



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:29 PM UTC

PDB ID : 1BPO / pdb_00001bpo
Title : CLATHRIN HEAVY-CHAIN TERMINAL DOMAIN AND LINKER
Authors : Harr, E.T.; Musacchio, A.; Harrison, S.C.; Kirchhausen, T.
Deposited on : 1998-08-11
Resolution : 2.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

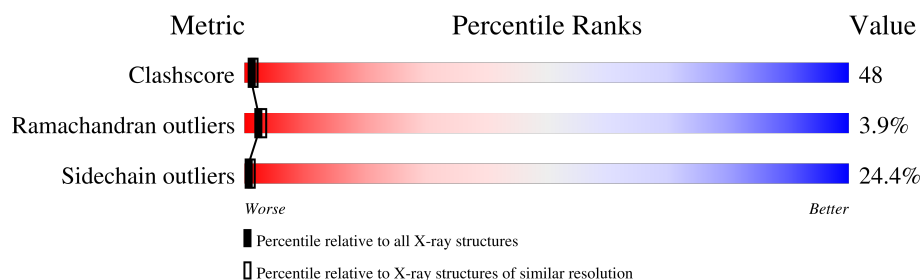
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

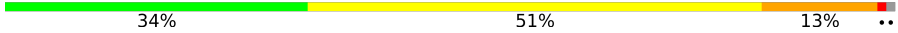
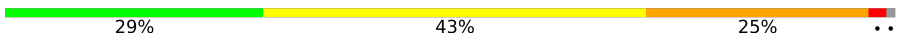
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	494	 34% 51% 13% ..
1	B	494	 36% 46% 16% .
1	C	494	 29% 43% 25% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11517 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 PROTEIN (CLATHRIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3812	2425	658	708	21			
1	B	493	Total	C	N	O	S	0	0	0
			3858	2456	665	715	22			
1	C	487	Total	C	N	O	S	0	0	0
			3812	2425	658	708	21			

- Molecule 2 is water.

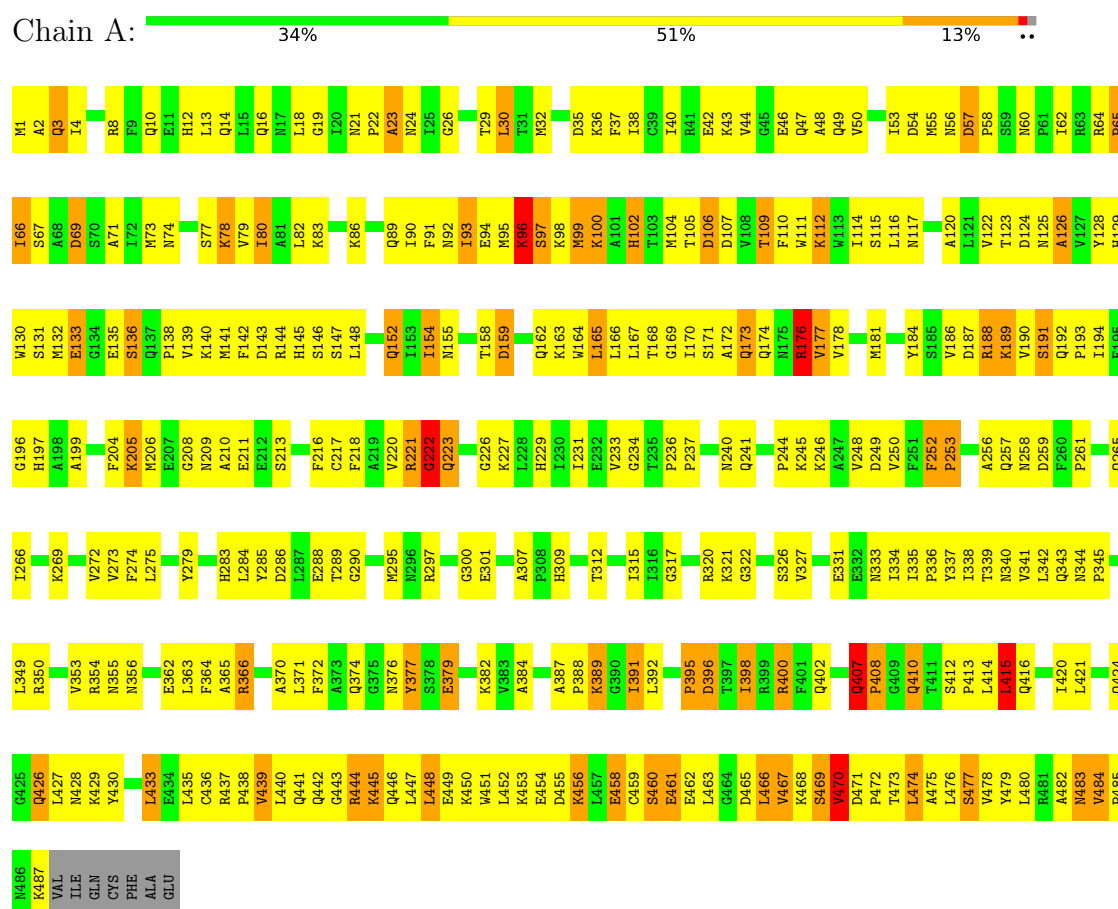
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	9	Total	O	0	0
			9	9		
2	C	10	Total	O	0	0
			10	10		

3 Residue-property plots

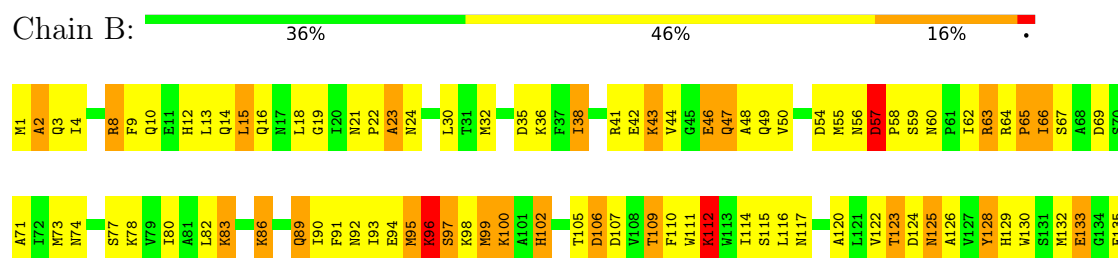
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

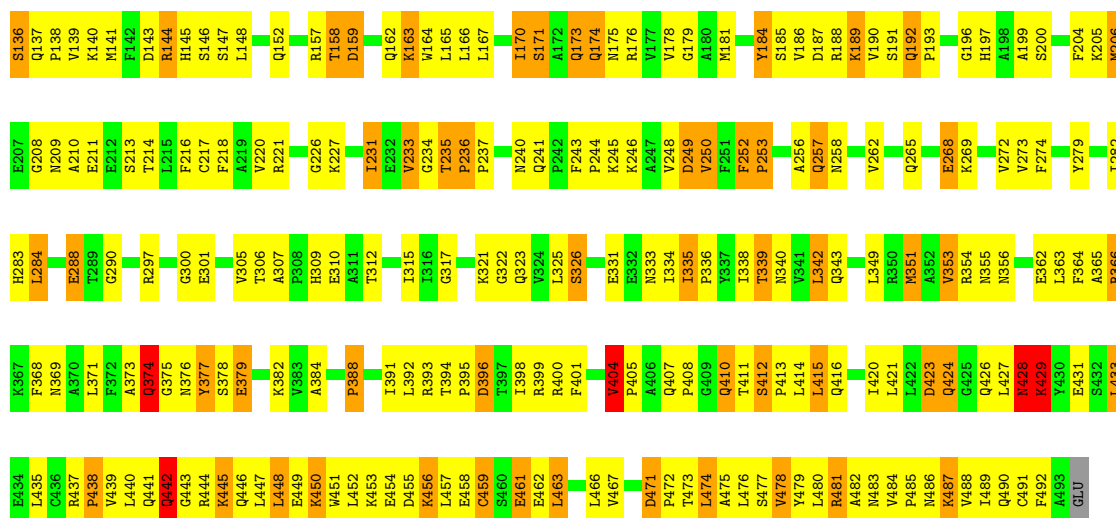
Note EDS was not executed.

• Molecule 1: PROTEIN (CLATHRIN)



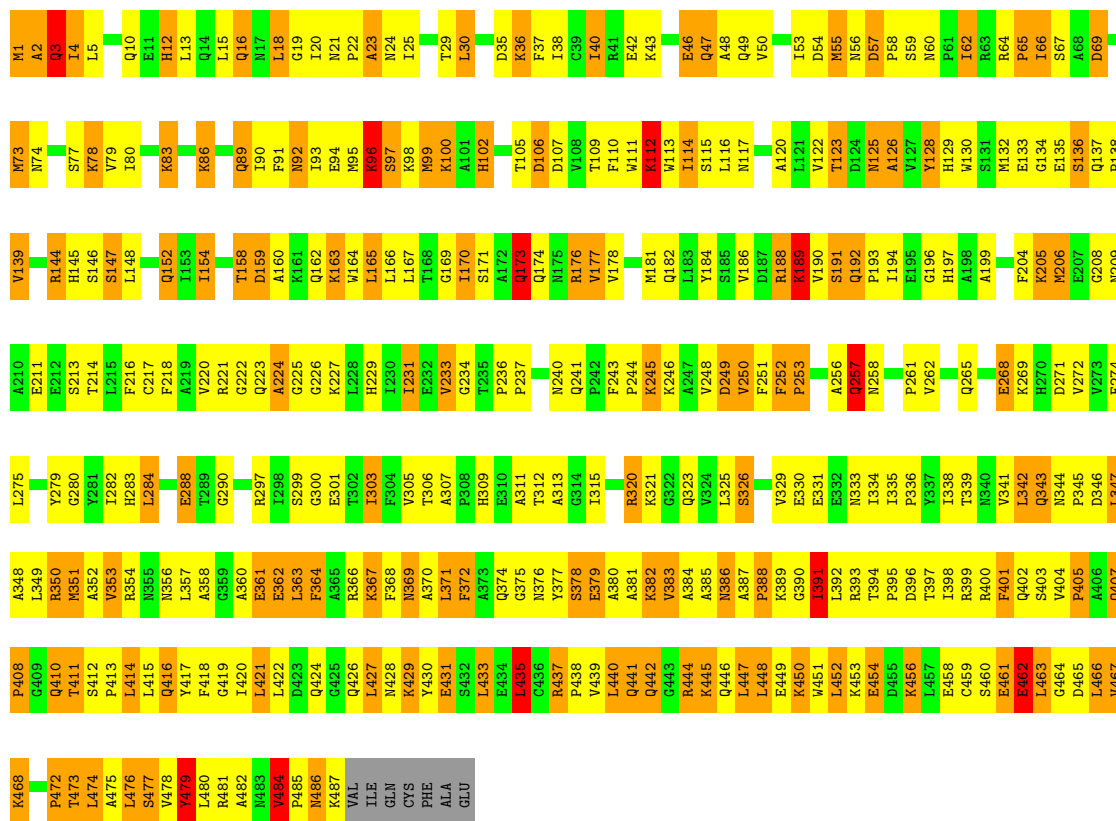
• Molecule 1: PROTEIN (CLATHRIN)





• Molecule 1: PROTEIN (CLATHRIN)

Chain C: 29% 43% 25% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	205.82Å 205.82Å 87.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.60	Depositor
% Data completeness (in resolution range)	95.0 (6.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.226 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11517	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

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	1.20	10/3889 (0.3%)	1.48	55/5270 (1.0%)
1	B	1.18	7/3936 (0.2%)	1.42	56/5334 (1.0%)
1	C	1.13	10/3889 (0.3%)	1.41	67/5270 (1.3%)
All	All	1.17	27/11714 (0.2%)	1.44	178/15874 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	GLN	CA-CB	-17.01	1.27	1.53
1	A	174	GLN	C-N	-12.67	1.16	1.33
1	A	222	GLY	C-N	-12.62	1.16	1.33
1	C	484	VAL	CB-CG2	9.69	1.84	1.52
1	C	484	VAL	C-N	9.66	1.45	1.33
1	C	4	ILE	CA-CB	7.06	1.60	1.55
1	B	95	MET	SD-CE	6.83	1.96	1.79
1	B	335	ILE	CA-CB	-6.82	1.50	1.54
1	B	353	VAL	CA-CB	-6.51	1.46	1.54
1	A	172	ALA	C-N	-6.36	1.23	1.33
1	C	329	VAL	CA-CB	6.20	1.62	1.54
1	B	273	VAL	CA-CB	6.18	1.61	1.54
1	B	339	THR	CA-CB	-6.15	1.43	1.53
1	C	122	VAL	CA-CB	-6.11	1.46	1.54
1	A	80	ILE	CA-CB	6.04	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	MET	SD-CE	5.81	1.94	1.79
1	A	38	ILE	CA-CB	-5.76	1.46	1.54
1	C	311	ALA	CA-CB	-5.43	1.45	1.53
1	C	40	ILE	CA-CB	5.42	1.61	1.54
1	C	303	ILE	CA-CB	5.41	1.60	1.53
1	C	10	GLN	CA-C	-5.29	1.46	1.52
1	A	327	VAL	CA-CB	-5.16	1.46	1.55
1	A	93	ILE	CA-CB	5.15	1.60	1.54
1	B	307	ALA	CA-C	-5.13	1.45	1.53
1	C	120	ALA	CA-CB	-5.02	1.46	1.53
1	B	236	PRO	CA-C	-5.02	1.47	1.52
1	A	40	ILE	CA-CB	5.00	1.61	1.54

