



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:43 AM UTC

PDB ID : 5ELP / pdb_00005elp
Title : Ketosynthase from module 1 of the bacillaene synthase from *Bacillus amyloliquefaciens* FZB42
Authors : Wagner, D.T.; Gay, D.C.; Keatinge-Clay, A.T.; Zogzas, C.E.
Deposited on : 2015-11-04
Resolution : 2.93 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
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

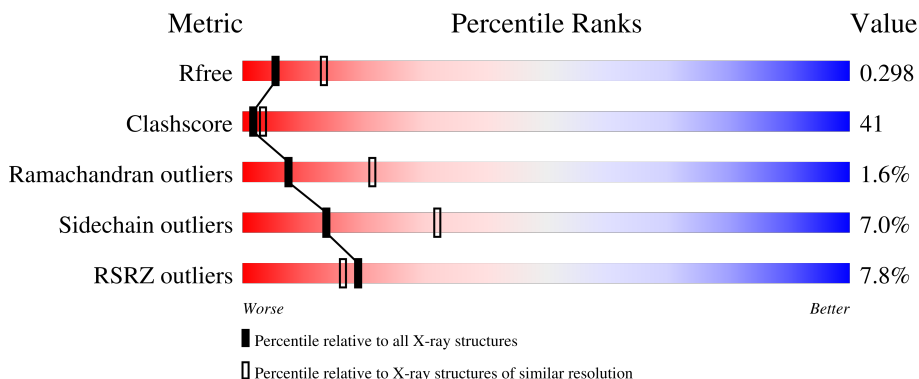
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	622	 3% 46% 35% 5% • 13%
1	B	622	 5% 41% 39% 6% • 12%
1	C	622	 9% 45% 35% 8% • 10%
1	D	622	 9% 37% 37% 9% • 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16749 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 NRPS/PKS protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	557	Total	C	N	O	S	0	0	0
			4317	2757	722	821	17			
1	A	540	Total	C	N	O	S	0	0	0
			4169	2656	704	792	17			
1	B	547	Total	C	N	O	S	0	0	0
			4213	2691	699	806	17			
1	D	523	Total	C	N	O	S	0	0	0
			4050	2591	677	766	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	MET	-	initiating methionine	UNP Q1RS73
C	-15	GLY	-	expression tag	UNP Q1RS73
C	-14	SER	-	expression tag	UNP Q1RS73
C	-13	SER	-	expression tag	UNP Q1RS73
C	-12	HIS	-	expression tag	UNP Q1RS73
C	-11	HIS	-	expression tag	UNP Q1RS73
C	-10	HIS	-	expression tag	UNP Q1RS73
C	-9	HIS	-	expression tag	UNP Q1RS73
C	-8	HIS	-	expression tag	UNP Q1RS73
C	-7	HIS	-	expression tag	UNP Q1RS73
C	-6	SER	-	expression tag	UNP Q1RS73
C	-5	SER	-	expression tag	UNP Q1RS73
C	-4	GLY	-	expression tag	UNP Q1RS73
C	-3	LEU	-	expression tag	UNP Q1RS73
C	-2	VAL	-	expression tag	UNP Q1RS73
C	-1	PRO	-	expression tag	UNP Q1RS73
C	0	ARG	-	expression tag	UNP Q1RS73
C	1	GLY	-	expression tag	UNP Q1RS73
C	2	SER	-	expression tag	UNP Q1RS73
C	3	SER	-	expression tag	UNP Q1RS73
A	-16	MET	-	initiating methionine	UNP Q1RS73

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	expression tag	UNP Q1RS73
A	-14	SER	-	expression tag	UNP Q1RS73
A	-13	SER	-	expression tag	UNP Q1RS73
A	-12	HIS	-	expression tag	UNP Q1RS73
A	-11	HIS	-	expression tag	UNP Q1RS73
A	-10	HIS	-	expression tag	UNP Q1RS73
A	-9	HIS	-	expression tag	UNP Q1RS73
A	-8	HIS	-	expression tag	UNP Q1RS73
A	-7	HIS	-	expression tag	UNP Q1RS73
A	-6	SER	-	expression tag	UNP Q1RS73
A	-5	SER	-	expression tag	UNP Q1RS73
A	-4	GLY	-	expression tag	UNP Q1RS73
A	-3	LEU	-	expression tag	UNP Q1RS73
A	-2	VAL	-	expression tag	UNP Q1RS73
A	-1	PRO	-	expression tag	UNP Q1RS73
A	0	ARG	-	expression tag	UNP Q1RS73
A	1	GLY	-	expression tag	UNP Q1RS73
A	2	SER	-	expression tag	UNP Q1RS73
A	3	SER	-	expression tag	UNP Q1RS73
B	-16	MET	-	initiating methionine	UNP Q1RS73
B	-15	GLY	-	expression tag	UNP Q1RS73
B	-14	SER	-	expression tag	UNP Q1RS73
B	-13	SER	-	expression tag	UNP Q1RS73
B	-12	HIS	-	expression tag	UNP Q1RS73
B	-11	HIS	-	expression tag	UNP Q1RS73
B	-10	HIS	-	expression tag	UNP Q1RS73
B	-9	HIS	-	expression tag	UNP Q1RS73
B	-8	HIS	-	expression tag	UNP Q1RS73
B	-7	HIS	-	expression tag	UNP Q1RS73
B	-6	SER	-	expression tag	UNP Q1RS73
B	-5	SER	-	expression tag	UNP Q1RS73
B	-4	GLY	-	expression tag	UNP Q1RS73
B	-3	LEU	-	expression tag	UNP Q1RS73
B	-2	VAL	-	expression tag	UNP Q1RS73
B	-1	PRO	-	expression tag	UNP Q1RS73
B	0	ARG	-	expression tag	UNP Q1RS73
B	1	GLY	-	expression tag	UNP Q1RS73
B	2	SER	-	expression tag	UNP Q1RS73
B	3	SER	-	expression tag	UNP Q1RS73
D	-16	MET	-	initiating methionine	UNP Q1RS73
D	-15	GLY	-	expression tag	UNP Q1RS73
D	-14	SER	-	expression tag	UNP Q1RS73

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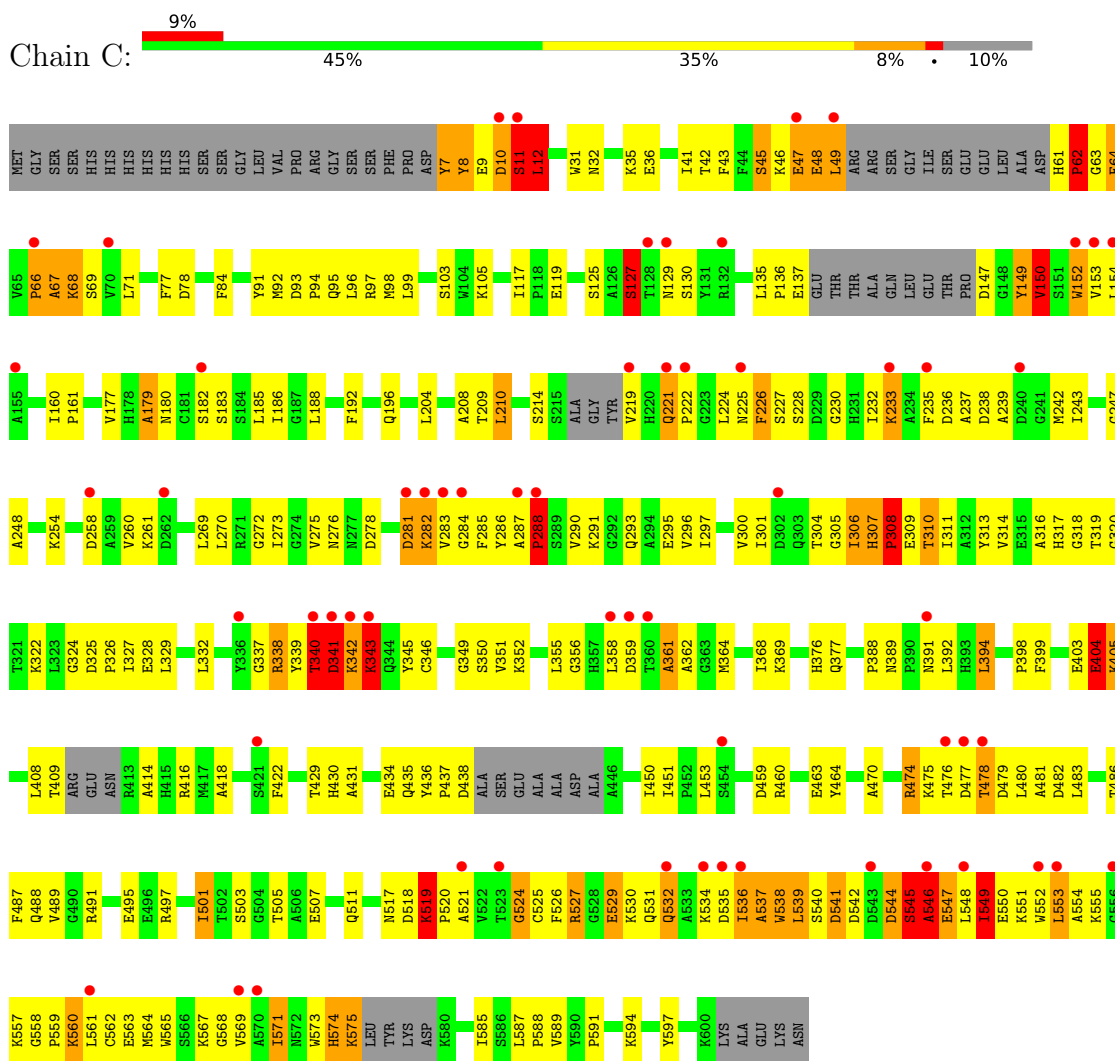
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-13	SER	-	expression tag	UNP Q1RS73
D	-12	HIS	-	expression tag	UNP Q1RS73
D	-11	HIS	-	expression tag	UNP Q1RS73
D	-10	HIS	-	expression tag	UNP Q1RS73
D	-9	HIS	-	expression tag	UNP Q1RS73
D	-8	HIS	-	expression tag	UNP Q1RS73
D	-7	HIS	-	expression tag	UNP Q1RS73
D	-6	SER	-	expression tag	UNP Q1RS73
D	-5	SER	-	expression tag	UNP Q1RS73
D	-4	GLY	-	expression tag	UNP Q1RS73
D	-3	LEU	-	expression tag	UNP Q1RS73
D	-2	VAL	-	expression tag	UNP Q1RS73
D	-1	PRO	-	expression tag	UNP Q1RS73
D	0	ARG	-	expression tag	UNP Q1RS73
D	1	GLY	-	expression tag	UNP Q1RS73
D	2	SER	-	expression tag	UNP Q1RS73
D	3	SER	-	expression tag	UNP Q1RS73

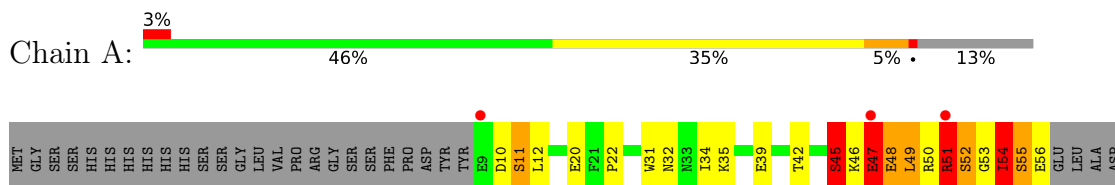
3 Residue-property plots

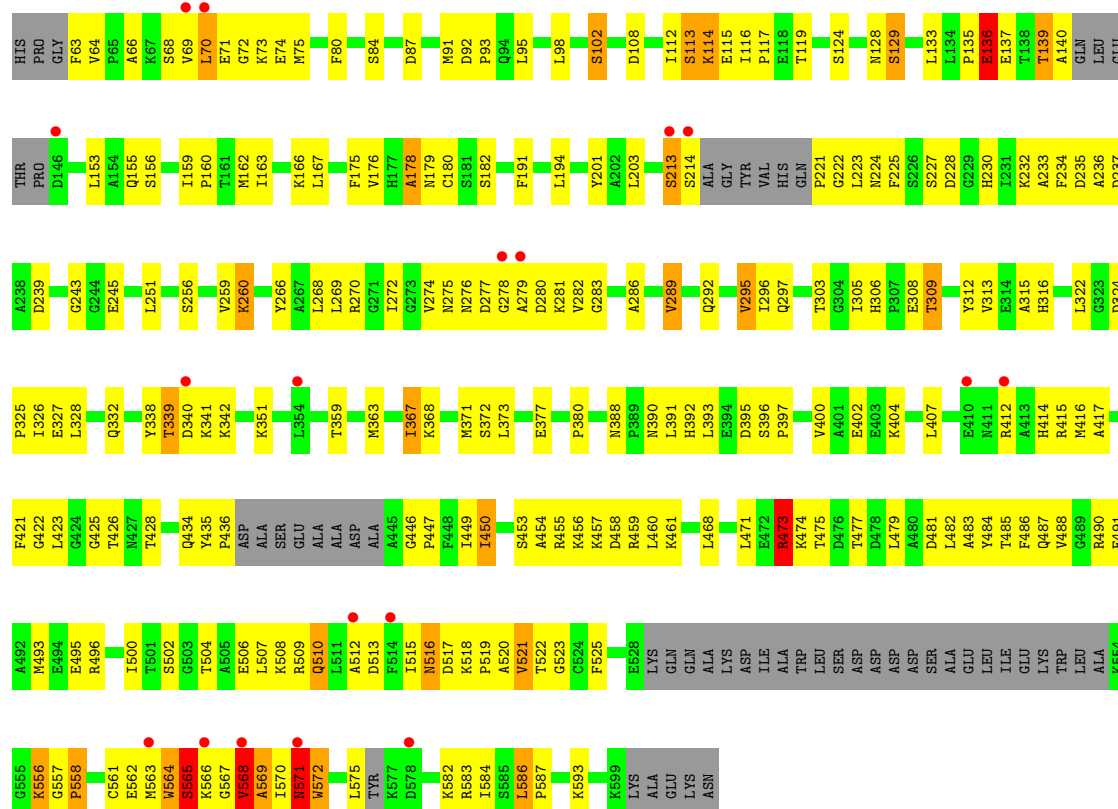
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NRPS/PKS protein

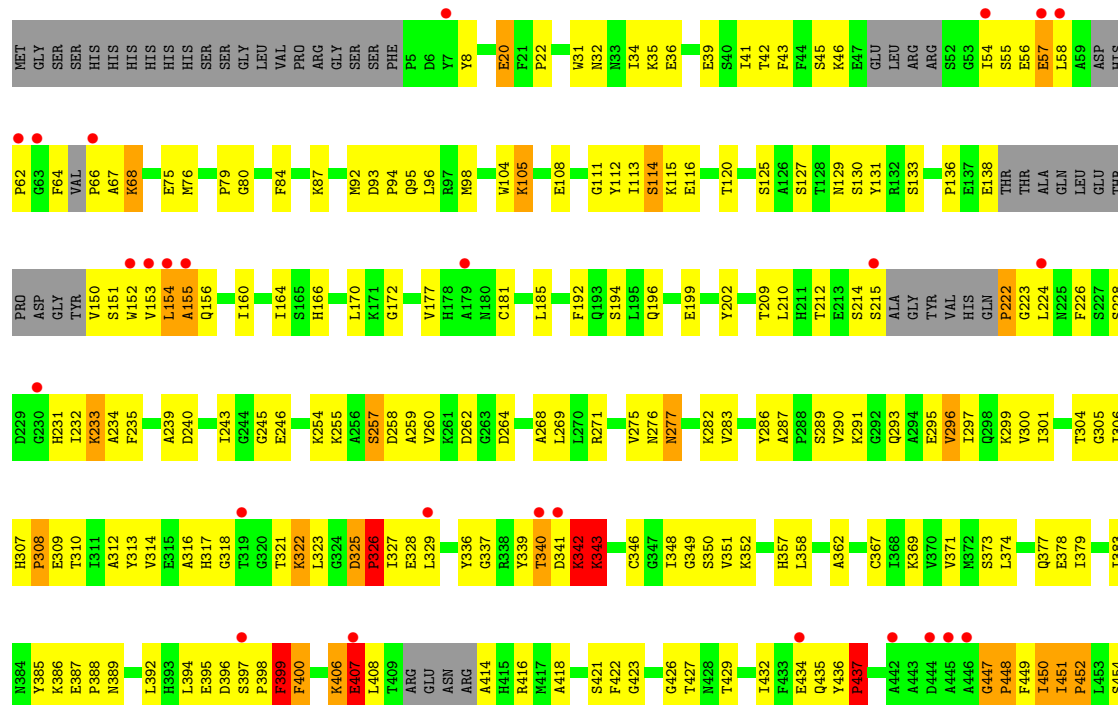


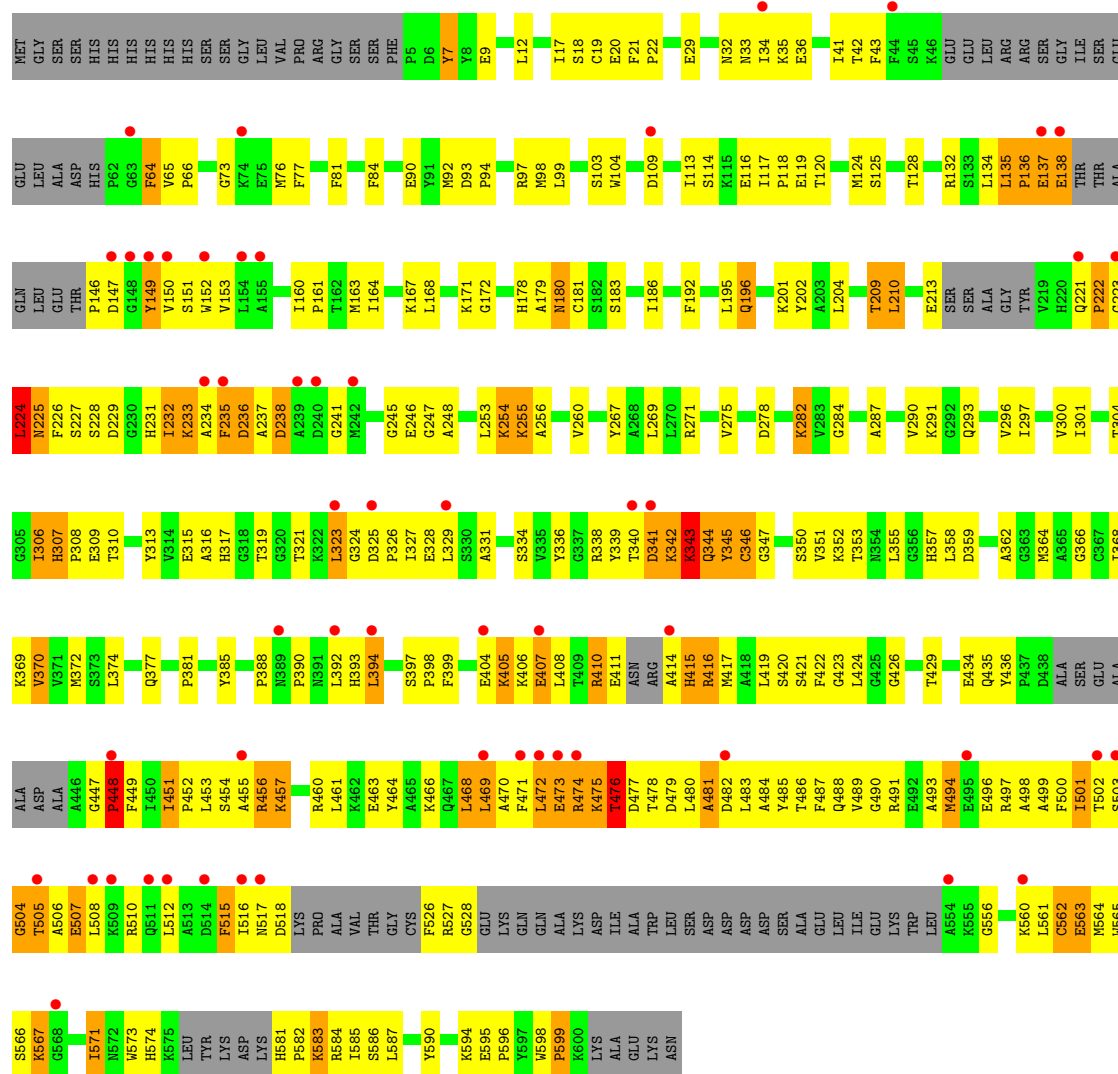
• Molecule 1: NRPS/PKS protein





- Molecule 1: NRPS/PKS protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.62Å 99.95Å 100.84Å 91.93° 88.18° 96.04°	Depositor
Resolution (Å)	99.35 – 2.93 99.35 – 2.93	Depositor EDS
% Data completeness (in resolution range)	94.9 (99.35-2.93) 94.9 (99.35-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.270 , 0.303 0.269 , 0.298	Depositor DCC
R_{free} test set	2426 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	16749	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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 ⓘ

