1.13	1.06
1:G:18:GLN:HA	1:G:19:ALA:HB3	1.30	1.06
1:I:24:ILE:CD1	1:I:37:PRO:HD3	1.84	1.05
1:F:108:LEU:CD2	1:F:302:GLY:HA3	1.83	1.05
1:A:253:MSE:CG	1:A:277:PHE:HE2	1.51	1.05
1:G:18:GLN:CA	1:G:19:ALA:HB3	1.86	1.04
1:F:87:LEU:H	1:F:87:LEU:CD1	1.67	1.04
1:G:18:GLN:HA	1:G:19:ALA:HB2	1.36	1.04
1:F:17:THR:OG1	1:F:18:GLN:NE2	1.90	1.03
1:E:22:GLU:OE2	1:E:22:GLU:HA	1.58	1.03
1:F:78:VAL:HG23	1:F:88:LEU:HD13	1.35	1.03
1:F:79:PHE:CE1	1:F:86:PRO:HB3	1.93	1.03
1:A:253:MSE:HG3	1:A:277:PHE:CE2	1.89	1.03
1:B:21:PRO:HD3	1:B:88:LEU:HD12	1.36	1.03
1:A:83:ALA:C	1:A:85:THR:N	2.17	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:THR:CG2	1:C:86:PRO:CD	2.37	1.02
1:I:317:ILE:HA	1:I:333:VAL:CG2	1.87	1.02
1:H:145:TYR:HB3	1:H:148:ILE:HD11	1.41	1.02
1:A:76:ILE:HD12	1:A:76:ILE:H	1.22	1.02
1:G:18:GLN:CA	1:G:19:ALA:CB	2.36	1.02
1:L:21:PRO:HG2	1:L:87:LEU:HD22	1.39	1.02
1:F:87:LEU:HD12	1:F:87:LEU:H	0.86	1.01
1:G:22:GLU:CG	1:G:24:ILE:HD12	1.89	1.01
1:K:40:LYS:HD3	1:K:60:ASP:OD1	1.59	1.01
1:A:276:ASP:HB2	1:A:278:THR:HG23	1.02	1.00
1:C:85:THR:CG2	1:C:86:PRO:HD2	1.90	1.00
1:F:79:PHE:CZ	1:F:86:PRO:HG3	1.95	1.00
1:C:10:ILE:HG23	1:C:11:THR:H	1.23	1.00
1:D:78:VAL:HG22	1:D:88:LEU:HB3	1.39	1.00
1:G:18:GLN:O	1:G:25:PHE:CB	2.08	1.00
1:L:21:PRO:HG3	1:L:87:LEU:HD23	1.43	1.00
1:C:38:GLU:OE1	1:C:39:GLY:N	1.95	0.99
1:L:233:ASN:H	1:L:371:THR:HB	1.24	0.99
1:B:34:VAL:HG12	1:B:64:VAL:CG2	1.91	0.99
1:L:18:GLN:O	1:L:25:PHE:C	2.06	0.99
1:F:78:VAL:HG23	1:F:88:LEU:HD12	1.42	0.99
1:L:21:PRO:HG3	1:L:87:LEU:CD2	1.91	0.99
1:L:19:ALA:HA	1:L:25:PHE:HA	1.42	0.98
1:D:277:PHE:O	1:D:286:ARG:NH2	1.96	0.98
1:C:85:THR:HG22	1:C:86:PRO:HD2	1.01	0.98
1:G:23:ASN:O	1:G:25:PHE:CE1	2.16	0.97
1:K:10:ILE:O	1:K:166:ARG:NH1	1.97	0.97
1:A:253:MSE:HG2	1:A:277:PHE:CD2	1.99	0.97
1:J:108:LEU:CG	1:J:302:GLY:HA3	1.93	0.97
1:G:24:ILE:CG2	1:G:36:LEU:HA	1.94	0.97
1:L:322:LEU:HD23	1:L:344:ASP:CG	1.90	0.97
1:G:34:VAL:CG2	1:G:64:VAL:CG1	2.42	0.97
1:A:133:MSE:CE	1:A:137:ILE:CG2	2.42	0.97
1:B:34:VAL:CG1	1:B:64:VAL:CG2	2.43	0.96
1:E:35:LEU:HA	1:E:62:GLY:O	1.64	0.96
1:L:231:TYR:O	1:L:371:THR:HG21	1.65	0.96
1:F:79:PHE:CZ	1:F:86:PRO:CG	2.47	0.95
1:J:108:LEU:HD21	1:J:302:GLY:HA3	1.38	0.95
1:C:10:ILE:O	1:C:166:ARG:NH1	1.99	0.95
1:J:108:LEU:HD11	1:J:302:GLY:CA	1.95	0.95
1:A:276:ASP:OD2	1:A:278:THR:HG23	1.64	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LYS:HE3	1:C:60:ASP:OD1	1.66	0.95
1:A:276:ASP:CA	1:A:277:PHE:HB2	1.94	0.95
1:C:16:PRO:CG	1:C:35:LEU:HD21	1.97	0.95
1:E:21:PRO:O	1:E:24:ILE:CD1	2.15	0.95
1:F:122:GLN:CB	1:F:129:LEU:HD23	1.96	0.95
1:L:94:LEU:HD12	1:L:125:HIS:CD2	2.01	0.94
1:L:314:VAL:O	1:L:329:THR:HG21	1.65	0.94
1:A:276:ASP:HA	1:A:277:PHE:CB	1.91	0.94
1:I:20:GLY:HA3	1:I:24:ILE:CG2	1.97	0.94
1:L:22:GLU:C	1:L:22:GLU:CD	2.32	0.94
1:I:317:ILE:HG12	1:I:333:VAL:HG21	1.47	0.94
1:G:80:ARG:HG3	1:G:80:ARG:HH11	1.32	0.94
1:L:322:LEU:CD2	1:L:344:ASP:OD2	2.14	0.94
1:J:108:LEU:HD13	1:J:109:GLY:N	1.82	0.94
1:A:253:MSE:HE2	1:A:253:MSE:N	1.81	0.93
1:G:133:MSE:HE3	1:G:137:ILE:CB	1.98	0.93
1:C:35:LEU:CD2	1:C:63:TRP:CZ3	2.50	0.93
1:C:16:PRO:CD	1:C:35:LEU:HD21	1.99	0.93
1:A:253:MSE:HG3	1:A:277:PHE:CD2	2.01	0.93
1:E:130:GLU:OE1	1:E:158:THR:HG23	1.69	0.93
1:F:26:TYR:CA	1:F:34:VAL:HA	1.98	0.93
1:L:16:PRO:HB3	1:L:27:ASP:CB	1.99	0.93
1:H:145:TYR:CB	1:H:148:ILE:HD11	1.98	0.92
1:B:29:ASN:O	1:B:164:THR:HB	1.69	0.92
1:F:78:VAL:CG2	1:F:88:LEU:HD12	1.93	0.92
1:C:93:LYS:HE3	1:C:93:LYS:HA	1.49	0.92
1:B:218:TYR:HB2	1:B:253:MSE:HE1	1.51	0.91
1:G:29:ASN:O	1:G:164:THR:HB	1.70	0.91
1:J:10:ILE:O	1:J:166:ARG:NH1	2.03	0.91
1:A:76:ILE:CD1	1:A:90:GLU:O	2.18	0.91
1:C:33:ARG:HG2	1:C:65:THR:HG22	1.50	0.91
1:I:20:GLY:N	1:I:24:ILE:O	2.03	0.91
1:L:133:MSE:CE	1:L:137:ILE:CB	2.49	0.91
1:E:18:GLN:OE1	1:E:97:ARG:NH2	2.04	0.91
1:E:19:ALA:HB1	1:E:20:GLY:HA3	1.51	0.91
1:F:122:GLN:HB3	1:F:129:LEU:CD2	2.01	0.91
1:I:20:GLY:HA3	1:I:24:ILE:HG22	1.51	0.90
1:E:35:LEU:HD23	1:E:62:GLY:C	1.97	0.90
1:A:363:ASN:H	1:A:367:GLN:NE2	1.70	0.90
1:I:24:ILE:CD1	1:I:37:PRO:CD	2.50	0.89
1:K:78:VAL:CG2	1:K:88:LEU:HB2	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLN:HE21	1:A:81:GLN:N	1.70	0.89
1:C:27:ASP:OD2	1:C:33:ARG:NH2	2.05	0.89
1:L:133:MSE:HE2	1:L:137:ILE:HB	1.55	0.89
1:C:252:VAL:C	1:C:253:MSE:HE3	1.98	0.89
1:F:79:PHE:CZ	1:F:86:PRO:HB3	2.07	0.89
1:G:18:GLN:O	1:G:25:PHE:CA	2.21	0.89
1:G:218:TYR:HB2	1:G:253:MSE:HE3	1.53	0.89
1:G:34:VAL:CG2	1:G:64:VAL:HG12	2.03	0.89
1:G:224:GLN:NE2	1:G:231:TYR:OH	2.06	0.88
1:D:206:LEU:O	1:D:208:LEU:HD13	1.73	0.88
1:G:34:VAL:HG22	1:G:64:VAL:HG13	1.55	0.88
1:L:100:LEU:HG	1:L:130:GLU:OE2	1.72	0.88
1:B:45:LEU:HD21	1:B:55:PHE:HB3	1.55	0.88
1:F:122:GLN:CB	1:F:129:LEU:CD2	2.51	0.88
1:F:73:ARG:HA	1:F:92:LEU:CD2	2.03	0.88
1:F:251:ARG:HB3	1:F:253:MSE:HE1	1.53	0.88
1:A:218:TYR:HB2	1:A:253:MSE:HE1	1.55	0.88
1:B:92:LEU:HD23	1:B:92:LEU:C	1.98	0.88
1:E:35:LEU:HD23	1:E:62:GLY:O	1.73	0.87
1:G:24:ILE:CG2	1:G:37:PRO:HD2	2.04	0.87
1:F:114:TRP:HZ2	1:F:169:LEU:HD13	1.37	0.87
1:H:21:PRO:HG2	1:H:87:LEU:CD2	2.04	0.87
1:L:18:GLN:O	1:L:25:PHE:HA	1.75	0.87
1:J:218:TYR:HB2	1:J:253:MSE:HE3	1.57	0.87
1:A:276:ASP:CB	1:A:278:THR:CG2	2.30	0.87
1:L:149:GLN:OE1	1:L:157:ARG:NH2	2.08	0.87
1:D:88:LEU:HD12	1:D:89:ASP:N	1.88	0.87
1:I:141:LEU:CD2	1:I:204:VAL:HG11	2.04	0.87
1:D:144:GLN:HE21	1:D:207:ASP:HB2	1.40	0.87
1:G:24:ILE:HG22	1:G:37:PRO:HD3	0.87	0.87
1:L:322:LEU:HD21	1:L:344:ASP:HB2	1.57	0.87
1:B:17:THR:C	1:B:18:GLN:OE1	2.19	0.86
1:F:81:GLN:H	1:F:81:GLN:HE21	1.17	0.86
1:A:276:ASP:HB2	1:A:278:THR:HG22	1.52	0.86
1:D:144:GLN:NE2	1:D:207:ASP:HB2	1.90	0.86
1:A:100:LEU:HB3	1:A:164:THR:HG22	1.58	0.86
1:C:75:ARG:CG	1:C:91:THR:HG22	2.04	0.86
1:B:34:VAL:CG1	1:B:64:VAL:HG22	2.05	0.86
1:G:24:ILE:HG23	1:G:37:PRO:HD3	1.54	0.86
1:I:149:GLN:OE1	1:I:157:ARG:HD3	1.75	0.86
1:F:42:HIS:O	1:F:79:PHE:N	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:HG3	1:A:91:THR:HG22	1.56	0.86
1:I:24:ILE:HD11	1:I:36:LEU:HA	1.58	0.86
1:G:27:ASP:O	1:G:32:ALA:HA	1.76	0.85
1:H:251:ARG:HB3	1:H:253:MSE:HE1	1.57	0.85
1:F:108:LEU:HD23	1:F:109:GLY:N	1.91	0.85
1:G:34:VAL:HG22	1:G:64:VAL:CG1	2.03	0.85
1:H:253:MSE:CG	1:H:277:PHE:CE1	2.60	0.85
1:L:251:ARG:CG	1:L:253:MSE:HE1	2.06	0.85
1:I:29:ASN:OD1	1:I:164:THR:OG1	1.93	0.85
1:L:41:TRP:N	1:L:41:TRP:CD1	2.44	0.85
1:C:36:LEU:HD21	1:C:61:LYS:O	1.76	0.85
1:C:40:LYS:CE	1:C:60:ASP:OD1	2.25	0.85
1:E:19:ALA:HB1	1:E:20:GLY:CA	2.07	0.85
1:H:145:TYR:HB3	1:H:148:ILE:CD1	2.06	0.84
1:D:254:CYS:SG	1:D:256:ASP:OD1	2.35	0.84
1:G:32:ALA:O	1:G:33:ARG:HG3	1.77	0.84
1:I:27:ASP:CG	1:I:29:ASN:HD22	1.85	0.84
1:K:218:TYR:HB2	1:K:253:MSE:HE3	1.60	0.84
1:L:133:MSE:HE1	1:L:137:ILE:CG2	2.07	0.84
1:E:49:ASP:OD1	1:E:73:ARG:NH1	2.09	0.83
1:H:277:PHE:O	1:H:286:ARG:NH2	2.11	0.83
1:G:388:ARG:HG2	1:G:388:ARG:HH11	1.42	0.83
1:G:18:GLN:CB	1:G:19:ALA:HB3	2.07	0.83
1:D:87:LEU:HD12	1:D:87:LEU:O	1.78	0.83
1:D:251:ARG:HB3	1:D:253:MSE:HE1	1.60	0.83
1:G:284:GLN:HA	1:G:287:VAL:HG12	1.59	0.83
1:B:277:PHE:O	1:B:286:ARG:NH2	2.11	0.83
1:J:155:LYS:HG3	1:J:155:LYS:O	1.76	0.83
1:L:218:TYR:HB2	1:L:253:MSE:HE3	1.58	0.83
1:B:19:ALA:O	1:B:25:PHE:N	2.12	0.83
1:B:253:MSE:N	1:B:253:MSE:HE2	1.94	0.83
1:F:43:VAL:HG12	1:F:78:VAL:HG13	1.59	0.83
1:I:218:TYR:HB2	1:I:253:MSE:HE3	1.60	0.83
1:D:291:ARG:HH11	1:D:292:HIS:CE1	1.95	0.82
1:I:141:LEU:HD22	1:I:204:VAL:HG11	1.60	0.82
1:F:282:PRO:CD	1:F:285:GLU:OE2	2.25	0.82
1:G:389:SER:OG	1:G:398:THR:HG22	1.79	0.82
1:B:21:PRO:HD3	1:B:88:LEU:CD1	2.10	0.82
1:B:34:VAL:HG13	1:B:64:VAL:HG22	1.61	0.82
1:B:45:LEU:H	1:B:45:LEU:HD22	1.43	0.82
1:F:13:PRO:O	1:F:14:ASP:HB3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:GLU:OE1	1:H:158:THR:CG2	2.23	0.81
1:L:284:GLN:O	1:L:287:VAL:HG12	1.80	0.81
1:H:253:MSE:HG3	1:H:277:PHE:CE1	2.14	0.81
1:L:133:MSE:HE1	1:L:137:ILE:HG22	1.62	0.81
1:B:130:GLU:HB2	1:B:149:GLN:HE21	1.44	0.81
1:L:16:PRO:HB3	1:L:27:ASP:HB2	1.62	0.81
1:F:218:TYR:HB2	1:F:253:MSE:HE3	1.63	0.81
1:A:270:ILE:CD1	1:A:276:ASP:HB3	2.11	0.81
1:F:79:PHE:CE1	1:F:86:PRO:CB	2.63	0.81
1:D:46:LEU:CD2	1:D:53:ILE:HD13	2.11	0.80
1:F:79:PHE:CZ	1:F:86:PRO:CB	2.64	0.80
1:E:61:LYS:HG2	1:E:62:GLY:N	1.94	0.80
1:F:78:VAL:HG21	1:F:88:LEU:CD1	2.09	0.80
1:F:79:PHE:CD1	1:F:86:PRO:HB3	2.16	0.80
1:G:25:PHE:CD1	1:G:25:PHE:N	2.48	0.80
1:F:73:ARG:HA	1:F:92:LEU:HD23	1.61	0.80
1:G:18:GLN:NE2	1:G:97:ARG:HH22	1.79	0.80
1:G:244:HIS:O	1:G:248:LEU:CD2	2.30	0.80
1:L:277:PHE:O	1:L:286:ARG:NH2	2.15	0.80
1:A:276:ASP:OD2	1:A:278:THR:CG2	2.30	0.80
1:C:35:LEU:N	1:C:35:LEU:HD23	1.97	0.80
1:G:251:ARG:HB3	1:G:253:MSE:HE1	1.64	0.80
1:C:35:LEU:HD22	1:C:63:TRP:CH2	2.16	0.80
1:L:133:MSE:CE	1:L:137:ILE:CG2	2.60	0.80
1:D:218:TYR:HB2	1:D:253:MSE:HE3	1.63	0.80
1:F:108:LEU:HD21	1:F:302:GLY:CA	2.10	0.80
1:G:36:LEU:HD12	1:G:36:LEU:H	1.45	0.80
1:B:27:ASP:CG	1:B:29:ASN:HD22	1.89	0.79
1:I:24:ILE:HD11	1:I:36:LEU:HD23	1.64	0.79
1:J:108:LEU:CD1	1:J:302:GLY:CA	2.53	0.79
1:J:251:ARG:HB3	1:J:253:MSE:HE1	1.65	0.79
1:I:281:LEU:HB2	1:I:282:PRO:HD2	1.64	0.79
1:F:81:GLN:H	1:F:81:GLN:NE2	1.79	0.79
1:J:108:LEU:HD21	1:J:302:GLY:O	1.82	0.79
1:L:251:ARG:HG2	1:L:253:MSE:CE	2.09	0.79
1:E:21:PRO:O	1:E:24:ILE:HG12	1.83	0.79
1:K:326:GLU:OE1	1:K:332:ARG:NH2	2.14	0.79
1:C:119:GLU:OE1	1:C:205:ARG:NH2	2.16	0.79
1:E:21:PRO:HG2	1:E:88:LEU:HG	1.65	0.78
1:L:18:GLN:O	1:L:25:PHE:CA	2.30	0.78