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	GLY	CA-C-N	18.45	156.78	121.54
1	A	222	GLY	C-N-CA	18.45	156.78	121.54
1	B	174	GLN	CB-CA-C	15.03	133.23	111.89
1	A	387	ALA	CA-C-N	12.40	132.53	119.76
1	A	387	ALA	C-N-CA	12.40	132.53	119.76
1	C	484	VAL	CA-CB-CG2	-10.79	92.06	110.40
1	A	222	GLY	O-C-N	-10.36	102.51	123.02
1	C	3	GLN	N-CA-C	-10.28	100.76	113.20
1	A	176	ARG	N-CA-C	10.14	124.55	109.95
1	C	407	GLN	CA-C-N	10.10	132.47	119.84
1	C	407	GLN	C-N-CA	10.10	132.47	119.84
1	B	174	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	A	223	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	A	173	GLN	OE1-CD-NE2	-9.74	112.86	122.60
1	C	18	LEU	N-CA-C	-9.64	101.73	112.72
1	C	334	ILE	N-CA-C	9.14	119.19	110.42
1	A	18	LEU	N-CA-C	-9.08	101.75	112.92
1	C	379	GLU	N-CA-C	-8.98	102.45	113.50
1	B	382	LYS	N-CA-C	-8.97	101.07	111.03
1	B	18	LEU	N-CA-C	-8.91	101.39	112.88
1	C	414	LEU	N-CA-C	-8.69	101.89	111.36
1	B	307	ALA	CA-C-N	-8.68	111.08	119.85
1	B	307	ALA	C-N-CA	-8.68	111.08	119.85
1	C	416	GLN	N-CA-C	-8.46	102.14	111.36
1	A	340	ASN	N-CA-C	8.38	121.62	111.40
1	A	382	LYS	N-CA-C	-8.18	102.31	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	THR	CA-C-N	8.18	127.86	119.19
1	B	394	THR	C-N-CA	8.18	127.86	119.19
1	C	38	ILE	N-CA-C	-7.95	96.69	108.45
1	B	173	GLN	OE1-CD-NE2	-7.92	114.68	122.60
1	C	23	ALA	N-CA-C	-7.88	103.12	112.89
1	A	23	ALA	N-CA-C	-7.87	103.47	113.23
1	A	334	ILE	N-CA-C	7.87	117.98	110.42
1	C	346	ASP	N-CA-C	-7.86	102.65	111.14
1	C	382	LYS	N-CA-C	-7.76	102.76	111.07
1	B	173	GLN	CG-CD-NE2	7.63	127.84	116.40
1	C	388	PRO	N-CA-C	7.46	123.07	111.21
1	C	435	LEU	N-CA-C	-7.46	102.75	111.03
1	C	69	ASP	N-CA-C	-7.45	103.18	111.82
1	C	241	GLN	N-CA-C	-7.38	99.89	110.08
1	C	307	ALA	CA-C-N	-7.38	112.39	119.85
1	C	307	ALA	C-N-CA	-7.38	112.39	119.85
1	A	252	PHE	CA-C-N	-7.35	112.81	120.38
1	A	252	PHE	C-N-CA	-7.35	112.81	120.38
1	C	441	GLN	N-CA-C	-7.34	102.45	111.33
1	C	65	PRO	N-CA-C	-7.30	98.65	110.55
1	C	387	ALA	CA-C-N	7.29	127.29	119.78
1	C	387	ALA	C-N-CA	7.29	127.29	119.78
1	A	46	GLU	N-CA-C	-7.02	103.90	113.30
1	A	407	GLN	CA-C-N	7.01	128.60	119.84
1	A	407	GLN	C-N-CA	7.01	128.60	119.84
1	C	350	ARG	N-CA-C	-6.98	103.36	110.97
1	B	65	PRO	N-CA-C	-6.95	99.23	110.55
1	B	334	ILE	N-CA-C	6.90	117.04	110.42
1	C	461	GLU	N-CA-C	-6.86	103.91	112.90
1	B	23	ALA	N-CA-C	-6.81	104.44	112.89
1	B	388	PRO	N-CA-C	6.81	121.89	111.34
1	C	252	PHE	CA-C-N	-6.78	113.40	120.38
1	C	252	PHE	C-N-CA	-6.78	113.40	120.38
1	C	223	GLN	N-CA-C	-6.76	104.76	112.87
1	A	377	TYR	N-CA-C	6.75	120.62	112.38
1	B	174	GLN	N-CA-CB	-6.75	101.71	111.70
1	B	241	GLN	N-CA-C	-6.73	100.42	110.24
1	A	241	GLN	N-CA-C	-6.70	100.83	110.08
1	B	252	PHE	CA-C-N	-6.68	113.50	120.38
1	B	252	PHE	C-N-CA	-6.68	113.50	120.38
1	A	223	GLN	CG-CD-NE2	6.67	126.41	116.40
1	A	99	MET	N-CA-C	6.65	119.54	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	GLN	CG-CD-NE2	6.63	126.35	116.40
1	A	320	ARG	N-CA-C	6.56	119.26	111.71
1	A	223	GLN	CA-C-O	-6.53	111.17	120.51
1	C	482	ALA	CA-C-N	6.53	134.01	121.54
1	C	482	ALA	C-N-CA	6.53	134.01	121.54
1	A	79	VAL	N-CA-C	-6.49	99.13	108.48
1	C	114	ILE	N-CA-C	-6.48	106.68	112.90
1	B	15	LEU	N-CA-C	6.46	119.14	111.33
1	A	391	ILE	N-CA-C	6.45	117.19	110.62
1	C	10	GLN	N-CA-C	6.44	119.50	109.52
1	C	99	MET	N-CA-C	6.41	119.26	111.82
1	C	12	HIS	N-CA-C	-6.40	105.77	113.97
1	B	174	GLN	CG-CD-NE2	6.34	125.91	116.40
1	A	365	ALA	N-CA-C	-6.33	104.29	111.07
1	C	440	LEU	N-CA-C	-6.31	104.28	112.23
1	C	139	VAL	N-CA-C	6.29	116.72	106.72
1	C	213	SER	N-CA-C	-6.28	101.23	110.52
1	A	152	GLN	N-CA-C	-6.26	98.97	108.67
1	B	99	MET	N-CA-C	6.25	119.07	111.82
1	B	2	ALA	N-CA-C	-6.19	101.78	110.50
1	C	159	ASP	N-CA-C	-6.17	101.33	110.46
1	A	65	PRO	N-CA-C	-6.14	100.54	110.55
1	C	224	ALA	N-CA-C	-6.14	105.37	112.92
1	B	213	SER	N-CA-C	-6.07	101.79	110.59
1	A	38	ILE	N-CA-C	-6.00	99.53	108.46
1	B	395	PRO	N-CA-C	-5.97	105.75	113.57
1	B	365	ALA	N-CA-C	-5.96	104.69	111.07
1	C	174	GLN	N-CA-C	-5.96	98.11	110.80
1	A	174	GLN	O-C-N	-5.93	113.86	121.33
1	B	46	GLU	N-CA-C	-5.93	105.36	113.30
1	A	3	GLN	N-CA-C	-5.89	105.18	112.90
1	A	484	VAL	N-CA-C	5.88	121.59	108.88
1	C	79	VAL	N-CA-C	-5.85	99.92	108.11
1	C	62	ILE	N-CA-C	-5.80	100.00	108.11
1	A	253	PRO	CA-C-N	5.77	125.90	119.32
1	A	253	PRO	C-N-CA	5.77	125.90	119.32
1	A	307	ALA	CA-C-N	-5.76	114.03	119.85
1	A	307	ALA	C-N-CA	-5.76	114.03	119.85
1	B	235	THR	CA-C-N	5.71	126.26	120.38
1	B	235	THR	C-N-CA	5.71	126.26	120.38
1	A	126	ALA	N-CA-C	5.68	117.71	109.07
1	A	69	ASP	N-CA-C	-5.68	105.23	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	ILE	N-CA-C	-5.67	100.02	108.46
1	C	387	ALA	N-CA-C	-5.66	101.33	109.48
1	C	46	GLU	N-CA-C	-5.65	105.73	113.30
1	B	253	PRO	CA-C-N	5.63	125.74	119.32
1	B	253	PRO	C-N-CA	5.63	125.74	119.32
1	C	92	ASN	CA-C-N	5.62	127.86	120.60
1	C	92	ASN	C-N-CA	5.62	127.86	120.60
1	C	55	MET	CA-C-N	-5.61	113.75	122.67
1	C	55	MET	C-N-CA	-5.61	113.75	122.67
1	A	379	GLU	N-CA-C	-5.59	105.27	111.36
1	B	491	CYS	N-CA-C	-5.47	105.47	111.82
1	C	192	GLN	CA-C-N	5.47	125.89	119.99
1	C	192	GLN	C-N-CA	5.47	125.89	119.99
1	A	213	SER	N-CA-C	-5.46	103.18	110.55
1	B	268	GLU	N-CA-C	-5.46	105.36	112.23
1	C	251	PHE	N-CA-C	5.46	118.19	110.50
1	A	475	ALA	N-CA-C	-5.44	105.78	112.90
1	B	322	GLY	N-CA-C	-5.42	107.55	115.63
1	B	184	TYR	N-CA-C	5.39	118.03	109.24
1	C	152	GLN	N-CA-C	-5.39	100.31	108.67
1	A	174	GLN	CA-C-N	5.39	131.83	121.54
1	A	174	GLN	C-N-CA	5.39	131.83	121.54
1	B	192	GLN	CA-C-N	5.36	126.54	119.84
1	B	192	GLN	C-N-CA	5.36	126.54	119.84
1	C	320	ARG	N-CA-C	5.34	117.86	111.71
1	A	400	ARG	N-CA-C	-5.33	105.64	111.82
1	A	415	LEU	N-CA-C	-5.32	105.48	111.28
1	B	241	GLN	CA-C-N	-5.32	115.10	120.31
1	B	241	GLN	C-N-CA	-5.32	115.10	120.31
1	B	429	LYS	N-CA-C	-5.29	105.65	112.68
1	B	8	ARG	N-CA-C	-5.28	100.80	109.40
1	A	62	ILE	N-CA-C	-5.28	100.72	108.11
1	B	423	ASP	N-CA-C	-5.27	104.45	111.24
1	B	189	LYS	N-CA-C	5.25	121.99	110.80
1	A	420	ILE	CB-CA-C	-5.24	105.17	111.88
1	B	126	ALA	N-CA-C	5.24	117.03	109.07
1	B	340	ASN	N-CA-C	5.24	119.73	112.45
1	C	134	GLY	N-CA-C	5.23	124.25	112.01
1	A	159	ASP	N-CA-C	-5.23	103.01	110.59
1	B	3	GLN	N-CA-C	5.23	118.72	111.71
1	B	310	GLU	N-CA-C	5.22	116.97	111.28
1	A	395	PRO	N-CA-C	-5.22	106.73	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	268	GLU	N-CA-C	-5.22	105.66	112.23
1	C	139	VAL	CB-CA-C	-5.21	105.02	111.32
1	C	484	VAL	CG1-CB-CG2	-5.18	99.40	110.80
1	C	126	ALA	N-CA-C	5.17	116.92	109.07
1	C	73	MET	CG-SD-CE	-5.15	89.57	100.90
1	C	253	PRO	CA-C-N	5.15	125.19	119.32
1	C	253	PRO	C-N-CA	5.15	125.19	119.32
1	B	404	VAL	CA-C-N	5.13	125.04	119.76
1	B	404	VAL	C-N-CA	5.13	125.04	119.76
1	B	463	LEU	N-CA-C	-5.13	105.81	111.71
1	A	398	ILE	CB-CA-C	-5.11	105.43	111.97
1	B	41	ARG	N-CA-C	-5.11	100.20	108.52
1	A	322	GLY	N-CA-C	-5.10	108.20	115.64
1	B	152	GLN	N-CA-C	-5.08	100.79	108.67
1	B	159	ASP	N-CA-C	-5.08	103.22	110.59
1	B	396	ASP	N-CA-C	-5.08	105.82	111.36
1	C	330	GLU	N-CA-C	-5.07	99.06	107.99
1	C	378	SER	N-CA-C	-5.06	108.13	114.56
1	A	436	CYS	N-CA-C	5.05	117.90	111.69
1	B	57	ASP	N-CA-C	-5.05	98.64	109.81
1	C	189	LYS	N-CA-C	5.04	121.53	110.80
1	A	467	VAL	N-CA-C	5.03	115.80	110.72
1	C	445	LYS	N-CA-C	-5.03	107.28	113.41
1	C	2	ALA	N-CA-C	5.02	116.92	108.73
1	C	15	LEU	N-CA-C	5.02	118.17	111.75
1	B	420	ILE	CB-CA-C	-5.01	105.48	112.04

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	GLY	Peptide,Mainchain
1	C	479	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3812	0	3848	341	0
1	B	3858	0	3897	331	1
1	C	3812	0	3850	454	0
2	A	16	0	0	1	0
2	B	9	0	0	0	0
2	C	10	0	0	1	0
All	All	11517	0	11595	1106	1

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 48.