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	0.86	3/4264 (0.1%)	1.42	38/5749 (0.7%)
1	B	0.77	2/4311 (0.0%)	1.16	38/5813 (0.7%)
1	C	0.89	7/4421 (0.2%)	1.53	87/5968 (1.5%)
1	D	0.84	9/4148 (0.2%)	1.41	68/5595 (1.2%)
All	All	0.84	21/17144 (0.1%)	1.39	231/23125 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	4
1	D	0	1
All	All	0	11

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	THR	CB-OG1	15.78	1.69	1.43
1	C	308	PRO	N-CD	13.55	1.66	1.47
1	C	288	PRO	N-CD	10.16	1.61	1.47
1	D	415	HIS	CA-C	10.00	1.66	1.52
1	D	414	ALA	CA-C	8.65	1.71	1.52
1	D	415	HIS	N-CA	-7.87	1.35	1.45
1	C	569	VAL	N-CA	7.39	1.55	1.46
1	D	416	ARG	N-CA	7.12	1.54	1.45
1	D	414	ALA	N-CA	-6.80	1.33	1.46
1	C	11	SER	C-N	-6.57	1.23	1.33
1	C	66	PRO	N-CD	6.48	1.56	1.47
1	D	448	PRO	N-CD	6.16	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	136	PRO	N-CD	6.14	1.56	1.47
1	C	531	GLN	CA-C	5.84	1.59	1.52
1	D	468	LEU	C-N	-5.82	1.24	1.33
1	A	225	PHE	CA-C	-5.66	1.46	1.52
1	B	326	PRO	N-CD	5.66	1.55	1.47
1	B	599	PRO	C-O	5.38	1.30	1.24
1	D	574	HIS	N-CA	5.35	1.53	1.46
1	A	48	GLU	N-CA	-5.30	1.40	1.46
1	C	8	TYR	C-N	-5.06	1.24	1.34

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	SER	N-CA-C	34.17	148.22	110.97
1	A	309	THR	CA-CB-OG1	34.17	160.85	109.60
1	C	150	VAL	N-CA-C	31.08	141.19	111.67
1	A	45	SER	CA-C-N	23.90	162.05	122.14
1	A	45	SER	C-N-CA	23.90	162.05	122.14
1	D	476	THR	N-CA-C	-19.58	84.27	111.87
1	D	474	ARG	N-CA-C	-19.49	79.78	109.60
1	D	475	LYS	N-CA-CB	-19.24	82.75	110.45
1	C	569	VAL	N-CA-C	18.44	147.69	109.34
1	A	565	SER	CB-CA-C	18.17	141.57	110.68
1	C	477	ASP	CB-CA-C	-17.19	78.93	109.86
1	D	473	GLU	N-CA-C	-16.99	89.75	114.39
1	B	57	GLU	CB-CA-C	16.52	143.30	110.42
1	C	150	VAL	N-CA-CB	-16.40	87.55	110.68
1	C	524	GLY	N-CA-C	-16.37	96.07	113.58
1	D	574	HIS	N-CA-C	16.20	132.65	112.23
1	C	340	THR	CB-CA-C	-15.77	85.30	109.90
1	A	309	THR	OG1-CB-CG2	-15.34	78.61	109.30
1	C	547	GLU	N-CA-CB	15.25	136.26	110.49
1	C	569	VAL	CB-CA-C	-15.22	86.32	111.29
1	D	469	LEU	N-CA-C	-15.10	92.49	114.39
1	D	468	LEU	N-CA-C	15.04	127.39	111.14
1	B	56	GLU	N-CA-C	14.97	131.88	112.72
1	A	563	MET	CB-CA-C	-14.92	85.00	110.81
1	C	478	THR	N-CA-C	-14.78	87.83	108.23
1	C	574	HIS	N-CA-C	14.61	129.08	112.57
1	D	137	GLU	N-CA-C	-14.50	89.25	110.42
1	D	405	LYS	N-CA-CB	-14.29	88.63	110.49
1	C	340	THR	N-CA-C	-13.38	90.17	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	404	GLU	N-CA-C	-12.44	91.33	108.86
1	C	9	GLU	N-CA-C	-12.38	88.07	108.49
1	B	57	GLU	N-CA-C	-12.04	85.14	110.80
1	D	137	GLU	CB-CA-C	11.86	126.19	109.71
1	A	225	PHE	N-CA-C	-11.82	90.81	109.72
1	C	547	GLU	N-CA-C	-11.80	85.66	110.80
1	C	404	GLU	N-CA-C	11.51	126.11	108.96
1	A	213	SER	N-CA-C	-11.37	90.13	108.55
1	C	530	LYS	N-CA-C	-11.35	90.48	108.63
1	B	155	ALA	N-CA-C	-11.28	90.02	108.41
1	A	565	SER	N-CA-C	-11.19	97.80	111.33
1	B	599	PRO	CB-CA-C	-11.01	93.40	111.56
1	B	154	LEU	CB-CA-C	-11.00	88.54	110.42
1	C	341	ASP	N-CA-C	-10.87	87.65	110.80
1	D	506	ALA	N-CA-C	-10.84	99.89	113.55
1	A	50	ARG	N-CA-C	-10.75	97.51	112.45
1	D	323	LEU	CB-CA-C	-10.57	93.90	111.02
1	C	12	LEU	N-CA-C	10.40	125.91	110.52
1	D	405	LYS	N-CA-C	10.39	126.47	110.36
1	C	477	ASP	N-CA-CB	-10.34	92.68	110.99
1	C	541	ASP	N-CA-C	-10.31	94.84	110.30
1	C	68	LYS	N-CA-C	10.29	125.26	110.14
1	C	180	ASN	N-CA-C	10.14	123.78	111.40
1	B	54	ILE	N-CA-C	-9.95	88.65	109.34
1	C	530	LYS	CB-CA-C	-9.73	95.31	110.88
1	B	222	PRO	N-CA-C	-9.40	88.60	112.10
1	C	68	LYS	N-CA-CB	-9.29	96.86	110.70
1	A	556	LYS	N-CA-C	9.24	124.80	109.46
1	D	235	PHE	CB-CA-C	-9.17	92.17	110.42
1	D	180	ASN	N-CA-C	9.10	130.19	110.80
1	D	475	LYS	N-CA-C	9.09	123.97	109.79
1	C	149	TYR	N-CA-C	9.00	124.89	113.55
1	D	468	LEU	CB-CA-C	-8.99	96.70	110.90
1	D	138	GLU	N-CA-C	-8.96	85.91	111.00
1	A	45	SER	CB-CA-C	-8.93	97.21	110.96
1	C	285	PHE	N-CA-CB	-8.84	95.56	110.49
1	D	475	LYS	CB-CA-C	8.81	133.25	113.33
1	C	214	SER	N-CA-C	8.81	122.03	111.02
1	D	447	GLY	C-N-CD	-8.72	89.24	125.00
1	C	285	PHE	N-CA-C	8.58	129.07	110.80
1	C	8	TYR	N-CA-C	-8.53	91.94	107.98
1	D	468	LEU	O-C-N	-8.38	113.04	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	TYR	CB-CA-C	8.35	122.28	109.34
1	D	416	ARG	N-CA-C	8.22	122.88	109.72
1	B	487	PHE	N-CA-C	-8.19	103.42	113.41
1	C	12	LEU	N-CA-CB	-8.17	97.39	110.46
1	C	545	SER	N-CA-C	-8.10	93.54	110.80
1	D	209	THR	CB-CA-C	-8.01	99.85	111.23
1	B	528	GLY	N-CA-C	8.01	117.50	110.21
1	A	179	ASN	CB-CA-C	-7.91	95.47	109.62
1	C	45	SER	CB-CA-C	7.89	123.97	109.46
1	C	307	HIS	CB-CA-C	7.89	125.71	110.17
1	C	546	ALA	N-CA-C	7.88	127.59	110.80
1	A	47	GLU	N-CA-C	-7.87	104.63	112.97
1	B	156	GLN	N-CA-C	-7.85	97.79	108.86
1	A	52	SER	N-CA-C	7.82	120.61	108.96
1	C	549	ILE	N-CA-C	-7.79	102.67	110.62
1	D	19	CYS	N-CA-C	7.78	120.69	108.79
1	A	564	TRP	CB-CA-C	-7.77	96.13	109.65
1	C	477	ASP	N-CA-C	-7.74	96.01	108.55
1	C	537	ALA	N-CA-C	-7.71	102.81	111.14
1	D	487	PHE	N-CA-C	-7.69	100.96	112.04
1	A	136	GLU	N-CA-C	7.66	121.97	109.72
1	A	54	ILE	N-CA-C	7.65	125.26	109.34
1	C	476	THR	N-CA-C	7.62	122.16	113.01
1	A	49	LEU	N-CA-C	7.56	120.17	110.65
1	C	282	LYS	N-CA-C	-7.54	94.73	110.80
1	B	399	PHE	CB-CA-C	-7.53	96.47	109.65
1	A	473	ARG	N-CA-C	7.52	119.16	110.97
1	C	308	PRO	CA-N-CD	-7.43	101.59	112.00
1	D	407	GLU	N-CA-C	-7.31	100.19	110.50
1	D	472	LEU	CB-CA-C	-7.26	95.97	110.42
1	C	66	PRO	CB-CA-C	-7.14	99.77	111.56
1	C	11	SER	O-C-N	-7.11	113.38	122.20
1	B	518	ASP	N-CA-C	7.05	125.81	110.80
1	D	507	GLU	N-CA-C	-7.01	100.18	111.04
1	C	288	PRO	N-CA-CB	6.99	110.59	103.25
1	A	10	ASP	N-CA-C	-6.99	103.33	112.41
1	C	521	ALA	N-CA-C	-6.98	103.10	111.69
1	C	536	ILE	CB-CA-C	-6.97	102.73	111.94
1	C	150	VAL	CB-CA-C	-6.97	103.57	111.80
1	D	414	ALA	N-CA-CB	6.96	120.84	110.40
1	D	469	LEU	N-CA-CB	6.91	120.10	110.98
1	B	468	LEU	N-CA-C	-6.89	103.45	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	288	PRO	CA-N-CD	-6.87	102.38	112.00
1	D	138	GLU	N-CA-CB	6.86	122.16	110.50
1	A	521	VAL	N-CA-C	6.85	117.64	110.72
1	C	179	ALA	N-CA-C	-6.82	99.04	109.41
1	D	515	PHE	N-CA-CB	6.82	120.55	110.53
1	C	536	ILE	N-CA-C	6.79	116.92	110.74
1	D	226	PHE	CB-CA-C	-6.77	97.44	109.70
1	C	11	SER	CB-CA-C	-6.76	96.91	111.78
1	B	325	ASP	CB-CA-C	-6.73	96.92	110.17
1	C	474	ARG	N-CA-C	6.68	120.53	112.38
1	A	412	ARG	CB-CA-C	-6.64	97.48	110.11
1	C	495	GLU	N-CA-C	6.62	119.05	111.11
1	D	415	HIS	O-C-N	6.61	130.46	123.06
1	D	415	HIS	N-CA-CB	6.61	121.18	110.41
1	C	538	TRP	N-CA-C	6.54	124.74	110.80
1	C	210	LEU	N-CA-C	-6.54	99.17	109.50
1	C	571	ILE	N-CA-C	-6.53	99.37	108.12
1	C	67	ALA	N-CA-CB	-6.52	100.69	110.60
1	C	525	CYS	N-CA-C	6.43	119.66	109.50
1	D	505	THR	CB-CA-C	-6.43	98.47	110.36
1	D	236	ASP	N-CA-C	-6.40	97.36	108.69
1	B	524	GLY	N-CA-C	-6.37	98.08	113.18
1	D	415	HIS	CA-C-N	6.36	132.80	122.81
1	D	415	HIS	C-N-CA	6.36	132.80	122.81
1	B	399	PHE	N-CA-C	6.33	119.90	108.69
1	C	67	ALA	N-CA-C	6.32	119.05	109.95
1	D	346	CYS	N-CA-C	6.32	119.24	109.07
1	D	307	HIS	CA-C-N	6.30	126.21	119.28
1	D	307	HIS	C-N-CA	6.30	126.21	119.28
1	C	208	ALA	N-CA-C	6.28	118.62	108.32
1	D	414	ALA	N-CA-C	-6.26	93.47	111.00
1	C	539	LEU	N-CA-C	-6.25	104.12	112.94
1	C	8	TYR	O-C-N	-6.25	114.31	122.43
1	A	339	THR	N-CA-C	6.25	118.01	108.52
1	C	127	SER	CB-CA-C	6.24	120.03	109.80
1	A	55	SER	N-CA-C	6.23	117.70	108.60
1	C	10	ASP	CB-CA-C	6.23	119.48	109.02
1	B	560	LYS	CB-CA-C	6.19	118.67	110.06
1	B	255	LYS	N-CA-C	-6.18	101.14	110.28
1	C	394	LEU	N-CA-C	6.17	120.42	113.01
1	C	67	ALA	CB-CA-C	-6.17	99.70	111.48
1	C	208	ALA	CB-CA-C	-6.16	99.47	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	437	PRO	CB-CA-C	-6.16	101.40	111.56
1	D	476	THR	N-CA-CB	6.15	120.98	111.39
1	D	253	LEU	N-CA-C	6.11	119.45	109.06
1	D	472	LEU	N-CA-C	-6.09	97.82	110.80
1	C	307	HIS	C-N-CD	-6.08	100.08	125.00
1	C	180	ASN	CB-CA-C	-6.07	100.59	110.79
1	A	178	ALA	N-CA-C	-6.07	97.95	108.69
1	D	180	ASN	CB-CA-C	-6.06	98.36	110.42
1	C	544	ASP	N-CA-C	-6.05	107.13	114.75
1	D	512	LEU	N-CA-C	-6.04	104.05	112.45
1	D	583	LYS	N-CA-C	6.01	118.69	108.90
1	B	574	HIS	N-CA-C	-6.00	107.78	114.62
1	C	306	ILE	N-CA-C	-5.97	99.82	108.36
1	A	572	TRP	N-CA-C	-5.88	106.02	113.43
1	C	531	GLN	N-CA-C	5.86	123.17	113.50
1	D	473	GLU	N-CA-CB	5.86	118.71	110.98
1	D	562	CYS	N-CA-C	-5.83	104.83	111.07
1	C	532	GLN	N-CA-C	5.83	118.78	110.68
1	C	47	GLU	N-CA-CB	-5.83	100.48	111.43
1	D	341	ASP	O-C-N	5.78	132.25	123.00
1	B	152	TRP	CA-C-N	5.77	130.37	121.19
1	B	152	TRP	C-N-CA	5.77	130.37	121.19
1	B	481	ALA	N-CA-C	-5.76	105.00	111.28
1	C	519	LYS	CA-C-N	-5.74	113.79	119.99
1	C	519	LYS	C-N-CA	-5.74	113.79	119.99
1	C	64	PHE	N-CA-C	-5.69	97.52	107.20
1	B	559	PRO	N-CA-C	5.68	124.17	112.47
1	D	152	TRP	N-CA-C	-5.67	101.91	110.70
1	B	340	THR	O-C-N	5.64	129.82	122.38
1	D	341	ASP	CA-C-N	5.62	133.67	123.27
1	D	341	ASP	C-N-CA	5.62	133.67	123.27
1	B	447	GLY	N-CA-C	5.61	123.79	112.34
1	D	504	GLY	N-CA-C	5.61	121.55	110.83
1	C	45	SER	N-CA-C	-5.60	102.19	110.48
1	B	342	LYS	N-CA-C	-5.59	98.89	110.80
1	C	531	GLN	CB-CA-C	-5.56	98.77	110.45
1	B	599	PRO	N-CA-C	5.55	123.91	112.47
1	B	527	ARG	N-CA-C	-5.55	103.21	110.53
1	C	62	PRO	CA-N-CD	-5.54	104.24	112.00
1	C	91	TYR	CB-CA-C	-5.53	101.25	110.81
1	A	557	GLY	N-CA-C	5.52	123.61	112.34
1	D	344	GLN	N-CA-C	-5.49	104.49	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	278	ASP	N-CA-C	5.47	117.33	111.36
1	C	66	PRO	CA-N-CD	-5.46	104.35	112.00
1	C	546	ALA	N-CA-CB	5.46	119.72	110.49
1	D	222	PRO	CB-CA-C	-5.40	102.65	111.56
1	A	556	LYS	CB-CA-C	-5.40	100.94	109.80
1	A	51	ARG	CB-CA-C	5.39	121.16	110.42
1	D	254	LYS	N-CA-CB	-5.38	102.34	111.69
1	B	517	ASN	N-CA-C	-5.36	107.05	113.21
1	A	565	SER	O-C-N	5.31	127.75	122.12
1	B	312	ALA	N-CA-C	5.31	116.87	111.14
1	D	135	LEU	CA-C-N	-5.29	114.54	120.14
1	D	135	LEU	C-N-CA	-5.29	114.54	120.14
1	C	9	GLU	N-CA-CB	5.28	119.31	111.23
1	B	407	GLU	N-CA-C	-5.28	100.30	108.90
1	A	49	LEU	CA-CB-CG	-5.26	97.88	116.30
1	B	548	LEU	N-CA-C	5.21	116.67	107.61
1	D	370	VAL	CB-CA-C	-5.21	105.04	112.22
1	A	48	GLU	CA-C-N	-5.17	114.70	122.24
1	A	48	GLU	C-N-CA	-5.17	114.70	122.24
1	D	415	HIS	CA-C-O	-5.16	115.16	121.36
1	B	514	ASP	N-CA-C	-5.15	105.12	111.40
1	D	253	LEU	CB-CA-C	-5.13	98.97	109.38
1	B	488	GLN	N-CA-C	-5.11	105.60	111.07
1	C	361	ALA	CB-CA-C	-5.10	102.52	110.37
1	C	281	ASP	N-CA-C	-5.09	100.58	108.42
1	A	558	PRO	N-CA-C	5.08	122.94	112.47
1	D	451	ILE	CB-CA-C	-5.08	104.88	110.52
1	A	289	VAL	CB-CA-C	-5.07	105.48	111.97
1	D	481	ALA	N-CA-C	-5.06	105.65	111.07
1	B	400	PHE	N-CA-C	5.05	118.44	109.96
1	D	556	GLY	N-CA-C	-5.04	106.09	112.54
1	B	296	VAL	N-CA-C	-5.01	105.50	110.62
1	C	306	ILE	CB-CA-C	-5.00	104.04	110.84
1	A	295	VAL	CB-CA-C	-5.00	105.32	112.22