1:A:133:MSE:CE	1:A:137:ILE:HG22	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:130:GLU:OE2	1:L:130:GLU:O	2.01	0.78
1:G:39:GLY:O	1:G:41:TRP:NE1	2.17	0.78
1:B:88:LEU:CD2	1:B:90:GLU:HG2	2.14	0.78
1:B:221:ILE:O	1:B:255:ILE:HD13	1.83	0.78
1:B:21:PRO:O	1:B:24:ILE:HD12	1.83	0.78
1:G:24:ILE:HG22	1:G:36:LEU:HA	1.62	0.77
1:E:21:PRO:O	1:E:24:ILE:HD13	1.85	0.77
1:A:253:MSE:HE2	1:A:253:MSE:H	1.47	0.77
1:J:60:ASP:O	1:J:61:LYS:HG3	1.84	0.77
1:L:94:LEU:HD12	1:L:125:HIS:HD2	1.43	0.77
1:B:21:PRO:CD	1:B:88:LEU:HD12	2.14	0.77
1:E:326:GLU:OE1	1:E:332:ARG:NH2	2.17	0.77
1:L:28:PHE:CD2	1:L:92:LEU:HD12	2.19	0.77
1:G:22:GLU:HG2	1:G:24:ILE:CD1	2.14	0.77
1:H:253:MSE:HG2	1:H:277:PHE:CE1	2.19	0.77
1:I:251:ARG:HB3	1:I:253:MSE:HE1	1.67	0.77
1:K:205:ARG:HG2	1:K:205:ARG:HH11	1.49	0.77
1:F:78:VAL:CG2	1:F:88:LEU:HD13	2.04	0.76
1:A:252:VAL:O	1:A:275:GLU:HG3	1.85	0.76
1:B:64:VAL:HG23	1:B:64:VAL:O	1.86	0.76
1:F:94:LEU:O	1:F:97:ARG:HG3	1.85	0.76
1:H:21:PRO:HG2	1:H:87:LEU:HD21	1.66	0.76
1:C:10:ILE:HG23	1:C:11:THR:N	2.00	0.76
1:G:22:GLU:HG3	1:G:23:ASN:N	1.98	0.76
1:K:394:GLY:CA	1:K:395:VAL:HG22	2.12	0.76
1:C:277:PHE:O	1:C:286:ARG:NH2	2.18	0.76
1:G:24:ILE:HG21	1:G:36:LEU:HA	1.67	0.76
1:K:78:VAL:HG22	1:K:88:LEU:CB	2.11	0.76
1:L:322:LEU:HD22	1:L:322:LEU:H	1.51	0.76
1:D:124:LEU:HD23	1:D:125:HIS:NE2	2.01	0.76
1:J:49:ASP:OD1	1:J:73:ARG:NH1	2.19	0.76
1:K:394:GLY:O	1:K:397:ALA:HB2	1.86	0.76
1:H:49:ASP:OD1	1:H:73:ARG:NH1	2.18	0.75
1:D:65:THR:HG21	1:D:69:LYS:NZ	2.02	0.75
1:L:322:LEU:CD2	1:L:344:ASP:HB2	2.17	0.75
1:C:22:GLU:O	1:C:22:GLU:OE1	2.03	0.75
1:F:89:ASP:CG	1:F:89:ASP:O	2.30	0.75
1:L:284:GLN:O	1:L:287:VAL:CG1	2.34	0.75
1:B:45:LEU:HD22	1:B:45:LEU:N	2.01	0.75
1:L:22:GLU:C	1:L:22:GLU:OE2	2.30	0.75
1:L:72:VAL:HG13	1:L:74:PHE:CE2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:115:PHE:HZ	1:H:148:ILE:HD12	1.51	0.75
1:D:119:GLU:OE1	1:D:145:TYR:CE2	2.40	0.75
1:G:18:GLN:OE1	1:G:26:TYR:OH	2.05	0.75
1:L:75:ARG:HG2	1:L:91:THR:OG1	1.87	0.75
1:G:22:GLU:CG	1:G:24:ILE:CD1	2.65	0.74
1:I:396:GLU:O	1:I:398:THR:N	2.20	0.74
1:E:252:VAL:C	1:E:253:MSE:HE2	2.12	0.74
1:H:145:TYR:HB3	1:H:148:ILE:CG1	2.17	0.74
1:E:22:GLU:OE2	1:E:22:GLU:CA	2.36	0.74
1:C:135:GLN:NE2	1:C:138:ILE:HG21	2.02	0.74
1:F:94:LEU:HD23	1:F:162:TYR:CD2	2.22	0.74
1:L:114:TRP:HZ2	1:L:169:LEU:HD13	1.52	0.74
1:L:22:GLU:CD	1:L:22:GLU:O	2.30	0.74
1:L:100:LEU:HD12	1:L:158:THR:HG21	1.69	0.74
1:G:34:VAL:HG23	1:G:64:VAL:HG12	1.66	0.74
1:L:20:GLY:O	1:L:23:ASN:O	2.06	0.74
1:B:24:ILE:HD11	1:B:87:LEU:HD23	1.69	0.74
1:D:79:PHE:CE1	1:D:86:PRO:N	2.55	0.74
1:G:18:GLN:OE1	1:G:26:TYR:CZ	2.41	0.74
1:K:49:ASP:OD1	1:K:73:ARG:NH1	2.20	0.74
1:C:78:VAL:HG22	1:C:88:LEU:HB3	1.68	0.74
1:A:78:VAL:CG2	1:A:88:LEU:HB3	2.17	0.73
1:E:21:PRO:O	1:E:24:ILE:CG1	2.35	0.73
1:F:44:ARG:NH1	1:F:77:GLN:OE1	2.21	0.73
1:I:130:GLU:OE1	1:I:158:THR:OG1	2.06	0.73
1:K:284:GLN:O	1:K:287:VAL:CG2	2.36	0.73
1:G:24:ILE:HG23	1:G:37:PRO:CD	2.14	0.73
1:E:38:GLU:O	1:E:41:TRP:CZ2	2.40	0.73
1:F:17:THR:HG1	1:F:18:GLN:NE2	1.83	0.73
1:J:277:PHE:O	1:J:286:ARG:NH1	2.21	0.73
1:C:16:PRO:HG2	1:C:35:LEU:CD2	2.18	0.73
1:G:28:PHE:HA	1:G:32:ALA:HA	1.71	0.73
1:I:317:ILE:CG1	1:I:333:VAL:HG21	2.18	0.73
1:F:280:LYS:HE3	1:F:280:LYS:O	1.89	0.73
1:K:89:ASP:OD1	1:K:89:ASP:C	2.30	0.73
1:E:22:GLU:HB2	1:E:24:ILE:HD11	1.69	0.72
1:C:35:LEU:HD22	1:C:63:TRP:CE3	2.23	0.72
1:I:94:LEU:HD12	1:I:125:HIS:ND1	2.04	0.72
1:B:357:TRP:CZ2	1:B:359:PRO:HG3	2.24	0.72
1:D:65:THR:CG2	1:D:69:LYS:NZ	2.51	0.72
1:A:133:MSE:CE	1:A:137:ILE:HG21	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ASN:OD1	1:C:161:PRO:O	2.07	0.72
1:E:16:PRO:HD3	1:E:63:TRP:HH2	1.54	0.72
1:E:87:LEU:HD23	1:E:87:LEU:N	2.03	0.72
1:D:83:ALA:HB1	1:D:84:ALA:HA	0.80	0.72
1:E:251:ARG:HB3	1:E:253:MSE:HE1	1.70	0.72
1:B:357:TRP:CE2	1:B:359:PRO:HG3	2.25	0.72
1:B:34:VAL:HG12	1:B:64:VAL:HG23	1.72	0.71
1:C:92:LEU:C	1:C:92:LEU:HD23	2.14	0.71
1:K:394:GLY:HA2	1:K:395:VAL:CG2	2.14	0.71
1:C:253:MSE:HE2	1:C:275:GLU:HB2	1.72	0.71
1:F:87:LEU:N	1:F:87:LEU:CD1	2.38	0.71
1:G:284:GLN:HA	1:G:287:VAL:CG1	2.20	0.71
1:L:233:ASN:H	1:L:371:THR:CB	2.02	0.71
1:L:233:ASN:N	1:L:371:THR:HB	2.00	0.71
1:B:10:ILE:HG21	1:B:102:SER:OG	1.90	0.71
1:A:363:ASN:H	1:A:367:GLN:HE22	1.37	0.71
1:K:29:ASN:O	1:K:164:THR:HB	1.90	0.71
1:L:133:MSE:HE1	1:L:137:ILE:CB	2.20	0.71
1:A:133:MSE:HE2	1:A:137:ILE:HB	1.72	0.71
1:K:284:GLN:HA	1:K:287:VAL:HG22	1.71	0.71
1:H:145:TYR:CG	1:H:148:ILE:HD11	2.25	0.71
1:C:36:LEU:HD22	1:C:62:GLY:HA2	1.73	0.71
1:J:242:ILE:HG23	1:J:252:VAL:HG21	1.73	0.71
1:C:135:GLN:O	1:C:138:ILE:HG22	1.91	0.71
1:I:21:PRO:HG2	1:I:87:LEU:HD13	1.73	0.71
1:I:24:ILE:HD13	1:I:37:PRO:CD	2.21	0.71
1:J:39:GLY:O	1:J:60:ASP:HB3	1.90	0.71
1:L:16:PRO:CB	1:L:27:ASP:HB2	2.21	0.71
1:F:39:GLY:O	1:F:60:ASP:HA	1.91	0.70
1:G:22:GLU:HG3	1:G:24:ILE:HD12	1.71	0.70
1:B:10:ILE:CG2	1:B:102:SER:OG	2.39	0.70
1:I:49:ASP:OD1	1:I:73:ARG:NH1	2.24	0.70
1:C:114:TRP:HZ2	1:C:169:LEU:HD13	1.56	0.70
1:C:138:ILE:HD11	1:C:150:PHE:HB3	0.74	0.70
1:C:198:ASP:OD2	1:C:200:ARG:NH1	2.25	0.70
1:E:22:GLU:CB	1:E:24:ILE:CD1	2.70	0.70
1:K:26:TYR:OH	1:K:90:GLU:HG3	1.92	0.70
1:L:18:GLN:O	1:L:26:TYR:N	2.25	0.70
1:L:310:THR:CG2	1:L:310:THR:O	2.38	0.70
1:B:49:ASP:OD1	1:B:73:ARG:NH1	2.25	0.70
1:G:244:HIS:O	1:G:248:LEU:HD22	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:284:GLN:O	1:K:287:VAL:HG22	1.92	0.70
1:L:100:LEU:HG	1:L:130:GLU:CD	2.16	0.70
1:A:94:LEU:HD12	1:A:125:HIS:CG	2.27	0.70
1:B:72:VAL:HB	1:B:74:PHE:CE2	2.26	0.70
1:C:17:THR:HG22	1:C:160:ALA:HB1	1.71	0.70
1:C:135:GLN:NE2	1:C:138:ILE:CG2	2.55	0.70
1:A:81:GLN:HE21	1:A:81:GLN:CA	2.03	0.70
1:G:24:ILE:HG21	1:G:37:PRO:HD2	1.73	0.70
1:J:20:GLY:N	1:J:24:ILE:O	2.24	0.70
1:L:252:VAL:C	1:L:253:MSE:HE2	2.15	0.70
1:E:255:ILE:HB	1:E:286:ARG:HH21	1.56	0.69
1:F:91:THR:HG22	1:F:92:LEU:N	2.06	0.69
1:G:28:PHE:HA	1:G:32:ALA:H	1.57	0.69
1:L:24:ILE:HG22	1:L:25:PHE:N	2.07	0.69
1:L:133:MSE:HE1	1:L:137:ILE:HB	1.72	0.69
1:E:16:PRO:HD3	1:E:63:TRP:CH2	2.26	0.69
1:G:25:PHE:N	1:G:25:PHE:HD1	1.87	0.69
1:L:21:PRO:CB	1:L:87:LEU:CD2	2.47	0.69
1:B:222:ALA:HA	1:B:256:ASP:OD1	1.92	0.69
1:D:119:GLU:OE1	1:D:145:TYR:HE2	1.74	0.69
1:F:26:TYR:HB3	1:F:34:VAL:HG23	1.74	0.69
1:C:16:PRO:CG	1:C:35:LEU:CD2	2.70	0.69
1:F:49:ASP:OD1	1:F:73:ARG:NH1	2.25	0.69
1:B:30:ASP:OD1	1:B:31:GLY:N	2.24	0.69
1:F:108:LEU:HD23	1:F:109:GLY:H	1.57	0.69
1:G:18:GLN:O	1:G:25:PHE:HA	1.90	0.69
1:B:38:GLU:O	1:B:60:ASP:O	2.11	0.69
1:C:35:LEU:CA	1:C:62:GLY:O	2.30	0.69
1:G:36:LEU:HD12	1:G:36:LEU:N	2.07	0.69
1:L:41:TRP:N	1:L:41:TRP:HD1	1.89	0.69
1:C:138:ILE:CD1	1:C:150:PHE:CB	2.37	0.69
1:F:79:PHE:CE1	1:F:86:PRO:HG3	2.27	0.68
1:A:76:ILE:HD12	1:A:76:ILE:N	2.04	0.68
1:D:10:ILE:O	1:D:166:ARG:NH1	2.26	0.68
1:F:94:LEU:HD23	1:F:162:TYR:CE2	2.28	0.68
1:B:17:THR:HG21	1:B:161:PRO:O	1.94	0.68
1:E:394:GLY:O	1:E:395:VAL:HG22	1.93	0.68
1:K:40:LYS:CD	1:K:60:ASP:OD1	2.40	0.68
1:K:252:VAL:C	1:K:253:MSE:HE2	2.18	0.68
1:D:252:VAL:C	1:D:253:MSE:HE2	2.18	0.68
1:I:141:LEU:HD22	1:I:204:VAL:CG1	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:HD12	1:A:75:ARG:HD3	1.74	0.68
1:F:252:VAL:C	1:F:253:MSE:HE2	2.18	0.68
1:A:133:MSE:HE3	1:A:137:ILE:HG21	1.75	0.68
1:E:17:THR:HG21	1:E:161:PRO:O	1.94	0.68
1:F:73:ARG:HA	1:F:92:LEU:HD22	1.73	0.68
1:L:299:LEU:HB3	1:L:300:PRO:HD2	1.75	0.68
1:B:36:LEU:H	1:B:36:LEU:HD12	1.58	0.68
1:I:24:ILE:CD1	1:I:36:LEU:HA	2.24	0.68
1:K:75:ARG:HG3	1:K:91:THR:OG1	1.94	0.68
1:A:208:LEU:O	1:A:291:ARG:NH1	2.27	0.67
1:G:40:LYS:HE2	1:G:60:ASP:OD2	1.93	0.67
1:I:253:MSE:HB3	1:I:277:PHE:CD1	2.29	0.67
1:L:207:ASP:OD1	1:L:209:SER:OG	2.13	0.67
1:L:394:GLY:O	1:L:395:VAL:HG23	1.95	0.67
1:K:40:LYS:HB3	1:K:81:GLN:HG3	1.76	0.67
1:E:101:ILE:HG12	1:E:129:LEU:HD11	1.75	0.67
1:G:41:TRP:CD1	1:G:41:TRP:N	2.61	0.67
1:L:311:ARG:HG3	1:L:311:ARG:O	1.94	0.67
1:C:93:LYS:O	1:C:162:TYR:HE2	1.78	0.67
1:I:317:ILE:CA	1:I:333:VAL:CG2	2.68	0.67
1:A:35:LEU:HD12	1:A:62:GLY:O	1.95	0.67
1:C:253:MSE:HE1	1:C:275:GLU:CD	2.20	0.67
1:J:61:LYS:HD2	1:J:61:LYS:O	1.95	0.67
1:L:16:PRO:CA	1:L:27:ASP:HB2	2.24	0.67
1:A:94:LEU:HD12	1:A:125:HIS:ND1	2.10	0.67
1:D:79:PHE:CE1	1:D:85:THR:C	2.73	0.67
1:H:100:LEU:HD12	1:H:100:LEU:H	1.60	0.67
1:D:46:LEU:HD21	1:D:53:ILE:HD13	1.76	0.67
1:G:31:GLY:O	1:G:32:ALA:HB3	1.94	0.67
1:J:137:ILE:HG22	1:J:141:LEU:HD22	1.76	0.67
1:K:396:GLU:OE2	1:K:396:GLU:N	2.27	0.67
1:L:322:LEU:HD22	1:L:322:LEU:N	2.10	0.67
1:G:80:ARG:HG3	1:G:80:ARG:NH1	2.04	0.66
1:F:114:TRP:CZ2	1:F:169:LEU:HD13	2.27	0.66
1:E:29:ASN:O	1:E:33:ARG:HD3	1.95	0.66
1:I:326:GLU:OE1	1:I:332:ARG:NH1	2.28	0.66
1:D:80:ARG:O	1:D:83:ALA:N	2.29	0.66
1:J:39:GLY:O	1:J:60:ASP:CB	2.44	0.66
1:H:129:LEU:HD13	1:H:148:ILE:HG22	1.77	0.66
1:I:141:LEU:HD21	1:I:204:VAL:HG11	1.77	0.66
1:C:36:LEU:CD2	1:C:61:LYS:O	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:ALA:O	1:G:33:ARG:CB	2.43	0.66
1:A:133:MSE:HE2	1:A:137:ILE:CG2	2.24	0.66
1:F:392:GLU:O	1:F:393:GLN:HG2	1.95	0.66
1:L:322:LEU:CD2	1:L:344:ASP:CB	2.74	0.66
1:D:22:GLU:CG	1:D:87:LEU:HD21	2.25	0.66
1:F:281:LEU:CB	1:F:285:GLU:OE2	2.41	0.66
1:H:29:ASN:O	1:H:166:ARG:NH2	2.28	0.66
1:E:59:VAL:HG11	1:E:61:LYS:HE2	1.78	0.66
1:K:251:ARG:CB	1:K:253:MSE:HE1	2.25	0.65
1:G:284:GLN:CA	1:G:287:VAL:HG12	2.26	0.65
1:L:23:ASN:O	1:L:24:ILE:HB	1.97	0.65
1:L:75:ARG:NH1	1:L:77:GLN:OE1	2.29	0.65