All (1106) 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:C:484:VAL:CG2	1:C:484:VAL:CB	1.84	1.55
1:A:181:MET:HE2	1:A:196:GLY:HA3	1.30	1.12
1:B:21:ASN:HD21	1:B:23:ALA:HB3	1.12	1.12
1:C:173:GLN:OE1	1:C:173:GLN:HA	1.47	1.12
1:A:444:ARG:HH11	1:A:444:ARG:HB2	1.05	1.10
1:C:181:MET:HE2	1:C:196:GLY:HA3	1.33	1.07
1:C:438:PRO:HA	1:C:441:GLN:HB2	1.37	1.06
1:A:21:ASN:HD21	1:A:23:ALA:HB3	1.20	1.04
1:B:21:ASN:ND2	1:B:23:ALA:HB3	1.75	1.02
1:C:442:GLN:HB3	1:C:444:ARG:CD	1.89	1.02
1:C:401:PHE:O	1:C:404:VAL:HB	1.61	1.01
1:B:1:MET:SD	1:C:1:MET:HA	2.03	0.99
1:C:361:GLU:H	1:C:361:GLU:CD	1.70	0.99
1:C:374:GLN:HE21	1:C:376:ASN:HB2	1.28	0.97
1:A:73:MET:HE2	1:A:80:ILE:HB	1.48	0.96
1:B:181:MET:HE2	1:B:196:GLY:HA3	1.48	0.95
1:C:64:ARG:HH11	1:C:96:LYS:HE3	1.32	0.94
1:C:484:VAL:CG2	1:C:484:VAL:CA	2.45	0.94
1:C:164:TRP:CE2	1:C:233:VAL:HG13	2.02	0.94
1:B:123:THR:HG22	1:B:125:ASN:H	1.32	0.94
1:A:64:ARG:HH11	1:A:96:LYS:HE3	1.31	0.93
1:B:64:ARG:HH11	1:B:96:LYS:HE3	1.33	0.93
1:B:24:ASN:ND2	1:B:42:GLU:HG2	1.82	0.93
1:B:371:LEU:HD13	1:B:379:GLU:HB3	1.48	0.93
1:A:24:ASN:ND2	1:A:42:GLU:HG2	1.82	0.93
1:C:21:ASN:HD21	1:C:23:ALA:HB3	1.30	0.93
1:A:21:ASN:ND2	1:A:23:ALA:HB3	1.83	0.93
1:A:444:ARG:HH11	1:A:444:ARG:CB	1.81	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:MET:CE	1:A:80:ILE:HB	2.00	0.92
1:A:123:THR:HG22	1:A:125:ASN:H	1.34	0.90
1:C:407:GLN:HE22	1:C:410:GLN:HE21	1.15	0.90
1:C:24:ASN:ND2	1:C:42:GLU:HG2	1.86	0.90
1:C:374:GLN:HG2	1:C:375:GLY:H	1.36	0.90
1:A:100:LYS:HE2	1:A:130:TRP:NE1	1.86	0.90
1:C:484:VAL:CG2	1:C:484:VAL:CG1	2.51	0.89
1:A:64:ARG:NH1	1:A:96:LYS:HE3	1.87	0.89
1:A:164:TRP:CE2	1:A:233:VAL:HG13	2.07	0.88
1:C:439:VAL:HG21	1:C:451:TRP:HH2	1.37	0.88
1:B:374:GLN:H	1:B:374:GLN:NE2	1.71	0.87
1:A:444:ARG:HB2	1:A:444:ARG:NH1	1.88	0.87
1:B:374:GLN:H	1:B:374:GLN:HE21	1.18	0.87
1:C:64:ARG:NH1	1:C:96:LYS:HE3	1.90	0.87
1:A:398:ILE:HD12	1:A:430:TYR:CD2	2.09	0.86
1:C:407:GLN:HE22	1:C:410:GLN:NE2	1.73	0.86
1:C:13:LEU:HD11	1:C:58:PRO:HB2	1.57	0.86
1:B:64:ARG:NH1	1:B:96:LYS:HE3	1.89	0.85
1:C:21:ASN:ND2	1:C:23:ALA:HB3	1.92	0.85
1:A:377:TYR:HB3	1:A:413:PRO:HB3	1.56	0.85
1:C:2:ALA:HB1	1:C:4:ILE:O	1.75	0.85
1:C:442:GLN:HB3	1:C:444:ARG:HD3	1.57	0.85
1:B:374:GLN:HE21	1:B:374:GLN:N	1.73	0.85
1:B:1:MET:SD	1:C:1:MET:HG2	2.16	0.84
1:C:50:VAL:HG23	1:C:66:ILE:HB	1.59	0.84
1:A:24:ASN:HD22	1:A:42:GLU:HG2	1.40	0.84
1:C:353:VAL:HG23	1:C:364:PHE:CZ	2.12	0.84
1:A:73:MET:HE2	1:A:80:ILE:CB	2.06	0.84
1:C:396:ASP:HA	1:C:399:ARG:NH1	1.93	0.84
1:C:173:GLN:HG2	1:C:178:VAL:HG21	1.56	0.84
1:A:309:HIS:HD2	1:A:312:THR:OG1	1.59	0.83
1:A:100:LYS:HE2	1:A:130:TRP:HE1	1.42	0.83
1:A:398:ILE:HD12	1:A:430:TYR:CE2	2.13	0.83
1:B:24:ASN:HD22	1:B:42:GLU:HG2	1.38	0.83
1:C:452:LEU:HD21	1:C:478:VAL:HG22	1.59	0.83
1:C:89:GLN:NE2	1:C:98:LYS:HD2	1.94	0.83
1:B:73:MET:HE2	1:B:80:ILE:HG13	1.61	0.82
1:B:471:ASP:HB3	1:B:474:LEU:HB2	1.60	0.82
1:C:477:SER:O	1:C:481:ARG:HG2	1.80	0.82
1:C:89:GLN:HE21	1:C:98:LYS:HD2	1.45	0.82
1:C:398:ILE:HG23	1:C:414:LEU:HD11	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:PRO:CA	1:C:441:GLN:HB2	2.10	0.82
1:C:123:THR:HG22	1:C:125:ASN:H	1.43	0.81
1:A:456:LYS:HZ2	1:A:456:LYS:HB3	1.46	0.81
1:C:438:PRO:HA	1:C:441:GLN:NE2	1.96	0.81
1:B:407:GLN:HG2	1:B:408:PRO:HD2	1.62	0.81
1:C:345:PRO:HA	1:C:348:ALA:HB3	1.63	0.81
1:A:216:PHE:HD2	1:A:231:ILE:HD11	1.47	0.80
1:B:9:PHE:CD2	1:C:5:LEU:HD23	2.16	0.80
1:C:176:ARG:HD3	1:C:177:VAL:H	1.45	0.80
1:C:394:THR:O	1:C:397:THR:HB	1.81	0.80
1:C:450:LYS:O	1:C:454:GLU:HG3	1.82	0.80
1:C:374:GLN:NE2	1:C:376:ASN:HB2	1.95	0.80
1:C:271:ASP:HB2	1:C:354:ARG:NH2	1.96	0.79
1:B:73:MET:HE2	1:B:80:ILE:CG1	2.13	0.79
1:B:477:SER:O	1:B:481:ARG:HG2	1.81	0.79
1:C:386:ASN:HD22	1:C:386:ASN:N	1.79	0.79
1:A:92:ASN:OD1	1:A:94:GLU:HB3	1.83	0.78
1:C:412:SER:O	1:C:416:GLN:HG3	1.83	0.78
1:B:50:VAL:HG23	1:B:66:ILE:HB	1.65	0.78
1:C:448:LEU:HD21	1:C:474:LEU:HG	1.65	0.78
1:B:439:VAL:HG13	1:B:444:ARG:HB2	1.63	0.78
1:C:74:ASN:HD22	1:C:77:SER:H	1.31	0.78
1:C:413:PRO:HA	1:C:416:GLN:HB2	1.65	0.78
1:B:175:ASN:O	1:B:176:ARG:HD3	1.84	0.77
1:C:24:ASN:HD22	1:C:42:GLU:HG2	1.47	0.77
1:C:271:ASP:HB2	1:C:354:ARG:HH21	1.49	0.77
1:B:450:LYS:O	1:B:454:GLU:HG3	1.85	0.77
1:C:363:LEU:HD12	1:C:363:LEU:H	1.49	0.77
1:A:449:GLU:HG3	1:A:474:LEU:HD11	1.65	0.77
1:C:176:ARG:HD3	1:C:177:VAL:N	1.99	0.77
1:C:484:VAL:CG2	1:C:484:VAL:C	2.58	0.77
1:B:453:LYS:C	1:B:455:ASP:H	1.92	0.77
1:C:382:LYS:HA	1:C:420:ILE:HD13	1.66	0.77
1:A:89:GLN:NE2	1:A:98:LYS:HD2	1.99	0.76
1:C:364:PHE:C	1:C:366:ARG:H	1.93	0.76
1:A:221:ARG:HG3	1:A:252:PHE:CE1	2.20	0.76
1:C:428:ASN:OD1	1:C:431:GLU:HB2	1.86	0.76
1:B:73:MET:CE	1:B:80:ILE:HB	2.15	0.76
1:C:412:SER:C	1:C:416:GLN:HG3	2.11	0.76
1:A:50:VAL:HG23	1:A:66:ILE:HB	1.68	0.76
1:C:371:LEU:HD13	1:C:380:ALA:HA	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LYS:HE2	1:B:130:TRP:NE1	2.02	0.75
1:C:438:PRO:HA	1:C:441:GLN:CB	2.15	0.75
1:C:353:VAL:HG23	1:C:364:PHE:HZ	1.49	0.75
1:B:12:HIS:NE2	1:B:326:SER:HB3	2.02	0.75
1:A:74:ASN:HD22	1:A:77:SER:H	1.32	0.75
1:B:216:PHE:HD2	1:B:231:ILE:HD11	1.48	0.74
1:C:361:GLU:HA	1:C:391:ILE:HD12	1.68	0.74
1:A:89:GLN:HE21	1:A:98:LYS:HD2	1.51	0.74
1:B:171:SER:OG	1:B:173:GLN:NE2	2.20	0.74
1:C:73:MET:HE2	1:C:80:ILE:HG13	1.69	0.74
1:C:216:PHE:HD2	1:C:231:ILE:HD11	1.51	0.74
1:C:92:ASN:OD1	1:C:94:GLU:HB3	1.87	0.74
1:A:301:GLU:HG3	1:A:321:LYS:HD3	1.67	0.74
1:C:73:MET:HE2	1:C:80:ILE:CG1	2.17	0.74
1:C:391:ILE:HG23	1:C:392:LEU:HG	1.70	0.74
1:A:176:ARG:CG	1:A:177:VAL:H	1.99	0.74
1:C:417:TYR:C	1:C:419:GLY:H	1.94	0.74
1:C:484:VAL:C	1:C:484:VAL:HG23	2.13	0.74
1:C:413:PRO:HG3	1:C:416:GLN:NE2	2.03	0.73
1:A:412:SER:OG	1:A:415:LEU:HD23	1.88	0.73
1:A:170:ILE:HB	1:A:177:VAL:HG12	1.69	0.73
1:A:220:VAL:O	1:A:226:GLY:HA2	1.88	0.73
1:A:12:HIS:NE2	1:A:326:SER:HB3	2.04	0.73
1:B:90:ILE:O	1:B:99:MET:HB2	1.88	0.73
1:A:86:LYS:HE3	1:A:107:ASP:CG	2.13	0.73
1:A:171:SER:O	1:A:178:VAL:HG22	1.88	0.73
1:B:164:TRP:CE2	1:B:233:VAL:HG13	2.23	0.72
1:A:473:THR:HG23	1:C:171:SER:HA	1.71	0.72
1:B:373:ALA:O	1:B:375:GLY:N	2.22	0.72
1:C:433:LEU:O	1:C:437:ARG:HB2	1.89	0.72
1:C:442:GLN:HB3	1:C:444:ARG:HD2	1.71	0.72
1:A:442:GLN:CB	1:A:444:ARG:HH12	2.02	0.72
1:C:407:GLN:NE2	1:C:410:GLN:HE21	1.87	0.72
1:B:309:HIS:HD2	1:B:312:THR:OG1	1.71	0.72
1:C:222:GLY:O	1:C:225:GLY:N	2.23	0.72
1:A:148:LEU:HD22	1:A:167:LEU:HD23	1.73	0.71
1:C:338:ILE:HA	1:C:342:LEU:HB2	1.71	0.71
1:B:92:ASN:OD1	1:B:94:GLU:HB3	1.90	0.71