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	SER	Peptide
1	A	51	ARG	Peptide
1	A	516	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	154	LEU	Peptide
1	B	517	ASN	Peptide
1	B	599	PRO	Mainchain
1	C	11	SER	Mainchain
1	C	546	ALA	Peptide
1	C	568	GLY	Peptide
1	C	8	TYR	Mainchain
1	D	468	LEU	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4169	0	4098	253	1
1	B	4213	0	4124	347	6
1	C	4317	0	4213	343	4
1	D	4050	0	3958	406	3
All	All	16749	0	16393	1343	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (1343) 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:309:THR:OG1	1:A:309:THR:CB	1.69	1.37
1:D:308:PRO:O	1:D:345:TYR:OH	1.54	1.23
1:D:345:TYR:N	1:D:398:PRO:O	1.78	1.15
1:D:340:THR:HA	1:D:341:ASP:HB2	1.18	1.14
1:D:342:LYS:HD3	1:D:342:LYS:H	1.13	1.13
1:D:340:THR:OG1	1:D:342:LYS:HB3	1.49	1.12
1:C:541:ASP:HB2	1:C:545:SER:CB	1.81	1.10
1:A:570:ILE:O	1:A:572:TRP:N	1.83	1.10
1:A:309:THR:OG1	1:A:309:THR:CG2	1.99	1.09
1:A:309:THR:HG21	1:A:415:ARG:HE	0.93	1.08
1:C:553:LEU:HG	1:C:574:HIS:HB2	1.28	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:PRO:HG2	1:C:327:ILE:HD12	1.35	1.06
1:A:309:THR:CG2	1:A:415:ARG:HE	1.71	1.03
1:C:541:ASP:CB	1:C:545:SER:HB3	1.90	1.01
1:A:570:ILE:HG22	1:A:572:TRP:HB2	1.37	1.00
1:C:541:ASP:HB2	1:C:545:SER:HB3	1.02	0.99
1:C:307:HIS:CE1	1:C:340:THR:OG1	2.18	0.96
1:A:309:THR:HG21	1:A:415:ARG:NE	1.79	0.96
1:B:482:ASP:OD1	1:B:582:PRO:HB2	1.66	0.96
1:D:340:THR:HB	1:D:342:LYS:N	1.80	0.95
1:D:308:PRO:HG2	1:D:339:TYR:CD2	2.01	0.95
1:A:309:THR:OG1	1:A:309:THR:HG21	1.65	0.94
1:D:598:TRP:CD1	1:D:599:PRO:HD2	2.01	0.94
1:C:541:ASP:CB	1:C:545:SER:CB	2.45	0.94
1:B:386:LYS:HG3	1:B:387:GLU:HG2	1.50	0.94
1:C:48:GLU:OE2	1:C:48:GLU:N	2.01	0.94
1:C:553:LEU:CG	1:C:574:HIS:HB2	1.97	0.94
1:D:340:THR:CA	1:D:341:ASP:HB2	1.98	0.93
1:D:342:LYS:CA	1:D:343:LYS:HE3	1.98	0.93
1:D:245:GLY:C	1:D:358:LEU:HD23	1.93	0.93
1:C:478:THR:HG22	1:C:479:ASP:H	1.32	0.93
1:C:474:ARG:NH2	1:A:339:THR:HA	1.84	0.93
1:D:34:ILE:HD13	1:D:369:LYS:HG3	1.49	0.92
1:D:381:PRO:HD3	1:D:405:LYS:HG2	1.47	0.92
1:D:502:THR:HG22	1:D:503:SER:H	1.33	0.91
1:B:416:ARG:HG2	1:B:434:GLU:OE1	1.70	0.91
1:C:12:LEU:HD12	1:C:270:LEU:HD23	1.52	0.91
1:D:561:LEU:HG	1:D:563:GLU:CB	2.00	0.91
1:D:209:THR:C	1:D:210:LEU:HD23	1.96	0.91
1:D:342:LYS:HA	1:D:343:LYS:HE3	1.53	0.91
1:D:340:THR:HB	1:D:341:ASP:C	1.95	0.90
1:D:377:GLN:OE1	1:D:435:GLN:NE2	2.03	0.90
1:B:511:GLN:NE2	1:B:523:THR:HA	1.87	0.90
1:D:473:GLU:C	1:D:474:ARG:O	1.90	0.90
1:D:561:LEU:HG	1:D:563:GLU:HB2	1.51	0.90
1:B:310:THR:HG21	1:B:416:ARG:HE	1.35	0.90
1:D:499:ALA:C	1:D:500:PHE:HD1	1.79	0.89
1:D:344:GLN:H	1:D:398:PRO:HA	1.37	0.89
1:B:480:LEU:O	1:B:484:ALA:N	2.05	0.89
1:D:136:PRO:O	1:D:137:GLU:C	2.15	0.89
1:D:310:THR:HG21	1:D:416:ARG:HH11	1.36	0.89
1:C:307:HIS:HE1	1:C:340:THR:OG1	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:TRP:CD1	1:C:557:LYS:CE	2.56	0.88
1:C:529:GLU:O	1:C:567:LYS:HD3	1.72	0.88
1:A:315:ALA:HB1	1:A:327:GLU:OE2	1.73	0.88
1:B:486:THR:O	1:B:489:VAL:O	1.90	0.88
1:C:545:SER:OG	1:C:549:ILE:HG21	1.72	0.88
1:A:338:TYR:O	1:A:339:THR:OG1	1.91	0.88
1:B:192:PHE:CE2	1:B:196:GLN:NE2	2.41	0.88
1:B:551:LYS:HD3	1:B:552:TRP:CZ3	2.08	0.87
1:C:403:GLU:C	1:C:404:GLU:HG3	1.99	0.87
1:A:341:LYS:HD3	1:A:395:ASP:OD1	1.75	0.87
1:B:307:HIS:NE2	1:B:340:THR:HB	1.89	0.87
1:D:317:HIS:N	1:D:328:GLU:OE2	2.07	0.87
1:B:75:GLU:OE1	1:B:75:GLU:N	2.05	0.87
1:B:480:LEU:HA	1:B:483:LEU:HB3	1.55	0.86
1:C:290:VAL:HG22	1:C:327:ILE:HG23	1.55	0.86
1:A:496:ARG:HD2	1:A:565:SER:O	1.74	0.86
1:D:561:LEU:CD1	1:D:563:GLU:HB2	2.06	0.86
1:C:233:LYS:HD3	1:C:238:ASP:O	1.74	0.86
1:B:58:LEU:CD1	1:B:62:PRO:HB3	2.04	0.86
1:D:232:ILE:HG23	1:D:353:THR:HA	1.57	0.85
1:B:277:ASN:OD1	1:B:427:THR:OG1	1.95	0.84
1:D:232:ILE:CG2	1:D:353:THR:HA	2.07	0.84
1:D:515:PHE:HE1	1:D:518:ASP:CG	1.85	0.84
1:B:504:GLY:O	1:B:507:GLU:HB3	1.76	0.84
1:D:515:PHE:HE1	1:D:518:ASP:OD1	1.61	0.84
1:B:447:GLY:O	1:B:503:SER:OG	1.94	0.83
1:C:185:LEU:CD2	1:C:429:THR:OG1	2.25	0.83
1:B:296:VAL:O	1:B:300:VAL:HG23	1.79	0.83
1:B:495:GLU:N	1:B:495:GLU:OE1	2.11	0.83
1:A:508:LYS:O	1:A:512:ALA:N	2.10	0.83
1:D:278:ASP:OD1	1:D:426:GLY:O	1.96	0.83
1:C:11:SER:HB2	1:C:270:LEU:O	1.79	0.83
1:C:486:THR:O	1:C:489:VAL:O	1.94	0.83
1:D:344:GLN:HA	1:D:398:PRO:C	2.03	0.83
1:D:357:HIS:CD2	1:D:359:ASP:OD1	2.32	0.82
1:C:546:ALA:O	1:C:550:GLU:HB2	1.79	0.82
1:A:136:GLU:C	1:A:137:GLU:HG3	2.03	0.82
1:C:552:TRP:CD1	1:C:557:LYS:HE2	2.14	0.82
1:A:289:VAL:HG22	1:A:326:ILE:HG23	1.59	0.82
1:B:112:TYR:CE1	1:B:584:ARG:NH1	2.47	0.82
1:D:293:GLN:O	1:D:296:VAL:HG12	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ILE:HG12	1:C:431:ALA:HB2	1.62	0.82
1:B:58:LEU:HD12	1:B:62:PRO:HB3	1.59	0.82
1:B:394:LEU:O	1:B:397:SER:HB3	1.78	0.82
1:B:194:SER:CB	1:B:199:GLU:OE2	2.27	0.82
1:C:389:ASN:OD1	1:C:391:ASN:N	2.12	0.82
1:A:564:TRP:CD2	1:A:564:TRP:O	2.33	0.82
1:C:281:ASP:C	1:C:282:LYS:O	2.11	0.81
1:C:288:PRO:HG2	1:C:327:ILE:CD1	2.09	0.81
1:D:456:ARG:NH1	1:D:494:MET:SD	2.53	0.81
1:D:561:LEU:CG	1:D:563:GLU:HB2	2.09	0.81
1:B:93:ASP:OD1	1:B:94:PRO:HD2	1.80	0.81
1:B:584:ARG:O	1:B:585:ILE:HD13	1.80	0.81
1:C:288:PRO:O	1:C:327:ILE:HD13	1.81	0.81
1:B:511:GLN:HE22	1:B:523:THR:HA	1.45	0.81
1:D:309:GLU:HA	1:D:345:TYR:CZ	2.16	0.81
1:C:306:ILE:HG22	1:C:307:HIS:O	1.80	0.80
1:C:546:ALA:N	1:C:549:ILE:HG22	1.96	0.80
1:A:221:PRO:HG3	1:A:227:SER:HA	1.62	0.80
1:A:388:ASN:HB3	1:A:391:LEU:HG	1.61	0.80
1:D:342:LYS:HE2	1:D:342:LYS:O	1.80	0.80
1:A:308:GLU:OE2	1:A:339:THR:HG21	1.80	0.80
1:D:246:GLU:N	1:D:358:LEU:CD2	2.45	0.80
1:D:357:HIS:HD2	1:D:359:ASP:OD1	1.64	0.80
1:D:499:ALA:C	1:D:500:PHE:CD1	2.59	0.80
1:A:316:HIS:O	1:A:351:LYS:HE2	1.81	0.80
1:A:98:LEU:O	1:A:102:SER:OG	1.98	0.80
1:C:185:LEU:HD22	1:C:429:THR:OG1	1.82	0.80
1:C:332:LEU:HG	1:C:399:PHE:HZ	1.47	0.80
1:B:564:MET:O	1:B:568:GLY:HA3	1.82	0.80
1:C:553:LEU:HG	1:C:574:HIS:CB	2.10	0.79
1:A:506:GLU:O	1:A:510:GLN:HG3	1.82	0.79
1:B:497:ARG:O	1:B:528:GLY:HA3	1.83	0.79
1:C:392:LEU:HB2	1:C:394:LEU:HG	1.63	0.79
1:B:76:MET:SD	1:B:596:PRO:HB3	2.23	0.79
1:B:245:GLY:C	1:B:358:LEU:HD23	2.08	0.79
1:D:32:ASN:HA	1:D:35:LYS:HG2	1.64	0.79
1:B:389:ASN:HB3	1:B:392:LEU:HG	1.64	0.79
1:C:222:PRO:HG3	1:C:228:SER:HA	1.64	0.79
1:C:364:MET:HA	1:C:364:MET:HE3	1.64	0.79
1:B:96:LEU:HD13	1:B:160:ILE:HA	1.64	0.79
1:C:332:LEU:HG	1:C:399:PHE:CZ	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ARG:NH1	1:B:271:ARG:HB3	1.99	0.78
1:B:282:LYS:HG2	1:B:287:ALA:HB1	1.64	0.78
1:C:552:TRP:CD1	1:C:557:LYS:HE3	2.18	0.78
1:B:523:THR:OG1	1:B:525:CYS:HB2	1.84	0.78
1:D:308:PRO:C	1:D:345:TYR:OH	2.26	0.78
1:C:10:ASP:O	1:C:196:GLN:OE1	2.01	0.78
1:D:209:THR:O	1:D:210:LEU:HD23	1.83	0.78
1:B:42:THR:HG22	1:B:68:LYS:O	1.82	0.78
1:B:462:LYS:NZ	1:B:518:ASP:OD1	2.15	0.78
1:D:304:THR:HB	1:D:306:ILE:HG13	1.65	0.78
1:D:342:LYS:C	1:D:343:LYS:HE3	2.07	0.78
1:B:595:GLU:OE1	1:B:597:TYR:OH	2.00	0.78
1:D:321:THR:HG22	1:D:323:LEU:H	1.48	0.78
1:A:457:LYS:O	1:A:461:LYS:HG3	1.83	0.77
1:D:300:VAL:O	1:D:304:THR:HG23	1.84	0.77
1:D:227:SER:HB2	1:D:241:GLY:O	1.84	0.77
1:D:598:TRP:CG	1:D:599:PRO:HD2	2.18	0.77
1:B:43:PHE:CD1	1:B:67:ALA:HB2	2.19	0.77
1:C:307:HIS:ND1	1:C:309:GLU:HG2	1.99	0.77
1:B:111:GLY:O	1:B:584:ARG:NH2	2.17	0.77
1:D:479:ASP:OD1	1:D:481:ALA:N	2.16	0.77
1:C:338:ARG:HG3	1:C:338:ARG:HH11	1.49	0.77
1:B:194:SER:HB2	1:B:199:GLU:OE2	1.85	0.77
1:A:136:GLU:O	1:A:137:GLU:HG3	1.85	0.76
1:B:482:ASP:OD1	1:B:582:PRO:CB	2.33	0.76
1:C:270:LEU:HD21	1:C:273:ILE:HD12	1.67	0.76
1:B:484:ALA:O	1:B:488:GLN:HG3	1.85	0.76
1:C:233:LYS:HB2	1:C:239:ALA:HA	1.66	0.76
1:C:549:ILE:O	1:C:552:TRP:HB2	1.85	0.76
1:D:201:LYS:HG2	1:D:202:TYR:CE1	2.20	0.76
1:D:310:THR:HG21	1:D:416:ARG:NH1	1.99	0.76
1:D:342:LYS:HD3	1:D:342:LYS:N	1.94	0.76
1:B:513:ALA:O	1:B:517:ASN:HB2	1.85	0.76
1:B:547:GLU:O	1:B:548:LEU:CD2	2.34	0.76
1:C:105:LYS:HG2	1:C:589:VAL:HG21	1.66	0.76
1:C:535:ASP:O	1:C:539:LEU:HB2	1.86	0.76
1:B:231:HIS:O	1:B:233:LYS:HD2	1.86	0.76
1:D:394:LEU:O	1:D:397:SER:OG	2.03	0.75
1:B:523:THR:OG1	1:B:525:CYS:CB	2.34	0.75
1:D:499:ALA:O	1:D:500:PHE:HD1	1.70	0.75
1:D:502:THR:HG22	1:D:503:SER:N	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:515:PHE:CE1	1:D:518:ASP:CG	2.64	0.75
1:C:41:ILE:CD1	1:C:69:SER:HB2	2.16	0.75
1:C:488:GLN:OE1	1:C:575:LYS:NZ	2.16	0.75
1:D:466:LYS:O	1:D:470:ALA:HB3	1.86	0.75
1:B:20:GLU:OE1	1:B:98:MET:HE1	1.86	0.75
1:C:553:LEU:C	1:C:555:LYS:H	1.94	0.75
1:D:366:GLY:O	1:D:370:VAL:HG23	1.87	0.75
1:D:474:ARG:NH1	1:D:587:LEU:HD23	2.01	0.75
1:C:341:ASP:OD2	1:C:398:PRO:HG3	1.87	0.75
1:C:553:LEU:CD1	1:C:574:HIS:HB2	2.15	0.74
1:B:282:LYS:HG2	1:B:287:ALA:CB	2.17	0.74
1:D:310:THR:CG2	1:D:416:ARG:HD2	2.16	0.74
1:A:449:ILE:C	1:A:450:ILE:HD13	2.11	0.74
1:D:340:THR:HA	1:D:341:ASP:CB	2.07	0.74
1:A:306:HIS:O	1:A:309:THR:HB	1.87	0.74
1:B:547:GLU:C	1:B:548:LEU:HG	2.13	0.74
1:C:288:PRO:CG	1:C:327:ILE:HD12	2.15	0.74
1:C:541:ASP:HB3	1:C:545:SER:HB2	1.69	0.74
1:C:179:ALA:O	1:C:183:SER:OG	2.05	0.74
1:C:332:LEU:CD2	1:C:399:PHE:CZ	2.71	0.74
1:B:456:ARG:HA	1:B:495:GLU:OE2	1.88	0.74
1:B:547:GLU:O	1:B:548:LEU:HG	1.88	0.74
1:A:586:LEU:HB3	1:A:587:PRO:HD2	1.69	0.74
1:B:394:LEU:HA	1:B:397:SER:HB3	1.68	0.74
1:A:482:LEU:HD23	1:A:486:PHE:HD2	1.52	0.74
1:C:49:LEU:HD23	1:C:49:LEU:N	2.03	0.73
1:C:152:TRP:O	1:C:153:VAL:HG22	1.87	0.73
1:B:352:LYS:NZ	1:B:357:HIS:ND1	2.32	0.73
1:C:552:TRP:HD1	1:C:557:LYS:HE2	1.52	0.73
1:D:227:SER:HB2	1:D:241:GLY:C	2.13	0.73
1:D:471:PHE:O	1:D:473:GLU:N	2.21	0.73
1:B:497:ARG:O	1:B:528:GLY:CA	2.37	0.73
1:D:501:ILE:HG21	1:D:560:LYS:HD3	1.69	0.73
1:C:541:ASP:OD1	1:C:541:ASP:O	2.06	0.73
1:B:547:GLU:O	1:B:548:LEU:HD23	1.89	0.73
1:C:11:SER:CB	1:C:270:LEU:O	2.36	0.73
1:C:254:LYS:HE2	1:C:258:ASP:O	1.89	0.73
1:C:343:LYS:O	1:C:345:TYR:HD1	1.72	0.73
1:D:346:CYS:HB3	1:D:399:PHE:CD1	2.23	0.73
1:A:481:ASP:HB3	1:A:584:ILE:CG1	2.19	0.73
1:B:495:GLU:CD	1:B:495:GLU:H	1.95	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:THR:C	1:D:342:LYS:HD3	2.14	0.73
1:A:390:ASN:O	1:A:392:HIS:CE1	2.42	0.73
1:D:469:LEU:HD23	1:D:472:LEU:HB2	1.70	0.73
1:C:478:THR:HG22	1:C:479:ASP:N	2.03	0.72
1:C:541:ASP:CB	1:C:545:SER:HB2	2.17	0.72
1:A:482:LEU:HD23	1:A:482:LEU:O	1.89	0.72
1:B:308:PRO:HB3	1:B:336:TYR:CD2	2.24	0.72
1:C:233:LYS:O	1:C:320:GLY:HA2	1.88	0.72
1:B:414:ALA:HB3	1:B:435:GLN:HB3	1.70	0.72
1:C:224:LEU:HD23	1:C:224:LEU:O	1.89	0.72
1:C:518:ASP:C	1:C:520:PRO:HD3	2.14	0.72
1:D:151:SER:CA	1:D:153:VAL:HG13	2.20	0.72
1:A:11:SER:HB2	1:A:269:LEU:O	1.89	0.72
1:A:281:LYS:HD2	1:A:286:ALA:O	1.89	0.72
1:D:201:LYS:HE3	1:D:254:LYS:HE3	1.72	0.72
1:A:582:LYS:HE3	1:A:584:ILE:HD11	1.70	0.72
1:D:224:LEU:N	1:D:224:LEU:HD12	2.04	0.72
1:D:317:HIS:O	1:D:352:LYS:CE	2.37	0.72
1:A:80:PHE:CD1	1:A:455:ARG:HG3	2.24	0.71
1:B:394:LEU:HA	1:B:397:SER:CB	2.19	0.71
1:C:273:ILE:HG12	1:C:431:ALA:CB	2.19	0.71
1:D:235:PHE:O	1:D:385:TYR:HE1	1.73	0.71
1:D:515:PHE:CE1	1:D:518:ASP:CB	2.72	0.71
1:B:310:THR:HG21	1:B:416:ARG:NE	2.06	0.71
1:C:559:PRO:O	1:C:562:CYS:N	2.24	0.71
1:D:394:LEU:HA	1:D:397:SER:OG	1.90	0.71
1:B:125:SER:HB3	1:B:177:VAL:O	1.90	0.71
1:B:181:CYS:HB2	1:B:423:GLY:HA2	1.72	0.71
1:B:511:GLN:O	1:B:514:ASP:HB2	1.91	0.71
1:D:34:ILE:CD1	1:D:369:LYS:HG3	2.21	0.71
1:B:511:GLN:HA	1:B:514:ASP:HB2	1.71	0.71
1:B:551:LYS:HD3	1:B:552:TRP:HZ3	1.51	0.70
1:D:224:LEU:O	1:D:225:ASN:HB2	1.90	0.70
1:C:340:THR:OG1	1:C:340:THR:O	1.96	0.70
1:C:511:GLN:NE2	1:C:524:GLY:HA3	2.06	0.70
1:D:293:GLN:HG2	1:D:422:PHE:CE2	2.27	0.70
1:C:474:ARG:HH21	1:A:339:THR:HA	1.54	0.70
1:D:507:GLU:O	1:D:510:ARG:HB2	1.91	0.70
1:C:537:ALA:HA	1:C:540:SER:OG	1.92	0.70
1:A:390:ASN:O	1:A:392:HIS:ND1	2.25	0.70
1:B:394:LEU:C	1:B:397:SER:HB3	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ARG:HB3	1:D:271:ARG:HH11	1.56	0.70
1:C:487:PHE:HD1	1:C:491:ARG:HG3	1.57	0.70
1:A:292:GLN:HG2	1:A:421:PHE:CZ	2.27	0.70
1:D:76:MET:SD	1:D:594:LYS:HB3	2.32	0.70
1:D:474:ARG:HH12	1:D:587:LEU:HD23	1.56	0.70
1:A:484:TYR:O	1:A:488:VAL:HG22	1.91	0.70
1:D:466:LYS:O	1:D:470:ALA:CB	2.39	0.70
1:B:528:GLY:O	1:B:566:SER:O	2.10	0.70
1:D:344:GLN:C	1:D:398:PRO:O	2.34	0.70
1:C:405:LYS:O	1:C:405:LYS:HG2	1.92	0.69
1:A:51:ARG:HG2	1:A:52:SER:H	1.55	0.69
1:D:344:GLN:N	1:D:398:PRO:HA	2.07	0.69
1:B:379:ILE:HB	1:B:406:LYS:HB2	1.73	0.69
1:D:113:ILE:HD12	1:D:116:GLU:CD	2.17	0.69
1:B:511:GLN:NE2	1:B:523:THR:HG22	2.06	0.69
1:D:421:SER:HB3	1:D:429:THR:OG1	1.91	0.69
1:D:410:ARG:O	1:D:411:GLU:HG3	1.91	0.69
1:C:209:THR:OG1	1:C:359:ASP:HB2	1.92	0.69
1:C:474:ARG:NH2	1:A:339:THR:CA	2.55	0.69
1:D:358:LEU:O	1:D:362:ALA:N	2.26	0.69
1:A:564:TRP:O	1:A:564:TRP:CG	2.43	0.69
1:A:583:ARG:O	1:A:584:ILE:HD13	1.93	0.69
1:D:342:LYS:H	1:D:342:LYS:CD	1.98	0.69
1:C:317:HIS:O	1:C:352:LYS:HE2	1.92	0.69
1:D:151:SER:C	1:D:153:VAL:HG13	2.18	0.69
1:D:340:THR:CB	1:D:342:LYS:HB3	2.23	0.69
1:D:394:LEU:HA	1:D:397:SER:CB	2.23	0.69
1:D:485:TYR:HH	1:D:573:TRP:HZ3	1.41	0.68
1:B:104:TRP:NE1	1:B:108:GLU:OE2	2.25	0.68
1:B:502:THR:HG21	1:B:508:LEU:HA	1.74	0.68
1:D:271:ARG:HB3	1:D:271:ARG:NH1	2.08	0.68
1:B:293:GLN:O	1:B:297:ILE:HG13	1.93	0.68
1:B:480:LEU:HA	1:B:483:LEU:CB	2.22	0.68
1:D:343:LYS:HD2	1:D:343:LYS:N	2.08	0.68
1:C:236:ASP:OD1	1:C:237:ALA:N	2.27	0.68
1:B:317:HIS:N	1:B:328:GLU:OE2	2.22	0.68
1:C:338:ARG:HH11	1:C:338:ARG:CG	2.07	0.68
1:D:341:ASP:N	1:D:342:LYS:HD3	2.07	0.68
1:D:480:LEU:HD11	1:D:505:THR:HB	1.74	0.68
1:C:316:ALA:HB1	1:C:328:GLU:OE2	1.94	0.68
1:D:35:LYS:HG3	1:D:36:GLU:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:501:ILE:CG2	1:D:560:LYS:HD3	2.23	0.68
1:D:293:GLN:HG2	1:D:422:PHE:CZ	2.29	0.68
1:D:132:ARG:NH1	1:D:153:VAL:HG22	2.09	0.68
1:C:358:LEU:HD23	1:C:361:ALA:C	2.18	0.67
1:C:529:GLU:O	1:C:567:LYS:CD	2.41	0.67
1:B:228:SER:HB3	1:B:240:ASP:OD2	1.95	0.67
1:D:309:GLU:HA	1:D:345:TYR:OH	1.93	0.67
1:C:270:LEU:HD11	1:C:273:ILE:HG13	1.77	0.67
1:C:416:ARG:NH1	1:C:434:GLU:OE1	2.28	0.67
1:A:11:SER:CB	1:A:269:LEU:O	2.43	0.67
1:C:185:LEU:HD23	1:C:429:THR:OG1	1.94	0.67
1:C:338:ARG:HG3	1:C:338:ARG:NH1	2.07	0.67
1:A:34:ILE:HD12	1:A:368:LYS:HG3	1.77	0.67
1:A:278:GLY:C	1:A:280:ASP:H	2.03	0.67
1:A:457:LYS:CG	1:A:495:GLU:OE1	2.43	0.67
1:C:358:LEU:HD23	1:C:361:ALA:CB	2.25	0.67
1:C:532:GLN:HB3	1:C:535:ASP:HB3	1.75	0.67
1:D:331:ALA:O	1:D:334:SER:OG	2.13	0.67
1:D:394:LEU:CA	1:D:397:SER:OG	2.42	0.67
1:C:497:ARG:NH2	1:C:565:TRP:O	2.26	0.67
1:A:485:THR:O	1:A:488:VAL:O	2.11	0.67
1:D:475:LYS:HB3	1:D:477:ASP:HB2	1.77	0.67
1:B:341:ASP:CG	1:B:342:LYS:H	2.03	0.66
1:A:12:LEU:HD11	1:A:191:PHE:HA	1.75	0.66
1:C:270:LEU:HD21	1:C:273:ILE:CD1	2.26	0.66
1:A:277:ASP:N	1:A:425:GLY:O	2.18	0.66
1:B:483:LEU:HD23	1:B:483:LEU:C	2.21	0.66
1:C:358:LEU:HB3	1:C:362:ALA:N	2.10	0.66
1:A:95:LEU:HD13	1:A:159:ILE:HA	1.77	0.66