1:L:329:THR:HG22	1:L:331:TRP:H	1.59	0.65
1:C:85:THR:CG2	1:C:86:PRO:HD3	2.24	0.65
1:J:252:VAL:C	1:J:253:MSE:HE2	2.21	0.65
1:D:10:ILE:HG21	1:D:102:SER:OG	1.96	0.65
1:I:291:ARG:HA	1:I:310:THR:CG2	2.26	0.65
1:A:253:MSE:HG3	1:A:277:PHE:HE2	1.42	0.65
1:K:78:VAL:HG23	1:K:87:LEU:HD12	1.79	0.65
1:B:21:PRO:HG2	1:B:24:ILE:HD13	1.77	0.65
1:G:24:ILE:HG21	1:G:37:PRO:CD	2.21	0.65
1:L:18:GLN:CB	1:L:26:TYR:O	2.44	0.65
1:C:299:LEU:HB3	1:C:300:PRO:HD2	1.79	0.65
1:E:21:PRO:CG	1:E:88:LEU:HG	2.27	0.65
1:G:279:GLY:O	1:G:286:ARG:NH2	2.25	0.65
1:D:22:GLU:HG3	1:D:87:LEU:HD21	1.78	0.64
1:E:24:ILE:HG22	1:E:36:LEU:HA	1.78	0.64
1:E:114:TRP:HZ2	1:E:169:LEU:HD13	1.62	0.64
1:G:252:VAL:C	1:G:253:MSE:HE2	2.21	0.64
1:L:16:PRO:HB3	1:L:27:ASP:HB3	1.78	0.64
1:F:122:GLN:HB3	1:F:129:LEU:HD21	1.80	0.64
1:G:133:MSE:HE1	1:G:137:ILE:HG22	1.78	0.64
1:K:40:LYS:NZ	1:K:60:ASP:OD2	2.30	0.64
1:F:90:GLU:HA	1:F:90:GLU:OE1	1.96	0.64
1:K:189:ARG:NH1	1:K:201:GLU:OE1	2.30	0.64
1:L:75:ARG:NH1	1:L:89:ASP:OD2	2.30	0.64
1:L:154:ASP:OD1	1:L:154:ASP:N	2.30	0.64
1:A:27:ASP:HB3	1:A:33:ARG:HG2	1.80	0.64
1:C:136:ASP:N	1:C:136:ASP:OD1	2.30	0.64
1:D:17:THR:OG1	1:D:160:ALA:HB1	1.98	0.64
1:L:27:ASP:OD1	1:L:28:PHE:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:189:ARG:NH1	1:I:201:GLU:OE1	2.30	0.64
1:B:22:GLU:O	1:B:23:ASN:CG	2.40	0.64
1:B:45:LEU:CD2	1:B:55:PHE:HB3	2.26	0.64
1:G:81:GLN:HA	1:G:81:GLN:HE21	1.63	0.64
1:L:149:GLN:HG3	1:L:157:ARG:HH21	1.62	0.64
1:A:133:MSE:HE3	1:A:137:ILE:CG2	2.26	0.63
1:A:326:GLU:OE1	1:A:332:ARG:NH1	2.31	0.63
1:E:281:LEU:HD22	1:E:286:ARG:NH1	2.11	0.63
1:B:92:LEU:O	1:B:92:LEU:CD2	2.30	0.63
1:G:23:ASN:O	1:G:25:PHE:CD1	2.52	0.63
1:K:189:ARG:NH2	1:K:324:ASN:O	2.31	0.63
1:G:28:PHE:HA	1:G:32:ALA:CA	2.26	0.63
1:H:189:ARG:NH2	1:H:324:ASN:O	2.32	0.63
1:B:88:LEU:HD22	1:B:90:GLU:HG2	1.79	0.63
1:F:91:THR:CG2	1:F:92:LEU:N	2.62	0.63
1:C:35:LEU:CD2	1:C:63:TRP:CH2	2.80	0.63
1:E:101:ILE:CG1	1:E:129:LEU:HD11	2.29	0.63
1:G:72:VAL:HG13	1:G:74:PHE:CE2	2.33	0.63
1:H:253:MSE:HE3	1:H:275:GLU:CD	2.23	0.63
1:L:18:GLN:HB2	1:L:26:TYR:O	1.98	0.63
1:D:41:TRP:N	1:D:81:GLN:NE2	2.47	0.63
1:D:206:LEU:C	1:D:208:LEU:HD12	2.24	0.63
1:L:284:GLN:C	1:L:287:VAL:HG12	2.23	0.63
1:D:78:VAL:CG2	1:D:88:LEU:HB3	2.24	0.63
1:F:34:VAL:HG22	1:F:35:LEU:HG	1.81	0.63
1:A:133:MSE:HE2	1:A:137:ILE:CB	2.29	0.62
1:B:36:LEU:HD12	1:B:36:LEU:N	2.13	0.62
1:H:253:MSE:CG	1:H:277:PHE:CD1	2.82	0.62
1:I:20:GLY:CA	1:I:24:ILE:HG22	2.27	0.62
1:D:101:ILE:HG13	1:D:129:LEU:HD11	1.80	0.62
1:I:20:GLY:HA3	1:I:24:ILE:HG23	1.77	0.62
1:B:253:MSE:HG3	1:B:277:PHE:CE1	2.34	0.62
1:E:136:ASP:OD1	1:E:136:ASP:N	2.31	0.62
1:F:28:PHE:CZ	1:F:92:LEU:CD1	2.82	0.62
1:F:40:LYS:O	1:F:81:GLN:NE2	2.33	0.62
1:G:28:PHE:HA	1:G:32:ALA:N	2.14	0.62
1:A:40:LYS:O	1:A:81:GLN:NE2	2.30	0.62
1:C:189:ARG:NE	3:C:502:EDO:O1	2.32	0.62
1:L:393:GLN:N	1:L:393:GLN:OE1	2.31	0.62
1:A:83:ALA:O	1:A:85:THR:N	2.32	0.62
1:G:18:GLN:HB3	1:G:19:ALA:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:GLU:HB3	1:E:24:ILE:CD1	2.29	0.62
1:I:189:ARG:NH2	1:I:324:ASN:O	2.32	0.62
1:L:133:MSE:HE3	1:L:137:ILE:HB	1.73	0.62
1:B:220:CYS:HB3	1:B:255:ILE:HD12	1.81	0.62
1:L:124:LEU:HD22	1:L:125:HIS:CE1	2.34	0.62
1:F:29:ASN:HD22	1:F:33:ARG:HH11	1.47	0.62
1:I:242:ILE:HG23	1:I:252:VAL:HG11	1.82	0.62
1:B:60:ASP:OD1	1:B:60:ASP:N	2.31	0.62
1:C:92:LEU:HD23	1:C:92:LEU:O	1.99	0.62
1:E:95:LYS:O	1:E:97:ARG:HG2	2.00	0.62
1:E:335:ASN:HB2	1:E:374:ILE:HD13	1.82	0.62
1:I:251:ARG:CB	1:I:253:MSE:HE1	2.30	0.62
1:B:85:THR:CG2	1:B:86:PRO:HD2	2.30	0.61
1:E:78:VAL:HG12	1:E:88:LEU:CB	2.30	0.61
1:K:394:GLY:HA3	1:K:395:VAL:C	2.24	0.61
1:J:251:ARG:CB	1:J:253:MSE:HE1	2.30	0.61
1:D:189:ARG:NH1	1:D:201:GLU:OE1	2.34	0.61
1:D:189:ARG:NH2	1:D:324:ASN:O	2.33	0.61
1:D:208:LEU:HD12	1:D:208:LEU:N	2.15	0.61
1:D:228:GLN:HG2	1:D:355:PHE:CE2	2.35	0.61
1:E:281:LEU:HD22	1:E:286:ARG:HH11	1.65	0.61
1:F:251:ARG:CB	1:F:253:MSE:HE1	2.30	0.61
1:A:133:MSE:CE	1:A:137:ILE:HB	2.29	0.61
1:G:16:PRO:HB3	1:G:27:ASP:HB2	1.81	0.61
1:G:284:GLN:O	1:G:287:VAL:CG1	2.48	0.61
1:K:299:LEU:HB3	1:K:300:PRO:HD2	1.82	0.61
1:L:326:GLU:OE1	1:L:332:ARG:NH2	2.33	0.61
1:A:253:MSE:CG	1:A:277:PHE:HD2	2.09	0.61
1:C:23:ASN:O	1:C:37:PRO:HD3	2.01	0.61
1:D:87:LEU:HD12	1:D:87:LEU:C	2.25	0.61
1:F:44:ARG:HG2	1:F:77:GLN:HB2	1.83	0.61
1:F:108:LEU:HD23	1:F:302:GLY:HA3	1.81	0.61
1:C:40:LYS:HE3	1:C:60:ASP:CG	2.24	0.61
1:A:75:ARG:CG	1:A:91:THR:HG22	2.27	0.61
1:F:37:PRO:HG2	1:F:38:GLU:H	1.66	0.61
1:G:188:HIS:HE1	1:G:325:SER:O	1.83	0.61
1:L:24:ILE:CG2	1:L:25:PHE:N	2.64	0.61
1:B:88:LEU:HD23	1:B:89:ASP:H	1.63	0.61
1:F:26:TYR:HB3	1:F:34:VAL:CG2	2.31	0.61
1:I:316:LEU:O	1:I:333:VAL:CG2	2.49	0.61
1:C:253:MSE:HE1	1:C:275:GLU:OE2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:ILE:HD13	1:I:37:PRO:HD2	1.81	0.61
1:B:253:MSE:HE2	1:B:253:MSE:H	1.63	0.60
1:D:65:THR:HG21	1:D:69:LYS:HZ1	1.66	0.60
1:J:89:ASP:CG	1:J:89:ASP:O	2.44	0.60
1:L:322:LEU:CD2	1:L:344:ASP:CG	2.66	0.60
1:F:190:SER:O	1:F:194:ILE:HG12	2.01	0.60
1:L:19:ALA:HB2	1:L:25:PHE:CE1	2.36	0.60
1:A:33:ARG:HB3	1:A:65:THR:HG23	1.83	0.60
1:F:252:VAL:HG23	1:F:252:VAL:O	2.00	0.60
1:H:189:ARG:NH1	1:H:201:GLU:OE1	2.34	0.60
1:I:16:PRO:HB3	1:I:27:ASP:HB2	1.83	0.60
1:D:79:PHE:CD1	1:D:85:THR:C	2.79	0.60
1:L:322:LEU:CD2	1:L:322:LEU:H	2.13	0.60
1:D:144:GLN:NE2	1:D:207:ASP:H	1.99	0.60
1:F:79:PHE:CE1	1:F:86:PRO:CG	2.85	0.60
1:K:284:GLN:C	1:K:287:VAL:HG22	2.26	0.60
1:G:18:GLN:HB2	1:G:26:TYR:O	2.02	0.60
1:B:18:GLN:O	1:B:25:PHE:HA	2.01	0.60
1:D:83:ALA:CB	1:D:84:ALA:CA	2.46	0.60
1:G:81:GLN:HE21	1:G:81:GLN:CA	2.15	0.60
1:H:23:ASN:O	1:H:37:PRO:HG3	2.02	0.60
1:K:284:GLN:NE2	1:K:287:VAL:HG21	2.17	0.60
1:D:46:LEU:HD23	1:D:53:ILE:HD13	1.84	0.59
1:F:130:GLU:OE2	1:F:157:ARG:CB	2.28	0.59
1:H:61:LYS:HG2	1:H:62:GLY:N	2.17	0.59
1:H:87:LEU:HD23	1:H:87:LEU:O	2.02	0.59
1:B:21:PRO:HG2	1:B:87:LEU:HD21	1.84	0.59
1:B:34:VAL:CG1	1:B:64:VAL:HG21	2.32	0.59
1:B:64:VAL:CG2	1:B:64:VAL:O	2.49	0.59
1:F:225:SER:OG	1:F:301:SER:OG	2.17	0.59
1:J:27:ASP:OD1	1:J:33:ARG:HG3	2.01	0.59
1:K:395:VAL:HG23	1:K:395:VAL:O	2.01	0.59
1:C:138:ILE:CG1	1:C:150:PHE:HB3	2.29	0.59
1:L:149:GLN:OE1	1:L:157:ARG:CZ	2.49	0.59
1:A:275:GLU:O	1:A:277:PHE:HB2	2.02	0.59
1:F:26:TYR:HB3	1:F:34:VAL:CB	2.31	0.59
1:A:27:ASP:OD2	1:A:33:ARG:NH1	2.36	0.59
1:H:101:ILE:HG12	1:H:129:LEU:HD21	1.84	0.59
1:I:252:VAL:C	1:I:253:MSE:HE2	2.27	0.59
1:B:27:ASP:OD2	1:B:29:ASN:ND2	2.32	0.59
1:G:24:ILE:CB	1:G:35:LEU:O	2.40	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:393:GLN:HB3	1:G:397:ALA:HB3	1.85	0.59
1:K:61:LYS:HG3	1:K:62:GLY:N	2.17	0.59
1:B:326:GLU:OE1	1:B:332:ARG:NH1	2.36	0.59
1:F:122:GLN:HB2	1:F:129:LEU:CD2	2.17	0.59
1:L:28:PHE:CE2	1:L:92:LEU:HA	2.38	0.59
1:A:253:MSE:CB	1:A:277:PHE:CD2	2.86	0.58
1:D:41:TRP:CA	1:D:81:GLN:HE21	2.15	0.58
1:A:46:LEU:HD22	1:A:53:ILE:HG13	1.85	0.58
1:A:133:MSE:CE	1:A:137:ILE:CB	2.81	0.58
1:A:152:THR:HG22	1:A:153:PRO:HD2	1.83	0.58
1:B:18:GLN:O	1:B:26:TYR:N	2.34	0.58
1:F:72:VAL:O	1:F:92:LEU:CD2	2.51	0.58
1:A:46:LEU:CD2	1:A:53:ILE:HG13	2.33	0.58
1:C:181:ASP:HB3	1:C:184:LYS:HD2	1.84	0.58
1:I:316:LEU:O	1:I:333:VAL:HG22	2.03	0.58
1:D:299:LEU:HB3	1:D:300:PRO:HD2	1.85	0.58
1:G:100:LEU:HD12	1:G:158:THR:HG21	1.84	0.58
1:B:18:GLN:OE1	1:B:18:GLN:N	2.36	0.58
1:C:36:LEU:N	1:C:36:LEU:HD13	2.18	0.58
1:D:20:GLY:N	1:D:24:ILE:O	2.36	0.58
1:H:325:SER:HB3	1:H:326:GLU:OE1	2.02	0.58
1:J:108:LEU:CD2	1:J:302:GLY:O	2.44	0.58
1:K:251:ARG:HB3	1:K:253:MSE:HE1	1.85	0.58
1:G:281:LEU:HB2	1:G:286:ARG:NH1	2.19	0.58
1:K:223:THR:N	1:K:256:ASP:OD2	2.34	0.58
1:I:18:GLN:O	1:I:25:PHE:HA	2.03	0.58
1:G:299:LEU:HB3	1:G:300:PRO:HD2	1.86	0.58
1:K:27:ASP:OD2	1:K:29:ASN:ND2	2.34	0.58
1:C:40:LYS:CD	1:C:60:ASP:OD1	2.51	0.58
1:H:88:LEU:C	1:H:88:LEU:HD23	2.29	0.58
1:J:145:TYR:HB3	1:J:148:ILE:HD13	1.85	0.58
1:A:76:ILE:H	1:A:76:ILE:CD1	2.02	0.57
1:C:93:LYS:O	1:C:162:TYR:CE2	2.56	0.57
1:L:133:MSE:HE3	1:L:137:ILE:CG2	2.34	0.57
1:G:119:GLU:OE2	1:G:205:ARG:NH2	2.36	0.57
1:L:324:ASN:HD22	1:L:324:ASN:H	1.50	0.57
1:G:16:PRO:HD3	1:G:63:TRP:CH2	2.40	0.57
1:K:40:LYS:N	1:K:80:ARG:HH12	2.02	0.57
1:A:253:MSE:HG3	1:A:277:PHE:HD2	1.66	0.57
1:B:17:THR:O	1:B:18:GLN:OE1	2.21	0.57
1:C:40:LYS:HD2	1:C:60:ASP:OD1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:ARG:CB	1:G:253:MSE:HE1	2.32	0.57
1:H:136:ASP:N	1:H:136:ASP:OD1	2.37	0.57
1:A:130:GLU:OE1	1:A:158:THR:OG1	2.20	0.57
1:A:363:ASN:N	1:A:367:GLN:NE2	2.47	0.57
1:B:184:LYS:HE3	1:F:322:LEU:HD11	1.86	0.57
1:B:299:LEU:HB3	1:B:300:PRO:HD2	1.86	0.57
1:L:21:PRO:O	1:L:22:GLU:C	2.47	0.57
1:F:79:PHE:CZ	1:F:86:PRO:CD	2.87	0.57
1:I:152:THR:HG22	1:I:153:PRO:HD2	1.87	0.57
1:C:16:PRO:HD3	1:C:35:LEU:HD21	1.83	0.57
1:G:22:GLU:HG3	1:G:24:ILE:CD1	2.33	0.57
1:G:244:HIS:O	1:G:248:LEU:HD23	2.03	0.57
1:B:38:GLU:HB2	1:B:41:TRP:HE1	1.70	0.57
1:G:22:GLU:CG	1:G:23:ASN:N	2.68	0.57
1:H:100:LEU:HD11	1:H:161:PRO:CG	2.34	0.57
1:L:18:GLN:HG2	1:L:26:TYR:CZ	2.39	0.57
1:F:77:GLN:HB3	1:F:79:PHE:HE1	1.69	0.57
1:F:115:PHE:HE2	1:F:145:TYR:CE2	2.22	0.57
1:G:388:ARG:HG2	1:G:388:ARG:NH1	2.12	0.57
1:D:95:LYS:O	1:D:97:ARG:HG2	2.05	0.56
1:E:10:ILE:HG22	1:E:166:ARG:NH1	2.19	0.56
1:E:35:LEU:CD2	1:E:62:GLY:CA	2.83	0.56
1:G:284:GLN:O	1:G:287:VAL:HG13	2.05	0.56
1:K:284:GLN:CA	1:K:287:VAL:HG22	2.34	0.56
1:L:310:THR:HG22	1:L:312:ILE:HG23	1.87	0.56