1:C:435:LEU:O	1:C:438:PRO:HD2	1.90	0.71
1:C:426:GLN:CD	1:C:458:GLU:HB2	2.16	0.71
1:A:166:LEU:HD22	1:A:216:PHE:HE1	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:GLN:HE21	1:C:376:ASN:CB	2.01	0.71
1:C:407:GLN:O	1:C:410:GLN:HG2	1.90	0.71
1:B:373:ALA:C	1:B:375:GLY:N	2.46	0.70
1:B:453:LYS:O	1:B:455:ASP:OD2	2.08	0.70
1:A:301:GLU:HG3	1:A:321:LYS:CD	2.20	0.70
1:C:253:PRO:HD2	1:C:256:ALA:CB	2.21	0.70
1:B:407:GLN:HG2	1:B:408:PRO:CD	2.21	0.70
1:C:439:VAL:HG21	1:C:451:TRP:CH2	2.24	0.70
1:B:73:MET:HE2	1:B:80:ILE:CB	2.21	0.70
1:B:116:LEU:HD22	1:B:116:LEU:H	1.56	0.70
1:C:402:GLN:C	1:C:404:VAL:H	1.99	0.70
1:B:73:MET:HE2	1:B:80:ILE:HB	1.72	0.69
1:B:440:LEU:HD21	1:B:448:LEU:HD22	1.72	0.69
1:A:181:MET:CE	1:A:196:GLY:HA3	2.16	0.69
1:A:412:SER:O	1:A:416:GLN:HG3	1.92	0.69
1:B:158:THR:HG22	1:B:159:ASP:O	1.92	0.69
1:B:272:VAL:HG11	1:B:284:LEU:HD13	1.75	0.69
1:C:486:ASN:O	1:C:487:LYS:HG3	1.92	0.69
1:C:445:LYS:O	1:C:449:GLU:HG3	1.91	0.69
1:A:158:THR:HG21	1:A:162:GLN:HG2	1.74	0.69
1:B:428:ASN:OD1	1:B:428:ASN:N	2.23	0.69
1:A:173:GLN:CD	1:A:178:VAL:HG21	2.18	0.69
1:C:476:LEU:HD23	1:C:476:LEU:C	2.18	0.69
1:C:486:ASN:O	1:C:487:LYS:CG	2.41	0.69
1:B:297:ARG:HH21	1:B:300:GLY:HA2	1.58	0.68
1:B:439:VAL:HA	1:B:442:GLN:HE21	1.59	0.68
1:C:145:HIS:NE2	1:C:193:PRO:HG3	2.09	0.68
1:B:301:GLU:HG3	1:B:321:LYS:HD3	1.75	0.68
1:A:471:ASP:HB3	1:A:474:LEU:HB2	1.75	0.68
1:A:476:LEU:HD21	1:C:170:ILE:HD12	1.75	0.68
1:B:91:PHE:CE2	1:B:96:LYS:HE2	2.29	0.68
1:B:373:ALA:C	1:B:375:GLY:H	2.01	0.68
1:C:468:LYS:HD3	1:C:475:ALA:HB3	1.76	0.68
1:B:220:VAL:O	1:B:226:GLY:HA2	1.94	0.68
1:A:117:ASN:HB2	1:A:132:MET:HG2	1.76	0.68
1:B:396:ASP:HA	1:B:399:ARG:HD2	1.74	0.68
1:B:297:ARG:NH2	1:B:300:GLY:HA2	2.09	0.68
1:A:73:MET:HE2	1:A:80:ILE:CG1	2.25	0.67
1:A:100:LYS:HG2	1:A:130:TRP:CZ2	2.30	0.67
1:A:476:LEU:HD11	1:C:177:VAL:HG22	1.76	0.67
1:C:73:MET:HE2	1:C:80:ILE:HB	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:LYS:HA	1:C:420:ILE:CD1	2.24	0.67
1:B:166:LEU:HD22	1:B:216:PHE:HE1	1.59	0.67
1:C:139:VAL:O	1:C:139:VAL:HG12	1.94	0.67
1:B:376:ASN:O	1:B:378:SER:N	2.27	0.67
1:C:100:LYS:HE2	1:C:130:TRP:NE1	2.10	0.67
1:C:417:TYR:C	1:C:419:GLY:N	2.52	0.67
1:C:363:LEU:H	1:C:363:LEU:CD1	2.04	0.67
1:C:269:LYS:HE2	1:C:331:GLU:OE2	1.95	0.67
1:C:467:VAL:HG11	1:C:474:LEU:HD12	1.77	0.67
1:A:91:PHE:CE2	1:A:96:LYS:HE2	2.29	0.67
1:B:158:THR:HG21	1:B:162:GLN:HG2	1.77	0.67
1:B:197:HIS:HD2	1:B:221:ARG:H	1.42	0.67
1:B:450:LYS:HG2	1:B:454:GLU:CD	2.20	0.67
1:C:73:MET:CE	1:C:80:ILE:HB	2.25	0.67
1:A:176:ARG:HG2	1:A:177:VAL:H	1.60	0.66
1:B:371:LEU:HD13	1:B:379:GLU:CB	2.21	0.66
1:C:16:GLN:OE1	1:C:22:PRO:HB3	1.94	0.66
1:A:269:LYS:HE2	1:A:331:GLU:OE2	1.96	0.66
1:B:86:LYS:HE3	1:B:107:ASP:CG	2.20	0.66
1:B:428:ASN:OD1	1:B:431:GLU:OE1	2.13	0.66
1:B:1:MET:CG	1:C:1:MET:HA	2.26	0.66
1:B:477:SER:O	1:B:481:ARG:CG	2.43	0.66
1:C:86:LYS:HE3	1:C:107:ASP:CG	2.20	0.66
1:B:301:GLU:HG3	1:B:321:LYS:CD	2.26	0.66
1:C:421:LEU:HD13	1:C:431:GLU:OE1	1.96	0.66
1:C:220:VAL:O	1:C:226:GLY:HA2	1.96	0.66
1:C:117:ASN:HB2	1:C:132:MET:HG2	1.78	0.66
1:B:128:TYR:O	1:B:129:HIS:HD2	1.78	0.66
1:C:421:LEU:HA	1:C:424:GLN:HB2	1.78	0.66
1:B:148:LEU:HD22	1:B:167:LEU:HD23	1.76	0.65
1:A:227:LYS:HD3	1:A:249:ASP:HA	1.76	0.65
1:B:117:ASN:HB2	1:B:132:MET:HG2	1.77	0.65
1:B:439:VAL:HA	1:B:442:GLN:NE2	2.11	0.65
1:C:166:LEU:HD22	1:C:216:PHE:HE1	1.61	0.65
1:C:447:LEU:HD23	1:C:451:TRP:CZ2	2.31	0.65
1:A:90:ILE:O	1:A:99:MET:HB2	1.95	0.65
1:A:154:ILE:HD13	1:A:170:ILE:HG12	1.79	0.65
1:C:438:PRO:O	1:C:441:GLN:HB2	1.95	0.65
1:C:211:GLU:HB2	1:C:240:ASN:OD1	1.97	0.65
1:C:438:PRO:C	1:C:441:GLN:HB2	2.21	0.65
1:C:158:THR:HG22	1:C:159:ASP:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:GLU:O	1:C:463:LEU:C	2.40	0.65
1:B:463:LEU:O	1:B:467:VAL:HG23	1.97	0.65
1:C:181:MET:CE	1:C:196:GLY:HA3	2.21	0.65
1:B:190:VAL:HG12	1:B:191:SER:N	2.12	0.65
1:A:181:MET:HE2	1:A:196:GLY:CA	2.19	0.65
1:A:91:PHE:HE2	1:A:96:LYS:HE2	1.62	0.64
1:B:211:GLU:HB2	1:B:240:ASN:OD1	1.97	0.64
1:A:73:MET:HE1	1:A:93:ILE:HG13	1.78	0.64
1:A:158:THR:HG22	1:A:159:ASP:O	1.97	0.64
1:C:385:ALA:C	1:C:386:ASN:HD22	2.05	0.64
1:A:190:VAL:HG12	1:A:191:SER:N	2.11	0.64
1:A:410:GLN:N	1:A:410:GLN:CD	2.55	0.64
1:A:461:GLU:HG3	1:A:484:VAL:HG11	1.80	0.64
1:A:350:ARG:NH2	2:A:505:HOH:O	2.30	0.64
1:A:211:GLU:HB2	1:A:240:ASN:OD1	1.96	0.64
1:A:1:MET:O	1:A:3:GLN:OE1	2.14	0.64
1:A:86:LYS:HE3	1:A:107:ASP:OD1	1.98	0.64
1:A:116:LEU:HD22	1:A:116:LEU:H	1.62	0.64
1:A:343:GLN:O	1:A:345:PRO:HD3	1.98	0.64
1:B:16:GLN:OE1	1:B:22:PRO:HB3	1.97	0.64
1:C:158:THR:HG21	1:C:162:GLN:HG2	1.79	0.64
1:C:309:HIS:HD2	1:C:312:THR:OG1	1.81	0.64
1:C:362:GLU:HG2	1:C:363:LEU:N	2.12	0.64
1:C:413:PRO:CG	1:C:416:GLN:HE21	2.11	0.64
1:C:440:LEU:HD11	1:C:467:VAL:HG22	1.80	0.64
1:A:439:VAL:HG11	1:A:447:LEU:HD23	1.80	0.64
1:B:158:THR:HG23	1:B:162:GLN:HA	1.80	0.64
1:B:384:ALA:HA	1:B:392:LEU:HD12	1.80	0.64
1:C:301:GLU:HG3	1:C:321:LYS:HD3	1.80	0.64
1:C:73:MET:HE2	1:C:80:ILE:CB	2.29	0.63
1:C:116:LEU:H	1:C:116:LEU:HD22	1.63	0.63
1:C:158:THR:HG23	1:C:162:GLN:HA	1.79	0.63
1:C:347:LEU:O	1:C:347:LEU:HD12	1.98	0.63
1:A:272:VAL:HG11	1:A:284:LEU:HD13	1.80	0.63
1:A:339:THR:O	1:A:343:GLN:HA	1.98	0.63
1:C:301:GLU:HG3	1:C:321:LYS:CD	2.29	0.63
1:C:353:VAL:HG22	1:C:386:ASN:O	1.99	0.63
1:C:91:PHE:CE2	1:C:96:LYS:HE2	2.34	0.63
1:C:413:PRO:HG3	1:C:416:GLN:HE21	1.61	0.63
1:B:117:ASN:HB3	1:B:132:MET:HE2	1.79	0.63
1:C:369:ASN:OD1	1:C:369:ASN:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:THR:HG23	1:A:162:GLN:HA	1.80	0.63
1:B:73:MET:HE1	1:B:93:ILE:HG13	1.81	0.63
1:B:393:ARG:NH2	1:B:431:GLU:OE1	2.29	0.63
1:C:485:PRO:C	1:C:487:LYS:H	2.06	0.63
1:A:188:ARG:O	1:A:190:VAL:N	2.31	0.63
1:B:95:MET:HG3	1:B:97:SER:OG	1.99	0.63
1:C:197:HIS:HD2	1:C:221:ARG:H	1.45	0.63
1:B:145:HIS:NE2	1:B:193:PRO:HG3	2.14	0.62
1:B:231:ILE:HG12	1:B:231:ILE:O	1.97	0.62
1:B:269:LYS:HE2	1:B:331:GLU:OE2	1.99	0.62
1:A:442:GLN:HB3	1:A:444:ARG:HH12	1.64	0.62
1:B:24:ASN:HD22	1:B:42:GLU:CG	2.11	0.62
1:C:208:GLY:C	1:C:209:ASN:HD22	2.06	0.62
1:A:73:MET:HE2	1:A:80:ILE:HG13	1.81	0.62
1:A:237:PRO:HD2	1:A:240:ASN:OD1	1.99	0.62
1:C:372:PHE:CE2	1:C:400:ARG:HD2	2.34	0.62
1:A:145:HIS:NE2	1:A:193:PRO:HG3	2.14	0.62
1:A:371:LEU:HD13	1:A:379:GLU:HB3	1.80	0.62
1:B:221:ARG:HA	1:B:226:GLY:HA2	1.81	0.62
1:A:274:PHE:CD2	1:A:284:LEU:HD22	2.35	0.62
1:B:65:PRO:O	1:B:66:ILE:HG13	1.98	0.62
1:B:237:PRO:HD2	1:B:240:ASN:OD1	1.99	0.62
1:C:417:TYR:O	1:C:419:GLY:N	2.33	0.62