1:B:120:THR:O	1:B:172:GLY:HA3	1.96	0.66
1:D:482:ASP:OD1	1:D:483:LEU:N	2.29	0.66
1:C:41:ILE:HD13	1:C:69:SER:HB2	1.77	0.66
1:B:160:ILE:O	1:B:164:ILE:HG13	1.95	0.66
1:A:481:ASP:HB3	1:A:584:ILE:HG13	1.78	0.66
1:D:132:ARG:HH11	1:D:153:VAL:HG23	1.61	0.66
1:D:246:GLU:C	1:D:358:LEU:HD22	2.20	0.66
1:D:475:LYS:C	1:D:477:ASP:H	1.96	0.66
1:C:224:LEU:O	1:C:225:ASN:HB2	1.96	0.66
1:B:64:PHE:HE1	1:B:226:PHE:HB3	1.61	0.66
1:D:344:GLN:HA	1:D:398:PRO:O	1.96	0.66
1:D:344:GLN:CA	1:D:398:PRO:O	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:ARG:NH1	1:D:463:GLU:OE1	2.28	0.66
1:B:571:ILE:O	1:B:571:ILE:HG13	1.96	0.65
1:D:132:ARG:NH1	1:D:153:VAL:CG2	2.59	0.65
1:B:58:LEU:HD11	1:B:62:PRO:HB3	1.79	0.65
1:A:235:ASP:OD1	1:A:236:ALA:N	2.29	0.65
1:B:112:TYR:CZ	1:B:584:ARG:NH1	2.63	0.65
1:B:310:THR:CG2	1:B:416:ARG:HE	2.09	0.65
1:D:497:ARG:HB3	1:D:565:TRP:CZ3	2.31	0.65
1:B:394:LEU:CA	1:B:397:SER:HB3	2.26	0.65
1:C:519:LYS:N	1:C:520:PRO:HD3	2.11	0.65
1:C:527:ARG:CG	1:C:527:ARG:HH11	2.10	0.65
1:C:553:LEU:O	1:C:555:LYS:N	2.29	0.65
1:B:301:ILE:O	1:B:305:GLY:N	2.28	0.65
1:B:451:ILE:N	1:B:451:ILE:HD13	2.11	0.65
1:D:103:SER:HB3	1:D:204:LEU:HD21	1.79	0.65
1:B:472:LEU:O	1:B:475:LYS:O	2.15	0.65
1:D:151:SER:HA	1:D:153:VAL:HG13	1.78	0.65
1:C:540:SER:O	1:C:541:ASP:C	2.39	0.65
1:A:571:ASN:ND2	1:A:571:ASN:H	1.94	0.65
1:D:485:TYR:OH	1:D:573:TRP:HZ3	1.80	0.65
1:D:448:PRO:C	1:D:449:PHE:CD1	2.75	0.64
1:A:519:PRO:HB2	1:A:521:VAL:HG23	1.78	0.64
1:B:290:VAL:HG22	1:B:327:ILE:HG23	1.77	0.64
1:C:296:VAL:O	1:C:300:VAL:HG23	1.96	0.64
1:B:84:PHE:CZ	1:B:92:MET:HE1	2.31	0.64
1:B:526:PHE:CE2	1:B:562:CYS:HB2	2.32	0.64
1:D:515:PHE:CD1	1:D:518:ASP:HA	2.33	0.64
1:C:291:LYS:O	1:C:295:GLU:HG3	1.98	0.64
1:C:342:LYS:O	1:C:343:LYS:HB3	1.95	0.64
1:A:482:LEU:HD21	1:A:486:PHE:CE2	2.32	0.64
1:B:93:ASP:OD1	1:B:94:PRO:CD	2.44	0.64
1:C:358:LEU:CB	1:C:362:ALA:N	2.61	0.64
1:C:550:GLU:O	1:C:551:LYS:C	2.40	0.64
1:B:202:TYR:CE2	1:B:254:LYS:HE3	2.33	0.64
1:A:490:ARG:HG2	1:A:490:ARG:HH11	1.63	0.64
1:B:519:LYS:N	1:B:520:PRO:CD	2.60	0.64
1:B:526:PHE:CD2	1:B:562:CYS:HB2	2.33	0.64
1:D:76:MET:HA	1:D:595:GLU:O	1.98	0.64
1:D:310:THR:HG21	1:D:416:ARG:HD2	1.80	0.64
1:C:392:LEU:HD13	1:C:394:LEU:HD21	1.80	0.64
1:A:203:LEU:HD13	1:A:251:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:MET:HG3	1:B:210:LEU:HD11	1.78	0.64
1:D:321:THR:HG22	1:D:323:LEU:N	2.11	0.64
1:C:553:LEU:CD1	1:C:574:HIS:CB	2.76	0.63
1:D:138:GLU:C	1:D:146:PRO:HD2	2.22	0.63
1:D:410:ARG:C	1:D:411:GLU:HG3	2.23	0.63
1:D:486:THR:HG22	1:D:486:THR:O	1.97	0.63
1:C:182:SER:O	1:C:186:ILE:HG12	1.97	0.63
1:C:536:ILE:O	1:C:540:SER:N	2.30	0.63
1:A:12:LEU:HD22	1:A:194:LEU:CD1	2.27	0.63
1:B:112:TYR:OH	1:B:264:ASP:OD1	2.10	0.63
1:D:310:THR:HG22	1:D:416:ARG:HD2	1.80	0.63
1:C:233:LYS:HD2	1:C:239:ALA:HA	1.80	0.63
1:A:45:SER:HB3	1:A:47:GLU:HG2	1.80	0.63
1:A:53:GLY:C	1:A:54:ILE:HG23	2.23	0.63
1:B:209:THR:O	1:B:210:LEU:HD23	1.98	0.63
1:B:282:LYS:CG	1:B:287:ALA:CB	2.75	0.63
1:D:340:THR:HG1	1:D:342:LYS:HB3	1.62	0.63
1:C:558:GLY:O	1:C:561:LEU:HB3	1.98	0.63
1:C:98:MET:HE2	1:C:248:ALA:HB3	1.81	0.63
1:D:132:ARG:HH11	1:D:153:VAL:CG2	2.10	0.63
1:C:318:GLY:HA3	1:C:350:SER:OG	1.98	0.63
1:C:341:ASP:CG	1:C:342:LYS:H	2.05	0.63
1:A:124:SER:HB3	1:A:176:VAL:O	1.99	0.63
1:B:517:ASN:O	1:B:520:PRO:HD3	1.99	0.63
1:B:129:ASN:HB2	1:B:212:THR:HG23	1.80	0.63
1:B:282:LYS:CG	1:B:287:ALA:HB1	2.29	0.63
1:B:396:ASP:O	1:B:398:PRO:HD3	1.99	0.63
1:C:587:LEU:HB3	1:C:588:PRO:HD2	1.81	0.63
1:D:293:GLN:O	1:D:296:VAL:CG1	2.47	0.63
1:D:293:GLN:O	1:D:297:ILE:HG13	1.99	0.63
1:C:358:LEU:HD23	1:C:361:ALA:O	1.99	0.62
1:D:308:PRO:HG2	1:D:339:TYR:HD2	1.63	0.62
1:C:358:LEU:HB2	1:C:362:ALA:HA	1.80	0.62
1:A:564:TRP:O	1:A:564:TRP:CE3	2.52	0.62
1:D:479:ASP:O	1:D:482:ASP:OD1	2.17	0.62
1:D:598:TRP:CG	1:D:599:PRO:CD	2.82	0.62
1:C:103:SER:HB3	1:C:204:LEU:HD21	1.82	0.62
1:C:358:LEU:HB2	1:C:362:ALA:CA	2.29	0.62
1:C:464:TYR:HD1	1:C:591:PRO:HD3	1.63	0.62
1:A:506:GLU:HG2	1:A:510:GLN:OE1	1.99	0.62
1:B:108:GLU:O	1:B:491:ARG:NH1	2.22	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:TRP:C	1:C:153:VAL:HG22	2.24	0.62
1:C:293:GLN:O	1:C:297:ILE:HG13	2.00	0.62
1:A:482:LEU:CD2	1:A:486:PHE:CD2	2.82	0.62
1:B:108:GLU:C	1:B:491:ARG:HH12	2.08	0.62
1:A:504:THR:HG22	1:A:508:LYS:HE2	1.81	0.62
1:A:570:ILE:C	1:A:572:TRP:N	2.53	0.62
1:C:41:ILE:HD12	1:C:69:SER:HB2	1.81	0.62
1:C:480:LEU:HD11	1:C:505:THR:HG22	1.81	0.62
1:A:479:LEU:HD11	1:A:504:THR:OG1	1.99	0.62
1:A:481:ASP:HB3	1:A:584:ILE:HG12	1.82	0.62
1:B:483:LEU:HD23	1:B:483:LEU:O	1.99	0.62
1:C:99:LEU:O	1:C:103:SER:OG	2.14	0.62
1:A:482:LEU:HD23	1:A:482:LEU:C	2.24	0.61
1:D:326:PRO:HA	1:D:392:LEU:HD23	1.81	0.61
1:D:563:GLU:CG	1:D:564:MET:H	2.14	0.61
1:B:551:LYS:CA	1:B:552:TRP:HE3	2.12	0.61
1:C:152:TRP:O	1:C:153:VAL:CG2	2.48	0.61
1:C:332:LEU:CG	1:C:399:PHE:CZ	2.83	0.61
1:A:407:LEU:HB3	1:A:414:HIS:CE1	2.35	0.61
1:B:45:SER:C	1:B:46:LYS:HD3	2.25	0.61
1:D:394:LEU:HA	1:D:397:SER:HB3	1.81	0.61
1:C:527:ARG:HH11	1:C:527:ARG:HG2	1.65	0.61
1:A:561:CYS:O	1:A:565:SER:N	2.34	0.61
1:B:406:LYS:HG3	1:B:407:GLU:H	1.64	0.61
1:D:571:ILE:HG23	1:D:571:ILE:O	2.00	0.61
1:C:594:LYS:HG3	1:C:594:LYS:O	2.00	0.61
1:A:482:LEU:HD23	1:A:486:PHE:CD2	2.35	0.61
1:D:469:LEU:HD23	1:D:469:LEU:O	2.00	0.61
1:D:476:THR:O	1:D:476:THR:HG22	1.99	0.61
1:D:499:ALA:H	1:D:526:PHE:N	1.99	0.61
1:A:564:TRP:C	1:A:566:LYS:N	2.53	0.61
1:B:348:ILE:HG23	1:B:399:PHE:CB	2.31	0.61
1:D:76:MET:CE	1:D:594:LYS:HD2	2.31	0.61
1:D:246:GLU:N	1:D:358:LEU:HD23	2.14	0.61
1:B:64:PHE:CE1	1:B:226:PHE:HB3	2.35	0.61
1:B:222:PRO:O	1:B:222:PRO:CD	2.38	0.61
1:B:485:TYR:CG	1:B:582:PRO:HG2	2.36	0.61
1:D:326:PRO:HA	1:D:392:LEU:CD2	2.30	0.61
1:A:482:LEU:CD2	1:A:486:PHE:HD2	2.13	0.61
1:B:271:ARG:HB3	1:B:271:ARG:HH11	1.66	0.61
1:A:12:LEU:HD22	1:A:194:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:O	1:A:342:LYS:HG3	2.01	0.60
1:D:448:PRO:C	1:D:449:PHE:HD1	2.08	0.60
1:C:281:ASP:O	1:C:282:LYS:O	2.20	0.60
1:B:511:GLN:NE2	1:B:523:THR:CA	2.63	0.60
1:D:502:THR:CG2	1:D:503:SER:H	2.10	0.60
1:D:563:GLU:O	1:D:566:SER:HB2	2.01	0.60
1:A:228:ASP:OD2	1:A:232:LYS:HE3	2.01	0.60
1:B:562:CYS:O	1:B:566:SER:N	2.33	0.60
1:D:368:ILE:O	1:D:372:MET:HG2	2.01	0.60
1:C:364:MET:O	1:C:368:ILE:HG13	2.00	0.60
1:C:532:GLN:CD	1:C:567:LYS:HG3	2.26	0.60
1:A:74:GLU:OE2	1:A:75:MET:HE2	2.01	0.60
1:A:136:GLU:HA	1:A:136:GLU:OE1	2.02	0.60
1:C:553:LEU:C	1:C:555:LYS:N	2.60	0.60
1:A:570:ILE:O	1:A:570:ILE:HG22	2.01	0.60
1:B:450:ILE:C	1:B:451:ILE:HD13	2.26	0.60
1:B:547:GLU:O	1:B:548:LEU:CG	2.49	0.60
1:D:296:VAL:HG13	1:D:297:ILE:N	2.16	0.60
1:D:515:PHE:CE1	1:D:518:ASP:HB2	2.36	0.60
1:C:301:ILE:O	1:C:305:GLY:N	2.33	0.60
1:C:389:ASN:HB3	1:C:392:LEU:HG	1.83	0.60
1:D:374:LEU:HD22	1:D:435:GLN:HB2	1.84	0.60
1:D:501:ILE:HG21	1:D:560:LYS:CD	2.32	0.60
1:D:99:LEU:O	1:D:103:SER:OG	2.17	0.60
1:C:63:GLY:C	1:C:64:PHE:CG	2.80	0.59
1:C:550:GLU:O	1:C:553:LEU:N	2.34	0.59
1:D:278:ASP:OD1	1:D:426:GLY:CA	2.51	0.59
1:B:105:LYS:HG2	1:B:589:VAL:HG21	1.85	0.59
1:B:246:GLU:N	1:B:358:LEU:CD2	2.65	0.59
1:B:509:LYS:O	1:B:512:LEU:HB2	2.01	0.59
1:B:525:CYS:SG	1:B:526:PHE:N	2.74	0.59
1:B:549:ILE:CG2	1:B:553:LEU:HD12	2.33	0.59
1:C:392:LEU:HB3	1:C:394:LEU:CD2	2.32	0.59
1:C:48:GLU:C	1:C:49:LEU:HD23	2.28	0.59
1:C:95:GLN:NE2	1:C:129:ASN:OD1	2.35	0.59
1:C:392:LEU:CB	1:C:394:LEU:HG	2.32	0.59
1:C:474:ARG:NH2	1:A:339:THR:N	2.51	0.59
1:C:536:ILE:O	1:C:540:SER:OG	2.19	0.59
1:A:556:LYS:O	1:A:556:LYS:HG3	2.02	0.59
1:B:511:GLN:CA	1:B:514:ASP:HB2	2.33	0.59
1:C:281:ASP:O	1:C:282:LYS:C	2.46	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD12	1:A:167:LEU:N	2.17	0.59
1:D:163:MET:O	1:D:167:LYS:HG2	2.02	0.59
1:A:484:TYR:HD1	1:A:575:LEU:HD12	1.66	0.59
1:B:136:PRO:O	1:B:138:GLU:OE1	2.21	0.59
1:D:35:LYS:O	1:D:405:LYS:HD3	2.03	0.59
1:B:113:ILE:O	1:B:114:SER:C	2.44	0.58
1:A:457:LYS:CE	1:A:495:GLU:OE1	2.51	0.58
1:B:504:GLY:O	1:B:507:GLU:CB	2.50	0.58
1:D:210:LEU:HD23	1:D:210:LEU:N	2.17	0.58
1:D:491:ARG:HG2	1:D:491:ARG:HH11	1.68	0.58
1:C:346:CYS:O	1:C:399:PHE:HA	2.03	0.58
1:A:450:ILE:HD13	1:A:450:ILE:N	2.15	0.58
1:B:192:PHE:HE2	1:B:196:GLN:HE22	1.48	0.58
1:D:98:MET:HE2	1:D:248:ALA:HB3	1.83	0.58
1:C:351:VAL:HB	1:C:369:LYS:HD2	1.85	0.58
1:A:32:ASN:HA	1:A:35:LYS:HE2	1.86	0.58
1:C:7:TYR:N	1:C:7:TYR:CD1	2.71	0.58
1:C:341:ASP:C	1:C:342:LYS:HG3	2.29	0.58
1:A:316:HIS:O	1:A:351:LYS:CE	2.51	0.58
1:C:96:LEU:HD13	1:C:160:ILE:HA	1.86	0.58
1:C:288:PRO:HB2	1:C:293:GLN:HE22	1.67	0.58
1:C:545:SER:C	1:C:549:ILE:CG2	2.77	0.58
1:B:246:GLU:C	1:B:358:LEU:HD22	2.29	0.58
1:A:34:ILE:CD1	1:A:368:LYS:HG3	2.34	0.58
1:A:458:ASP:OD1	1:A:459:ARG:N	2.37	0.58
1:D:528:GLY:C	1:D:566:SER:O	2.46	0.58
1:C:329:LEU:HD22	1:C:392:LEU:HD22	1.86	0.58
1:A:203:LEU:CD1	1:A:251:LEU:HD13	2.34	0.58
1:B:473:GLU:HB2	1:B:509:LYS:HE3	1.84	0.58
1:D:41:ILE:HG22	1:D:42:THR:N	2.17	0.58
1:B:120:THR:HB	1:B:170:LEU:HD22	1.86	0.58
1:A:481:ASP:CB	1:A:584:ILE:HG13	2.34	0.57
1:A:233:ALA:O	1:A:234:PHE:HB2	2.04	0.57
1:C:403:GLU:O	1:C:404:GLU:HG3	2.04	0.57
1:A:80:PHE:HD1	1:A:455:ARG:HG3	1.69	0.57
1:B:414:ALA:N	1:B:434:GLU:OE2	2.37	0.57
1:D:343:LYS:O	1:D:344:GLN:HB3	2.04	0.57
1:D:246:GLU:CA	1:D:358:LEU:CD2	2.83	0.57
1:C:185:LEU:HD23	1:C:429:THR:CB	2.35	0.57
1:B:511:GLN:O	1:B:514:ASP:CB	2.53	0.57
1:C:408:LEU:O	1:C:409:THR:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASP:HB2	1:B:326:PRO:HD3	1.86	0.57
1:A:32:ASN:OD1	1:A:35:LYS:NZ	2.30	0.57
1:A:309:THR:HG22	1:A:415:ARG:HG3	1.87	0.57
1:D:385:TYR:OH	1:D:388:PRO:HB3	2.04	0.57
1:C:546:ALA:N	1:C:549:ILE:CG2	2.68	0.57
1:D:342:LYS:O	1:D:343:LYS:HB3	2.05	0.57
1:B:223:GLY:O	1:B:224:LEU:HG	2.04	0.57
1:B:228:SER:CB	1:B:240:ASP:OD2	2.52	0.57
1:B:245:GLY:C	1:B:358:LEU:CD2	2.77	0.57
1:D:364:MET:HE3	1:D:364:MET:HA	1.86	0.57
1:B:185:LEU:HD23	1:B:429:THR:HB	1.87	0.57
1:C:233:LYS:CD	1:C:238:ASP:O	2.51	0.56
1:D:21:PHE:HB3	1:D:22:PRO:CD	2.35	0.56
1:D:232:ILE:HG21	1:D:353:THR:HA	1.87	0.56
1:D:235:PHE:O	1:D:385:TYR:CE1	2.57	0.56
1:C:551:LYS:O	1:C:555:LYS:HB2	2.05	0.56
1:A:159:ILE:O	1:A:163:ILE:HG13	2.05	0.56
1:A:496:ARG:NH2	1:A:566:LYS:HA	2.20	0.56
1:D:278:ASP:OD1	1:D:426:GLY:C	2.48	0.56
1:C:63:GLY:C	1:C:64:PHE:CD2	2.83	0.56
1:C:93:ASP:OD1	1:C:94:PRO:HD2	2.04	0.56
1:C:233:LYS:CB	1:C:239:ALA:HA	2.33	0.56
1:A:282:VAL:HG13	1:A:282:VAL:O	2.05	0.56
1:A:487:GLN:HB3	1:A:571:ASN:HB2	1.87	0.56
1:A:566:LYS:O	1:A:566:LYS:HG2	2.03	0.56
1:B:192:PHE:O	1:B:196:GLN:HG3	2.05	0.56
1:B:323:LEU:O	1:B:327:ILE:HG13	2.06	0.56
1:B:549:ILE:CG2	1:B:553:LEU:CD1	2.83	0.56
1:D:21:PHE:HB3	1:D:22:PRO:HD2	1.88	0.56
1:D:301:ILE:HG23	1:D:306:ILE:O	2.04	0.56
1:D:452:PRO:HB3	1:D:565:TRP:CZ2	2.40	0.56
1:C:32:ASN:O	1:C:36:GLU:HG2	2.05	0.56
1:C:480:LEU:CD1	1:C:505:THR:HG22	2.35	0.56
1:B:283:VAL:HG13	1:B:283:VAL:O	2.06	0.56
1:D:344:GLN:O	1:D:344:GLN:HG2	2.04	0.56
1:D:351:VAL:HB	1:D:369:LYS:HD2	1.87	0.56
1:C:311:ILE:HD12	1:C:311:ILE:N	2.21	0.56
1:B:482:ASP:OD1	1:B:583:LYS:N	2.38	0.56
1:D:151:SER:HA	1:D:153:VAL:CG1	2.35	0.56
1:D:246:GLU:C	1:D:358:LEU:CD2	2.78	0.56
1:B:39:GLU:OE1	1:B:231:HIS:CE1	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:HIS:CD2	1:D:319:THR:HG22	2.41	0.56
1:C:544:ASP:O	1:C:546:ALA:N	2.39	0.56
1:A:292:GLN:O	1:A:296:ILE:HG13	2.06	0.56
1:B:313:TYR:OH	1:B:349:GLY:HA3	2.06	0.56
1:D:325:ASP:O	1:D:392:LEU:HD21	2.06	0.56
1:C:464:TYR:CD1	1:C:591:PRO:HD3	2.41	0.56
1:B:111:GLY:O	1:B:490:GLY:HA3	2.06	0.56
1:C:518:ASP:CG	1:C:518:ASP:O	2.48	0.56
1:C:559:PRO:O	1:C:560:LYS:C	2.49	0.56
1:B:511:GLN:C	1:B:514:ASP:HB2	2.30	0.56
1:D:147:ASP:C	1:D:149:TYR:H	2.14	0.56
1:D:564:MET:O	1:D:567:LYS:N	2.34	0.56
1:C:552:TRP:CD1	1:C:552:TRP:N	2.72	0.55
1:B:515:PHE:CD1	1:B:515:PHE:C	2.84	0.55
1:C:358:LEU:CG	1:C:361:ALA:HB3	2.37	0.55
1:B:348:ILE:HG23	1:B:399:PHE:HB2	1.88	0.55
1:B:549:ILE:HG22	1:B:549:ILE:O	2.05	0.55
1:B:341:ASP:O	1:B:342:LYS:HB2	2.07	0.55
1:D:345:TYR:C	1:D:345:TYR:CD1	2.84	0.55
1:D:469:LEU:CD2	1:D:472:LEU:HB2	2.35	0.55
1:B:434:GLU:OE1	1:B:434:GLU:HA	2.06	0.55
1:D:81:PHE:CE1	1:D:456:ARG:NH1	2.69	0.55
1:C:358:LEU:O	1:C:362:ALA:HB2	2.07	0.55
1:A:182:SER:OG	1:A:359:THR:HG23	2.07	0.55
1:D:584:ARG:O	1:D:585:ILE:HD13	2.06	0.55
1:C:339:TYR:O	1:C:340:THR:C	2.47	0.55
1:A:128:ASN:O	1:A:129:SER:OG	2.24	0.55
1:A:393:LEU:HD21	1:A:400:VAL:HG23	1.88	0.55
1:D:35:LYS:HE2	1:D:36:GLU:HG2	1.88	0.55
1:C:358:LEU:HD23	1:C:361:ALA:HB3	1.89	0.55
1:A:313:VAL:HG22	1:A:417:ALA:HB3	1.88	0.55
1:B:150:VAL:HG12	1:B:151:SER:N	2.21	0.55
1:B:523:THR:OG1	1:B:525:CYS:HB3	2.06	0.55
1:D:32:ASN:OD1	1:D:33:ASN:N	2.40	0.55
1:D:329:LEU:HD11	1:D:399:PHE:HD2	1.72	0.55
1:D:473:GLU:O	1:D:474:ARG:O	2.23	0.55
1:A:112:ILE:HG22	1:A:114:LYS:HG3	1.87	0.55
1:A:475:THR:O	1:A:477:THR:N	2.34	0.55
1:A:564:TRP:O	1:A:565:SER:C	2.48	0.55
1:B:323:LEU:C	1:B:326:PRO:HD2	2.32	0.55
1:D:132:ARG:HH12	1:D:153:VAL:HG22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:GLN:CA	1:D:398:PRO:C	2.78	0.55
1:C:63:GLY:O	1:C:64:PHE:CD1	2.60	0.55
1:A:324:ASP:HB2	1:A:325:PRO:HD3	1.88	0.55
1:B:551:LYS:HA	1:B:552:TRP:CE3	2.41	0.55
1:D:500:PHE:CD1	1:D:500:PHE:N	2.74	0.55
1:C:239:ALA:O	1:C:322:LYS:HG2	2.07	0.55
1:A:568:VAL:O	1:A:569:ALA:HB3	2.06	0.55
1:C:93:ASP:OD2	1:C:95:GLN:NE2	2.40	0.54
1:B:138:GLU:OE1	1:B:138:GLU:N	2.40	0.54
1:C:63:GLY:O	1:C:64:PHE:CG	2.59	0.54
1:A:69:VAL:HG12	1:A:70:LEU:N	2.21	0.54
1:A:488:VAL:HG11	1:A:572:TRP:CE2	2.41	0.54
1:D:117:ILE:O	1:D:117:ILE:HG13	2.08	0.54
1:C:288:PRO:HG3	1:C:324:GLY:HA2	1.90	0.54
1:D:485:TYR:OH	1:D:573:TRP:CZ3	2.53	0.54
1:A:339:THR:CG2	1:A:340:ASP:H	2.21	0.54
1:D:340:THR:O	1:D:342:LYS:HD2	2.08	0.54
1:D:451:ILE:N	1:D:500:PHE:O	2.31	0.54
1:D:585:ILE:HG22	1:D:586:SER:N	2.22	0.54
1:C:288:PRO:O	1:C:327:ILE:HG21	2.06	0.54
1:C:545:SER:C	1:C:549:ILE:HG21	2.33	0.54
1:D:232:ILE:HG23	1:D:232:ILE:O	2.07	0.54
1:D:329:LEU:HD11	1:D:399:PHE:CD2	2.42	0.54
1:D:410:ARG:O	1:D:411:GLU:CG	2.55	0.54
1:D:452:PRO:HB3	1:D:565:TRP:CH2	2.42	0.54
1:C:71:LEU:HD22	1:C:247:GLY:HA2	1.89	0.54
1:A:341:LYS:HD3	1:A:395:ASP:CG	2.31	0.54
1:B:471:PHE:CD1	1:B:471:PHE:C	2.85	0.54
1:B:35:LYS:HG3	1:B:36:GLU:HG2	1.89	0.54
1:B:306:ILE:HD13	1:B:416:ARG:HD2	1.90	0.54
1:C:539:LEU:O	1:C:540:SER:C	2.51	0.54
1:A:468:LEU:HD22	1:A:515:ILE:HD11	1.90	0.54
1:A:490:ARG:HG2	1:A:490:ARG:NH1	2.22	0.54
1:B:501:ILE:HD13	1:B:560:LYS:HG3	1.90	0.54
1:D:64:PHE:CD1	1:D:64:PHE:C	2.85	0.54
1:D:321:THR:N	1:D:325:ASP:OD2	2.41	0.54
1:A:64:VAL:HG23	1:A:64:VAL:O	2.07	0.54
1:A:504:THR:O	1:A:507:LEU:N	2.40	0.54
1:B:223:GLY:C	1:B:224:LEU:HG	2.32	0.54
1:D:113:ILE:HD12	1:D:116:GLU:OE2	2.08	0.54
1:C:64:PHE:O	1:C:221:GLN:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:PHE:CD1	1:B:67:ALA:CB	2.91	0.54
1:B:569:VAL:HG13	1:B:569:VAL:O	2.06	0.54
1:D:340:THR:C	1:D:342:LYS:CD	2.81	0.54