1:A:133:MSE:HE2	1:A:137:ILE:HG22	1.85	0.56
1:A:133:MSE:HE1	1:A:137:ILE:HG22	1.87	0.56
1:F:178:GLN:HA	1:F:194:ILE:HD13	1.87	0.56
1:G:222:ALA:HA	1:G:256:ASP:OD1	2.05	0.56
1:H:87:LEU:HD23	1:H:87:LEU:C	2.29	0.56
1:H:100:LEU:HD12	1:H:100:LEU:N	2.20	0.56
1:L:20:GLY:O	1:L:21:PRO:C	2.48	0.56
1:A:27:ASP:HB3	1:A:33:ARG:CG	2.35	0.56
1:A:76:ILE:HD13	1:A:90:GLU:HB3	1.87	0.56
1:D:88:LEU:HD12	1:D:88:LEU:C	2.28	0.56
1:G:99:VAL:HG21	1:G:127:CYS:SG	2.46	0.56
1:H:95:LYS:O	1:H:97:ARG:HG2	2.05	0.56
1:J:60:ASP:C	1:J:61:LYS:HG3	2.30	0.56
1:J:89:ASP:O	1:J:89:ASP:OD1	2.23	0.56
1:J:33:ARG:HB3	1:J:65:THR:HG22	1.86	0.56
1:J:228:GLN:HG2	1:J:355:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:251:ARG:HG3	1:L:275:GLU:OE1	2.05	0.56
1:A:14:ASP:O	1:A:63:TRP:HH2	1.88	0.56
1:A:16:PRO:HB3	1:A:27:ASP:HB2	1.88	0.56
1:B:24:ILE:CD1	1:B:87:LEU:HD23	2.35	0.56
1:D:253:MSE:HB3	1:D:277:PHE:CD1	2.41	0.56
1:G:27:ASP:O	1:G:32:ALA:CA	2.53	0.56
1:L:322:LEU:HD23	1:L:344:ASP:CB	2.35	0.56
1:E:22:GLU:O	1:E:24:ILE:HD13	2.05	0.56
1:G:24:ILE:N	1:G:24:ILE:HD13	2.21	0.56
1:J:108:LEU:HD11	1:J:302:GLY:N	2.20	0.56
1:A:299:LEU:HB3	1:A:300:PRO:HD2	1.87	0.56
1:B:136:ASP:OD1	1:B:136:ASP:N	2.36	0.56
1:G:80:ARG:HH11	1:G:80:ARG:CG	2.11	0.56
1:I:157:ARG:O	1:I:159:VAL:HG23	2.06	0.56
1:C:85:THR:HG22	1:C:86:PRO:N	2.19	0.56
1:C:90:GLU:OE2	1:C:90:GLU:HA	2.06	0.56
1:C:326:GLU:OE1	1:C:332:ARG:NH2	2.38	0.56
1:E:59:VAL:HG12	1:E:60:ASP:N	2.21	0.56
1:K:284:GLN:O	1:K:287:VAL:HG23	2.04	0.56
1:C:16:PRO:HG2	1:C:35:LEU:HD23	1.88	0.56
1:E:226:THR:OG1	1:E:230:LYS:NZ	2.34	0.56
1:A:79:PHE:CE1	1:A:86:PRO:HB3	2.41	0.56
1:C:17:THR:CG2	1:C:160:ALA:CB	2.72	0.56
1:F:28:PHE:CZ	1:F:92:LEU:HD13	2.41	0.56
1:F:30:ASP:HA	1:F:166:ARG:HH21	1.71	0.56
1:I:218:TYR:HB2	1:I:253:MSE:CE	2.35	0.56
1:E:367:GLN:O	1:E:372:ARG:NH2	2.39	0.55
1:G:284:GLN:C	1:G:287:VAL:HG12	2.30	0.55
1:I:317:ILE:CA	1:I:333:VAL:HG23	2.11	0.55
1:J:299:LEU:HB3	1:J:300:PRO:HD2	1.88	0.55
1:C:35:LEU:HD23	1:C:35:LEU:H	1.69	0.55
1:F:79:PHE:HZ	1:F:86:PRO:HG3	1.60	0.55
1:J:95:LYS:O	1:J:97:ARG:HG2	2.06	0.55
1:K:284:GLN:HA	1:K:287:VAL:CG2	2.35	0.55
1:D:41:TRP:CA	1:D:81:GLN:NE2	2.70	0.55
1:I:281:LEU:HB2	1:I:282:PRO:CD	2.33	0.55
1:I:299:LEU:HB3	1:I:300:PRO:HD2	1.89	0.55
1:B:27:ASP:HB2	1:B:29:ASN:ND2	2.22	0.55
1:C:33:ARG:CG	1:C:65:THR:HG22	2.29	0.55
1:C:138:ILE:HD12	1:C:150:PHE:HB3	1.72	0.55
1:H:100:LEU:HD13	1:H:164:THR:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:287:VAL:HG13	1:L:288:ASN:N	2.21	0.55
1:B:100:LEU:CD1	1:B:164:THR:HG23	2.37	0.55
1:C:10:ILE:CG2	1:C:11:THR:H	2.08	0.55
1:K:29:ASN:C	1:K:164:THR:HB	2.31	0.55
1:E:47:ASP:O	1:E:51:GLU:N	2.36	0.55
1:F:389:SER:O	1:F:392:GLU:O	2.25	0.55
1:I:158:THR:O	1:I:160:ALA:N	2.39	0.55
1:A:29:ASN:O	1:A:33:ARG:HD3	2.06	0.55
1:B:34:VAL:HG13	1:B:64:VAL:CG2	2.27	0.55
1:E:299:LEU:HB3	1:E:300:PRO:HD2	1.86	0.55
1:L:119:GLU:OE2	1:L:205:ARG:NH2	2.39	0.55
1:F:28:PHE:HZ	1:F:92:LEU:HD13	1.72	0.55
1:E:363:ASN:H	1:E:367:GLN:NE2	2.05	0.55
1:F:79:PHE:CE2	1:F:86:PRO:HB3	2.40	0.55
1:H:16:PRO:HB2	1:H:25:PHE:HB3	1.89	0.55
1:H:100:LEU:HD11	1:H:161:PRO:CB	2.36	0.55
1:L:22:GLU:OE2	1:L:22:GLU:CA	2.55	0.55
1:L:310:THR:O	1:L:310:THR:HG23	2.06	0.55
1:D:88:LEU:HD12	1:D:89:ASP:H	1.69	0.54
1:D:210:ALA:O	1:D:291:ARG:NH1	2.40	0.54
1:E:78:VAL:HG12	1:E:88:LEU:HB2	1.88	0.54
1:I:291:ARG:HA	1:I:310:THR:HG21	1.88	0.54
1:D:100:LEU:HB3	1:D:164:THR:HG23	1.88	0.54
1:F:78:VAL:HG21	1:F:88:LEU:HD11	1.90	0.54
1:K:137:ILE:HG22	1:K:141:LEU:HD22	1.90	0.54
1:L:252:VAL:CA	1:L:253:MSE:HE2	2.37	0.54
1:A:136:ASP:OD1	1:A:136:ASP:N	2.38	0.54
1:B:130:GLU:HB2	1:B:149:GLN:NE2	2.17	0.54
1:C:138:ILE:HD11	1:C:150:PHE:CA	2.31	0.54
1:D:251:ARG:CB	1:D:253:MSE:HE1	2.35	0.54
1:H:40:LYS:C	1:H:81:GLN:OE1	2.51	0.54
1:J:251:ARG:C	1:J:253:MSE:CE	2.80	0.54
1:C:92:LEU:O	1:C:93:LYS:HE3	2.07	0.54
1:F:394:GLY:O	1:F:395:VAL:C	2.50	0.54
1:A:181:ASP:HB3	1:A:184:LYS:HD2	1.90	0.54
1:F:45:LEU:HD23	1:F:55:PHE:HB3	1.90	0.54
1:G:25:PHE:HD1	1:G:25:PHE:H	1.54	0.54
1:H:129:LEU:HD13	1:H:148:ILE:CG2	2.37	0.54
1:I:136:ASP:OD1	1:I:136:ASP:N	2.36	0.54
1:L:42:HIS:NE2	1:L:56:CYS:SG	2.81	0.54
1:B:28:PHE:CE2	1:B:92:LEU:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:395:VAL:H	1:K:397:ALA:N	2.06	0.54
1:B:45:LEU:N	1:B:45:LEU:CD2	2.71	0.54
1:B:253:MSE:HG3	1:B:277:PHE:CD1	2.42	0.54
1:F:84:ALA:O	1:F:85:THR:HG22	2.07	0.54
1:D:101:ILE:CG1	1:D:129:LEU:HD11	2.38	0.54
1:E:26:TYR:CZ	1:E:90:GLU:HG2	2.43	0.54
1:F:94:LEU:O	1:F:95:LYS:C	2.49	0.54
1:G:158:THR:O	1:G:160:ALA:N	2.38	0.54
1:K:357:TRP:CE2	1:K:359:PRO:HD3	2.43	0.54
1:F:136:ASP:N	1:F:136:ASP:OD1	2.39	0.53
1:G:20:GLY:O	1:G:22:GLU:O	2.25	0.53
1:L:189:ARG:NH2	1:L:324:ASN:O	2.41	0.53
1:C:144:GLN:O	1:C:205:ARG:NH1	2.40	0.53
1:I:24:ILE:CD1	1:I:37:PRO:HD2	2.33	0.53
1:L:16:PRO:HA	1:L:27:ASP:HB2	1.90	0.53
1:F:26:TYR:HB3	1:F:34:VAL:HB	1.88	0.53
1:G:44:ARG:HB3	1:G:77:GLN:HB2	1.91	0.53
1:D:275:GLU:HB3	1:D:277:PHE:CE1	2.44	0.53
1:D:41:TRP:C	1:D:81:GLN:NE2	2.67	0.53
1:G:72:VAL:HG13	1:G:74:PHE:CZ	2.44	0.53
1:H:208:LEU:O	1:H:291:ARG:NE	2.36	0.53
1:I:158:THR:C	1:I:159:VAL:HG23	2.34	0.53
1:L:158:THR:HG23	1:L:159:VAL:N	2.23	0.53
1:E:22:GLU:C	1:E:24:ILE:HD13	2.34	0.53
1:I:60:ASP:N	1:I:60:ASP:OD1	2.41	0.53
1:E:26:TYR:OH	1:E:90:GLU:HG2	2.08	0.53
1:F:13:PRO:O	1:F:14:ASP:CB	2.52	0.53
1:J:189:ARG:HE	3:J:502:EDO:H21	1.73	0.53
1:K:95:LYS:O	1:K:97:ARG:HG2	2.09	0.53
1:K:252:VAL:CA	1:K:253:MSE:HE2	2.39	0.53
1:C:189:ARG:HE	3:C:502:EDO:HO1	1.56	0.53
1:F:300:PRO:HD3	1:F:318:SER:HB2	1.91	0.53
1:B:85:THR:HG22	1:B:86:PRO:HD2	1.90	0.53
1:F:357:TRP:CZ2	1:F:359:PRO:HG3	2.44	0.53
1:J:41:TRP:HD1	1:J:60:ASP:HA	1.74	0.53
1:L:368:PHE:O	1:L:372:ARG:HG3	2.08	0.53
1:B:24:ILE:HD11	1:B:87:LEU:CD2	2.38	0.53
1:C:161:PRO:O	1:C:162:TYR:C	2.52	0.53
1:E:40:LYS:HG2	1:E:60:ASP:OD1	2.09	0.53
1:F:326:GLU:OE1	1:F:332:ARG:NH2	2.42	0.53
1:H:253:MSE:HE2	1:H:275:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:227:CYS:SG	1:J:230:LYS:HG3	2.49	0.53
1:K:252:VAL:HG23	1:K:252:VAL:O	2.09	0.53
1:F:58:ASP:OD1	1:F:58:ASP:N	2.41	0.52
1:G:188:HIS:CE1	1:G:325:SER:O	2.62	0.52
1:L:22:GLU:O	1:L:22:GLU:CG	2.56	0.52
1:G:22:GLU:OE1	1:G:37:PRO:HG3	2.10	0.52
1:G:34:VAL:HG11	1:G:76:ILE:HG21	1.90	0.52
1:C:230:LYS:HE3	1:C:320:PHE:CZ	2.45	0.52
1:D:46:LEU:HD11	1:D:77:GLN:NE2	2.23	0.52
1:E:78:VAL:HG12	1:E:88:LEU:HB3	1.91	0.52
1:E:251:ARG:C	1:E:253:MSE:HE3	2.34	0.52
1:G:80:ARG:NH1	1:G:80:ARG:CG	2.71	0.52
1:L:75:ARG:CG	1:L:91:THR:OG1	2.57	0.52
1:A:255:ILE:HA	1:A:277:PHE:O	2.10	0.52
1:G:95:LYS:O	1:G:97:ARG:HG2	2.10	0.52
1:F:108:LEU:HD23	1:F:108:LEU:C	2.34	0.52
1:F:157:ARG:HG2	1:F:157:ARG:NH2	2.24	0.52
1:G:133:MSE:CE	1:G:137:ILE:HG22	2.39	0.52
1:C:95:LYS:O	1:C:97:ARG:HG3	2.09	0.52
1:G:18:GLN:C	1:G:25:PHE:HB3	2.29	0.52
1:I:251:ARG:C	1:I:253:MSE:CE	2.83	0.52
1:K:149:GLN:OE1	1:K:157:ARG:HD2	2.10	0.52
1:K:284:GLN:NE2	1:K:287:VAL:CG2	2.73	0.52
1:L:19:ALA:HB2	1:L:25:PHE:CZ	2.45	0.52
1:A:81:GLN:CA	1:A:81:GLN:NE2	2.69	0.52
1:B:95:LYS:O	1:B:97:ARG:HG2	2.09	0.52
1:E:24:ILE:HD13	1:E:24:ILE:H	1.75	0.52
1:H:72:VAL:HB	1:H:74:PHE:CE2	2.43	0.52
1:H:253:MSE:CE	1:H:275:GLU:CD	2.83	0.52
1:B:100:LEU:HD12	1:B:164:THR:HG23	1.91	0.52
1:C:17:THR:HG22	1:C:160:ALA:CB	2.39	0.52
1:E:38:GLU:O	1:E:41:TRP:HZ2	1.93	0.52
1:L:72:VAL:HG13	1:L:74:PHE:CZ	2.45	0.52
1:G:133:MSE:CE	1:G:137:ILE:CG2	2.87	0.52
1:L:130:GLU:OE2	1:L:130:GLU:C	2.53	0.52
1:B:218:TYR:HD2	1:B:253:MSE:HE3	1.75	0.52
1:C:16:PRO:HB3	1:C:27:ASP:HB2	1.92	0.52
1:E:300:PRO:HD3	1:E:318:SER:HB2	1.91	0.52
1:G:18:GLN:HE22	1:G:97:ARG:HH22	1.52	0.52
1:D:79:PHE:HE1	1:D:86:PRO:N	2.06	0.51
1:F:64:VAL:O	1:F:64:VAL:HG13	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:87:LEU:HD23	1:L:87:LEU:C	2.35	0.51
1:L:223:THR:HG22	1:L:238:TRP:CE2	2.45	0.51
1:E:29:ASN:O	1:E:33:ARG:CD	2.57	0.51
1:E:320:PHE:CE2	1:E:343:TRP:HB2	2.45	0.51
1:K:40:LYS:CB	1:K:81:GLN:HG3	2.40	0.51
1:L:100:LEU:HG	1:L:130:GLU:OE1	2.10	0.51
1:L:322:LEU:HD22	1:L:344:ASP:OD2	2.07	0.51
1:B:30:ASP:HB3	1:B:33:ARG:HD3	1.92	0.51
1:E:22:GLU:HB2	1:E:24:ILE:CD1	2.34	0.51
1:E:22:GLU:CB	1:E:24:ILE:HD13	2.40	0.51
1:F:26:TYR:CD1	1:F:26:TYR:N	2.79	0.51
1:H:44:ARG:NH1	1:H:77:GLN:OE1	2.42	0.51
1:H:299:LEU:HB3	1:H:300:PRO:HD2	1.92	0.51
1:F:299:LEU:HB3	1:F:300:PRO:HD2	1.92	0.51
1:G:16:PRO:HG2	1:G:25:PHE:O	2.11	0.51
1:D:41:TRP:HA	1:D:81:GLN:HE21	1.75	0.51
1:E:39:GLY:O	1:E:60:ASP:HB3	2.10	0.51
1:G:39:GLY:O	1:G:41:TRP:CD1	2.64	0.51
1:I:280:LYS:O	1:I:280:LYS:HG2	2.11	0.51
1:L:136:ASP:OD1	1:L:136:ASP:N	2.39	0.51
1:E:27:ASP:OD2	1:E:33:ARG:NH1	2.44	0.51
1:C:252:VAL:O	1:C:253:MSE:HE3	2.11	0.51
1:G:43:VAL:HG11	1:G:64:VAL:HG21	1.92	0.51
1:L:122:GLN:HG3	1:L:123:SER:N	2.24	0.51
1:B:21:PRO:HG2	1:B:87:LEU:CD2	2.41	0.51
1:F:74:PHE:H	1:F:92:LEU:HD22	1.76	0.51
1:G:133:MSE:HE3	1:G:137:ILE:CG2	2.39	0.51
1:K:29:ASN:HA	1:K:164:THR:N	2.26	0.51
1:D:291:ARG:O	1:D:292:HIS:HB2	2.10	0.51
1:D:331:TRP:HZ3	1:D:385:LYS:HG2	1.76	0.51
1:G:31:GLY:O	1:G:32:ALA:CB	2.59	0.51
1:G:158:THR:HG23	1:G:159:VAL:N	2.25	0.51
1:K:100:LEU:HB3	1:K:164:THR:HG23	1.93	0.51
1:L:284:GLN:HA	1:L:287:VAL:HG12	1.93	0.51
1:D:65:THR:HG22	1:D:69:LYS:HZ3	1.76	0.51
1:E:61:LYS:CG	1:E:62:GLY:N	2.72	0.51
1:H:43:VAL:HG11	1:H:64:VAL:HG21	1.92	0.51
1:H:79:PHE:CE1	1:H:85:THR:C	2.88	0.51
1:I:204:VAL:HG12	1:I:205:ARG:N	2.26	0.51
1:J:108:LEU:CD2	1:J:302:GLY:HA2	2.30	0.51