1:B:91:PHE:HE2	1:B:96:LYS:HE2	1.63	0.62
1:C:363:LEU:HD12	1:C:363:LEU:N	2.14	0.62
1:C:368:PHE:HD2	1:C:400:ARG:CZ	2.13	0.62
1:C:117:ASN:HB3	1:C:132:MET:HE2	1.80	0.62
1:C:368:PHE:HD2	1:C:400:ARG:NH2	1.97	0.62
1:C:440:LEU:HD12	1:C:466:LEU:HD23	1.81	0.62
1:B:208:GLY:C	1:B:209:ASN:HD22	2.07	0.61
1:B:438:PRO:HG2	1:B:439:VAL:H	1.65	0.61
1:C:90:ILE:O	1:C:99:MET:HB2	1.98	0.61
1:C:361:GLU:CD	1:C:361:GLU:N	2.49	0.61
1:C:466:LEU:O	1:C:468:LYS:N	2.33	0.61
1:B:100:LYS:HE2	1:B:130:TRP:HE1	1.65	0.61
1:C:323:GLN:OE1	1:C:325:LEU:HD21	2.00	0.61
1:B:412:SER:O	1:B:416:GLN:HG3	1.99	0.61
1:B:454:GLU:HB3	1:B:456:LYS:HZ1	1.65	0.61
1:A:106:ASP:N	1:A:106:ASP:OD2	2.34	0.61
1:A:197:HIS:HD2	1:A:221:ARG:H	1.48	0.61
1:A:204:PHE:CZ	1:A:288:GLU:HB2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ALA:O	1:A:374:GLN:HG3	2.00	0.61
1:C:73:MET:HE1	1:C:93:ILE:HG13	1.81	0.61
1:C:106:ASP:N	1:C:106:ASP:OD2	2.33	0.61
1:A:442:GLN:HB2	1:A:444:ARG:HH12	1.65	0.61
1:C:145:HIS:ND1	1:C:146:SER:N	2.49	0.61
1:C:253:PRO:HD2	1:C:256:ALA:HB3	1.82	0.61
1:C:364:PHE:C	1:C:366:ARG:N	2.57	0.61
1:C:99:MET:O	1:C:100:LYS:HB2	2.01	0.61
1:C:16:GLN:NE2	1:C:22:PRO:HG3	2.15	0.61
1:C:372:PHE:C	1:C:374:GLN:H	2.09	0.61
1:A:449:GLU:O	1:A:453:LYS:HE3	2.01	0.60
1:A:176:ARG:HG2	1:A:177:VAL:HG23	1.83	0.60
1:B:166:LEU:HD22	1:B:216:PHE:CE1	2.36	0.60
1:A:429:LYS:HG3	1:A:458:GLU:OE2	2.01	0.60
1:C:227:LYS:HD3	1:C:249:ASP:HA	1.81	0.60
1:C:438:PRO:HA	1:C:441:GLN:HE21	1.66	0.60
1:A:99:MET:O	1:A:100:LYS:HB2	2.00	0.60
1:B:211:GLU:CB	1:B:237:PRO:HG2	2.31	0.60
1:C:407:GLN:NE2	1:C:408:PRO:O	2.34	0.60
1:C:462:GLU:C	1:C:464:GLY:N	2.58	0.60
1:A:102:HIS:CE1	1:A:138:PRO:HD2	2.36	0.60
1:B:197:HIS:CD2	1:B:221:ARG:H	2.19	0.60
1:B:166:LEU:CD2	1:B:216:PHE:HE1	2.14	0.60
1:A:145:HIS:ND1	1:A:146:SER:N	2.50	0.60
1:B:99:MET:O	1:B:100:LYS:HB2	2.01	0.60
1:A:188:ARG:O	1:A:190:VAL:HG23	2.01	0.60
1:C:91:PHE:HE2	1:C:96:LYS:HE2	1.66	0.60
1:C:102:HIS:CE1	1:C:138:PRO:HD2	2.37	0.60
1:B:106:ASP:OD2	1:B:106:ASP:N	2.35	0.60
1:B:253:PRO:HD2	1:B:256:ALA:CB	2.31	0.60
1:C:57:ASP:CG	1:C:60:ASN:HD22	2.09	0.59
1:A:24:ASN:HD22	1:A:42:GLU:CG	2.12	0.59
1:A:440:LEU:HD12	1:A:466:LEU:HD23	1.85	0.59
1:C:69:ASP:CB	1:C:83:LYS:HZ2	2.15	0.59
1:C:188:ARG:O	1:C:190:VAL:HG23	2.02	0.59
1:C:204:PHE:CZ	1:C:288:GLU:HB2	2.37	0.59
1:C:222:GLY:C	1:C:224:ALA:N	2.60	0.59
1:A:471:ASP:OD1	1:A:472:PRO:HD2	2.02	0.59
1:C:404:VAL:CG2	1:C:405:PRO:HD2	2.31	0.59
1:B:86:LYS:HE3	1:B:107:ASP:OD1	2.02	0.59
1:C:367:LYS:O	1:C:370:ALA:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:VAL:HG11	1:C:284:LEU:HD13	1.83	0.59
1:A:117:ASN:HB3	1:A:132:MET:HE2	1.83	0.59
1:A:338:ILE:HA	1:A:342:LEU:HB2	1.85	0.59
1:B:211:GLU:HB2	1:B:237:PRO:HG2	1.85	0.59
1:B:373:ALA:HB3	1:B:374:GLN:NE2	2.17	0.59
1:A:477:SER:HB2	1:C:152:GLN:OE1	2.02	0.59
1:C:197:HIS:CD2	1:C:221:ARG:H	2.21	0.59
1:B:16:GLN:NE2	1:B:22:PRO:HG3	2.18	0.59
1:C:413:PRO:HA	1:C:416:GLN:CB	2.31	0.59
1:B:472:PRO:O	1:B:492:PHE:CE2	2.56	0.59
1:B:73:MET:HE1	1:B:80:ILE:HB	1.85	0.58
1:B:248:VAL:HG21	1:B:290:GLY:O	2.02	0.58
1:C:371:LEU:O	1:C:374:GLN:HB3	2.02	0.58
1:A:170:ILE:HB	1:A:177:VAL:CG1	2.32	0.58
1:A:216:PHE:CD2	1:A:231:ILE:HD11	2.35	0.58
1:A:407:GLN:C	1:A:407:GLN:CD	2.71	0.58
1:B:216:PHE:CD2	1:B:231:ILE:HD11	2.36	0.58
1:A:128:TYR:CD1	1:A:128:TYR:N	2.71	0.58
1:A:244:PRO:O	1:A:246:LYS:HD2	2.04	0.58
1:C:221:ARG:HA	1:C:226:GLY:HA2	1.85	0.58
1:C:402:GLN:C	1:C:404:VAL:N	2.62	0.58
1:A:16:GLN:OE1	1:A:22:PRO:HB3	2.04	0.58
1:A:463:LEU:O	1:A:467:VAL:HG23	2.04	0.58
1:A:421:LEU:HB3	1:A:427:LEU:HD23	1.84	0.58
1:B:437:ARG:O	1:B:441:GLN:HG2	2.04	0.58
1:C:128:TYR:N	1:C:128:TYR:CD1	2.70	0.58
1:C:360:ALA:O	1:C:364:PHE:HB2	2.03	0.58
1:A:398:ILE:HD12	1:A:430:TYR:HD2	1.63	0.57
1:B:188:ARG:O	1:B:190:VAL:HG23	2.03	0.57
1:C:244:PRO:O	1:C:246:LYS:HD2	2.04	0.57
1:A:454:GLU:O	1:A:455:ASP:HB2	2.04	0.57
1:A:197:HIS:CD2	1:A:221:ARG:H	2.21	0.57
1:B:1:MET:SD	1:C:1:MET:CG	2.90	0.57
1:B:244:PRO:O	1:B:246:LYS:HD2	2.03	0.57
1:C:297:ARG:NH2	1:C:300:GLY:HA2	2.19	0.57
1:C:367:LYS:O	1:C:371:LEU:HD12	2.04	0.57
1:C:381:ALA:HB2	1:C:401:PHE:CZ	2.39	0.57
1:A:461:GLU:HG3	1:A:484:VAL:CG1	2.34	0.57
1:B:92:ASN:OD1	1:B:92:ASN:C	2.48	0.57
1:C:12:HIS:CD2	1:C:326:SER:HB3	2.39	0.57
1:C:372:PHE:CD1	1:C:377:TYR:HD2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ASN:O	1:B:458:GLU:HB3	2.05	0.57
1:C:164:TRP:C	1:C:165:LEU:HD23	2.29	0.57
1:C:402:GLN:O	1:C:404:VAL:N	2.32	0.57
1:A:455:ASP:HB3	1:C:69:ASP:OD1	2.04	0.57
1:B:145:HIS:ND1	1:B:147:SER:OG	2.36	0.57
1:B:482:ALA:O	1:B:483:ASN:HB3	2.04	0.57
1:B:117:ASN:CB	1:B:132:MET:HE2	2.33	0.57
1:A:297:ARG:NH2	1:A:300:GLY:HA2	2.20	0.57
1:B:9:PHE:HD2	1:C:5:LEU:HD23	1.67	0.57
1:C:222:GLY:C	1:C:224:ALA:H	2.12	0.57
1:C:231:ILE:O	1:C:231:ILE:HG12	2.03	0.57
1:A:57:ASP:CG	1:A:60:ASN:HD22	2.12	0.56
1:A:190:VAL:CG1	1:A:191:SER:N	2.68	0.56
1:A:476:LEU:HD21	1:C:170:ILE:CD1	2.34	0.56
1:B:475:ALA:HB3	1:B:492:PHE:HZ	1.69	0.56
1:B:114:ILE:O	1:B:115:SER:HB3	2.05	0.56
1:B:171:SER:CB	1:B:173:GLN:NE2	2.68	0.56
1:B:471:ASP:CB	1:B:474:LEU:HB2	2.34	0.56
1:A:148:LEU:CD2	1:A:167:LEU:HD23	2.35	0.56
1:A:454:GLU:CB	1:A:456:LYS:HD2	2.35	0.56
1:C:12:HIS:NE2	1:C:326:SER:HB3	2.20	0.56
1:C:377:TYR:CE1	1:C:405:PRO:HG2	2.40	0.56
1:C:412:SER:HB3	1:C:415:LEU:HD23	1.86	0.56
1:A:220:VAL:HG22	1:A:222:GLY:H	1.69	0.56
1:B:190:VAL:CG1	1:B:191:SER:N	2.69	0.56
1:C:412:SER:O	1:C:416:GLN:N	2.37	0.56
1:A:208:GLY:C	1:A:209:ASN:HD22	2.13	0.56
1:B:21:ASN:HD21	1:B:23:ALA:CB	2.02	0.56
1:B:354:ARG:HG2	1:B:355:ASN:ND2	2.20	0.56
1:C:148:LEU:HD22	1:C:167:LEU:HD23	1.87	0.56
1:C:227:LYS:HA	1:C:249:ASP:HA	1.88	0.56
1:A:199:ALA:HB2	1:A:218:PHE:CB	2.36	0.56
1:A:231:ILE:HG12	1:A:231:ILE:O	2.05	0.56
1:A:412:SER:OG	1:A:415:LEU:CD2	2.54	0.56
1:B:204:PHE:CZ	1:B:288:GLU:HB2	2.41	0.56
1:C:164:TRP:CD2	1:C:233:VAL:HG13	2.39	0.56
1:A:426:GLN:HG3	1:A:427:LEU:N	2.20	0.56
1:A:444:ARG:HG2	1:A:446:GLN:OE1	2.06	0.56
1:B:486:ASN:O	1:B:489:ILE:N	2.37	0.56
1:C:449:GLU:HG2	1:C:474:LEU:HD21	1.87	0.56
1:C:484:VAL:HB	1:C:485:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD22	1:A:216:PHE:CE1	2.38	0.56
1:A:454:GLU:HB3	1:A:456:LYS:HD2	1.87	0.56
1:B:16:GLN:CD	1:B:22:PRO:HG3	2.31	0.56
1:B:145:HIS:ND1	1:B:146:SER:N	2.53	0.56
1:C:309:HIS:CD2	1:C:312:THR:HG23	2.40	0.56
1:C:368:PHE:CD2	1:C:400:ARG:CZ	2.88	0.56
1:C:442:GLN:HG2	1:C:444:ARG:NH1	2.21	0.56
1:C:164:TRP:HZ2	1:C:234:GLY:CA	2.19	0.55
1:A:21:ASN:HD21	1:A:23:ALA:CB	2.08	0.55