1:D:561:LEU:HD12	1:D:563:GLU:HB2	1.89	0.54
1:C:12:LEU:HD11	1:C:192:PHE:HD1	1.73	0.53
1:C:534:LYS:O	1:C:538:TRP:CD2	2.61	0.53
1:B:465:ALA:O	1:B:469:LEU:HB2	2.08	0.53
1:C:283:VAL:O	1:C:284:GLY:C	2.50	0.53
1:D:323:LEU:O	1:D:327:ILE:HG13	2.07	0.53
1:D:483:LEU:HA	1:D:587:LEU:HD11	1.90	0.53
1:D:563:GLU:CG	1:D:564:MET:N	2.69	0.53
1:C:487:PHE:CD1	1:C:491:ARG:HG3	2.39	0.53
1:B:214:SER:O	1:B:215:SER:OG	2.23	0.53
1:A:309:THR:CG2	1:A:415:ARG:NE	2.55	0.53
1:A:481:ASP:OD2	1:A:582:LYS:CE	2.56	0.53
1:D:160:ILE:HB	1:D:161:PRO:CD	2.38	0.53
1:D:343:LYS:N	1:D:343:LYS:CD	2.71	0.53
1:C:534:LYS:O	1:C:538:TRP:CG	2.62	0.53
1:A:113:SER:OG	1:A:167:LEU:HB3	2.09	0.53
1:A:473:ARG:CG	1:A:474:LYS:N	2.72	0.53
1:B:456:ARG:HD3	1:B:495:GLU:OE2	2.09	0.53
1:B:504:GLY:O	1:B:507:GLU:N	2.42	0.53
1:C:537:ALA:CA	1:C:540:SER:OG	2.56	0.53
1:A:259:VAL:HG23	1:A:260:LYS:HG2	1.91	0.53
1:D:498:ALA:HB1	1:D:500:PHE:CE1	2.43	0.53
1:B:456:ARG:O	1:B:457:LYS:HG3	2.08	0.53
1:D:485:TYR:O	1:D:489:VAL:HG22	2.09	0.53
1:A:39:GLU:OE2	1:A:230:HIS:HD2	1.92	0.53
1:A:341:LYS:C	1:A:342:LYS:HG3	2.34	0.53
1:C:478:THR:CG2	1:C:479:ASP:H	2.12	0.53
1:B:42:THR:CG2	1:B:68:LYS:O	2.53	0.53
1:B:113:ILE:HB	1:B:116:GLU:HG3	1.90	0.53
1:D:336:TYR:C	1:D:338:ARG:H	2.16	0.53
1:D:304:THR:CB	1:D:306:ILE:HG13	2.37	0.52
1:C:42:THR:OG1	1:C:68:LYS:O	2.22	0.52
1:C:269:LEU:HD13	1:C:436:TYR:HB2	1.90	0.52
1:B:246:GLU:C	1:B:358:LEU:CD2	2.82	0.52
1:B:367:CYS:O	1:B:371:VAL:HG23	2.09	0.52
1:D:563:GLU:HG2	1:D:564:MET:N	2.23	0.52
1:C:460:ARG:NH1	1:C:463:GLU:OE1	2.42	0.52
1:D:98:MET:HE2	1:D:248:ALA:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ARG:HE	1:B:416:ARG:NH1	2.08	0.52
1:D:394:LEU:C	1:D:397:SER:OG	2.53	0.52
1:C:95:GLN:OE1	1:C:127:SER:O	2.27	0.52
1:C:501:ILE:HG23	1:C:501:ILE:O	2.09	0.52
1:A:292:GLN:O	1:A:295:VAL:HG22	2.09	0.52
1:A:340:ASP:O	1:A:342:LYS:HG3	2.09	0.52
1:B:307:HIS:HD2	1:B:309:GLU:H	1.58	0.52
1:C:474:ARG:HH22	1:A:339:THR:N	2.07	0.52
1:A:11:SER:HB3	1:A:270:ARG:HA	1.90	0.52
1:A:51:ARG:HG2	1:A:52:SER:N	2.24	0.52
1:A:482:LEU:HD21	1:A:486:PHE:CD2	2.44	0.52
1:B:328:GLU:HG3	1:B:422:PHE:HE2	1.74	0.52
1:D:282:LYS:CE	1:D:284:GLY:O	2.58	0.52
1:A:84:SER:OG	1:A:87:ASP:CG	2.52	0.52
1:A:485:THR:O	1:A:485:THR:HG22	2.09	0.52
1:A:561:CYS:O	1:A:565:SER:HB2	2.09	0.52
1:B:150:VAL:CG1	1:B:151:SER:N	2.72	0.52
1:B:317:HIS:CD2	1:B:422:PHE:H	2.27	0.52
1:C:332:LEU:HD21	1:C:399:PHE:CZ	2.45	0.52
1:A:115:GLU:C	1:A:117:PRO:HD3	2.35	0.52
1:A:457:LYS:HG2	1:A:495:GLU:OE1	2.09	0.52
1:A:513:ASP:O	1:A:519:PRO:HG3	2.10	0.52
1:B:346:CYS:O	1:B:399:PHE:HB3	2.10	0.52
1:D:419:LEU:HD12	1:D:420:SER:H	1.75	0.52
1:D:517:ASN:O	1:D:518:ASP:C	2.53	0.52
1:C:95:GLN:HG2	1:C:210:LEU:HB2	1.92	0.52
1:B:41:ILE:HG22	1:B:42:THR:N	2.25	0.52
1:B:587:LEU:HB3	1:B:588:PRO:HD2	1.92	0.52
1:D:12:LEU:HD13	1:D:192:PHE:CD2	2.45	0.52
1:D:419:LEU:HD12	1:D:420:SER:N	2.24	0.52
1:C:388:PRO:HB3	1:C:394:LEU:HD12	1.92	0.52
1:C:450:ILE:C	1:C:451:ILE:HD13	2.35	0.52
1:A:570:ILE:HG23	1:A:572:TRP:HD1	1.75	0.52
1:B:304:THR:C	1:B:306:ILE:H	2.18	0.52
1:D:449:PHE:CD1	1:D:449:PHE:N	2.76	0.52
1:A:457:LYS:HG3	1:A:495:GLU:OE1	2.10	0.51
1:D:81:PHE:CD1	1:D:456:ARG:HD2	2.45	0.51
1:D:293:GLN:CD	1:D:422:PHE:CE2	2.89	0.51
1:D:325:ASP:N	1:D:326:PRO:CD	2.73	0.51
1:D:326:PRO:HD2	1:D:327:ILE:H	1.75	0.51
1:C:559:PRO:O	1:C:561:LEU:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:THR:O	1:B:325:ASP:OD2	2.28	0.51
1:D:116:GLU:O	1:D:118:PRO:HD2	2.10	0.51
1:D:310:THR:HG22	1:D:310:THR:O	2.08	0.51
1:C:43:PHE:HA	1:C:67:ALA:CB	2.40	0.51
1:C:127:SER:OG	1:C:209:THR:CB	2.59	0.51
1:B:526:PHE:HZ	1:B:560:LYS:HD3	1.74	0.51
1:B:549:ILE:HG21	1:B:553:LEU:CD1	2.40	0.51
1:D:282:LYS:HD2	1:D:287:ALA:O	2.10	0.51
1:D:491:ARG:HG2	1:D:491:ARG:NH1	2.25	0.51
1:C:389:ASN:OD1	1:C:391:ASN:HB2	2.11	0.51
1:B:93:ASP:OD1	1:B:94:PRO:N	2.42	0.51
1:B:153:VAL:HG12	1:B:153:VAL:O	2.10	0.51
1:D:136:PRO:O	1:D:138:GLU:N	2.42	0.51
1:D:515:PHE:CE1	1:D:518:ASP:OD1	2.52	0.51
1:C:343:LYS:O	1:C:345:TYR:CD1	2.60	0.51
1:A:292:GLN:HG2	1:A:421:PHE:CE1	2.44	0.51
1:B:277:ASN:HA	1:B:426:GLY:O	2.09	0.51
1:D:181:CYS:HB2	1:D:423:GLY:HA2	1.91	0.51
1:D:338:ARG:HG2	1:D:338:ARG:O	2.10	0.51
1:D:475:LYS:HB3	1:D:477:ASP:CB	2.40	0.51
1:C:36:GLU:HA	1:C:36:GLU:OE1	2.10	0.51
1:B:31:TRP:O	1:B:34:ILE:HG12	2.10	0.51
1:D:98:MET:CE	1:D:248:ALA:HB3	2.40	0.51
1:D:246:GLU:N	1:D:358:LEU:HD21	2.24	0.51
1:D:317:HIS:O	1:D:352:LYS:HE2	2.09	0.51
1:C:286:TYR:O	1:C:287:ALA:HB2	2.10	0.51
1:C:377:GLN:O	1:C:408:LEU:HB2	2.11	0.51
1:B:194:SER:HA	1:B:199:GLU:OE2	2.11	0.51
1:D:221:GLN:O	1:D:221:GLN:HG3	2.11	0.51
1:D:501:ILE:HG21	1:D:560:LYS:CG	2.41	0.51
1:A:53:GLY:C	1:A:54:ILE:CG2	2.83	0.51
1:A:162:MET:O	1:A:166:LYS:HG2	2.09	0.51
1:A:309:THR:CB	1:A:309:THR:HG1	2.12	0.51
1:D:300:VAL:HG12	1:D:304:THR:HG21	1.92	0.51
1:C:276:ASN:CG	1:C:296:VAL:HG13	2.36	0.50
1:B:549:ILE:HG22	1:B:553:LEU:CD1	2.41	0.50
1:D:113:ILE:O	1:D:116:GLU:HB2	2.12	0.50
1:C:209:THR:OG1	1:C:359:ASP:CB	2.58	0.50
1:C:358:LEU:HB2	1:C:362:ALA:N	2.26	0.50
1:A:92:ASP:OD1	1:A:93:PRO:HD2	2.12	0.50
1:A:163:ILE:O	1:A:167:LEU:HD13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:SER:HB3	1:A:239:ASP:OD2	2.10	0.50
1:B:337:GLY:C	1:B:339:TYR:H	2.18	0.50
1:D:246:GLU:CA	1:D:358:LEU:HD22	2.42	0.50
1:D:405:LYS:O	1:D:406:LYS:HG2	2.11	0.50
1:C:519:LYS:N	1:C:520:PRO:CD	2.71	0.50
1:C:540:SER:O	1:C:542:ASP:N	2.44	0.50
1:B:307:HIS:O	1:B:310:THR:HB	2.12	0.50
1:B:480:LEU:O	1:B:484:ALA:CB	2.59	0.50
1:D:300:VAL:HG12	1:D:304:THR:CG2	2.41	0.50
1:C:11:SER:HB3	1:C:270:LEU:O	2.12	0.50
1:C:314:VAL:HG22	1:C:418:ALA:HB3	1.92	0.50
1:A:289:VAL:CG2	1:A:326:ILE:HG23	2.34	0.50
1:D:561:LEU:HG	1:D:563:GLU:HB3	1.91	0.50
1:C:84:PHE:CZ	1:C:92:MET:HE1	2.46	0.50
1:A:506:GLU:O	1:A:510:GLN:CG	2.57	0.50
1:B:282:LYS:CG	1:B:287:ALA:HB3	2.40	0.50
1:C:32:ASN:HA	1:C:35:LYS:HG2	1.93	0.50
1:C:153:VAL:HG23	1:C:153:VAL:O	2.12	0.50
1:C:233:LYS:HD3	1:C:238:ASP:C	2.35	0.50
1:A:509:ARG:HG3	1:A:510:GLN:N	2.27	0.50
1:C:127:SER:OG	1:C:209:THR:OG1	2.23	0.50
1:A:31:TRP:CD1	1:A:371:MET:HB3	2.47	0.50
1:B:549:ILE:HG22	1:B:553:LEU:HD12	1.92	0.50
1:C:62:PRO:O	1:C:63:GLY:C	2.54	0.50
1:B:351:VAL:HB	1:B:369:LYS:HD2	1.94	0.50
1:D:461:LEU:O	1:D:464:TYR:CB	2.59	0.50
1:D:471:PHE:C	1:D:473:GLU:N	2.69	0.50
1:D:490:GLY:O	1:D:491:ARG:NH1	2.43	0.50
1:A:128:ASN:C	1:A:129:SER:OG	2.55	0.50
1:A:341:LYS:O	1:A:342:LYS:CG	2.60	0.50
1:A:484:TYR:HD1	1:A:575:LEU:CD1	2.25	0.50
1:A:517:ASP:OD1	1:A:518:LYS:HG3	2.12	0.50
1:C:117:ILE:HG13	1:C:117:ILE:O	2.13	0.49
1:C:129:ASN:O	1:C:130:SER:C	2.53	0.49
1:B:480:LEU:HD11	1:B:505:THR:HG22	1.94	0.49
1:D:77:PHE:CD1	1:D:97:ARG:HB3	2.47	0.49
1:D:390:PRO:O	1:D:393:HIS:CD2	2.65	0.49
1:D:461:LEU:O	1:D:464:TYR:HB3	2.12	0.49
1:B:114:SER:O	1:B:116:GLU:N	2.45	0.49
1:B:150:VAL:CG1	1:B:151:SER:H	2.25	0.49
1:B:282:LYS:HG3	1:B:283:VAL:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ILE:HD11	1:D:369:LYS:NZ	2.27	0.49
1:C:483:LEU:HG	1:C:587:LEU:HD13	1.94	0.49
1:A:239:ASP:OD1	1:A:239:ASP:N	2.42	0.49
1:A:295:VAL:HG23	1:A:296:ILE:N	2.27	0.49
1:A:71:GLU:HG2	1:A:72:GLY:N	2.27	0.49
1:B:339:TYR:O	1:B:341:ASP:N	2.45	0.49
1:D:515:PHE:CE1	1:D:518:ASP:HA	2.46	0.49
1:C:47:GLU:N	1:C:48:GLU:OE2	2.45	0.49
1:B:514:ASP:HB3	1:B:523:THR:CG2	2.42	0.49
1:D:497:ARG:HD2	1:D:565:TRP:O	2.11	0.49
1:B:43:PHE:CE1	1:B:67:ALA:HB2	2.47	0.49
1:D:34:ILE:HD12	1:D:351:VAL:HG23	1.93	0.49
1:D:282:LYS:HE3	1:D:284:GLY:O	2.13	0.49
1:D:324:GLY:C	1:D:326:PRO:CD	2.86	0.49
1:D:501:ILE:HG21	1:D:560:LYS:HG2	1.93	0.49
1:A:68:SER:O	1:A:68:SER:OG	2.29	0.49
1:A:516:ASN:O	1:A:519:PRO:HD2	2.13	0.49
1:B:194:SER:CA	1:B:199:GLU:OE2	2.61	0.49
1:B:337:GLY:C	1:B:339:TYR:N	2.70	0.49
1:A:11:SER:HB3	1:A:269:LEU:O	2.13	0.49
1:A:108:ASP:OD2	1:A:266:TYR:OH	2.23	0.49
1:B:512:LEU:C	1:B:514:ASP:N	2.70	0.49
1:D:179:ALA:O	1:D:180:ASN:HB2	2.13	0.49
1:C:209:THR:O	1:C:209:THR:HG23	2.12	0.49
1:C:542:ASP:HB3	1:C:544:ASP:OD2	2.13	0.49
1:C:546:ALA:O	1:C:550:GLU:CB	2.57	0.49
1:B:448:PRO:O	1:B:449:PHE:CD1	2.65	0.49
1:B:468:LEU:O	1:B:471:PHE:HB3	2.13	0.49
1:D:17:ILE:HG22	1:D:18:SER:N	2.28	0.49
1:B:64:PHE:HA	1:B:66:PRO:CD	2.43	0.49
1:B:234:ALA:O	1:B:235:PHE:HB2	2.13	0.49
1:B:291:LYS:O	1:B:295:GLU:HG3	2.12	0.49
1:D:456:ARG:HB2	1:D:590:TYR:OH	2.13	0.49
1:D:515:PHE:HD1	1:D:518:ASP:HA	1.75	0.49
1:C:137:GLU:HA	1:C:137:GLU:OE1	2.13	0.48
1:A:473:ARG:HG3	1:A:474:LYS:N	2.28	0.48
1:B:114:SER:O	1:B:115:LYS:C	2.55	0.48
1:B:115:LYS:HB3	1:B:115:LYS:HE3	1.61	0.48
1:B:222:PRO:O	1:B:222:PRO:HD2	2.12	0.48
1:B:325:ASP:N	1:B:326:PRO:CD	2.76	0.48
1:D:415:HIS:O	1:D:435:GLN:N	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:LEU:CD1	1:C:394:LEU:HD21	2.43	0.48
1:A:102:SER:HB3	1:A:203:LEU:HD21	1.95	0.48
1:D:120:THR:O	1:D:172:GLY:HA3	2.13	0.48
1:D:502:THR:HB	1:D:508:LEU:HD12	1.95	0.48
1:C:260:VAL:HG23	1:C:261:LYS:N	2.28	0.48
1:A:268:LEU:HD13	1:A:435:TYR:HB2	1.96	0.48
1:A:570:ILE:CG2	1:A:572:TRP:HB2	2.28	0.48
1:D:120:THR:HG23	1:D:202:TYR:HB2	1.95	0.48
1:C:227:SER:OG	1:C:230:GLY:HA2	2.13	0.48
1:C:548:LEU:O	1:C:552:TRP:CD1	2.67	0.48
1:A:339:THR:CG2	1:A:340:ASP:N	2.76	0.48
1:A:341:LYS:CD	1:A:395:ASP:OD1	2.54	0.48
1:B:64:PHE:HA	1:B:66:PRO:N	2.27	0.48
1:D:316:ALA:HB1	1:D:328:GLU:OE2	2.12	0.48
1:C:317:HIS:CD2	1:C:319:THR:CG2	2.95	0.48
1:A:56:GLU:C	1:A:63:PHE:N	2.72	0.48
1:B:317:HIS:HD2	1:B:421:SER:HA	1.79	0.48
1:B:341:ASP:CG	1:B:342:LYS:N	2.69	0.48
1:B:458:LYS:HG2	1:B:496:GLU:CG	2.43	0.48
1:B:547:GLU:C	1:B:548:LEU:CG	2.86	0.48
1:D:231:HIS:O	1:D:233:LYS:HE3	2.14	0.48
1:D:309:GLU:CA	1:D:345:TYR:OH	2.62	0.48
1:C:71:LEU:HD23	1:C:210:LEU:HD21	1.96	0.48
1:C:483:LEU:HA	1:C:587:LEU:HD11	1.94	0.48
1:C:571:ILE:HG23	1:C:571:ILE:O	2.13	0.48
1:C:573:TRP:CD1	1:C:573:TRP:O	2.67	0.48
1:A:11:SER:CB	1:A:270:ARG:HA	2.44	0.48
1:A:69:VAL:CG1	1:A:70:LEU:N	2.77	0.48
1:A:446:GLY:O	1:A:502:SER:HA	2.14	0.48
1:B:458:LYS:HG2	1:B:496:GLU:HG2	1.95	0.48
1:C:325:ASP:O	1:C:329:LEU:HD13	2.14	0.48
1:A:519:PRO:O	1:A:520:ALA:HB3	2.13	0.48
1:A:525:PHE:CD1	1:A:525:PHE:N	2.81	0.48
1:B:337:GLY:HA2	1:B:341:ASP:OD2	2.14	0.48
1:D:32:ASN:CA	1:D:35:LYS:HG2	2.39	0.48
1:D:293:GLN:CG	1:D:422:PHE:CE2	2.96	0.48
1:D:300:VAL:O	1:D:304:THR:CG2	2.59	0.48
1:C:503:SER:OG	1:C:507:GLU:HG3	2.14	0.48
1:B:66:PRO:HD2	1:B:67:ALA:H	1.78	0.48
1:D:224:LEU:CD1	1:D:225:ASN:H	2.26	0.48
1:C:307:HIS:HE1	1:C:340:THR:HG1	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:PHE:CD2	1:B:562:CYS:CB	2.96	0.47
1:D:324:GLY:C	1:D:326:PRO:HD2	2.39	0.47
1:D:501:ILE:O	1:D:502:THR:OG1	2.31	0.47
1:C:392:LEU:HD12	1:C:394:LEU:HD11	1.95	0.47
1:A:256:SER:O	1:A:259:VAL:CG2	2.62	0.47
1:A:259:VAL:HG23	1:A:260:LYS:N	2.29	0.47
1:A:380:PRO:HD3	1:A:404:LYS:HB3	1.95	0.47
1:B:268:ALA:HB3	1:B:371:VAL:HG13	1.96	0.47
1:D:93:ASP:OD1	1:D:94:PRO:HD2	2.12	0.47
1:D:336:TYR:C	1:D:338:ARG:N	2.71	0.47
1:C:358:LEU:HG	1:C:361:ALA:HB3	1.95	0.47
1:C:545:SER:C	1:C:549:ILE:HG22	2.40	0.47
1:A:84:SER:O	1:A:87:ASP:HB2	2.14	0.47
1:B:22:PRO:HD3	1:B:246:GLU:O	2.15	0.47
1:B:348:ILE:O	1:B:348:ILE:HG13	2.13	0.47
1:D:76:MET:HE3	1:D:594:LYS:HD2	1.96	0.47
1:A:272:ILE:HG23	1:A:272:ILE:O	2.14	0.47
1:B:351:VAL:HG22	1:B:351:VAL:O	2.13	0.47
1:B:392:LEU:CD1	1:B:394:LEU:HD21	2.44	0.47
1:D:484:ALA:O	1:D:488:GLN:HG3	2.14	0.47
1:C:332:LEU:HD23	1:C:399:PHE:CE2	2.49	0.47
1:C:450:ILE:HB	1:C:488:GLN:HE21	1.80	0.47
1:C:460:ARG:CZ	1:C:463:GLU:OE1	2.63	0.47
1:C:559:PRO:C	1:C:561:LEU:N	2.72	0.47
1:A:112:ILE:HG23	1:A:491:GLU:HG3	1.95	0.47
1:A:564:TRP:HD1	1:A:568:VAL:O	1.98	0.47
1:B:95:GLN:OE1	1:B:127:SER:OG	2.29	0.47
1:B:307:HIS:CE1	1:B:340:THR:HB	2.49	0.47
1:D:29:GLU:O	1:D:32:ASN:OD1	2.32	0.47
1:D:109:ASP:OD2	1:D:267:TYR:OH	2.31	0.47
1:A:278:GLY:O	1:A:280:ASP:N	2.47	0.47
1:A:393:LEU:O	1:A:396:SER:OG	2.26	0.47
1:A:468:LEU:HD22	1:A:515:ILE:CD1	2.45	0.47
1:B:551:LYS:CB	1:B:552:TRP:HE3	2.28	0.47
1:D:336:TYR:N	1:D:336:TYR:CD1	2.81	0.47
1:D:381:PRO:HD3	1:D:405:LYS:CG	2.34	0.47
1:B:516:ILE:C	1:B:518:ASP:H	2.21	0.47
1:D:504:GLY:O	1:D:508:LEU:CB	2.62	0.47
1:C:474:ARG:NH2	1:A:338:TYR:C	2.73	0.47
1:C:536:ILE:O	1:C:540:SER:CA	2.63	0.47
1:D:275:VAL:HG22	1:D:429:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:THR:O	1:C:67:ALA:HB1	2.15	0.47
1:C:307:HIS:CE1	1:C:340:THR:HG1	2.29	0.47
1:A:373:LEU:HD22	1:A:434:GLN:HB2	1.97	0.47
1:B:58:LEU:HD12	1:B:62:PRO:CB	2.39	0.47
1:B:239:ALA:O	1:B:322:LYS:HG2	2.15	0.47
1:B:317:HIS:CD2	1:B:421:SER:HA	2.50	0.47
1:B:436:TYR:HA	1:B:437:PRO:HD3	1.51	0.47
1:D:160:ILE:O	1:D:164:ILE:HG13	2.15	0.47
1:D:515:PHE:HE1	1:D:518:ASP:CB	2.20	0.47
1:A:213:SER:O	1:A:214:SER:CB	2.63	0.47
1:A:276:ASN:HA	1:A:426:THR:HA	1.97	0.47
1:A:482:LEU:HD21	1:A:486:PHE:HE2	1.79	0.47
1:B:94:PRO:HD3	1:B:131:TYR:CE1	2.50	0.47
1:B:519:LYS:N	1:B:520:PRO:HD2	2.30	0.47
1:D:234:ALA:O	1:D:235:PHE:C	2.57	0.47
1:A:139:THR:O	1:A:140:ALA:O	2.33	0.46
1:B:454:SER:HB2	1:B:494:MET:HB2	1.97	0.46
1:D:364:MET:O	1:D:368:ILE:HG13	2.15	0.46
1:D:483:LEU:HG	1:D:587:LEU:HD13	1.97	0.46
1:D:493:ALA:HB1	1:D:497:ARG:HE	1.80	0.46
1:D:562:CYS:O	1:D:563:GLU:C	2.59	0.46
1:A:332:GLN:HG3	1:A:397:PRO:HD2	1.97	0.46
1:B:259:ALA:HA	1:B:264:ASP:OD2	2.15	0.46
1:D:421:SER:HB3	1:D:429:THR:HG1	1.78	0.46
1:C:49:LEU:N	1:C:49:LEU:CD2	2.72	0.46
1:C:304:THR:O	1:C:305:GLY:C	2.58	0.46
1:A:322:LEU:HD12	1:A:322:LEU:H	1.79	0.46
1:A:454:ALA:HB3	1:A:460:LEU:HB2	1.96	0.46
1:B:306:ILE:CD1	1:B:432:ILE:HG21	2.45	0.46
1:B:471:PHE:CE2	1:B:588:PRO:HD3	2.50	0.46
1:B:480:LEU:CD1	1:B:505:THR:HG22	2.46	0.46
1:D:290:VAL:HG13	1:D:291:LYS:N	2.29	0.46
1:D:317:HIS:O	1:D:352:LYS:HE3	2.14	0.46
1:D:457:LYS:HE2	1:D:457:LYS:HB3	1.60	0.46
1:D:507:GLU:O	1:D:510:ARG:N	2.39	0.46
1:D:515:PHE:CD1	1:D:515:PHE:O	2.69	0.46
1:C:479:ASP:OD2	1:C:481:ALA:HB3	2.16	0.46
1:A:276:ASN:HA	1:A:425:GLY:O	2.16	0.46
1:B:138:GLU:HB3	1:B:151:SER:OG	2.15	0.46
1:D:153:VAL:HG23	1:D:153:VAL:O	2.16	0.46
1:D:504:GLY:O	1:D:508:LEU:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:VAL:HG12	1:C:219:VAL:O	2.15	0.46
1:C:526:PHE:N	1:C:526:PHE:CD1	2.84	0.46
1:A:297:GLN:NE2	1:A:338:TYR:OH	2.46	0.46
1:B:527:ARG:O	1:B:566:SER:OG	2.34	0.46
1:D:326:PRO:CD	1:D:327:ILE:H	2.29	0.46
1:C:553:LEU:HD12	1:C:574:HIS:CB	2.44	0.46
1:B:293:GLN:O	1:B:296:VAL:HG22	2.16	0.46
1:C:308:PRO:HA	1:C:311:ILE:HD13	1.96	0.46
1:C:329:LEU:HD12	1:C:329:LEU:N	2.31	0.46
1:B:395:GLU:HG3	1:B:396:ASP:N	2.30	0.46
1:D:301:ILE:CG2	1:D:306:ILE:O	2.64	0.46
1:C:460:ARG:NH2	1:C:463:GLU:OE1	2.49	0.46
1:A:115:GLU:O	1:A:117:PRO:HD3	2.16	0.46
1:A:324:ASP:HB2	1:A:325:PRO:CD	2.45	0.46
1:B:471:PHE:CD1	1:B:472:LEU:N	2.84	0.46
1:B:553:LEU:HD23	1:B:554:ALA:O	2.15	0.46
1:C:527:ARG:CG	1:C:527:ARG:NH1	2.72	0.45
1:A:457:LYS:HE3	1:A:495:GLU:OE1	2.16	0.45
1:B:41:ILE:HG22	1:B:42:THR:H	1.82	0.45
1:B:348:ILE:CG2	1:B:399:PHE:CB	2.94	0.45