1:A:44:ARG:HG3	1:A:79:PHE:HE2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TYR:HB2	1:A:253:MSE:CE	2.36	0.50
1:C:35:LEU:HD13	1:C:63:TRP:CZ2	2.46	0.50
1:E:357:TRP:CZ2	1:E:359:PRO:HG3	2.46	0.50
1:G:24:ILE:CD1	1:G:24:ILE:N	2.74	0.50
1:G:34:VAL:CG1	1:G:76:ILE:HG21	2.41	0.50
1:G:252:VAL:CA	1:G:253:MSE:HE2	2.42	0.50
1:L:389:SER:O	1:L:393:GLN:O	2.29	0.50
1:C:93:LYS:HA	1:C:93:LYS:CE	2.20	0.50
1:K:388:ARG:O	1:K:392:GLU:HG3	2.11	0.50
1:A:46:LEU:CD2	1:A:53:ILE:CG1	2.89	0.50
1:A:46:LEU:HB2	1:A:75:ARG:HB3	1.94	0.50
1:I:291:ARG:HA	1:I:310:THR:HG22	1.93	0.50
1:A:88:LEU:HD12	1:A:89:ASP:N	2.26	0.50
1:B:19:ALA:O	1:B:24:ILE:N	2.45	0.50
1:F:85:THR:HG23	1:F:85:THR:O	2.11	0.50
1:G:284:GLN:O	1:G:287:VAL:HG12	2.11	0.50
1:L:18:GLN:CA	1:L:18:GLN:HE21	2.25	0.50
1:A:72:VAL:HB	1:A:74:PHE:CE2	2.46	0.50
1:A:357:TRP:CZ2	1:A:359:PRO:HG3	2.47	0.50
1:D:46:LEU:HB2	1:D:75:ARG:HB3	1.93	0.50
1:D:206:LEU:HD11	1:D:309:ALA:CB	2.41	0.50
1:E:142:ALA:HB3	1:E:143:PRO:HD3	1.92	0.50
1:F:252:VAL:HG23	1:F:274:ALA:HA	1.93	0.50
1:I:119:GLU:OE2	1:I:205:ARG:NH2	2.43	0.50
1:L:357:TRP:CZ2	1:L:359:PRO:HG3	2.46	0.50
1:A:276:ASP:OD1	1:A:276:ASP:O	2.30	0.50
1:K:159:VAL:HG12	1:K:159:VAL:O	2.12	0.50
1:D:251:ARG:C	1:D:253:MSE:CE	2.85	0.50
1:E:87:LEU:HD23	1:E:87:LEU:H	1.76	0.50
1:H:38:GLU:HG2	1:H:39:GLY:N	2.26	0.50
1:H:253:MSE:HG2	1:H:277:PHE:CD1	2.46	0.50
1:K:251:ARG:HB2	1:K:253:MSE:HE1	1.94	0.50
1:L:19:ALA:CA	1:L:25:PHE:HA	2.30	0.50
1:D:79:PHE:CE1	1:D:86:PRO:HD3	2.47	0.50
1:D:136:ASP:OD1	1:D:136:ASP:N	2.42	0.50
1:D:252:VAL:CA	1:D:253:MSE:HE2	2.42	0.50
1:I:27:ASP:OD2	1:I:29:ASN:ND2	2.40	0.50
1:A:270:ILE:HD12	1:A:276:ASP:HB3	1.90	0.50
1:D:18:GLN:HA	1:D:18:GLN:NE2	2.26	0.50
1:D:79:PHE:CE1	1:D:86:PRO:CD	2.95	0.50
1:D:175:THR:HG23	1:D:175:THR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:253:MSE:HG3	1:H:277:PHE:CD1	2.45	0.50
1:J:72:VAL:HB	1:J:74:PHE:CE2	2.47	0.50
1:K:90:GLU:OE1	1:K:90:GLU:HA	2.10	0.50
1:K:251:ARG:C	1:K:253:MSE:CE	2.85	0.50
1:K:395:VAL:N	1:K:397:ALA:N	2.60	0.50
1:A:36:LEU:HD11	1:A:59:VAL:CG1	2.41	0.49
1:C:138:ILE:CG1	1:C:150:PHE:CB	2.90	0.49
1:G:189:ARG:NH2	1:G:201:GLU:OE1	2.45	0.49
1:L:310:THR:O	1:L:310:THR:HG22	2.11	0.49
1:A:18:GLN:HB2	1:A:26:TYR:O	2.12	0.49
1:E:61:LYS:HG2	1:E:62:GLY:H	1.76	0.49
1:F:72:VAL:HB	1:F:74:PHE:CE2	2.47	0.49
1:G:256:ASP:OD1	1:G:256:ASP:N	2.45	0.49
1:L:20:GLY:O	1:L:21:PRO:O	2.30	0.49
1:L:23:ASN:O	1:L:24:ILE:CB	2.61	0.49
1:L:251:ARG:C	1:L:253:MSE:CE	2.85	0.49
1:C:131:CYS:HB3	1:C:133:MSE:CE	2.42	0.49
1:F:94:LEU:O	1:F:97:ARG:CG	2.57	0.49
1:F:115:PHE:N	1:F:116:PRO:CD	2.75	0.49
1:J:107:THR:OG1	1:J:108:LEU:HD12	2.12	0.49
1:K:26:TYR:CZ	1:K:90:GLU:HG3	2.47	0.49
1:D:82:GLY:O	1:D:83:ALA:HB3	2.13	0.49
1:I:252:VAL:CA	1:I:253:MSE:HE2	2.42	0.49
1:B:23:ASN:OD1	1:B:23:ASN:O	2.30	0.49
1:D:275:GLU:HB3	1:D:277:PHE:CD1	2.48	0.49
1:E:77:GLN:HA	1:E:88:LEU:O	2.13	0.49
1:G:300:PRO:HD3	1:G:318:SER:HB2	1.95	0.49
1:H:28:PHE:CD2	1:H:92:LEU:HD12	2.47	0.49
1:I:27:ASP:OD1	1:I:29:ASN:ND2	2.44	0.49
1:L:365:ASP:O	1:L:372:ARG:NH2	2.45	0.49
1:F:43:VAL:CG1	1:F:78:VAL:HG13	2.38	0.49
1:G:18:GLN:HE21	1:G:97:ARG:HH22	1.59	0.49
1:B:22:GLU:O	1:B:23:ASN:OD1	2.30	0.49
1:J:155:LYS:O	1:J:155:LYS:CG	2.55	0.49
1:K:136:ASP:OD1	1:K:136:ASP:N	2.38	0.49
1:K:230:LYS:HE3	1:K:320:PHE:CZ	2.48	0.49
1:B:223:THR:HG22	1:B:238:TRP:CE2	2.47	0.49
1:E:19:ALA:CB	1:E:20:GLY:CA	2.80	0.49
1:F:34:VAL:O	1:F:35:LEU:C	2.54	0.49
1:I:144:GLN:O	1:I:205:ARG:NH1	2.42	0.49
1:K:72:VAL:HB	1:K:74:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:THR:HG22	1:D:69:LYS:NZ	2.27	0.49
1:C:58:ASP:OD1	1:C:58:ASP:N	2.46	0.48
1:C:79:PHE:CE1	1:C:86:PRO:HB3	2.48	0.48
1:H:206:LEU:O	1:H:208:LEU:HD12	2.12	0.48
1:L:87:LEU:HD23	1:L:87:LEU:O	2.12	0.48
1:D:206:LEU:HD11	1:D:309:ALA:HB3	1.95	0.48
1:F:38:GLU:OE2	1:F:38:GLU:O	2.30	0.48
1:J:108:LEU:HD22	1:J:109:GLY:N	2.27	0.48
1:L:21:PRO:O	1:L:22:GLU:O	2.30	0.48
1:F:159:VAL:O	1:F:160:ALA:HB3	2.13	0.48
1:I:100:LEU:HB3	1:I:164:THR:HG23	1.94	0.48
1:K:205:ARG:HH11	1:K:205:ARG:CG	2.23	0.48
1:L:16:PRO:CB	1:L:27:ASP:CB	2.79	0.48
1:L:114:TRP:CZ2	1:L:169:LEU:HD13	2.42	0.48
1:B:19:ALA:C	1:B:25:PHE:H	2.16	0.48
1:B:357:TRP:CZ2	1:B:359:PRO:CG	2.95	0.48
1:D:208:LEU:CD1	1:D:208:LEU:N	2.76	0.48
1:F:12:PRO:O	1:F:13:PRO:C	2.56	0.48
1:F:14:ASP:O	1:F:14:ASP:CG	2.56	0.48
1:F:46:LEU:HB2	1:F:75:ARG:HB3	1.95	0.48
1:F:74:PHE:N	1:F:92:LEU:HD22	2.28	0.48
1:H:24:ILE:HG23	1:H:37:PRO:CD	2.44	0.48
1:J:18:GLN:HB2	1:J:26:TYR:O	2.14	0.48
1:L:24:ILE:HG22	1:L:25:PHE:H	1.76	0.48
1:A:133:MSE:HE1	1:A:137:ILE:CG2	2.37	0.48
1:A:366:ARG:O	1:A:369:GLU:HB2	2.14	0.48
1:H:87:LEU:CD2	1:H:87:LEU:C	2.87	0.48
1:J:252:VAL:CA	1:J:253:MSE:HE2	2.44	0.48
1:B:253:MSE:CG	1:B:277:PHE:CE1	2.96	0.48
1:C:149:GLN:OE1	1:C:157:ARG:HD3	2.14	0.48
1:C:357:TRP:CZ2	1:C:359:PRO:HG3	2.49	0.48
1:C:257:ARG:HD2	1:C:280:LYS:HD3	1.96	0.48
1:D:280:LYS:O	1:D:280:LYS:HG3	2.13	0.48
1:G:158:THR:O	1:G:159:VAL:HB	2.14	0.48
1:F:63:TRP:H	1:F:63:TRP:CD1	2.32	0.48
1:G:27:ASP:HB3	1:G:33:ARG:HE	1.79	0.48
1:I:10:ILE:HD11	1:I:102:SER:OG	2.14	0.48
1:L:95:LYS:O	1:L:97:ARG:HG2	2.14	0.48
1:G:179:PRO:HG2	1:G:193:TYR:HB3	1.96	0.48
1:C:340:TYR:CD1	1:C:340:TYR:C	2.91	0.47
1:B:43:VAL:HG11	1:B:64:VAL:HG11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:THR:HG23	1:B:86:PRO:HD2	1.95	0.47
1:E:14:ASP:O	1:E:63:TRP:HZ2	1.97	0.47
1:I:357:TRP:CZ2	1:I:359:PRO:HG3	2.49	0.47
1:J:357:TRP:CZ2	1:J:359:PRO:HG3	2.49	0.47
1:D:11:THR:HG22	1:D:12:PRO:O	2.15	0.47
1:E:47:ASP:HB3	1:E:50:SER:OG	2.14	0.47
1:F:144:GLN:NE2	1:F:207:ASP:HB2	2.29	0.47
1:G:108:LEU:HD11	1:G:283:LEU:HD22	1.97	0.47
1:L:22:GLU:O	1:L:23:ASN:C	2.57	0.47
1:C:35:LEU:CD2	1:C:35:LEU:N	2.73	0.47
1:C:85:THR:HG23	1:C:86:PRO:HD3	1.95	0.47
1:D:101:ILE:CD1	1:D:129:LEU:HD11	2.44	0.47
1:E:149:GLN:HE22	1:E:157:ARG:HD3	1.78	0.47
1:K:284:GLN:CD	1:K:287:VAL:HG21	2.40	0.47
1:D:83:ALA:HB1	1:D:84:ALA:CB	2.40	0.47
1:D:291:ARG:O	1:D:292:HIS:CB	2.62	0.47
1:F:157:ARG:HG2	1:F:157:ARG:HH21	1.78	0.47
1:F:252:VAL:CA	1:F:253:MSE:HE2	2.45	0.47
1:F:392:GLU:O	1:F:393:GLN:CG	2.61	0.47
1:G:218:TYR:HB2	1:G:253:MSE:CE	2.34	0.47
1:I:252:VAL:O	1:I:275:GLU:HG3	2.15	0.47
1:L:28:PHE:HE2	1:L:92:LEU:HA	1.79	0.47
1:F:160:ALA:N	1:F:161:PRO:HD3	2.29	0.47
1:I:316:LEU:O	1:I:333:VAL:HG23	2.15	0.47
1:J:230:LYS:HE3	1:J:320:PHE:CZ	2.49	0.47
1:L:133:MSE:HE3	1:L:137:ILE:HG21	1.96	0.47
1:L:158:THR:CG2	1:L:159:VAL:N	2.78	0.47
1:C:263:GLN:HG3	1:C:355:PHE:CB	2.45	0.47
1:D:65:THR:HG22	1:D:66:SER:O	2.14	0.47
1:D:79:PHE:HE1	1:D:85:THR:C	2.19	0.47
1:D:184:LYS:HZ3	1:L:184:LYS:HZ3	1.61	0.47
1:D:223:THR:HG22	1:D:238:TRP:CE2	2.50	0.47
1:F:79:PHE:CG	1:F:86:PRO:HB3	2.49	0.47
1:G:224:GLN:N	1:G:256:ASP:OD2	2.42	0.47
1:G:357:TRP:CZ2	1:G:359:PRO:HG3	2.49	0.47
1:J:85:THR:CG2	1:J:86:PRO:HD2	2.44	0.47
1:J:321:SER:HB2	1:J:325:SER:OG	2.15	0.47
1:K:80:ARG:HA	1:K:80:ARG:HD2	1.50	0.47
1:K:394:GLY:CA	1:K:395:VAL:CG2	2.85	0.47
1:B:38:GLU:HB2	1:B:41:TRP:NE1	2.28	0.47
1:D:72:VAL:HB	1:D:74:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:PHE:CE2	1:D:343:TRP:HB2	2.50	0.47
1:H:320:PHE:CE2	1:H:343:TRP:HB2	2.50	0.47
1:J:286:ARG:N	1:J:286:ARG:HD2	2.30	0.47
1:K:252:VAL:HG23	1:K:274:ALA:HA	1.97	0.47
1:L:29:ASN:O	1:L:30:ASP:CB	2.63	0.47
1:A:279:GLY:O	1:A:286:ARG:NH2	2.48	0.47
1:B:27:ASP:CG	1:B:29:ASN:ND2	2.66	0.47
1:B:115:PHE:HE2	1:B:145:TYR:CE2	2.33	0.47
1:C:66:SER:O	1:C:69:LYS:HE3	2.15	0.47
1:E:251:ARG:HB3	1:E:253:MSE:CE	2.40	0.47
1:E:252:VAL:C	1:E:253:MSE:CE	2.84	0.47
1:F:37:PRO:HG2	1:F:41:TRP:HE1	1.80	0.47
1:B:142:ALA:HB3	1:B:143:PRO:HD3	1.95	0.47
1:C:135:GLN:HE22	1:C:138:ILE:HG21	1.76	0.47
1:E:35:LEU:HD23	1:E:62:GLY:CA	2.45	0.47
1:B:88:LEU:HD23	1:B:89:ASP:N	2.30	0.46
1:B:124:LEU:HD23	1:B:125:HIS:CE1	2.50	0.46
1:E:328:TYR:HE2	1:E:399:LEU:HD11	1.80	0.46
1:F:75:ARG:HG3	1:F:90:GLU:O	2.15	0.46
1:G:350:PHE:HA	1:G:357:TRP:CZ2	2.50	0.46
1:L:324:ASN:H	1:L:324:ASN:ND2	2.12	0.46
1:D:18:GLN:HB2	1:D:26:TYR:O	2.16	0.46
1:D:144:GLN:O	1:D:205:ARG:NH1	2.40	0.46
1:J:350:PHE:HA	1:J:357:TRP:CZ2	2.50	0.46
1:K:320:PHE:CE2	1:K:343:TRP:HB2	2.50	0.46
1:B:27:ASP:CB	1:B:29:ASN:ND2	2.79	0.46
1:D:357:TRP:CZ2	1:D:359:PRO:HG3	2.50	0.46
1:E:158:THR:O	1:E:159:VAL:HB	2.16	0.46
1:F:37:PRO:CG	1:F:38:GLU:H	2.27	0.46
1:K:396:GLU:N	1:K:396:GLU:CD	2.73	0.46
1:L:253:MSE:HE2	1:L:253:MSE:N	2.31	0.46
1:D:119:GLU:OE1	1:D:145:TYR:CD2	2.69	0.46
1:E:22:GLU:HB3	1:E:24:ILE:HD13	1.96	0.46
1:H:158:THR:O	1:H:160:ALA:N	2.46	0.46
1:I:397:ALA:O	1:I:398:THR:C	2.58	0.46
1:G:59:VAL:CG1	1:G:61:LYS:O	2.62	0.46
1:J:108:LEU:CD1	1:J:109:GLY:N	2.68	0.46
1:A:24:ILE:HD11	1:A:34:VAL:CG2	2.46	0.46
1:B:174:ASP:OD1	1:B:174:ASP:C	2.58	0.46
1:D:385:LYS:HE3	1:D:385:LYS:HB2	1.40	0.46
1:E:35:LEU:CD2	1:E:62:GLY:C	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:ILE:HG12	1:E:129:LEU:CD1	2.43	0.46
1:F:41:TRP:HA	1:F:81:GLN:HE22	1.79	0.46
1:I:223:THR:HG22	1:I:238:TRP:CE2	2.50	0.46
1:K:23:ASN:O	1:K:37:PRO:HG3	2.15	0.46
1:K:398:THR:HG22	1:K:398:THR:O	2.16	0.46
1:L:158:THR:O	1:L:160:ALA:N	2.45	0.46
1:F:29:ASN:O	1:F:164:THR:HB	2.16	0.46
1:L:218:TYR:HB2	1:L:253:MSE:CE	2.38	0.46
1:I:149:GLN:CD	1:I:157:ARG:HD3	2.39	0.46
1:J:108:LEU:HD22	1:J:302:GLY:CA	2.37	0.46
1:K:142:ALA:N	1:K:143:PRO:HD2	2.30	0.46
1:K:205:ARG:HG2	1:K:205:ARG:NH1	2.26	0.46
1:L:149:GLN:CD	1:L:157:ARG:NH2	2.74	0.46