1:A:440:LEU:HD11	1:A:467:VAL:HG22	1.89	0.55
1:A:479:TYR:O	1:A:483:ASN:N	2.37	0.55
1:A:71:ALA:HB1	1:A:80:ILE:HD11	1.88	0.55
1:A:95:MET:HG3	1:A:97:SER:OG	2.06	0.55
1:A:69:ASP:HB2	1:A:83:LYS:HZ2	1.71	0.55
1:A:199:ALA:HB2	1:A:218:PHE:HB2	1.88	0.55
1:B:376:ASN:O	1:B:377:TYR:C	2.48	0.55
1:C:199:ALA:HB2	1:C:218:PHE:HB2	1.88	0.55
1:C:448:LEU:HG	1:C:449:GLU:N	2.20	0.55
1:B:13:LEU:HD11	1:B:15:LEU:CD2	2.37	0.55
1:A:221:ARG:HA	1:A:226:GLY:HA2	1.88	0.55
1:B:32:MET:HE1	1:B:317:GLY:HA2	1.88	0.55
1:B:99:MET:O	1:B:100:LYS:CB	2.55	0.55
1:C:216:PHE:CD2	1:C:231:ILE:HD11	2.39	0.55
1:C:379:GLU:OE1	1:C:379:GLU:HA	2.06	0.55
1:C:462:GLU:O	1:C:464:GLY:N	2.39	0.55
1:A:173:GLN:NE2	1:A:178:VAL:HG21	2.21	0.55
1:C:24:ASN:HD22	1:C:42:GLU:CG	2.18	0.55
1:C:86:LYS:HE3	1:C:107:ASP:OD1	2.06	0.55
1:C:117:ASN:CB	1:C:132:MET:HE2	2.36	0.55
1:C:438:PRO:CA	1:C:441:GLN:NE2	2.68	0.55
1:B:274:PHE:CD2	1:B:284:LEU:HD22	2.42	0.55
1:C:188:ARG:NH2	2:C:501:HOH:O	2.34	0.55
1:C:407:GLN:NE2	1:C:410:GLN:HG2	2.22	0.55
1:B:74:ASN:HD22	1:B:77:SER:H	1.55	0.54
1:B:453:LYS:C	1:B:455:ASP:N	2.56	0.54
1:A:164:TRP:CD2	1:A:233:VAL:HG13	2.42	0.54
1:B:8:ARG:HE	1:B:10:GLN:NE2	2.05	0.54
1:B:89:GLN:OE1	1:B:98:LYS:HD2	2.08	0.54
1:B:454:GLU:HB3	1:B:456:LYS:NZ	2.21	0.54
1:C:190:VAL:HG12	1:C:191:SER:N	2.22	0.54
1:A:309:HIS:CD2	1:A:312:THR:OG1	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ALA:HB2	1:C:218:PHE:CB	2.38	0.54
1:C:13:LEU:HD11	1:C:58:PRO:CB	2.33	0.54
1:C:188:ARG:O	1:C:190:VAL:N	2.40	0.54
1:C:377:TYR:O	1:C:413:PRO:HB3	2.07	0.54
1:B:137:GLN:HB3	1:B:138:PRO:HD2	1.89	0.54
1:B:373:ALA:O	1:B:374:GLN:C	2.50	0.54
1:C:442:GLN:OE1	1:C:444:ARG:NH1	2.41	0.54
1:A:128:TYR:O	1:A:129:HIS:HD2	1.91	0.54
1:B:209:ASN:HD22	1:B:209:ASN:N	2.06	0.54
1:A:16:GLN:NE2	1:A:22:PRO:HG3	2.23	0.54
1:A:100:LYS:CE	1:A:130:TRP:HE1	2.18	0.54
1:A:449:GLU:CG	1:A:474:LEU:HD11	2.35	0.54
1:A:139:VAL:HG12	1:A:139:VAL:O	2.06	0.54
1:A:141:MET:O	1:A:142:PHE:HB3	2.07	0.54
1:A:176:ARG:HH22	1:A:221:ARG:HD3	1.71	0.54
1:A:253:PRO:HD2	1:A:256:ALA:CB	2.38	0.54
1:C:137:GLN:HB3	1:C:138:PRO:HD2	1.90	0.54
1:C:465:ASP:OD1	1:C:479:TYR:OH	2.18	0.54
1:C:65:PRO:O	1:C:66:ILE:HG13	2.09	0.53
1:C:468:LYS:HD3	1:C:475:ALA:CB	2.38	0.53
1:A:16:GLN:CD	1:A:22:PRO:HG3	2.34	0.53
1:A:73:MET:HE1	1:A:80:ILE:HB	1.86	0.53
1:A:99:MET:O	1:A:100:LYS:CB	2.54	0.53
1:B:128:TYR:N	1:B:128:TYR:CD1	2.76	0.53
1:C:411:THR:O	1:C:416:GLN:NE2	2.42	0.53
1:A:114:ILE:O	1:A:115:SER:HB3	2.09	0.53
1:A:166:LEU:CD2	1:A:216:PHE:HE1	2.20	0.53
1:B:1:MET:HG3	1:C:1:MET:HA	1.88	0.53
1:C:438:PRO:HA	1:C:441:GLN:CD	2.33	0.53
1:A:3:GLN:HB2	1:A:341:VAL:HG22	1.90	0.53
1:A:433:LEU:HD13	1:A:463:LEU:HB2	1.91	0.53
1:B:335:ILE:HB	1:B:336:PRO:HD3	1.90	0.53
1:A:437:ARG:HB3	1:A:438:PRO:CD	2.38	0.53
1:B:158:THR:CG2	1:B:159:ASP:O	2.56	0.53
1:C:100:LYS:HE2	1:C:130:TRP:HE1	1.74	0.53
1:C:137:GLN:HB3	1:C:138:PRO:CD	2.38	0.53
1:C:362:GLU:C	1:C:364:PHE:H	2.15	0.53
1:C:420:ILE:O	1:C:424:GLN:HG3	2.09	0.53
1:B:12:HIS:NE2	1:B:326:SER:CB	2.72	0.53
1:C:123:THR:HB	1:C:126:ALA:O	2.09	0.53
1:C:444:ARG:HD2	1:C:444:ARG:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:LEU:C	1:C:468:LYS:H	2.16	0.53
1:A:12:HIS:CD2	1:A:326:SER:HB3	2.43	0.52
1:B:461:GLU:HG3	1:B:484:VAL:HG12	1.91	0.52
1:A:4:ILE:CG2	1:A:337:TYR:HB2	2.39	0.52
1:A:248:VAL:HG21	1:A:290:GLY:O	2.10	0.52
1:B:454:GLU:CB	1:B:456:LYS:HE3	2.38	0.52
1:C:111:TRP:O	1:C:112:LYS:CB	2.52	0.52
1:C:211:GLU:CB	1:C:237:PRO:HG2	2.38	0.52
1:C:445:LYS:HD3	1:C:449:GLU:CD	2.33	0.52
1:A:176:ARG:CG	1:A:177:VAL:N	2.72	0.52
1:A:372:PHE:HZ	1:A:400:ARG:O	1.93	0.52
1:B:71:ALA:HB1	1:B:80:ILE:HD11	1.90	0.52
1:C:437:ARG:O	1:C:441:GLN:HG3	2.09	0.52
1:C:466:LEU:C	1:C:468:LYS:N	2.66	0.52
1:A:442:GLN:HB3	1:A:444:ARG:NH1	2.24	0.52
1:B:376:ASN:OD1	1:B:379:GLU:HB2	2.09	0.52
1:C:173:GLN:CG	1:C:178:VAL:HG21	2.36	0.52
1:A:412:SER:HG	1:A:415:LEU:CD2	2.22	0.52
1:C:372:PHE:C	1:C:374:GLN:N	2.66	0.52
1:A:144:ARG:HD3	1:A:167:LEU:HD21	1.91	0.52
1:A:454:GLU:HB3	1:A:456:LYS:CG	2.40	0.52
1:C:16:GLN:CD	1:C:22:PRO:HG3	2.35	0.52
1:A:91:PHE:CZ	1:A:96:LYS:HA	2.44	0.52
1:A:117:ASN:CB	1:A:132:MET:HE2	2.40	0.52
1:B:1:MET:CG	1:B:2:ALA:H	2.22	0.52
1:C:347:LEU:HD12	1:C:347:LEU:C	2.35	0.52
1:C:394:THR:O	1:C:398:ILE:HD12	2.10	0.52
1:B:353:VAL:HG23	1:B:364:PHE:CZ	2.45	0.52
1:C:312:THR:O	1:C:313:ALA:HB3	2.10	0.52
1:A:110:PHE:C	1:A:110:PHE:CD2	2.88	0.52
1:A:111:TRP:O	1:A:112:LYS:CB	2.55	0.52
1:A:395:PRO:HB3	1:A:430:TYR:CZ	2.45	0.52
1:B:227:LYS:HD3	1:B:249:ASP:HA	1.92	0.52
1:C:209:ASN:HD22	1:C:209:ASN:N	2.07	0.52
1:A:47:GLN:NE2	1:A:65:PRO:HB3	2.25	0.51
1:A:123:THR:CG2	1:A:124:ASP:N	2.73	0.51
1:C:413:PRO:HA	1:C:416:GLN:CG	2.40	0.51
1:C:448:LEU:HD21	1:C:474:LEU:CG	2.39	0.51
1:C:485:PRO:O	1:C:487:LYS:N	2.43	0.51
1:A:253:PRO:HD2	1:A:256:ALA:HB3	1.91	0.51
1:A:211:GLU:CB	1:A:237:PRO:HG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ILE:HA	1:B:342:LEU:HB2	1.93	0.51
1:C:369:ASN:CG	1:C:400:ARG:HH12	2.19	0.51
1:C:374:GLN:HG2	1:C:375:GLY:N	2.16	0.51
1:C:437:ARG:O	1:C:441:GLN:N	2.43	0.51
1:A:140:LYS:NZ	1:A:143:ASP:OD2	2.42	0.51
1:B:445:LYS:HG2	1:B:449:GLU:OE2	2.11	0.51
1:B:376:ASN:O	1:B:379:GLU:N	2.43	0.51
1:B:227:LYS:HA	1:B:249:ASP:HA	1.93	0.51
1:B:323:GLN:OE1	1:B:325:LEU:HD21	2.10	0.51
1:C:383:VAL:HG12	1:C:384:ALA:N	2.25	0.51
1:B:139:VAL:HG12	1:B:139:VAL:O	2.09	0.51
1:A:476:LEU:HD11	1:C:177:VAL:CG2	2.41	0.51
1:B:437:ARG:HB3	1:B:438:PRO:CD	2.41	0.51
1:C:345:PRO:HA	1:C:348:ALA:CB	2.38	0.51
1:C:484:VAL:CG2	1:C:484:VAL:HG13	2.38	0.51
1:A:69:ASP:CB	1:A:83:LYS:HZ2	2.23	0.50
1:A:83:LYS:O	1:A:83:LYS:HG2	2.10	0.50
1:C:429:LYS:HE3	1:C:459:CYS:O	2.11	0.50
1:A:279:TYR:N	1:A:279:TYR:CD2	2.79	0.50
1:B:69:ASP:CB	1:B:83:LYS:HZ2	2.24	0.50
1:C:69:ASP:HB2	1:C:83:LYS:HZ2	1.75	0.50
1:C:144:ARG:HD3	1:C:167:LEU:HD21	1.92	0.50
1:C:237:PRO:HD2	1:C:240:ASN:OD1	2.12	0.50
1:C:253:PRO:HD2	1:C:256:ALA:HB2	1.94	0.50
1:A:456:LYS:HB3	1:A:456:LYS:NZ	2.21	0.50
1:C:110:PHE:C	1:C:110:PHE:CD2	2.89	0.50
1:A:173:GLN:OE1	1:A:178:VAL:HG11	2.11	0.50
1:A:362:GLU:O	1:A:366:ARG:HB2	2.11	0.50
1:B:13:LEU:HD23	1:B:58:PRO:CB	2.41	0.50
1:B:475:ALA:O	1:B:478:VAL:N	2.45	0.50
1:C:335:ILE:HB	1:C:336:PRO:HD3	1.94	0.50
1:C:391:ILE:HG23	1:C:392:LEU:N	2.26	0.50
1:B:140:LYS:NZ	1:B:143:ASP:OD2	2.41	0.50
1:B:253:PRO:HD2	1:B:256:ALA:HB3	1.93	0.50
1:C:89:GLN:NE2	1:C:98:LYS:CD	2.70	0.50
1:C:221:ARG:HG3	1:C:252:PHE:CE1	2.46	0.50
1:C:372:PHE:CD1	1:C:377:TYR:CD2	2.99	0.50
1:A:440:LEU:HD21	1:A:448:LEU:HD22	1.92	0.50