1:B:517:ASN:O	1:B:520:PRO:CD	2.62	0.45
1:D:301:ILE:HA	1:D:304:THR:HG1	1.81	0.45
1:D:336:TYR:N	1:D:336:TYR:HD1	2.13	0.45
1:C:185:LEU:HD23	1:C:429:THR:HB	1.98	0.45
1:C:254:LYS:CE	1:C:258:ASP:O	2.61	0.45
1:A:178:ALA:O	1:A:182:SER:HB3	2.15	0.45
1:B:296:VAL:HG23	1:B:297:ILE:N	2.31	0.45
1:D:138:GLU:C	1:D:146:PRO:CD	2.89	0.45
1:D:315:GLU:OE2	1:D:350:SER:HA	2.16	0.45
1:D:581:HIS:CD2	1:D:581:HIS:O	2.69	0.45
1:C:232:ILE:HD12	1:C:352:LYS:O	2.16	0.45
1:C:376:HIS:O	1:C:377:GLN:HB2	2.17	0.45
1:C:470:ALA:O	1:C:474:ARG:HG2	2.16	0.45
1:C:573:TRP:O	1:C:573:TRP:HD1	1.99	0.45
1:A:281:LYS:HE3	1:A:283:GLY:O	2.17	0.45
1:A:562:GLU:O	1:A:565:SER:CB	2.64	0.45
1:B:584:ARG:O	1:B:585:ILE:CD1	2.59	0.45
1:D:516:ILE:CG2	1:D:517:ASN:N	2.79	0.45
1:D:581:HIS:O	1:D:581:HIS:CG	2.70	0.45
1:C:597:TYR:N	1:C:597:TYR:CD1	2.85	0.45
1:B:96:LEU:HB2	1:B:160:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:TYR:CD1	1:B:584:ARG:NH1	2.69	0.45
1:D:296:VAL:CG1	1:D:297:ILE:N	2.79	0.45
1:D:504:GLY:O	1:D:508:LEU:HB2	2.16	0.45
1:B:471:PHE:HD1	1:B:472:LEU:N	2.14	0.45
1:D:9:GLU:O	1:D:9:GLU:HG2	2.16	0.45
1:C:68:LYS:HE3	1:C:219:VAL:HB	1.99	0.45
1:C:95:GLN:NE2	1:C:129:ASN:CG	2.75	0.45
1:C:235:PHE:HD1	1:C:325:ASP:HB3	1.82	0.45
1:A:156:SER:HB3	1:A:175:PHE:CG	2.52	0.45
1:A:482:LEU:CD2	1:A:482:LEU:C	2.89	0.45
1:B:483:LEU:C	1:B:483:LEU:CD2	2.89	0.45
1:D:479:ASP:OD1	1:D:480:LEU:N	2.50	0.45
1:C:188:LEU:HB3	1:C:273:ILE:CD1	2.46	0.45
1:C:316:ALA:HB1	1:C:328:GLU:CD	2.42	0.45
1:C:317:HIS:N	1:C:328:GLU:OE2	2.42	0.45
1:C:358:LEU:CD2	1:C:361:ALA:HB3	2.46	0.45
1:A:91:MET:HG3	1:A:153:LEU:HD13	1.99	0.45
1:A:116:ILE:HG13	1:A:116:ILE:O	2.17	0.45
1:B:79:PRO:HD2	1:B:80:GLY:H	1.82	0.45
1:B:348:ILE:CG2	1:B:399:PHE:HB2	2.46	0.45
1:B:377:GLN:O	1:B:408:LEU:HB2	2.16	0.45
1:D:256:ALA:O	1:D:260:VAL:HG22	2.16	0.45
1:A:42:THR:O	1:A:66:ALA:HA	2.17	0.45
1:B:358:LEU:O	1:B:362:ALA:N	2.50	0.45
1:D:84:PHE:CZ	1:D:92:MET:HE1	2.52	0.45
1:D:192:PHE:O	1:D:196:GLN:HB2	2.16	0.45
1:D:454:SER:HB2	1:D:494:MET:H	1.82	0.45
1:A:372:SER:HB3	1:A:377:GLU:O	2.16	0.45
1:B:394:LEU:HA	1:B:397:SER:HB2	1.96	0.45
1:D:93:ASP:OD1	1:D:94:PRO:CD	2.65	0.45
1:D:516:ILE:HG23	1:D:517:ASN:N	2.32	0.45
1:C:135:LEU:HA	1:C:136:PRO:HD3	1.86	0.45
1:C:535:ASP:OD1	1:C:539:LEU:HD12	2.16	0.45
1:B:456:ARG:O	1:B:457:LYS:CG	2.65	0.45
1:D:317:HIS:O	1:D:352:LYS:HD2	2.17	0.45
1:C:291:LYS:HD2	1:C:291:LYS:HA	1.68	0.44
1:C:538:TRP:CE3	1:C:539:LEU:HG	2.52	0.44
1:A:68:SER:HB3	1:A:243:GLY:O	2.17	0.44
1:D:388:PRO:HB2	1:D:394:LEU:HD21	1.99	0.44
1:C:125:SER:HB3	1:C:177:VAL:O	2.17	0.44
1:A:309:THR:HG22	1:A:309:THR:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:HIS:O	1:B:310:THR:CB	2.65	0.44
1:B:329:LEU:N	1:B:329:LEU:HD12	2.32	0.44
1:B:559:PRO:O	1:B:561:LEU:HG	2.16	0.44
1:D:291:LYS:HD3	1:D:291:LYS:HA	1.72	0.44
1:C:341:ASP:CG	1:C:342:LYS:N	2.73	0.44
1:A:223:LEU:O	1:A:224:ASN:HB2	2.18	0.44
1:B:32:ASN:HA	1:B:35:LYS:HG2	1.99	0.44
1:B:34:ILE:HD12	1:B:369:LYS:HG3	1.99	0.44
1:B:497:ARG:HB3	1:B:565:TRP:CZ3	2.53	0.44
1:B:504:GLY:O	1:B:508:LEU:N	2.41	0.44
1:B:573:TRP:O	1:B:573:TRP:CE3	2.71	0.44
1:D:329:LEU:CD1	1:D:399:PHE:CD2	3.00	0.44
1:C:233:LYS:CD	1:C:239:ALA:HA	2.47	0.44
1:B:31:TRP:CE3	1:B:34:ILE:HD11	2.53	0.44
1:B:153:VAL:O	1:B:155:ALA:N	2.47	0.44
1:B:516:ILE:C	1:B:518:ASP:N	2.75	0.44
1:D:269:LEU:HD13	1:D:436:TYR:HB2	1.99	0.44
1:D:313:TYR:HD1	1:D:347:GLY:O	1.99	0.44
1:A:167:LEU:N	1:A:167:LEU:CD1	2.80	0.44
1:A:292:GLN:HG2	1:A:421:PHE:CE2	2.52	0.44
1:B:346:CYS:O	1:B:399:PHE:CB	2.65	0.44
1:D:338:ARG:O	1:D:339:TYR:CD1	2.71	0.44
1:A:303:THR:HB	1:A:305:ILE:HG13	1.99	0.44
1:A:453:SER:HB2	1:A:493:MET:H	1.82	0.44
1:B:282:LYS:HG3	1:B:287:ALA:CB	2.48	0.44
1:B:282:LYS:HB2	1:B:289:SER:HB3	2.00	0.44
1:B:452:PRO:HD2	1:B:487:PHE:HB3	1.98	0.44
1:D:585:ILE:CG2	1:D:586:SER:N	2.81	0.44
1:C:61:HIS:O	1:C:61:HIS:CG	2.70	0.44
1:C:325:ASP:HB2	1:C:326:PRO:CD	2.48	0.44
1:C:541:ASP:HB3	1:C:545:SER:CB	2.30	0.44
1:A:31:TRP:CZ3	1:A:35:LYS:HD3	2.52	0.44
1:A:423:LEU:HD12	1:A:423:LEU:HA	1.84	0.44
1:B:43:PHE:CE1	1:B:67:ALA:CB	3.01	0.44
1:D:136:PRO:CD	1:D:138:GLU:OE2	2.65	0.44
1:C:548:LEU:O	1:C:551:LYS:HB2	2.18	0.44
1:A:274:VAL:HG22	1:A:428:THR:HG22	2.00	0.44
1:A:312:TYR:HB3	1:A:416:MET:HG2	1.98	0.44
1:B:39:GLU:HB2	1:B:383:ILE:HD12	1.98	0.44
1:B:526:PHE:CZ	1:B:560:LYS:HD3	2.52	0.44
1:C:93:ASP:CG	1:C:95:GLN:HE21	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:THR:C	1:A:477:THR:N	2.76	0.44
1:D:254:LYS:HG2	1:D:255:LYS:N	2.32	0.44
1:D:390:PRO:O	1:D:393:HIS:HD2	2.00	0.44
1:C:150:VAL:H	1:C:150:VAL:HG22	1.07	0.43
1:B:308:PRO:HB3	1:B:336:TYR:CE2	2.52	0.43
1:B:373:SER:O	1:B:377:GLN:N	2.51	0.43
1:D:135:LEU:HB3	1:D:136:PRO:CD	2.48	0.43
1:D:224:LEU:HD13	1:D:225:ASN:H	1.83	0.43
1:D:342:LYS:C	1:D:343:LYS:CE	2.84	0.43
1:D:346:CYS:HB3	1:D:399:PHE:HD1	1.78	0.43
1:D:595:GLU:HA	1:D:596:PRO:HD3	1.77	0.43
1:C:232:ILE:CD1	1:C:356:GLY:HA2	2.48	0.43
1:D:34:ILE:HD11	1:D:369:LYS:CE	2.48	0.43
1:D:282:LYS:HE2	1:D:284:GLY:O	2.18	0.43
1:D:408:LEU:HD23	1:D:408:LEU:HA	1.80	0.43
1:D:562:CYS:O	1:D:565:TRP:N	2.40	0.43
1:C:225:ASN:O	1:C:226:PHE:CG	2.70	0.43
1:C:310:THR:C	1:C:311:ILE:HD12	2.43	0.43
1:C:437:PRO:O	1:C:438:ASP:C	2.61	0.43
1:C:585:ILE:HD13	1:C:585:ILE:HA	1.84	0.43
1:A:46:LYS:C	1:A:48:GLU:H	2.24	0.43
1:A:453:SER:CB	1:A:493:MET:H	2.31	0.43
1:B:385:TYR:OH	1:B:388:PRO:HB3	2.18	0.43
1:D:168:LEU:N	1:D:168:LEU:HD12	2.33	0.43
1:D:296:VAL:O	1:D:300:VAL:HG23	2.18	0.43
1:D:448:PRO:O	1:D:449:PHE:HD1	2.01	0.43
1:D:482:ASP:OD2	1:D:585:ILE:HG13	2.18	0.43
1:C:311:ILE:N	1:C:311:ILE:CD1	2.80	0.43
1:C:364:MET:HA	1:C:364:MET:CE	2.42	0.43
1:C:414:ALA:HB1	1:C:435:GLN:HB3	2.00	0.43
1:A:166:LYS:C	1:A:167:LEU:HD12	2.43	0.43
1:A:237:ASP:OD1	1:A:237:ASP:O	2.36	0.43
1:B:275:VAL:HG22	1:B:429:THR:HG22	2.01	0.43
1:B:469:LEU:HD13	1:B:469:LEU:C	2.43	0.43
1:D:336:TYR:O	1:D:338:ARG:N	2.51	0.43
1:C:152:TRP:C	1:C:153:VAL:CG2	2.90	0.43
1:A:570:ILE:O	1:A:572:TRP:HB2	2.18	0.43
1:B:64:PHE:HA	1:B:66:PRO:HD3	1.99	0.43
1:B:584:ARG:C	1:B:585:ILE:HG12	2.44	0.43
1:D:293:GLN:CD	1:D:422:PHE:CD2	2.97	0.43
1:D:307:HIS:O	1:D:310:THR:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:THR:HG22	1:A:340:ASP:N	2.32	0.43
1:B:98:MET:HE3	1:B:98:MET:HB3	1.92	0.43
1:B:480:LEU:CA	1:B:483:LEU:HB3	2.37	0.43
1:C:332:LEU:HD23	1:C:399:PHE:CZ	2.53	0.43
1:A:459:ARG:HD3	1:A:459:ARG:HA	1.74	0.43
1:B:282:LYS:HG2	1:B:287:ALA:HB3	1.97	0.43
1:D:573:TRP:O	1:D:573:TRP:CG	2.71	0.43
1:C:548:LEU:HD22	1:C:551:LYS:HD2	2.00	0.43
1:A:22:PRO:HD3	1:A:245:GLU:O	2.19	0.43
1:B:68:LYS:HE3	1:B:68:LYS:HB3	1.74	0.43
1:D:455:ALA:HB3	1:D:461:LEU:HB2	2.00	0.43
1:A:119:THR:HG23	1:A:201:TYR:HB2	2.00	0.43
1:A:315:ALA:CB	1:A:327:GLU:OE2	2.57	0.43
1:B:232:ILE:HG13	1:B:243:ILE:HG22	2.00	0.43
1:B:271:ARG:HB3	1:B:271:ARG:CZ	2.47	0.43
1:B:551:LYS:HB3	1:B:552:TRP:HE3	1.83	0.43
1:D:150:VAL:O	1:D:150:VAL:HG12	2.18	0.43
1:C:270:LEU:HD11	1:C:273:ILE:CG1	2.47	0.43
1:A:481:ASP:OD2	1:A:582:LYS:HE2	2.19	0.43
1:A:483:ALA:O	1:A:487:GLN:HG3	2.19	0.43
1:A:504:THR:O	1:A:507:LEU:HB3	2.19	0.43
1:B:194:SER:O	1:B:199:GLU:HG2	2.18	0.43
1:C:84:PHE:CE1	1:C:92:MET:HE1	2.54	0.42
1:C:233:LYS:O	1:C:320:GLY:CA	2.63	0.42
1:C:358:LEU:HD23	1:C:361:ALA:HB1	2.01	0.42
1:C:545:SER:OG	1:C:549:ILE:HD13	2.19	0.42
1:A:363:MET:O	1:A:367:ILE:HG13	2.19	0.42
1:D:113:ILE:HD12	1:D:116:GLU:OE1	2.18	0.42
1:D:245:GLY:C	1:D:358:LEU:CD2	2.70	0.42
1:C:147:ASP:C	1:C:149:TYR:H	2.27	0.42
1:C:459:ASP:N	1:C:459:ASP:OD1	2.52	0.42
1:A:500:ILE:HG22	1:A:523:GLY:HA3	2.01	0.42
1:B:120:THR:O	1:B:172:GLY:CA	2.66	0.42
1:B:397:SER:C	1:B:399:PHE:H	2.26	0.42
1:D:313:TYR:HB3	1:D:417:MET:HG2	2.01	0.42
1:D:317:HIS:CB	1:D:328:GLU:OE2	2.67	0.42
1:D:485:TYR:HB2	1:D:582:PRO:HB2	2.01	0.42
1:C:317:HIS:CD2	1:C:319:THR:HG23	2.54	0.42
1:C:482:ASP:HB3	1:C:585:ILE:CG1	2.49	0.42
1:C:558:GLY:O	1:C:559:PRO:C	2.60	0.42
1:A:12:LEU:HD22	1:A:194:LEU:HD13	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HD12	1:A:133:LEU:N	2.33	0.42
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.76	0.42
1:B:318:GLY:HA3	1:B:350:SER:HB2	2.02	0.42
1:D:201:LYS:HE3	1:D:254:LYS:CE	2.47	0.42
1:D:237:ALA:O	1:D:238:ASP:CB	2.66	0.42
1:B:346:CYS:O	1:B:399:PHE:CA	2.67	0.42
1:D:43:PHE:N	1:D:43:PHE:CD1	2.87	0.42
1:D:134:LEU:HB3	1:D:599:PRO:HG2	2.00	0.42
1:D:564:MET:C	1:D:566:SER:N	2.77	0.42
1:C:547:GLU:O	1:C:551:LYS:HG3	2.20	0.42
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.86	0.42
1:B:257:SER:O	1:B:260:VAL:CG2	2.68	0.42
1:B:295:GLU:O	1:B:299:LYS:HB2	2.19	0.42
1:D:183:SER:O	1:D:186:ILE:HB	2.19	0.42
1:D:186:ILE:HD13	1:D:186:ILE:HA	1.89	0.42
1:D:473:GLU:O	1:D:474:ARG:C	2.53	0.42
1:C:552:TRP:NE1	1:C:557:LYS:CE	2.83	0.42
1:B:108:GLU:C	1:B:491:ARG:NH1	2.76	0.42
1:B:233:LYS:O	1:B:239:ALA:HB2	2.19	0.42
1:B:246:GLU:CA	1:B:358:LEU:CD2	2.97	0.42
1:B:373:SER:HB3	1:B:378:GLU:O	2.19	0.42
1:B:414:ALA:CB	1:B:435:GLN:HB3	2.45	0.42
1:D:7:TYR:CE1	1:D:434:GLU:OE2	2.72	0.42
1:D:64:PHE:CG	1:D:65:VAL:N	2.86	0.42
1:D:489:VAL:O	1:D:489:VAL:HG23	2.20	0.42
1:B:397:SER:HA	1:B:398:PRO:HD2	1.84	0.42
1:D:307:HIS:O	1:D:310:THR:CB	2.68	0.42
1:C:77:PHE:CD1	1:C:78:ASP:N	2.87	0.42
1:C:105:LYS:HG2	1:C:589:VAL:CG2	2.43	0.42
1:A:570:ILE:HG23	1:A:572:TRP:CD1	2.54	0.42
1:B:308:PRO:C	1:B:310:THR:N	2.76	0.42
1:B:488:GLN:HB3	1:B:572:ASN:HB3	2.01	0.42
1:D:22:PRO:HD2	1:D:355:LEU:HD22	2.02	0.42
1:D:515:PHE:O	1:D:515:PHE:CG	2.72	0.42
1:D:561:LEU:HD12	1:D:561:LEU:HA	1.77	0.42
1:D:583:LYS:O	1:D:585:ILE:HG12	2.20	0.42
1:C:12:LEU:CD1	1:C:192:PHE:HD1	2.32	0.42
1:C:272:GLY:O	1:C:273:ILE:HG13	2.19	0.42
1:C:297:ILE:HG23	1:C:430:HIS:CD2	2.54	0.42
1:A:521:VAL:HB	1:A:522:THR:HG23	2.02	0.42
1:D:73:GLY:HA3	1:D:76:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:MET:HG2	1:C:96:LEU:HD23	2.02	0.41
1:C:276:ASN:OD1	1:C:276:ASN:C	2.62	0.41
1:C:328:GLU:HG3	1:C:422:PHE:HE2	1.85	0.41
1:A:180:CYS:HB2	1:A:422:GLY:HA2	2.01	0.41
1:B:8:TYR:CZ	1:B:269:LEU:HD21	2.55	0.41
1:B:39:GLU:HB2	1:B:383:ILE:CD1	2.50	0.41
1:B:400:PHE:CD1	1:B:400:PHE:C	2.98	0.41
1:D:340:THR:O	1:D:342:LYS:CD	2.68	0.41
1:A:39:GLU:OE2	1:A:230:HIS:CD2	2.72	0.41
1:B:223:GLY:O	1:B:224:LEU:CG	2.68	0.41
1:B:594:LYS:HE3	1:B:594:LYS:HB2	1.76	0.41
1:D:136:PRO:O	1:D:138:GLU:HG3	2.20	0.41
1:D:342:LYS:HE2	1:D:342:LYS:C	2.45	0.41
1:D:474:ARG:NH1	1:D:586:SER:O	2.38	0.41
1:C:464:TYR:HH	1:C:487:PHE:HE1	1.66	0.41
1:D:41:ILE:CG2	1:D:42:THR:N	2.83	0.41
1:D:237:ALA:O	1:D:238:ASP:HB2	2.21	0.41
1:D:497:ARG:HD3	1:D:565:TRP:CE3	2.56	0.41
1:C:392:LEU:HB3	1:C:394:LEU:HD21	2.01	0.41
1:A:156:SER:HB3	1:A:175:PHE:CD1	2.55	0.41
1:B:282:LYS:HG3	1:B:287:ALA:HB3	2.02	0.41
1:B:497:ARG:H	1:B:528:GLY:HA3	1.84	0.41
1:B:557:LYS:HD3	1:B:574:HIS:CB	2.50	0.41
1:C:225:ASN:O	1:C:226:PHE:CB	2.69	0.41
1:C:351:VAL:O	1:C:351:VAL:HG22	2.19	0.41
1:D:34:ILE:HG23	1:D:35:LYS:N	2.36	0.41
1:D:313:TYR:HA	1:D:347:GLY:O	2.19	0.41
1:C:77:PHE:CD2	1:C:97:ARG:HD3	2.54	0.41
1:C:358:LEU:HB3	1:C:361:ALA:C	2.46	0.41
1:C:552:TRP:CZ3	1:C:564:MET:HG3	2.56	0.41
1:A:315:ALA:HB1	1:A:327:GLU:CD	2.44	0.41
1:C:77:PHE:CG	1:C:78:ASP:N	2.89	0.41
1:B:342:LYS:O	1:B:343:LYS:CB	2.69	0.41
1:B:374:LEU:HD22	1:B:435:GLN:HB2	2.02	0.41
1:B:501:ILE:HG23	1:B:501:ILE:O	2.20	0.41
1:D:526:PHE:O	1:D:527:ARG:C	2.63	0.41
1:C:160:ILE:HB	1:C:161:PRO:CD	2.50	0.41
1:A:159:ILE:HB	1:A:160:PRO:CD	2.50	0.41
1:A:516:ASN:O	1:A:519:PRO:CD	2.68	0.41
1:B:314:VAL:HG22	1:B:418:ALA:HB3	2.01	0.41
1:B:386:LYS:HB3	1:B:386:LYS:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:LYS:CG	1:D:202:TYR:CE1	2.98	0.41
1:C:31:TRP:CH2	1:C:35:LYS:HE3	2.56	0.41
1:C:61:HIS:O	1:C:61:HIS:CD2	2.74	0.41
1:C:127:SER:OG	1:C:209:THR:HA	2.21	0.41
1:A:388:ASN:O	1:A:391:LEU:HB2	2.21	0.41
1:A:456:LYS:O	1:A:459:ARG:HB2	2.20	0.41
1:B:342:LYS:O	1:B:343:LYS:CG	2.69	0.41
1:B:456:ARG:CD	1:B:495:GLU:OE2	2.68	0.41
1:B:512:LEU:O	1:B:515:PHE:N	2.54	0.41
1:B:551:LYS:HB3	1:B:552:TRP:CE3	2.56	0.41
1:D:486:THR:O	1:D:486:THR:CG2	2.68	0.41
1:D:515:PHE:CE1	1:D:518:ASP:CA	3.04	0.41
1:C:154:LEU:HA	1:C:154:LEU:HD23	1.81	0.41
1:C:337:GLY:C	1:C:339:TYR:H	2.28	0.41
1:C:553:LEU:HD12	1:C:574:HIS:O	2.20	0.41
1:B:185:LEU:CD2	1:B:429:THR:HB	2.51	0.41
1:B:246:GLU:CA	1:B:358:LEU:HD22	2.51	0.41
1:B:310:THR:O	1:B:310:THR:HG22	2.21	0.41
1:B:337:GLY:O	1:B:339:TYR:N	2.54	0.41
1:D:147:ASP:C	1:D:149:TYR:N	2.79	0.41
1:D:229:ASP:OD1	1:D:233:LYS:HE2	2.21	0.41
1:D:236:ASP:HB2	1:D:385:TYR:CD1	2.56	0.41
1:D:278:ASP:OD1	1:D:426:GLY:HA2	2.21	0.41
1:C:571:ILE:O	1:C:571:ILE:CG2	2.69	0.40
1:B:75:GLU:H	1:B:75:GLU:CD	2.14	0.40
1:B:138:GLU:N	1:B:138:GLU:CD	2.78	0.40
1:B:316:ALA:HB1	1:B:328:GLU:CD	2.47	0.40
1:D:64:PHE:CE1	1:D:66:PRO:HB3	2.56	0.40
1:D:160:ILE:HB	1:D:161:PRO:HD3	2.03	0.40
1:D:317:HIS:O	1:D:352:LYS:CD	2.68	0.40
1:D:410:ARG:C	1:D:411:GLU:CG	2.91	0.40
1:B:202:TYR:CZ	1:B:254:LYS:HE3	2.55	0.40
1:B:258:ASP:O	1:B:262:ASP:HB2	2.20	0.40
1:B:587:LEU:CB	1:B:588:PRO:CD	2.99	0.40
1:D:501:ILE:C	1:D:502:THR:OG1	2.65	0.40
1:C:313:TYR:OH	1:C:349:GLY:HA3	2.22	0.40
1:C:434:GLU:HG2	1:C:435:GLN:N	2.35	0.40
1:B:66:PRO:CD	1:B:67:ALA:H	2.35	0.40
1:B:286:TYR:CD1	1:B:286:TYR:N	2.89	0.40
1:D:317:HIS:CA	1:D:328:GLU:OE2	2.70	0.40
1:D:457:LYS:HA	1:D:496:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:TYR:HA	1:C:437:PRO:HD3	1.87	0.40
1:C:511:GLN:NE2	1:C:524:GLY:CA	2.80	0.40
1:C:517:ASN:O	1:C:518:ASP:HB3	2.21	0.40
1:C:553:LEU:HD12	1:C:574:HIS:HB3	2.02	0.40
1:A:51:ARG:CG	1:A:52:SER:N	2.84	0.40
1:B:114:SER:C	1:B:116:GLU:N	2.77	0.40
1:B:130:SER:O	1:B:133:SER:HB2	2.22	0.40
1:B:276:ASN:OD1	1:B:276:ASN:C	2.63	0.40
1:B:493:ALA:HB1	1:B:497:ARG:NH1	2.37	0.40
1:D:98:MET:HE2	1:D:98:MET:HB3	1.95	0.40
1:D:104:TRP:CD1	1:D:104:TRP:C	2.99	0.40
1:D:178:HIS:CE1	1:D:180:ASN:HA	2.56	0.40
1:D:247:GLY:N	1:D:358:LEU:HD22	2.36	0.40
1:D:290:VAL:HG23	1:D:331:ALA:HB2	2.03	0.40
1:C:232:ILE:HD12	1:C:356:GLY:HA2	2.03	0.40
1:C:275:VAL:HG22	1:C:429:THR:HG22	2.03	0.40
1:A:64:VAL:O	1:A:64:VAL:CG2	2.69	0.40
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.89	0.40
1:B:313:TYR:OH	1:B:349:GLY:CA	2.68	0.40
1:D:222:PRO:HG3	1:D:228:SER:HA	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLN:OE1	1:D:128:THR:OG1[1_556]	1.71	0.49
1:C:284:GLY:O	1:B:166:HIS:CD2[1_565]	1.78	0.42
1:B:477:ASP:OD2	1:D:223:GLY:O[1_655]	1.95	0.25
1:C:284:GLY:C	1:B:166:HIS:NE2[1_565]	2.03	0.17
1:C:284:GLY:O	1:B:166:HIS:CE1[1_565]	2.06	0.14
1:C:284:GLY:CA	1:B:166:HIS:NE2[1_565]	2.11	0.09
1:B:87:LYS:CD	1:D:507:GLU:OE2[1_545]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	526/622 (85%)	483 (92%)	34 (6%)	9 (2%)	7	20
1	B	529/622 (85%)	473 (89%)	48 (9%)	8 (2%)	8	23
1	C	543/622 (87%)	485 (89%)	48 (9%)	10 (2%)	6	19
1	D	505/622 (81%)	461 (91%)	38 (8%)	6 (1%)	10	27
All	All	2103/2488 (84%)	1902 (90%)	168 (8%)	33 (2%)	7	21