1:H:345:ASP:OD2	1:H:360:ARG:NH2	2.49	0.46
1:D:18:GLN:HB3	1:D:26:TYR:CE1	2.51	0.46
1:F:281:LEU:HB3	1:F:285:GLU:CD	2.34	0.46
1:J:39:GLY:O	1:J:60:ASP:HB2	2.14	0.46
1:A:276:ASP:CG	1:A:278:THR:CG2	2.66	0.45
1:E:38:GLU:O	1:E:41:TRP:CE2	2.68	0.45
1:G:133:MSE:HE2	1:G:138:ILE:HA	1.98	0.45
1:B:17:THR:OG1	1:B:160:ALA:HB1	2.16	0.45
1:B:17:THR:CG2	1:B:29:ASN:HD21	2.29	0.45
1:B:21:PRO:CD	1:B:88:LEU:CD1	2.87	0.45
1:E:80:ARG:O	1:E:81:GLN:C	2.60	0.45
1:E:396:GLU:N	1:E:396:GLU:OE2	2.49	0.45
1:F:84:ALA:O	1:F:85:THR:CG2	2.64	0.45
1:G:48:ALA:HB1	1:G:73:ARG:HH21	1.81	0.45
1:G:389:SER:HG	1:G:398:THR:HG22	1.81	0.45
1:K:40:LYS:HZ3	1:K:60:ASP:CG	2.24	0.45
1:L:16:PRO:HB3	1:L:27:ASP:N	2.30	0.45
1:L:19:ALA:HB2	1:L:25:PHE:CD1	2.52	0.45
1:A:36:LEU:HD11	1:A:59:VAL:HG11	1.97	0.45
1:A:276:ASP:OD2	1:A:278:THR:OG1	2.30	0.45
1:D:89:ASP:OD1	1:D:89:ASP:C	2.59	0.45
1:E:291:ARG:HG3	1:E:291:ARG:HH11	1.81	0.45
1:G:30:ASP:HB3	1:G:33:ARG:HD2	1.99	0.45
1:G:251:ARG:C	1:G:253:MSE:CE	2.89	0.45
1:H:24:ILE:HG23	1:H:37:PRO:HD3	1.98	0.45
1:I:28:PHE:CD2	1:I:92:LEU:HD12	2.51	0.45
1:K:114:TRP:CD1	1:K:191:ALA:HB2	2.51	0.45
1:K:395:VAL:N	1:K:396:GLU:C	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:144:GLN:O	1:L:205:ARG:NH1	2.46	0.45
1:L:206:LEU:O	1:L:208:LEU:HD12	2.16	0.45
1:E:59:VAL:HG11	1:E:61:LYS:CE	2.45	0.45
1:F:79:PHE:CZ	1:F:86:PRO:HD3	2.51	0.45
1:I:22:GLU:HB2	1:I:87:LEU:HD11	1.99	0.45
1:J:218:TYR:HB2	1:J:253:MSE:CE	2.36	0.45
1:K:36:LEU:HD22	1:K:41:TRP:CG	2.51	0.45
1:A:95:LYS:O	1:A:97:ARG:HG2	2.16	0.45
1:F:26:TYR:CB	1:F:34:VAL:HG23	2.43	0.45
1:F:90:GLU:OE1	1:F:90:GLU:CA	2.63	0.45
1:I:345:ASP:OD2	1:I:360:ARG:NH1	2.49	0.45
1:L:291:ARG:HA	1:L:310:THR:HG23	1.99	0.45
1:A:75:ARG:HG3	1:A:91:THR:CG2	2.37	0.45
1:C:30:ASP:O	1:C:69:LYS:HE2	2.16	0.45
1:F:223:THR:HG22	1:F:238:TRP:CE2	2.52	0.45
1:G:24:ILE:CD1	1:G:24:ILE:H	2.29	0.45
1:I:253:MSE:HB3	1:I:277:PHE:CE1	2.50	0.45
1:L:17:THR:OG1	1:L:18:GLN:NE2	2.50	0.45
1:A:106:GLY:O	1:A:107:THR:C	2.60	0.45
1:C:321:SER:HB2	1:C:325:SER:OG	2.17	0.45
1:G:16:PRO:HB2	1:G:25:PHE:C	2.42	0.45
1:I:174:ASP:OD1	1:I:174:ASP:C	2.60	0.45
1:D:224:GLN:N	1:D:256:ASP:OD2	2.41	0.45
1:F:40:LYS:C	1:F:81:GLN:HE22	2.24	0.45
1:G:158:THR:CG2	1:G:159:VAL:N	2.79	0.45
1:H:21:PRO:O	1:H:24:ILE:CG1	2.65	0.45
1:H:140:LEU:HD11	1:H:287:VAL:HG21	1.99	0.45
1:I:281:LEU:CB	1:I:282:PRO:HD2	2.42	0.45
1:K:38:GLU:OE1	1:K:38:GLU:HA	2.16	0.45
1:K:350:PHE:HA	1:K:357:TRP:CZ2	2.52	0.45
1:L:133:MSE:HE3	1:L:137:ILE:CB	2.36	0.45
1:L:155:LYS:HB2	1:L:155:LYS:HE2	1.73	0.45
1:A:12:PRO:O	1:A:13:PRO:C	2.59	0.45
1:B:221:ILE:O	1:B:255:ILE:CD1	2.61	0.45
1:K:40:LYS:NZ	1:K:60:ASP:CG	2.75	0.45
1:L:27:ASP:OD1	1:L:29:ASN:OD1	2.34	0.45
1:C:142:ALA:HB3	1:C:143:PRO:HD3	1.98	0.45
1:F:26:TYR:HA	1:F:33:ARG:O	2.17	0.45
1:J:320:PHE:CE2	1:J:343:TRP:HB2	2.52	0.45
1:F:33:ARG:O	1:F:33:ARG:HG2	2.16	0.44
1:G:42:HIS:ND1	1:G:58:ASP:OD1	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:357:TRP:CZ2	1:H:359:PRO:HG3	2.51	0.44
1:L:189:ARG:NH1	3:L:502:EDO:O1	2.41	0.44
1:C:138:ILE:CG2	1:C:139:ASP:N	2.79	0.44
1:G:40:LYS:C	1:G:41:TRP:CD1	2.96	0.44
1:H:350:PHE:HA	1:H:357:TRP:CZ2	2.52	0.44
1:D:197:VAL:O	1:D:198:ASP:C	2.61	0.44
1:E:100:LEU:HB3	1:E:164:THR:HG23	2.00	0.44
1:E:277:PHE:O	1:E:286:ARG:NH2	2.43	0.44
1:F:77:GLN:HB3	1:F:79:PHE:CE1	2.51	0.44
1:G:38:GLU:HG3	1:G:39:GLY:N	2.32	0.44
1:L:174:ASP:OD1	1:L:174:ASP:C	2.59	0.44
1:L:222:ALA:O	1:L:299:LEU:HD22	2.16	0.44
1:B:91:THR:HG22	1:B:91:THR:O	2.18	0.44
1:B:130:GLU:CB	1:B:149:GLN:HG3	2.48	0.44
1:C:18:GLN:HB2	1:C:26:TYR:O	2.16	0.44
1:C:198:ASP:OD1	1:C:200:ARG:HD3	2.18	0.44
1:E:223:THR:HG22	1:E:238:TRP:CE2	2.52	0.44
1:F:28:PHE:CE2	1:F:92:LEU:CD1	3.00	0.44
1:K:223:THR:HG22	1:K:238:TRP:CE2	2.53	0.44
1:B:218:TYR:HB2	1:B:253:MSE:CE	2.36	0.44
1:C:138:ILE:HD11	1:C:150:PHE:C	2.41	0.44
1:D:340:TYR:CD1	1:D:340:TYR:C	2.95	0.44
1:F:252:VAL:O	1:F:252:VAL:CG2	2.65	0.44
1:A:26:TYR:OH	1:A:90:GLU:HG2	2.18	0.44
1:D:133:MSE:HE3	1:D:137:ILE:CG2	2.47	0.44
1:F:73:ARG:CA	1:F:92:LEU:HD22	2.44	0.44
1:I:72:VAL:HB	1:I:74:PHE:CE2	2.53	0.44
1:J:108:LEU:HD11	1:J:302:GLY:H	1.81	0.44
1:J:108:LEU:HD22	1:J:108:LEU:C	2.42	0.44
1:K:124:LEU:HD23	1:K:125:HIS:CE1	2.53	0.44
1:L:28:PHE:HB2	1:L:162:TYR:O	2.18	0.44
1:L:149:GLN:CG	1:L:157:ARG:HH21	2.31	0.44
1:A:14:ASP:O	1:A:63:TRP:CH2	2.71	0.44
1:A:28:PHE:CD2	1:A:92:LEU:HD12	2.52	0.44
1:C:179:PRO:HG2	1:C:193:TYR:HB3	2.00	0.44
1:E:114:TRP:CD1	1:E:191:ALA:HB2	2.52	0.44
1:G:225:SER:OG	1:G:301:SER:OG	2.25	0.44
1:A:223:THR:HG22	1:A:238:TRP:CE2	2.52	0.44
1:B:320:PHE:CE2	1:B:343:TRP:HB2	2.52	0.44
1:C:92:LEU:C	1:C:92:LEU:CD2	2.86	0.44
1:F:17:THR:HG21	1:F:161:PRO:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:253:MSE:HG3	1:H:277:PHE:HE1	1.76	0.44
1:J:85:THR:HG23	1:J:86:PRO:HD2	2.00	0.44
1:A:29:ASN:O	1:A:33:ARG:CD	2.66	0.44
1:A:79:PHE:CD1	1:A:86:PRO:HB3	2.53	0.44
1:D:28:PHE:CD2	1:D:92:LEU:HD12	2.53	0.44
1:D:80:ARG:HA	1:D:80:ARG:HD2	1.78	0.44
1:E:189:ARG:NH2	1:E:324:ASN:O	2.51	0.44
1:F:251:ARG:HD2	1:F:275:GLU:OE1	2.18	0.44
1:H:20:GLY:N	1:H:24:ILE:O	2.41	0.44
1:H:148:ILE:HG13	1:H:150:PHE:HE1	1.83	0.44
1:H:181:ASP:HB3	1:H:184:LYS:HG3	2.00	0.44
1:I:365:ASP:OD1	1:I:365:ASP:C	2.61	0.44
1:B:115:PHE:N	1:B:116:PRO:CD	2.81	0.43
1:H:253:MSE:CE	1:H:275:GLU:OE1	2.65	0.43
1:B:17:THR:HG22	1:B:29:ASN:HD21	1.83	0.43
1:F:100:LEU:HB3	1:F:164:THR:HG23	2.00	0.43
1:H:114:TRP:CD1	1:H:191:ALA:HB2	2.53	0.43
1:H:223:THR:HG22	1:H:238:TRP:CE2	2.53	0.43
1:I:89:ASP:OD1	1:I:89:ASP:C	2.60	0.43
1:I:152:THR:CG2	1:I:153:PRO:HD2	2.48	0.43
1:C:101:ILE:HG13	1:C:129:LEU:HD11	2.00	0.43
1:D:291:ARG:HD2	1:D:292:HIS:NE2	2.34	0.43
1:K:40:LYS:N	1:K:80:ARG:NH1	2.65	0.43
1:D:252:VAL:O	1:D:275:GLU:HB2	2.18	0.43
1:E:394:GLY:C	1:E:395:VAL:HG13	2.42	0.43
1:J:28:PHE:CD2	1:J:92:LEU:HD12	2.53	0.43
1:K:394:GLY:CA	1:K:395:VAL:C	2.90	0.43
1:L:144:GLN:NE2	1:L:207:ASP:HB2	2.34	0.43
1:L:340:TYR:C	1:L:340:TYR:CD1	2.95	0.43
1:A:77:GLN:OE1	1:A:79:PHE:HZ	2.02	0.43
1:E:325:SER:OG	1:E:344:ASP:OD2	2.36	0.43
1:E:340:TYR:CD1	1:E:340:TYR:C	2.95	0.43
1:D:174:ASP:OD1	1:D:175:THR:N	2.51	0.43
1:E:130:GLU:OE1	1:E:158:THR:CG2	2.54	0.43
1:G:30:ASP:CB	1:G:33:ARG:HD2	2.48	0.43
1:H:174:ASP:OD1	1:H:174:ASP:C	2.61	0.43
1:J:368:PHE:O	1:J:372:ARG:HG3	2.18	0.43
1:K:50:SER:O	1:K:51:GLU:HB2	2.18	0.43
1:A:23:ASN:HB3	1:A:37:PRO:HG3	2.01	0.43
1:G:224:GLN:NE2	1:G:261:TYR:HB3	2.33	0.43
1:L:169:LEU:HD11	1:L:187:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:LYS:HD2	1:D:126:LYS:HA	1.58	0.43
1:E:61:LYS:HE2	1:E:61:LYS:HB3	1.76	0.43
1:F:258:ASP:OD1	1:F:258:ASP:N	2.51	0.43
1:F:320:PHE:CE2	1:F:343:TRP:HB2	2.53	0.43
1:H:18:GLN:O	1:H:25:PHE:HA	2.18	0.43
1:H:291:ARG:HG2	1:H:291:ARG:HH11	1.83	0.43
1:L:350:PHE:HA	1:L:357:TRP:CZ2	2.54	0.43
1:B:80:ARG:O	1:B:81:GLN:C	2.61	0.43
1:B:93:LYS:HB2	1:B:93:LYS:HE3	1.65	0.43
1:C:46:LEU:HB2	1:C:75:ARG:HB3	2.01	0.43
1:E:169:LEU:HD11	1:E:187:PHE:HB2	1.99	0.43
1:G:340:TYR:CD1	1:G:340:TYR:C	2.96	0.43
1:I:300:PRO:HD3	1:I:318:SER:HB2	2.00	0.43
1:J:61:LYS:O	1:J:61:LYS:CD	2.64	0.43
1:K:29:ASN:HA	1:K:164:THR:H	1.84	0.43
1:B:224:GLN:N	1:B:256:ASP:OD2	2.43	0.43
1:B:340:TYR:CD1	1:B:340:TYR:C	2.97	0.43
1:C:43:VAL:HG22	1:C:57:CYS:O	2.18	0.43
1:C:300:PRO:HD3	1:C:318:SER:HB2	2.00	0.43
1:F:131:CYS:HB3	1:F:133:MSE:HE3	2.01	0.43
1:G:64:VAL:HG13	1:G:64:VAL:O	2.18	0.43
1:G:99:VAL:HG12	1:G:163:ALA:HB3	2.00	0.43
1:B:21:PRO:O	1:B:24:ILE:CD1	2.62	0.42
1:B:59:VAL:HG12	1:B:60:ASP:N	2.33	0.42
1:C:140:LEU:O	1:C:140:LEU:HD22	2.19	0.42
1:D:291:ARG:NH1	1:D:292:HIS:CE1	2.76	0.42
1:D:361:HIS:CE1	1:D:366:ARG:HH21	2.37	0.42
1:E:44:ARG:NH1	1:E:77:GLN:OE1	2.52	0.42
1:F:84:ALA:C	1:F:85:THR:HG22	2.44	0.42
1:F:242:ILE:HG23	1:F:252:VAL:HG21	2.01	0.42
1:A:300:PRO:HD3	1:A:318:SER:HB2	2.01	0.42
1:C:16:PRO:HB2	1:C:25:PHE:HB3	2.01	0.42
1:C:263:GLN:HB2	1:C:355:PHE:CD2	2.55	0.42
1:G:133:MSE:CE	1:G:137:ILE:CB	2.84	0.42
1:G:287:VAL:HG23	1:G:310:THR:HG22	2.01	0.42
1:H:115:PHE:CZ	1:H:148:ILE:HD12	2.41	0.42
1:C:36:LEU:HD13	1:C:36:LEU:H	1.83	0.42
1:H:208:LEU:HD21	1:H:310:THR:HA	2.00	0.42
1:H:286:ARG:N	1:H:286:ARG:HD2	2.33	0.42
1:K:340:TYR:CD1	1:K:340:TYR:C	2.97	0.42
1:L:109:GLY:CA	1:L:302:GLY:HA2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:298:GLY:C	1:L:299:LEU:HD13	2.44	0.42
1:B:300:PRO:HD3	1:B:318:SER:HB2	2.01	0.42
1:C:253:MSE:CE	1:C:275:GLU:CD	2.91	0.42
1:C:350:PHE:HA	1:C:357:TRP:CZ2	2.54	0.42
1:F:114:TRP:CD1	1:F:191:ALA:HB2	2.54	0.42
1:I:29:ASN:OD1	1:I:161:PRO:HG2	2.19	0.42
1:L:99:VAL:HG23	1:L:163:ALA:O	2.20	0.42
1:F:197:VAL:O	1:F:198:ASP:C	2.62	0.42
1:I:78:VAL:HG23	1:I:88:LEU:HD23	2.01	0.42
1:L:233:ASN:HB2	1:L:371:THR:OG1	2.20	0.42
1:C:100:LEU:HB3	1:C:164:THR:HG23	2.02	0.42
1:D:174:ASP:OD1	1:D:174:ASP:C	2.62	0.42
1:D:252:VAL:N	1:D:253:MSE:HE2	2.33	0.42
1:E:42:HIS:CD2	1:E:58:ASP:OD1	2.73	0.42
1:L:19:ALA:HA	1:L:25:PHE:CA	2.31	0.42
1:B:23:ASN:OD1	1:B:23:ASN:C	2.63	0.42
1:B:93:LYS:O	1:B:162:TYR:HE2	2.02	0.42
1:G:37:PRO:O	1:G:41:TRP:HZ2	2.03	0.42
1:J:108:LEU:CD1	1:J:108:LEU:N	2.82	0.42
1:A:79:PHE:HE1	1:A:86:PRO:HG3	1.84	0.42
1:B:92:LEU:C	1:B:92:LEU:CD2	2.69	0.42
1:G:46:LEU:HB2	1:G:75:ARG:HB3	2.01	0.42
1:G:286:ARG:HG2	1:G:286:ARG:HH11	1.85	0.42
1:H:79:PHE:CE2	1:H:86:PRO:HB3	2.54	0.42
1:H:299:LEU:C	1:H:301:SER:H	2.28	0.42
1:I:115:PHE:N	1:I:116:PRO:CD	2.82	0.42