1:B:144:ARG:HD3	1:B:167:LEU:HD21	1.94	0.50
1:B:258:ASN:OD1	1:B:258:ASN:N	2.44	0.50
1:B:461:GLU:HG3	1:B:484:VAL:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:PRO:O	1:B:475:ALA:HB3	2.11	0.50
1:C:248:VAL:HG21	1:C:290:GLY:O	2.11	0.50
1:C:258:ASN:OD1	1:C:258:ASN:N	2.44	0.50
1:A:227:LYS:HA	1:A:249:ASP:HA	1.93	0.50
1:A:384:ALA:HA	1:A:392:LEU:HD12	1.94	0.50
1:B:487:LYS:HD2	1:B:487:LYS:O	2.12	0.50
1:C:54:ASP:O	1:C:56:ASN:N	2.45	0.50
1:C:480:LEU:C	1:C:480:LEU:HD23	2.36	0.50
1:B:148:LEU:CD2	1:B:167:LEU:HD23	2.42	0.50
1:B:188:ARG:O	1:B:190:VAL:N	2.45	0.50
1:C:164:TRP:NE1	1:C:233:VAL:HG13	2.25	0.50
1:A:353:VAL:HG23	1:A:364:PHE:CZ	2.46	0.49
1:B:47:GLN:HG3	1:B:48:ALA:N	2.25	0.49
1:B:111:TRP:O	1:B:112:LYS:CB	2.58	0.49
1:C:356:ASN:O	1:C:389:LYS:NZ	2.45	0.49
1:A:92:ASN:OD1	1:A:92:ASN:C	2.55	0.49
1:B:129:HIS:CD2	1:B:141:MET:HG3	2.47	0.49
1:B:279:TYR:N	1:B:279:TYR:CD2	2.77	0.49
1:B:353:VAL:HG23	1:B:364:PHE:HZ	1.76	0.49
1:B:376:ASN:ND2	1:B:378:SER:OG	2.45	0.49
1:B:377:TYR:HB3	1:B:413:PRO:HB3	1.93	0.49
1:C:166:LEU:HD22	1:C:216:PHE:CE1	2.45	0.49
1:A:356:ASN:CG	1:A:356:ASN:O	2.53	0.49
1:A:377:TYR:CB	1:A:413:PRO:HB3	2.36	0.49
1:B:439:VAL:HA	1:B:444:ARG:HD2	1.93	0.49
1:C:57:ASP:CG	1:C:60:ASN:ND2	2.69	0.49
1:C:245:LYS:O	1:C:245:LYS:HG3	2.08	0.49
1:A:335:ILE:HB	1:A:336:PRO:HD3	1.93	0.49
1:B:111:TRP:HA	1:B:120:ALA:O	2.13	0.49
1:C:372:PHE:CD2	1:C:400:ARG:HD2	2.48	0.49
1:A:91:PHE:CZ	1:A:96:LYS:C	2.90	0.49
1:A:164:TRP:HZ2	1:A:234:GLY:CA	2.25	0.49
1:A:168:THR:HG23	1:A:181:MET:HG2	1.94	0.49
1:A:173:GLN:HG3	1:A:178:VAL:HG21	1.93	0.49
1:A:454:GLU:HB3	1:A:456:LYS:CD	2.42	0.49
1:B:91:PHE:CZ	1:B:96:LYS:HA	2.47	0.49
1:B:398:ILE:HG23	1:B:414:LEU:HD11	1.95	0.49
1:C:352:ALA:HA	1:C:357:LEU:HB2	1.93	0.49
1:C:396:ASP:CG	1:C:399:ARG:HH12	2.20	0.49
1:A:412:SER:HG	1:A:415:LEU:HD23	1.78	0.49
1:C:395:PRO:C	1:C:397:THR:N	2.68	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:LEU:C	1:C:476:LEU:CD2	2.86	0.49
1:A:123:THR:HB	1:A:126:ALA:O	2.12	0.49
1:A:412:SER:OG	1:A:415:LEU:HB2	2.12	0.49
1:B:13:LEU:HD11	1:B:15:LEU:HD23	1.93	0.49
1:B:181:MET:CE	1:B:196:GLY:HA3	2.33	0.49
1:C:361:GLU:HA	1:C:391:ILE:CD1	2.40	0.49
1:A:427:LEU:O	1:A:458:GLU:HB2	2.13	0.49
1:B:137:GLN:HB3	1:B:138:PRO:CD	2.43	0.49
1:B:445:LYS:HE3	1:B:449:GLU:OE1	2.13	0.49
1:C:356:ASN:HA	1:C:388:PRO:HB3	1.95	0.49
1:A:451:TRP:O	1:A:456:LYS:HG3	2.12	0.49
1:C:188:ARG:O	1:C:188:ARG:CG	2.60	0.49
1:C:401:PHE:HB3	1:C:414:LEU:CD1	2.43	0.49
1:C:404:VAL:HG22	1:C:405:PRO:HD2	1.94	0.49
1:B:100:LYS:NZ	1:B:133:GLU:O	2.45	0.48
1:C:184:TYR:HD1	1:C:191:SER:HB2	1.77	0.48
1:C:279:TYR:N	1:C:279:TYR:CD2	2.80	0.48
1:C:415:LEU:N	1:C:415:LEU:HD22	2.28	0.48
1:C:433:LEU:HD21	1:C:462:GLU:CB	2.43	0.48
1:C:462:GLU:O	1:C:465:ASP:N	2.46	0.48
1:A:35:ASP:OD1	1:A:36:LYS:HD3	2.14	0.48
1:A:170:ILE:HA	1:A:178:VAL:O	2.12	0.48
1:C:2:ALA:C	1:C:4:ILE:H	2.20	0.48
1:C:102:HIS:CE1	1:C:138:PRO:CD	2.97	0.48
1:C:217:CYS:HA	1:C:229:HIS:O	2.14	0.48
1:C:401:PHE:O	1:C:404:VAL:CB	2.47	0.48
1:A:4:ILE:HG12	1:A:333:ASN:HB3	1.95	0.48
1:A:1:MET:CG	1:A:2:ALA:H	2.27	0.48
1:A:65:PRO:O	1:A:66:ILE:HG13	2.14	0.48
1:B:211:GLU:HB3	1:B:237:PRO:HG2	1.96	0.48
1:C:274:PHE:CD2	1:C:284:LEU:HD22	2.48	0.48
1:C:114:ILE:O	1:C:115:SER:HB3	2.14	0.48
1:C:188:ARG:O	1:C:188:ARG:HG3	2.13	0.48
1:B:12:HIS:CD2	1:B:326:SER:HB3	2.49	0.48
1:B:16:GLN:O	1:B:19:GLY:N	2.42	0.48
1:B:110:PHE:C	1:B:110:PHE:CD2	2.92	0.48
1:B:421:LEU:HB3	1:B:427:LEU:HD11	1.96	0.48
1:B:438:PRO:O	1:B:441:GLN:N	2.45	0.48
1:C:47:GLN:HG3	1:C:48:ALA:N	2.22	0.48
1:A:407:GLN:OE1	1:A:408:PRO:O	2.32	0.48
1:A:110:PHE:CD2	1:A:111:TRP:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LYS:NZ	1:A:456:LYS:CB	2.77	0.48
1:B:472:PRO:O	1:B:492:PHE:HE2	1.96	0.48
1:C:35:ASP:OD1	1:C:36:LYS:HD3	2.13	0.48
1:C:199:ALA:HB1	1:C:217:CYS:O	2.13	0.48
1:C:442:GLN:CD	1:C:444:ARG:HH11	2.22	0.48
1:A:438:PRO:O	1:A:439:VAL:C	2.56	0.48
1:C:372:PHE:HD1	1:C:377:TYR:HD2	1.60	0.48
1:C:363:LEU:HA	1:C:366:ARG:HB2	1.96	0.48
1:C:426:GLN:HA	1:C:456:LYS:O	2.14	0.48
1:A:188:ARG:O	1:A:188:ARG:HG3	2.14	0.47
1:B:123:THR:CG2	1:B:124:ASP:N	2.77	0.47
1:B:250:VAL:HG22	1:B:250:VAL:O	2.13	0.47
1:B:338:ILE:O	1:B:342:LEU:HB2	2.13	0.47
1:C:421:LEU:O	1:C:424:GLN:HB2	2.14	0.47
1:C:484:VAL:HG23	1:C:484:VAL:O	2.13	0.47
1:A:467:VAL:O	1:A:468:LYS:C	2.56	0.47
1:B:54:ASP:OD1	1:B:54:ASP:C	2.57	0.47
1:B:459:CYS:SG	1:B:478:VAL:CG1	3.02	0.47
1:C:99:MET:O	1:C:100:LYS:CB	2.57	0.47
1:C:392:LEU:C	1:C:394:THR:H	2.22	0.47
1:C:459:CYS:SG	1:C:478:VAL:HG13	2.54	0.47
1:A:78:LYS:HB3	1:A:78:LYS:HE3	1.56	0.47
1:A:258:ASN:OD1	1:A:258:ASN:N	2.47	0.47
1:A:286:ASP:OD2	1:A:289:THR:HG23	2.13	0.47
1:B:65:PRO:O	1:B:66:ILE:CG1	2.62	0.47
1:A:356:ASN:HA	1:A:388:PRO:HB3	1.96	0.47
1:B:199:ALA:HB2	1:B:218:PHE:HB2	1.97	0.47
1:B:250:VAL:HG22	1:B:252:PHE:CE1	2.50	0.47
1:C:391:ILE:HG12	1:C:392:LEU:HD23	1.96	0.47
1:C:393:ARG:NH2	1:C:431:GLU:OE1	2.48	0.47
1:A:54:ASP:O	1:A:56:ASN:N	2.47	0.47
1:A:181:MET:HE1	1:A:218:PHE:CD1	2.49	0.47
1:A:465:ASP:OD1	1:A:479:TYR:OH	2.22	0.47
1:B:35:ASP:OD1	1:B:36:LYS:HD3	2.15	0.47
1:C:152:GLN:O	1:C:169:GLY:HA2	2.14	0.47
1:C:227:LYS:HD3	1:C:249:ASP:CA	2.44	0.47
1:C:347:LEU:HD11	1:C:351:MET:CE	2.45	0.47
1:A:8:ARG:HE	1:A:10:GLN:NE2	2.12	0.47
1:A:363:LEU:HD23	1:A:366:ARG:NH1	2.29	0.47
1:B:459:CYS:SG	1:B:478:VAL:HG13	2.54	0.47
1:C:57:ASP:N	1:C:58:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:ASN:N	1:C:386:ASN:ND2	2.51	0.47
1:A:164:TRP:C	1:A:165:LEU:HD23	2.40	0.47
1:A:173:GLN:CG	1:A:178:VAL:HG21	2.45	0.47
1:B:69:ASP:HB2	1:B:83:LYS:HZ2	1.79	0.47
1:B:116:LEU:H	1:B:116:LEU:CD2	2.26	0.47
1:B:485:PRO:HD2	1:B:488:VAL:HG23	1.97	0.47
1:C:211:GLU:HB2	1:C:237:PRO:HG2	1.96	0.47
1:A:245:LYS:O	1:A:245:LYS:HG3	2.14	0.47
1:A:362:GLU:CD	1:A:366:ARG:HH22	2.22	0.47
1:C:54:ASP:C	1:C:56:ASN:H	2.22	0.47
1:C:371:LEU:HD13	1:C:380:ALA:CA	2.40	0.47
1:A:32:MET:HE1	1:A:317:GLY:HA2	1.96	0.47
1:C:2:ALA:C	1:C:4:ILE:N	2.72	0.47
1:C:47:GLN:NE2	1:C:65:PRO:HB3	2.30	0.47
1:C:78:LYS:HB3	1:C:78:LYS:HE3	1.44	0.47
1:B:100:LYS:HG2	1:B:130:TRP:CZ2	2.50	0.47
1:B:141:MET:HE3	1:B:141:MET:HB3	1.82	0.47
1:B:362:GLU:CD	1:B:366:ARG:HH22	2.23	0.47
1:C:358:ALA:N	1:C:389:LYS:HZ1	2.13	0.47
1:C:410:GLN:CD	1:C:410:GLN:N	2.71	0.47
1:A:26:GLY:O	1:A:30:LEU:N	2.38	0.46
1:A:227:LYS:HD3	1:A:249:ASP:CA	2.42	0.46
1:B:12:HIS:O	1:B:13:LEU:HB3	2.15	0.46
1:B:78:LYS:HE3	1:B:78:LYS:HB3	1.53	0.46
1:B:376:ASN:C	1:B:378:SER:N	2.71	0.46