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	226	PHE
1	C	288	PRO
1	C	554	ALA
1	A	447	PRO
1	A	571	ASN
1	B	343	LYS
1	B	448	PRO
1	B	452	PRO
1	D	225	ASN
1	D	343	LYS
1	C	62	PRO
1	C	343	LYS
1	B	342	LYS
1	C	342	LYS
1	C	560	LYS
1	A	279	ALA
1	A	558	PRO
1	A	568	VAL
1	B	559	PRO
1	D	224	LEU
1	C	308	PRO
1	C	341	ASP
1	B	437	PRO
1	A	569	ALA
1	B	326	PRO
1	D	238	ASP
1	D	448	PRO
1	A	135	PRO
1	A	567	GLY
1	D	599	PRO

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Mol	Chain	Res	Type
1	B	519	LYS
1	C	66	PRO
1	A	222	GLY

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	439/506 (87%)	411 (94%)	28 (6%)	16	36
1	B	442/506 (87%)	419 (95%)	23 (5%)	21	44
1	C	453/506 (90%)	418 (92%)	35 (8%)	12	28
1	D	425/506 (84%)	388 (91%)	37 (9%)	9	24
All	All	1759/2024 (87%)	1636 (93%)	123 (7%)	14	32

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	7	TYR
1	C	11	SER
1	C	12	LEU
1	C	45	SER
1	C	46	LYS
1	C	48	GLU
1	C	49	LEU
1	C	62	PRO
1	C	119	GLU
1	C	127	SER
1	C	150	VAL
1	C	152	TRP
1	C	221	GLN
1	C	233	LYS
1	C	242	MET
1	C	243	ILE
1	C	308	PRO
1	C	310	THR