1:K:174:ASP:OD1	1:K:174:ASP:C	2.62	0.42
1:A:26:TYR:CZ	1:A:90:GLU:HG2	2.54	0.42
1:A:291:ARG:HG2	1:A:291:ARG:HH11	1.85	0.42
1:F:80:ARG:O	1:F:81:GLN:C	2.62	0.42
1:F:251:ARG:C	1:F:253:MSE:CE	2.93	0.42
1:K:390:LEU:HD23	1:K:390:LEU:HA	1.88	0.42
1:A:253:MSE:HB3	1:A:277:PHE:CD2	2.55	0.41
1:A:320:PHE:CE2	1:A:343:TRP:HB2	2.55	0.41
1:B:115:PHE:CD1	1:B:133:MSE:HE1	2.55	0.41
1:B:286:ARG:N	1:B:286:ARG:HD2	2.35	0.41
1:C:286:ARG:N	1:C:286:ARG:HD2	2.34	0.41
1:D:101:ILE:HD12	1:D:129:LEU:HD11	2.01	0.41
1:E:35:LEU:CD2	1:E:62:GLY:O	2.57	0.41
1:E:368:PHE:HD2	1:L:265:PHE:CG	2.38	0.41
1:J:130:GLU:OE1	1:J:158:THR:OG1	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:42:HIS:ND1	1:K:58:ASP:OD1	2.52	0.41
1:K:300:PRO:HD3	1:K:318:SER:HB2	2.03	0.41
1:C:223:THR:HG22	1:C:238:TRP:CE2	2.55	0.41
1:D:17:THR:HG23	1:D:160:ALA:HB3	2.02	0.41
1:D:107:THR:O	1:D:110:ASP:HB2	2.21	0.41
1:G:29:ASN:HA	1:G:164:THR:H	1.85	0.41
1:J:107:THR:OG1	1:J:108:LEU:CD1	2.68	0.41
1:A:219:VAL:O	1:A:253:MSE:CE	2.68	0.41
1:B:59:VAL:CG1	1:B:60:ASP:N	2.83	0.41
1:D:22:GLU:HG2	1:D:87:LEU:HD21	2.02	0.41
1:E:72:VAL:HB	1:E:74:PHE:CE2	2.55	0.41
1:I:204:VAL:CG1	1:I:205:ARG:N	2.83	0.41
1:L:27:ASP:OD2	1:L:29:ASN:OD1	2.38	0.41
1:L:29:ASN:ND2	1:L:161:PRO:HG2	2.35	0.41
1:L:100:LEU:CD1	1:L:130:GLU:OE1	2.68	0.41
1:L:227:CYS:SG	1:L:230:LYS:HG3	2.60	0.41
1:A:340:TYR:CD1	1:A:340:TYR:C	2.98	0.41
1:B:20:GLY:HA3	1:B:24:ILE:HB	2.02	0.41
1:L:99:VAL:HG13	1:L:129:LEU:HD13	2.02	0.41
1:J:340:TYR:CD1	1:J:340:TYR:C	2.99	0.41
1:K:218:TYR:HB2	1:K:253:MSE:CE	2.39	0.41
1:A:180:VAL:HA	1:E:340:TYR:OH	2.21	0.41
1:D:350:PHE:HA	1:D:357:TRP:CZ2	2.55	0.41
1:F:218:TYR:HB2	1:F:253:MSE:CE	2.42	0.41
1:G:28:PHE:CA	1:G:32:ALA:H	2.31	0.41
1:G:30:ASP:HA	1:G:166:ARG:HH12	1.84	0.41
1:H:109:GLY:CA	1:H:302:GLY:HA2	2.51	0.41
1:L:29:ASN:ND2	1:L:164:THR:OG1	2.48	0.41
1:B:365:ASP:OD1	1:B:365:ASP:N	2.41	0.41
1:H:23:ASN:O	1:H:37:PRO:CG	2.69	0.41
1:H:78:VAL:HG23	1:H:88:LEU:HD22	2.02	0.41
1:K:20:GLY:N	1:K:24:ILE:O	2.36	0.41
1:K:29:ASN:OD1	1:K:161:PRO:HG2	2.21	0.41
1:L:284:GLN:O	1:L:287:VAL:HG13	2.17	0.41
1:B:19:ALA:O	1:B:24:ILE:HG22	2.20	0.41
1:E:17:THR:HG21	1:E:29:ASN:HD21	1.85	0.41
1:F:17:THR:HG1	1:F:18:GLN:HE22	1.64	0.41
1:F:40:LYS:C	1:F:81:GLN:NE2	2.79	0.41
1:G:133:MSE:HE2	1:G:138:ILE:N	2.36	0.41
1:K:149:GLN:HG2	1:K:157:ARG:NH1	2.35	0.41
1:L:284:GLN:HA	1:L:287:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:HD11	1:A:287:VAL:HG21	2.03	0.41
1:B:255:ILE:HD13	1:B:255:ILE:H	1.85	0.41
1:D:144:GLN:NE2	1:D:207:ASP:N	2.67	0.41
1:E:68:LYS:HA	1:E:68:LYS:HD3	1.81	0.41
1:E:354:ASP:OD2	1:E:362:LYS:NZ	2.46	0.41
1:F:103:PHE:CD2	1:F:133:MSE:HE2	2.56	0.41
1:G:28:PHE:CD2	1:G:92:LEU:HD12	2.56	0.41
1:G:144:GLN:O	1:G:205:ARG:NH1	2.46	0.41
1:G:147:GLN:HG2	1:G:148:ILE:HG13	2.02	0.41
1:I:18:GLN:HB2	1:I:26:TYR:O	2.21	0.41
1:I:21:PRO:HG2	1:I:87:LEU:CD1	2.45	0.41
1:I:320:PHE:CD1	1:I:320:PHE:C	2.97	0.41
1:I:340:TYR:CD1	1:I:340:TYR:C	2.98	0.41
1:L:26:TYR:CZ	1:L:90:GLU:HG3	2.55	0.41
1:L:197:VAL:O	1:L:198:ASP:C	2.64	0.41
1:L:284:GLN:CA	1:L:287:VAL:HG12	2.49	0.41
1:E:87:LEU:H	1:E:87:LEU:CD2	2.34	0.41
1:E:107:THR:OG1	1:E:108:LEU:N	2.53	0.41
1:F:80:ARG:H	1:F:80:ARG:HG2	1.64	0.41
1:G:100:LEU:HD22	1:G:164:THR:HG23	2.03	0.41
1:A:197:VAL:O	1:A:198:ASP:C	2.62	0.40
1:B:92:LEU:HA	1:B:162:TYR:OH	2.20	0.40
1:B:132:THR:C	1:B:133:MSE:HG2	2.47	0.40
1:B:253:MSE:CG	1:B:277:PHE:CD1	3.04	0.40
1:C:122:GLN:HG3	1:C:123:SER:N	2.37	0.40
1:C:161:PRO:HG2	1:C:164:THR:OG1	2.21	0.40
1:E:21:PRO:O	1:E:24:ILE:N	2.43	0.40
1:E:21:PRO:O	1:E:24:ILE:HD11	2.13	0.40
1:F:18:GLN:HB2	1:F:26:TYR:CE1	2.56	0.40
1:G:223:THR:HG22	1:G:238:TRP:CE2	2.56	0.40
1:I:107:THR:OG1	1:I:108:LEU:N	2.54	0.40
1:J:142:ALA:HB3	1:J:143:PRO:HD3	2.03	0.40
1:L:320:PHE:CE2	1:L:343:TRP:HB2	2.57	0.40
1:A:20:GLY:N	1:A:24:ILE:O	2.48	0.40
1:A:76:ILE:CD1	1:A:76:ILE:N	2.72	0.40
1:D:46:LEU:HD21	1:D:53:ILE:CD1	2.49	0.40
1:F:368:PHE:C	1:F:370:CYS:N	2.78	0.40
1:G:80:ARG:NH1	1:G:87:LEU:HD21	2.36	0.40
1:J:253:MSE:HE2	1:J:253:MSE:N	2.36	0.40
1:K:18:GLN:O	1:K:25:PHE:HA	2.21	0.40
1:K:252:VAL:N	1:K:253:MSE:HE2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ASP:C	1:C:89:ASP:OD1	2.63	0.40
1:J:20:GLY:CA	1:J:24:ILE:O	2.68	0.40
1:J:70:TYR:CE2	1:J:179:PRO:HA	2.56	0.40
1:L:21:PRO:HB2	1:L:87:LEU:CD2	2.13	0.40
1:L:87:LEU:CD2	1:L:87:LEU:C	2.94	0.40
1:C:197:VAL:O	1:C:198:ASP:C	2.65	0.40
1:D:286:ARG:N	1:D:286:ARG:HD2	2.37	0.40
1:E:299:LEU:C	1:E:301:SER:H	2.29	0.40
1:F:78:VAL:CB	1:F:88:LEU:HD12	2.48	0.40
1:F:140:LEU:HD11	1:F:287:VAL:HG21	2.04	0.40
1:G:393:GLN:HB3	1:G:397:ALA:CB	2.51	0.40
1:L:365:ASP:OD1	1:L:365:ASP:C	2.62	0.40
1:B:24:ILE:HG22	1:B:25:PHE:N	2.35	0.40
1:B:155:LYS:HE2	1:B:155:LYS:HB3	1.78	0.40
1:E:30:ASP:HB3	1:E:33:ARG:HD2	2.04	0.40
1:E:59:VAL:CG1	1:E:60:ASP:N	2.84	0.40
1:F:253:MSE:HE2	1:F:253:MSE:N	2.37	0.40
1:G:160:ALA:HA	1:G:161:PRO:HD3	1.86	0.40
1:H:300:PRO:HD3	1:H:318:SER:HB2	2.02	0.40
1:I:316:LEU:C	1:I:333:VAL:CG2	2.95	0.40
1:K:28:PHE:CD2	1:K:92:LEU:HD13	2.56	0.40
1:L:300:PRO:HD3	1:L:318:SER:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	377/406 (93%)	369 (98%)	8 (2%)	0	100	100
1	B	381/406 (94%)	368 (97%)	11 (3%)	2 (0%)	24	51
1	C	387/406 (95%)	373 (96%)	13 (3%)	1 (0%)	36	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
1	D	377/406 (93%)	363 (96%)	12 (3%)	2 (0%)	24	51	
1	E	388/406 (96%)	369 (95%)	15 (4%)	4 (1%)	12	35	
1	F	375/406 (92%)	358 (96%)	15 (4%)	2 (0%)	24	51	
1	G	387/406 (95%)	370 (96%)	12 (3%)	5 (1%)	9	29	
1	H	383/406 (94%)	370 (97%)	12 (3%)	1 (0%)	36	62	
1	I	387/406 (95%)	373 (96%)	13 (3%)	1 (0%)	36	62	
1	J	382/406 (94%)	371 (97%)	10 (3%)	1 (0%)	36	62	
1	K	387/406 (95%)	376 (97%)	9 (2%)	2 (0%)	24	51	
1	L	365/406 (90%)	345 (94%)	16 (4%)	4 (1%)	11	33	
All	All	4576/4872 (94%)	4405 (96%)	146 (3%)	25 (0%)	24	51	

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	21	PRO
1	E	23	ASN
1	E	395	VAL
1	G	33	ARG
1	I	397	ALA
1	F	62	GLY
1	L	21	PRO
1	L	22	GLU
1	B	25	PHE
1	C	161	PRO
1	G	161	PRO
1	L	161	PRO
1	E	161	PRO
1	F	95	LYS
1	G	31	GLY
1	J	81	GLN
1	B	62	GLY
1	D	207	ASP
1	G	19	ALA
1	G	32	ALA
1	K	21	PRO
1	L	23	ASN
1	D	83	ALA
1	K	37	PRO
1	H	161	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/347 (95%)	295 (89%)	36 (11%)	6	18
1	B	332/347 (96%)	307 (92%)	25 (8%)	12	34
1	C	336/347 (97%)	313 (93%)	23 (7%)	14	39
1	D	330/347 (95%)	299 (91%)	31 (9%)	8	24
1	E	337/347 (97%)	308 (91%)	29 (9%)	10	28
1	F	330/347 (95%)	283 (86%)	47 (14%)	3	10
1	G	336/347 (97%)	315 (94%)	21 (6%)	16	42
1	H	333/347 (96%)	309 (93%)	24 (7%)	13	36
1	I	336/347 (97%)	309 (92%)	27 (8%)	11	31
1	J	333/347 (96%)	308 (92%)	25 (8%)	12	34
1	K	336/347 (97%)	310 (92%)	26 (8%)	12	33
1	L	321/347 (92%)	286 (89%)	35 (11%)	6	18
All	All	3991/4164 (96%)	3642 (91%)	349 (9%)	9	27

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	23	ASN
1	A	24	ILE
1	A	36	LEU
1	A	53	ILE
1	A	59	VAL
1	A	65	THR
1	A	66	SER
1	A	76	ILE
1	A	80	ARG
1	A	81	GLN
1	A	87	LEU
1	A	92	LEU
1	A	105	THR

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Mol	Chain	Res	Type
1	A	107	THR
1	A	108	LEU
1	A	111	LEU
1	A	147	GLN
1	A	149	GLN
1	A	152	THR
1	A	158	THR
1	A	174	ASP
1	A	180	VAL
1	A	221	ILE
1	A	224	GLN
1	A	253	MSE
1	A	257	ARG
1	A	263	GLN
1	A	275	GLU
1	A	276	ASP
1	A	278	THR
1	A	290	LEU
1	A	320	PHE
1	A	339	CYS
1	A	371	THR
1	A	372	ARG
1	B	9	PHE
1	B	18	GLN
1	B	24	ILE
1	B	30	ASP
1	B	36	LEU
1	B	45	LEU
1	B	60	ASP
1	B	80	ARG
1	B	88	LEU
1	B	91	THR
1	B	92	LEU
1	B	93	LYS
1	B	100	LEU
1	B	133	MSE
1	B	158	THR
1	B	159	VAL
1	B	224	GLN
1	B	253	MSE
1	B	255	ILE
1	B	286	ARG

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Mol	Chain	Res	Type
1	B	291	ARG
1	B	316	LEU
1	B	320	PHE
1	B	339	CYS
1	B	371	THR
1	C	22	GLU
1	C	33	ARG
1	C	35	LEU
1	C	36	LEU
1	C	45	LEU
1	C	58	ASP
1	C	69	LYS
1	C	88	LEU
1	C	92	LEU
1	C	93	LYS
1	C	122	GLN
1	C	136	ASP
1	C	138	ILE
1	C	140	LEU
1	C	157	ARG
1	C	169	LEU
1	C	174	ASP
1	C	200	ARG
1	C	226	THR
1	C	253	MSE
1	C	286	ARG
1	C	320	PHE
1	C	339	CYS
1	D	18	GLN
1	D	22	GLU
1	D	41	TRP
1	D	45	LEU
1	D	53	ILE
1	D	59	VAL
1	D	81	GLN
1	D	87	LEU
1	D	88	LEU
1	D	92	LEU
1	D	95	LYS
1	D	100	LEU
1	D	111	LEU
1	D	122	GLN

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Mol	Chain	Res	Type
1	D	126	LYS
1	D	133	MSE
1	D	147	GLN
1	D	157	ARG
1	D	175	THR
1	D	206	LEU
1	D	224	GLN
1	D	228	GLN
1	D	253	MSE
1	D	275	GLU
1	D	281	LEU
1	D	286	ARG
1	D	291	ARG
1	D	320	PHE
1	D	339	CYS
1	D	348	LEU
1	D	391	THR
1	E	10	ILE
1	E	15	THR
1	E	17	THR
1	E	22	GLU
1	E	23	ASN
1	E	24	ILE
1	E	35	LEU
1	E	38	GLU
1	E	54	LEU
1	E	60	ASP
1	E	61	LYS
1	E	87	LEU
1	E	88	LEU
1	E	107	THR
1	E	111	LEU
1	E	119	GLU
1	E	136	ASP
1	E	169	LEU
1	E	253	MSE
1	E	263	GLN
1	E	281	LEU
1	E	290	LEU
1	E	320	PHE
1	E	326	GLU
1	E	339	CYS

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Mol	Chain	Res	Type
1	E	348	LEU
1	E	367	GLN
1	E	395	VAL
1	E	396	GLU
1	F	9	PHE
1	F	10	ILE
1	F	11	THR
1	F	15	THR
1	F	26	TYR
1	F	28	PHE
1	F	30	ASP
1	F	33	ARG
1	F	38	GLU
1	F	45	LEU
1	F	54	LEU
1	F	56	CYS
1	F	57	CYS
1	F	58	ASP
1	F	63	TRP
1	F	76	ILE
1	F	78	VAL
1	F	80	ARG
1	F	81	GLN
1	F	87	LEU
1	F	89	ASP
1	F	90	GLU
1	F	92	LEU
1	F	93	LYS
1	F	107	THR
1	F	108	LEU
1	F	111	LEU
1	F	122	GLN
1	F	129	LEU
1	F	147	GLN
1	F	149	GLN
1	F	151	SER
1	F	155	LYS
1	F	157	ARG
1	F	158	THR
1	F	169	LEU
1	F	224	GLN
1	F	226	THR

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Mol	Chain	Res	Type
1	F	253	MSE
1	F	258	ASP
1	F	280	LYS
1	F	290	LEU
1	F	306	LEU
1	F	320	PHE
1	F	371	THR
1	F	390	LEU
1	F	393	GLN
1	G	22	GLU
1	G	24	ILE
1	G	25	PHE
1	G	35	LEU
1	G	36	LEU
1	G	38	GLU
1	G	40	LYS
1	G	41	TRP
1	G	61	LYS
1	G	72	VAL
1	G	80	ARG
1	G	81	GLN
1	G	92	LEU
1	G	111	LEU
1	G	253	MSE
1	G	281	LEU
1	G	320	PHE
1	G	339	CYS
1	G	356	LEU
1	G	371	THR
1	G	388	ARG
1	H	22	GLU
1	H	24	ILE
1	H	43	VAL
1	H	45	LEU
1	H	80	ARG
1	H	81	GLN
1	H	87	LEU
1	H	92	LEU
1	H	100	LEU
1	H	107	THR
1	H	108	LEU
1	H	111	LEU

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Mol	Chain	Res	Type
1	H	129	LEU
1	H	148	ILE
1	H	166	ARG
1	H	174	ASP
1	H	180	VAL
1	H	253	MSE
1	H	257	ARG
1	H	281	LEU
1	H	286	ARG
1	H	320	PHE
1	H	360	ARG
1	H	393	GLN
1	I	11	THR
1	I	35	LEU
1	I	40	LYS
1	I	56	CYS
1	I	60	ASP
1	I	61	LYS
1	I	65	THR
1	I	81	GLN
1	I	87	LEU
1	I	92	LEU
1	I	100	LEU
1	I	107	THR
1	I	108	LEU
1	I	152	THR
1	I	158	THR
1	I	159	VAL
1	I	247	SER
1	I	252	VAL
1	I	253	MSE
1	I	280	LYS
1	I	281	LEU
1	I	289	LEU
1	I	290	LEU
1	I	320	PHE
1	I	333	VAL
1	I	339	CYS
1	I	371	THR
1	J	24	ILE
1	J	33	ARG
1	J	34	VAL

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Mol	Chain	Res	Type
1	J	35	LEU
1	J	60	ASP
1	J	61	LYS
1	J	89	ASP
1	J	99	VAL
1	J	108	LEU
1	J	136	ASP
1	J	141	LEU
1	J	147	GLN
1	J	158	THR
1	J	166	ARG
1	J	180	VAL
1	J	226	THR
1	J	253	MSE
1	J	270	ILE
1	J	281	LEU
1	J	286	ARG
1	J	316	LEU
1	J	320	PHE
1	J	326	GLU
1	J	356	LEU
1	J	372	ARG
1	K	10	ILE
1	K	18	GLN
1	K	24	ILE
1	K	38	GLU
1	K	61	LYS
1	K	68	LYS
1	K	80	ARG
1	K	87	LEU
1	K	89	ASP
1	K	90	GLU
1	K	100	LEU
1	K	107	THR
1	K	141	LEU
1	K	166	ARG
1	K	174	ASP
1	K	180	VAL
1	K	205	ARG
1	K	226	THR
1	K	253	MSE
1	K	263	GLN

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Mol	Chain	Res	Type
1	K	281	LEU
1	K	291	ARG
1	K	320	PHE
1	K	326	GLU
1	K	382	VAL
1	K	396	GLU
1	L	17	THR
1	L	18	GLN
1	L	22	GLU
1	L	24	ILE
1	L	41	TRP
1	L	65	THR
1	L	72	VAL
1	L	75	ARG
1	L	88	LEU
1	L	107	THR
1	L	111	LEU
1	L	122	GLN
1	L	130	GLU
1	L	154	ASP
1	L	155	LYS
1	L	169	LEU
1	L	180	VAL
1	L	245	LEU
1	L	247	SER
1	L	248	LEU
1	L	251	ARG
1	L	253	MSE
1	L	281	LEU
1	L	286	ARG
1	L	299	LEU
1	L	303	LEU
1	L	310	THR
1	L	320	PHE
1	L	322	LEU
1	L	324	ASN
1	L	333	VAL
1	L	339	CYS
1	L	369	GLU
1	L	371	THR
1	L	395	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	81	GLN
1	A	149	GLN
1	A	177	ASN
1	A	284	GLN
1	A	349	ASN
1	A	367	GLN
1	B	23	ASN
1	B	29	ASN
1	B	122	GLN
1	B	125	HIS
1	B	149	GLN
1	B	178	GLN
1	B	284	GLN
1	B	349	ASN
1	C	81	GLN
1	C	135	GLN
1	C	337	HIS
1	C	349	ASN
1	C	393	GLN
1	D	18	GLN
1	D	77	GLN
1	D	81	GLN
1	D	144	GLN
1	D	149	GLN
1	D	177	ASN
1	D	349	ASN
1	E	42	HIS
1	E	149	GLN
1	E	349	ASN
1	E	367	GLN
1	F	18	GLN
1	F	29	ASN
1	F	42	HIS
1	F	81	GLN
1	F	144	GLN
1	F	149	GLN
1	F	176	ASN
1	F	177	ASN
1	F	284	GLN
1	F	337	HIS
1	F	349	ASN

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Mol	Chain	Res	Type
1	G	23	ASN
1	G	81	GLN
1	G	144	GLN
1	G	177	ASN
1	G	224	GLN
1	G	288	ASN
1	G	349	ASN
1	H	177	ASN
1	H	228	GLN
1	H	244	HIS
1	H	268	ASN
1	H	349	ASN
1	I	144	GLN
1	I	177	ASN
1	I	337	HIS
1	I	349	ASN
1	J	18	GLN
1	J	177	ASN
1	J	349	ASN
1	K	23	ASN
1	K	125	HIS
1	K	228	GLN
1	K	233	ASN
1	K	244	HIS
1	K	268	ASN
1	K	284	GLN
1	K	349	ASN
1	L	18	GLN
1	L	29	ASN
1	L	81	GLN
1	L	177	ASN
1	L	228	GLN
1	L	268	ASN
1	L	324	ASN
1	L	349	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
3	EDO	I	502	-	3,3,3	0.29	0	2,2,2	0.61	0
3	EDO	J	502	-	3,3,3	0.30	0	2,2,2	0.66	0
3	EDO	L	502	-	3,3,3	0.25	0	2,2,2	0.91	0
3	EDO	I	503	-	3,3,3	0.57	0	2,2,2	0.46	0
3	EDO	C	502	-	3,3,3	0.28	0	2,2,2	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	I	502	-	-	1/1/1/1	-
3	EDO	J	502	-	-	1/1/1/1	-
3	EDO	L	502	-	-	1/1/1/1	-
3	EDO	I	503	-	-	1/1/1/1	-
3	EDO	C	502	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	502	EDO	O1-C1-C2-O2
3	L	502	EDO	O1-C1-C2-O2
3	I	503	EDO	O1-C1-C2-O2
3	J	502	EDO	O1-C1-C2-O2
3	C	502	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	502	EDO	1	0
3	L	502	EDO	1	0
3	C	502	EDO	2	0

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	379/406 (93%)	0.12	12 (3%) 50 41	44, 69, 108, 132	0
1	B	381/406 (93%)	0.06	17 (4%) 38 30	42, 64, 114, 148	0
1	C	387/406 (95%)	-0.03	16 (4%) 41 33	34, 56, 114, 146	0
1	D	379/406 (93%)	0.10	16 (4%) 40 32	25, 66, 108, 129	0
1	E	388/406 (95%)	0.01	16 (4%) 41 33	26, 59, 109, 131	0
1	F	380/406 (93%)	0.35	42 (11%) 10 9	25, 66, 125, 151	0
1	G	387/406 (95%)	0.13	23 (5%) 28 22	30, 65, 114, 150	0
1	H	383/406 (94%)	0.03	9 (2%) 61 52	44, 66, 106, 128	0
1	I	387/406 (95%)	0.02	12 (3%) 51 42	40, 65, 108, 125	0
1	J	382/406 (94%)	-0.15	8 (2%) 63 55	35, 59, 97, 117	0
1	K	387/406 (95%)	-0.13	9 (2%) 61 52	37, 57, 98, 124	0
1	L	369/406 (90%)	0.32	30 (8%) 18 15	37, 67, 116, 132	0
All	All	4589/4872 (94%)	0.07	210 (4%) 37 29	25, 64, 112, 151	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	35	LEU	8.3
1	F	34	VAL	6.7
1	L	31	GLY	6.3
1	G	21	PRO	6.1
1	K	10	ILE	6.1
1	G	32	ALA	6.0
1	I	30	ASP	5.9
1	E	21	PRO	5.7
1	G	62	GLY	5.6
1	A	79	PHE	5.3
1	C	159	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	G	324	ASN	5.1
1	G	395	VAL	5.0
1	F	87	LEU	5.0
1	A	342	CYS	4.8
1	L	342	CYS	4.8
1	F	92	LEU	4.8
1	F	29	ASN	4.7
1	F	88	LEU	4.7
1	F	9	PHE	4.6
1	F	28	PHE	4.5
1	L	12	PRO	4.5
1	E	22	GLU	4.5
1	F	395	VAL	4.4
1	B	88	LEU	4.4
1	C	160	ALA	4.4
1	F	22	GLU	4.3
1	L	57	CYS	4.3
1	G	325	SER	4.3
1	G	61	LYS	4.3
1	H	342	CYS	4.1
1	F	31	GLY	4.1
1	C	161	PRO	4.1
1	F	37	PRO	4.1
1	G	20	GLY	4.0
1	A	10	ILE	4.0
1	D	24	ILE	4.0
1	E	342	CYS	4.0
1	D	342	CYS	4.0
1	B	9	PHE	3.9
1	D	85	THR	3.9
1	G	23	ASN	3.9
1	L	371	THR	3.9
1	B	342	CYS	3.9
1	F	342	CYS	3.9
1	E	20	GLY	3.8
1	F	89	ASP	3.8
1	I	342	CYS	3.8
1	K	29	ASN	3.8
1	D	25	PHE	3.7
1	G	342	CYS	3.7
1	F	79	PHE	3.7
1	H	10	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	18	GLN	3.7
1	I	398	THR	3.7
1	K	342	CYS	3.6
1	B	370	CYS	3.6
1	H	370	CYS	3.5
1	A	159	VAL	3.5
1	K	397	ALA	3.5
1	A	370	CYS	3.5
1	C	342	CYS	3.5
1	J	342	CYS	3.5
1	F	39	GLY	3.4
1	E	370	CYS	3.4
1	G	25	PHE	3.4
1	G	159	VAL	3.4
1	A	83	ALA	3.4
1	C	158	THR	3.3
1	D	207	ASP	3.3
1	F	94	LEU	3.3
1	G	22	GLU	3.2
1	D	84	ALA	3.2
1	G	59	VAL	3.2
1	L	85	THR	3.2
1	E	399	LEU	3.2
1	F	78	VAL	3.2
1	F	33	ARG	3.2
1	F	159	VAL	3.2
1	E	24	ILE	3.2
1	G	24	ILE	3.2
1	C	357	TRP	3.1
1	C	370	CYS	3.1
1	D	370	CYS	3.1
1	E	18	GLN	3.1
1	F	158	THR	3.1
1	B	24	ILE	3.0
1	G	31	GLY	3.0
1	H	38	GLU	3.0
1	C	21	PRO	3.0
1	F	394	GLY	2.9
1	F	370	CYS	2.9
1	G	370	CYS	2.9
1	L	25	PHE	2.9
1	C	61	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	158	THR	2.9
1	I	10	ILE	2.9
1	F	62	GLY	2.9
1	D	391	THR	2.9
1	F	63	TRP	2.8
1	B	37	PRO	2.8
1	G	63	TRP	2.8
1	L	43	VAL	2.8
1	L	159	VAL	2.8
1	F	93	LYS	2.8
1	H	339	CYS	2.8
1	H	160	ALA	2.8
1	I	370	CYS	2.7
1	F	76	ILE	2.7
1	J	10	ILE	2.7
1	D	82	GLY	2.7
1	E	339	CYS	2.7
1	L	130	GLU	2.7
1	L	370	CYS	2.7
1	F	26	TYR	2.7
1	E	159	VAL	2.7
1	I	87	LEU	2.7
1	L	86	PRO	2.7
1	F	43	VAL	2.7
1	L	27	ASP	2.6
1	F	80	ARG	2.6
1	B	339	CYS	2.6
1	I	339	CYS	2.6
1	J	370	CYS	2.6
1	K	370	CYS	2.6
1	B	62	GLY	2.6
1	H	340	TYR	2.6
1	C	59	VAL	2.6
1	I	27	ASP	2.6
1	F	64	VAL	2.6
1	E	25	PHE	2.6
1	D	160	ALA	2.5
1	F	82	GLY	2.5
1	H	159	VAL	2.5
1	G	81	GLN	2.5
1	G	160	ALA	2.5
1	A	339	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	256	ASP	2.4
1	K	395	VAL	2.4
1	G	19	ALA	2.4
1	L	160	ALA	2.4
1	D	20	GLY	2.4
1	L	28	PHE	2.4
1	F	15	THR	2.4
1	D	21	PRO	2.4
1	E	61	LYS	2.4
1	L	83	ALA	2.4
1	B	147	GLN	2.4
1	E	87	LEU	2.4
1	F	30	ASP	2.4
1	L	395	VAL	2.3
1	B	25	PHE	2.3
1	D	131	CYS	2.3
1	L	56	CYS	2.3
1	F	90	GLU	2.3
1	B	87	LEU	2.3
1	I	159	VAL	2.3
1	C	88	LEU	2.3
1	F	16	PRO	2.3
1	L	24	ILE	2.3
1	B	157	ARG	2.3
1	L	157	ARG	2.3
1	L	79	PHE	2.3
1	F	154	ASP	2.3
1	L	96	ASP	2.3
1	G	40	LYS	2.3
1	L	17	THR	2.3
1	L	158	THR	2.3
1	B	173	GLY	2.3
1	B	23	ASN	2.2
1	F	91	THR	2.2
1	K	39	GLY	2.2
1	A	277	PHE	2.2
1	E	30	ASP	2.2
1	F	128	ARG	2.2
1	D	339	CYS	2.2
1	J	340	TYR	2.2
1	A	82	GLY	2.2
1	L	19	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	31	GLY	2.2
1	A	85	THR	2.2
1	L	105	THR	2.2
1	C	79	PHE	2.2
1	K	339	CYS	2.2
1	C	10	ILE	2.1
1	C	86	PRO	2.1
1	K	17	THR	2.1
1	L	394	GLY	2.1
1	L	339	CYS	2.1
1	A	37	PRO	2.1
1	F	59	VAL	2.1
1	B	391	THR	2.1
1	D	132	THR	2.1
1	I	105	THR	2.1
1	F	19	ALA	2.1
1	L	16	PRO	2.1
1	E	96	ASP	2.1
1	E	396	GLU	2.1
1	F	339	CYS	2.0
1	J	393	GLN	2.0
1	H	394	GLY	2.0
1	J	25	PHE	2.0
1	B	105	THR	2.0
1	I	397	ALA	2.0
1	L	41	TRP	2.0
1	J	80	ARG	2.0
1	I	39	GLY	2.0
1	A	276	ASP	2.0
1	B	38	GLU	2.0
1	C	27	ASP	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($\text{\AA}^2$)	Q<0.9
3	EDO	I	503	4/4	0.81	0.19	61,75,76,77	0
3	EDO	I	502	4/4	0.87	0.18	57,59,72,80	0
2	FE	B	501	1/1	0.87	0.35	60,60,60,60	0
2	FE	E	1400	1/1	0.89	0.34	57,57,57,57	0
2	FE	K	501	1/1	0.89	0.34	59,59,59,59	0
2	FE	H	501	1/1	0.90	0.37	60,60,60,60	0
2	FE	G	1400	1/1	0.90	0.36	57,57,57,57	0
2	FE	D	501	1/1	0.91	0.34	63,63,63,63	0
2	FE	A	501	1/1	0.91	0.34	59,59,59,59	0
2	FE	I	501	1/1	0.91	0.35	58,58,58,58	0
2	FE	F	501	1/1	0.92	0.33	55,55,55,55	0
2	FE	L	501	1/1	0.92	0.35	55,55,55,55	0
2	FE	C	501	1/1	0.92	0.36	54,54,54,54	0
2	FE	J	501	1/1	0.92	0.38	56,56,56,56	0
3	EDO	L	502	4/4	0.92	0.14	51,52,59,62	0
3	EDO	C	502	4/4	0.94	0.13	40,43,48,59	0
3	EDO	J	502	4/4	0.96	0.11	48,49,52,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.