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Mol	Chain	Res	Type
1	C	338	ARG
1	C	340	THR
1	C	343	LYS
1	C	355	LEU
1	C	404	GLU
1	C	405	LYS
1	C	453	LEU
1	C	475	LYS
1	C	501	ILE
1	C	519	LYS
1	C	527	ARG
1	C	529	GLU
1	C	545	SER
1	C	549	ILE
1	C	553	LEU
1	C	563	GLU
1	C	575	LYS
1	A	11	SER
1	A	20	GLU
1	A	47	GLU
1	A	49	LEU
1	A	54	ILE
1	A	55	SER
1	A	70	LEU
1	A	73	LYS
1	A	102	SER
1	A	113	SER
1	A	114	LYS
1	A	129	SER
1	A	136	GLU
1	A	139	THR
1	A	260	LYS
1	A	275	ASN
1	A	328	LEU
1	A	367	ILE
1	A	402	GLU
1	A	436	PRO
1	A	450	ILE
1	A	473	ARG
1	A	510	GLN
1	A	565	SER
1	A	568	VAL

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Mol	Chain	Res	Type
1	A	571	ASN
1	A	586	LEU
1	A	593	LYS
1	B	20	GLU
1	B	55	SER
1	B	57	GLU
1	B	68	LYS
1	B	105	LYS
1	B	114	SER
1	B	233	LYS
1	B	257	SER
1	B	277	ASN
1	B	308	PRO
1	B	322	LYS
1	B	343	LYS
1	B	399	PHE
1	B	406	LYS
1	B	407	GLU
1	B	450	ILE
1	B	451	ILE
1	B	471	PHE
1	B	476	THR
1	B	495	GLU
1	B	572	ASN
1	B	587	LEU
1	B	594	LYS
1	D	7	TYR
1	D	20	GLU
1	D	64	PHE
1	D	90	GLU
1	D	114	SER
1	D	119	GLU
1	D	124	MET
1	D	125	SER
1	D	149	TYR
1	D	171	LYS
1	D	195	LEU
1	D	196	GLN
1	D	210	LEU
1	D	213	GLU
1	D	224	LEU
1	D	232	ILE

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Mol	Chain	Res	Type
1	D	233	LYS
1	D	255	LYS
1	D	282	LYS
1	D	306	ILE
1	D	342	LYS
1	D	343	LYS
1	D	345	TYR
1	D	394	LEU
1	D	407	GLU
1	D	410	ARG
1	D	424	LEU
1	D	453	LEU
1	D	456	ARG
1	D	457	LYS
1	D	476	THR
1	D	478	THR
1	D	494	MET
1	D	501	ILE
1	D	563	GLU
1	D	567	LYS
1	D	571	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	61	HIS
1	C	95	GLN
1	C	221	GLN
1	C	307	HIS
1	C	317	HIS
1	C	354	ASN
1	C	376	HIS
1	C	511	GLN
1	A	177	HIS
1	A	188	HIS
1	A	230	HIS
1	A	292	GLN
1	A	297	GLN
1	A	302	GLN
1	A	375	HIS
1	A	466	GLN
1	A	571	ASN

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Mol	Chain	Res	Type
1	B	156	GLN
1	B	178	HIS
1	B	196	GLN
1	B	231	HIS
1	B	317	HIS
1	B	435	GLN
1	B	511	GLN
1	D	27	HIS
1	D	178	HIS
1	D	221	GLN
1	D	303	GLN
1	D	307	HIS
1	D	317	HIS
1	D	391	ASN
1	D	393	HIS
1	D	428	ASN
1	D	488	GLN
1	D	581	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	540/622 (86%)	0.34	21 (3%) 43 35	23, 48, 87, 109	0
1	B	547/622 (87%)	0.67	34 (6%) 26 22	24, 62, 100, 121	0
1	C	557/622 (89%)	0.70	59 (10%) 11 11	23, 55, 104, 162	0
1	D	523/622 (84%)	0.79	54 (10%) 12 11	24, 63, 108, 133	0
All	All	2167/2488 (87%)	0.62	168 (7%) 19 16	23, 57, 101, 162	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	341	ASP	7.2
1	D	469	LEU	5.3
1	D	341	ASP	5.0
1	C	548	LEU	4.7
1	C	523	THR	4.6
1	C	340	THR	4.6
1	C	288	PRO	4.5
1	B	340	THR	4.5
1	D	472	LEU	4.5
1	B	341	ASP	4.5
1	D	240	ASP	4.4
1	B	572	ASN	4.3
1	C	258	ASP	4.3
1	B	58	LEU	4.3
1	C	233	LYS	4.1
1	C	182	SER	4.0
1	C	360	THR	4.0
1	D	495	GLU	4.0
1	C	153	VAL	4.0
1	B	547	GLU	3.9
1	C	221	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	512	LEU	3.9
1	D	325	ASP	3.8
1	C	476	THR	3.8
1	C	155	ALA	3.7
1	B	224	LEU	3.7
1	D	505	THR	3.7
1	D	471	PHE	3.6
1	C	478	THR	3.6
1	C	358	LEU	3.5
1	B	62	PRO	3.5
1	C	532	GLN	3.4
1	C	132	ARG	3.4
1	B	66	PRO	3.4
1	D	221	GLN	3.3
1	D	63	GLY	3.3
1	A	146	ASP	3.2
1	C	49	LEU	3.2
1	D	404	GLU	3.2
1	D	74	LYS	3.2
1	C	128	THR	3.2
1	C	154	LEU	3.1
1	B	511	GLN	3.1
1	C	283	VAL	3.1
1	D	235	PHE	3.1
1	D	155	ALA	3.0
1	C	552	TRP	3.0
1	A	70	LEU	3.0
1	D	517	ASN	3.0
1	B	155	ALA	3.0
1	D	147	ASP	3.0
1	D	482	ASP	3.0
1	C	281	ASP	3.0
1	C	477	ASP	3.0
1	A	340	ASP	3.0
1	C	222	PRO	3.0
1	A	69	VAL	3.0
1	A	278	GLY	2.9
1	C	359	ASP	2.9
1	D	516	ILE	2.9
1	D	474	ARG	2.8
1	D	503	SER	2.8
1	A	47	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	44	PHE	2.8
1	C	570	ALA	2.8
1	D	394	LEU	2.8
1	C	302	ASP	2.8
1	C	282	LYS	2.8
1	B	319	THR	2.8
1	B	567	LYS	2.8
1	D	508	LEU	2.7
1	D	150	VAL	2.7
1	B	154	LEU	2.7
1	C	343	LYS	2.7
1	B	434	GLU	2.7
1	B	7	TYR	2.7
1	B	230	GLY	2.6
1	D	448	PRO	2.6
1	D	389	ASN	2.6
1	D	560	LYS	2.6
1	B	397	SER	2.6
1	C	336	TYR	2.6
1	A	410	GLU	2.6
1	B	501	ILE	2.6
1	C	553	LEU	2.6
1	A	512	ALA	2.6
1	D	568	GLY	2.6
1	D	137	GLU	2.6
1	D	511	GLN	2.6
1	C	391	ASN	2.6
1	C	152	TRP	2.5
1	C	225	ASN	2.5
1	C	10	ASP	2.5
1	C	543	ASP	2.5
1	A	578	ASP	2.5
1	B	63	GLY	2.5
1	B	480	LEU	2.5
1	B	407	GLU	2.5
1	A	412	ARG	2.5
1	A	51	ARG	2.4
1	C	569	VAL	2.4
1	C	454	SER	2.4
1	D	340	THR	2.4
1	D	323	LEU	2.4
1	C	47	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	514	PHE	2.4
1	C	536	ILE	2.4
1	C	342	LYS	2.4
1	C	556	GLY	2.4
1	D	109	ASP	2.4
1	D	473	GLU	2.4
1	D	234	ALA	2.4
1	C	11	SER	2.4
1	B	329	LEU	2.3
1	D	329	LEU	2.3
1	D	502	THR	2.3
1	C	284	GLY	2.3
1	C	240	ASP	2.3
1	C	535	ASP	2.3
1	D	239	ALA	2.3
1	D	554	ALA	2.3
1	B	445	ALA	2.3
1	C	521	ALA	2.3
1	D	414	ALA	2.3
1	A	354	LEU	2.3
1	B	153	VAL	2.3
1	B	54	ILE	2.2
1	D	242	MET	2.2
1	D	138	GLU	2.2
1	D	407	GLU	2.2
1	D	509	LYS	2.2
1	C	70	VAL	2.2
1	A	213	SER	2.2
1	A	214	SER	2.2
1	C	561	LEU	2.2
1	C	262	ASP	2.2
1	D	392	LEU	2.2
1	C	129	ASN	2.2
1	C	219	VAL	2.2
1	B	559	PRO	2.2
1	D	148	GLY	2.2
1	C	421	SER	2.2
1	C	546	ALA	2.2
1	B	446	ALA	2.2
1	A	563	MET	2.1
1	B	57	GLU	2.1
1	A	571	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	514	ASP	2.1
1	B	152	TRP	2.1
1	B	215	SER	2.1
1	D	34	ILE	2.1
1	A	279	ALA	2.1
1	A	568	VAL	2.1
1	D	223	GLY	2.1
1	C	287	ALA	2.1
1	D	154	LEU	2.0
1	B	179	ALA	2.0
1	C	534	LYS	2.0
1	A	566	LYS	2.0
1	C	66	PRO	2.0
1	C	235	PHE	2.0
1	B	442	ALA	2.0
1	D	455	ALA	2.0
1	A	9	GLU	2.0
1	B	444	ASP	2.0
1	B	529	GLU	2.0
1	D	152	TRP	2.0
1	D	149	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.