1:B:447:LEU:HD12	1:B:447:LEU:O	2.15	0.46
1:C:117:ASN:HB2	1:C:132:MET:CG	2.43	0.46
1:A:170:ILE:CB	1:A:177:VAL:HG12	2.43	0.46
1:A:188:ARG:O	1:A:188:ARG:CG	2.62	0.46
1:C:362:GLU:C	1:C:364:PHE:N	2.73	0.46
1:B:43:LYS:HA	1:B:47:GLN:O	2.15	0.46
1:B:371:LEU:CD1	1:B:379:GLU:HG3	2.44	0.46
1:B:478:VAL:HA	1:B:481:ARG:HG3	1.98	0.46
1:C:154:ILE:HD13	1:C:170:ILE:HG12	1.96	0.46
1:C:472:PRO:O	1:C:475:ALA:N	2.49	0.46
1:A:112:LYS:HE2	1:A:155:ASN:OD1	2.15	0.46
1:A:139:VAL:O	1:A:140:LYS:C	2.56	0.46
1:A:181:MET:HE1	1:A:218:PHE:CG	2.50	0.46
1:B:157:ARG:NH1	1:B:200:SER:HB2	2.30	0.46
1:C:166:LEU:CD2	1:C:216:PHE:HE1	2.25	0.46
1:C:265:GLN:HG3	1:C:315:ILE:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ASN:C	1:C:336:PRO:HD2	2.41	0.46
1:A:297:ARG:HH21	1:A:300:GLY:HA2	1.81	0.46
1:B:57:ASP:CG	1:B:60:ASN:HD22	2.24	0.46
1:B:487:LYS:HD2	1:B:487:LYS:C	2.40	0.46
1:C:92:ASN:OD1	1:C:92:ASN:C	2.59	0.46
1:C:297:ARG:HH21	1:C:300:GLY:HA2	1.80	0.46
1:C:413:PRO:N	1:C:416:GLN:HE21	2.14	0.46
1:C:158:THR:CG2	1:C:159:ASP:O	2.62	0.46
1:A:176:ARG:HD3	1:A:177:VAL:HG23	1.98	0.46
1:A:485:PRO:HA	1:C:320:ARG:NH1	2.30	0.46
1:B:184:TYR:HD1	1:B:191:SER:HB2	1.80	0.46
1:B:199:ALA:HB2	1:B:218:PHE:CB	2.46	0.46
1:A:37:PHE:HA	1:A:53:ILE:O	2.16	0.46
1:A:57:ASP:CG	1:A:60:ASN:ND2	2.74	0.46
1:A:184:TYR:HD1	1:A:191:SER:HB2	1.81	0.46
1:B:401:PHE:HD2	1:B:413:PRO:HB2	1.79	0.46
1:B:486:ASN:HB3	1:B:490:GLN:OE1	2.16	0.46
1:C:145:HIS:ND1	1:C:147:SER:OG	2.44	0.46
1:C:145:HIS:CD2	1:C:193:PRO:HG3	2.50	0.46
1:C:236:PRO:O	1:C:237:PRO:C	2.59	0.46
1:A:158:THR:CG2	1:A:159:ASP:O	2.61	0.46
1:A:473:THR:CG2	1:C:171:SER:HA	2.41	0.46
1:C:100:LYS:HG2	1:C:130:TRP:CZ2	2.51	0.46
1:A:250:VAL:HG22	1:A:252:PHE:CE1	2.51	0.46
1:A:266:ILE:HG12	1:A:273:VAL:HG22	1.97	0.46
1:A:349:LEU:HD21	1:A:363:LEU:HB2	1.98	0.46
1:B:86:LYS:HE2	1:B:106:ASP:HA	1.98	0.46
1:B:164:TRP:HZ2	1:B:234:GLY:CA	2.29	0.46
1:B:206:MET:SD	1:B:243:PHE:HB2	2.56	0.46
1:B:362:GLU:O	1:B:366:ARG:HB2	2.15	0.46
1:C:54:ASP:C	1:C:56:ASN:N	2.73	0.46
1:C:74:ASN:OD1	1:C:113:TRP:CZ3	2.69	0.46
1:C:445:LYS:HG3	1:C:446:GLN:N	2.29	0.46
1:A:57:ASP:N	1:A:58:PRO:CD	2.79	0.45
1:A:485:PRO:HB2	1:A:487:LYS:CG	2.46	0.45
1:B:147:SER:H	1:B:147:SER:HG	1.19	0.45
1:C:102:HIS:NE2	1:C:138:PRO:HG2	2.31	0.45
1:C:301:GLU:HG3	1:C:321:LYS:HE2	1.99	0.45
1:C:421:LEU:CA	1:C:424:GLN:HB2	2.44	0.45
1:A:54:ASP:C	1:A:54:ASP:OD1	2.57	0.45
1:A:141:MET:HB3	1:A:141:MET:HE3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ILE:HG22	1:A:344:ASN:O	2.17	0.45
1:A:396:ASP:OD2	1:A:396:ASP:N	2.49	0.45
1:B:109:THR:N	1:B:122:VAL:O	2.44	0.45
1:B:250:VAL:O	1:B:250:VAL:CG2	2.62	0.45
1:C:374:GLN:NE2	1:C:376:ASN:CB	2.69	0.45
1:C:404:VAL:HG23	1:C:405:PRO:HD2	1.97	0.45
1:A:444:ARG:HH11	1:A:444:ARG:CG	2.27	0.45
1:B:489:ILE:O	1:B:492:PHE:HB2	2.16	0.45
1:C:372:PHE:CE2	1:C:400:ARG:HB3	2.52	0.45
1:A:16:GLN:O	1:A:19:GLY:N	2.46	0.45
1:B:475:ALA:O	1:B:476:LEU:C	2.60	0.45
1:C:211:GLU:HB3	1:C:237:PRO:HG2	1.98	0.45
1:C:280:GLY:HA3	1:C:299:SER:O	2.16	0.45
1:A:438:PRO:HG2	1:A:439:VAL:H	1.80	0.45
1:B:14:GLN:HE21	1:B:16:GLN:H	1.65	0.45
1:B:47:GLN:NE2	1:B:65:PRO:HB3	2.32	0.45
1:B:192:GLN:HA	1:B:193:PRO:HD3	1.73	0.45
1:A:218:PHE:CZ	1:A:229:HIS:CD2	3.05	0.45
1:A:433:LEU:HD21	1:A:462:GLU:CD	2.41	0.45
1:B:44:VAL:N	1:B:47:GLN:O	2.49	0.45
1:C:164:TRP:CZ2	1:C:234:GLY:CA	2.99	0.45
1:A:216:PHE:HD2	1:A:231:ILE:CD1	2.23	0.45
1:A:236:PRO:O	1:A:237:PRO:C	2.58	0.45
1:B:433:LEU:HD21	1:B:462:GLU:CD	2.42	0.45
1:C:73:MET:HE1	1:C:80:ILE:HB	1.97	0.45
1:C:190:VAL:CG1	1:C:191:SER:N	2.79	0.45
1:C:227:LYS:HD3	1:C:249:ASP:HB3	1.97	0.45
1:A:455:ASP:CB	1:C:69:ASP:OD1	2.64	0.45
1:A:474:LEU:O	1:A:478:VAL:HG23	2.16	0.45
1:B:54:ASP:C	1:B:56:ASN:H	2.25	0.45
1:B:102:HIS:CE1	1:B:138:PRO:HD2	2.51	0.45
1:B:339:THR:O	1:B:343:GLN:HA	2.16	0.45
1:C:438:PRO:HB3	1:C:441:GLN:NE2	2.32	0.45
1:C:442:GLN:CG	1:C:444:ARG:NH1	2.80	0.45
1:A:211:GLU:HB3	1:A:237:PRO:HG2	1.99	0.45
1:B:454:GLU:HB3	1:B:456:LYS:HE3	1.98	0.45
1:C:167:LEU:O	1:C:181:MET:HA	2.17	0.45
1:C:392:LEU:O	1:C:394:THR:N	2.44	0.45
1:C:396:ASP:CA	1:C:399:ARG:NH1	2.75	0.45
1:A:211:GLU:HB2	1:A:237:PRO:HG2	1.99	0.45
1:A:265:GLN:HG3	1:A:315:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASN:C	1:A:376:ASN:HD22	2.25	0.45
1:A:398:ILE:HD12	1:A:430:TYR:HE2	1.73	0.45
1:B:145:HIS:CE1	1:B:147:SER:OG	2.70	0.45
1:B:475:ALA:HB1	1:B:479:TYR:CE1	2.52	0.45
1:C:145:HIS:CE1	1:C:147:SER:OG	2.70	0.45
1:B:186:VAL:HG12	1:B:187:ASP:N	2.32	0.44
1:B:446:GLN:HA	1:B:449:GLU:OE2	2.16	0.44
1:C:57:ASP:OD1	1:C:60:ASN:ND2	2.50	0.44
1:C:438:PRO:HA	1:C:441:GLN:CG	2.47	0.44
1:C:463:LEU:HD12	1:C:463:LEU:HA	1.77	0.44
1:A:89:GLN:NE2	1:A:98:LYS:CD	2.76	0.44
1:A:407:GLN:HA	1:A:408:PRO:HD2	1.63	0.44
1:B:57:ASP:N	1:B:58:PRO:CD	2.78	0.44
1:B:199:ALA:HB1	1:B:217:CYS:O	2.17	0.44
1:C:54:ASP:C	1:C:54:ASP:OD1	2.61	0.44
1:C:163:LYS:O	1:C:186:VAL:HB	2.18	0.44
1:C:253:PRO:O	1:C:256:ALA:HB3	2.16	0.44
1:A:86:LYS:HG3	1:A:107:ASP:OD1	2.18	0.44
1:A:452:LEU:C	1:A:454:GLU:N	2.75	0.44
1:C:279:TYR:O	1:C:297:ARG:NH2	2.50	0.44
1:C:339:THR:HG23	1:C:345:PRO:HG3	1.99	0.44
1:C:392:LEU:C	1:C:394:THR:N	2.74	0.44
1:A:167:LEU:O	1:A:181:MET:HA	2.18	0.44
1:A:471:ASP:HA	1:A:472:PRO:HD3	1.79	0.44
1:B:197:HIS:HD2	1:B:221:ARG:N	2.13	0.44
1:C:3:GLN:HB2	1:C:341:VAL:HG22	1.99	0.44
1:C:145:HIS:CE1	1:C:147:SER:HG	2.34	0.44
1:C:368:PHE:C	1:C:370:ALA:N	2.73	0.44
1:A:13:LEU:HD13	1:A:58:PRO:HB2	1.99	0.44
1:A:476:LEU:CD1	1:C:177:VAL:HG22	2.44	0.44
1:B:396:ASP:OD1	1:B:396:ASP:N	2.50	0.44
1:B:442:GLN:O	1:B:444:ARG:HG3	2.17	0.44
1:C:16:GLN:O	1:C:19:GLY:N	2.47	0.44
1:C:145:HIS:H	1:C:182:GLN:CD	2.25	0.44
1:C:415:LEU:HD13	1:C:415:LEU:HA	1.67	0.44
1:C:428:ASN:O	1:C:429:LYS:C	2.60	0.44
1:C:486:ASN:C	1:C:487:LYS:HG3	2.42	0.44
1:A:109:THR:HG23	1:A:109:THR:O	2.16	0.44
1:A:176:ARG:NH2	1:A:221:ARG:HD3	2.33	0.44
1:B:57:ASP:N	1:B:58:PRO:HD3	2.33	0.44
1:C:407:GLN:OE1	1:C:410:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLN:HG3	1:A:48:ALA:N	2.25	0.44
1:A:91:PHE:CE2	1:A:96:LYS:HA	2.53	0.44
1:A:145:HIS:ND1	1:A:147:SER:OG	2.47	0.44
1:A:445:LYS:HE2	1:A:445:LYS:HB2	1.65	0.44
1:B:449:GLU:O	1:B:453:LYS:HE3	2.18	0.44
1:B:454:GLU:HB3	1:B:456:LYS:CE	2.48	0.44
1:C:95:MET:HG3	1:C:97:SER:OG	2.18	0.44
1:A:54:ASP:C	1:A:56:ASN:H	2.26	0.44
1:A:176:ARG:CD	1:A:177:VAL:H	2.30	0.44
1:A:217:CYS:HA	1:A:229:HIS:O	2.18	0.44
1:A:471:ASP:OD1	1:A:472:PRO:CD	2.66	0.44
1:B:253:PRO:HD2	1:B:256:ALA:HB2	2.00	0.44
1:C:158:THR:CG2	1:C:159:ASP:N	2.81	0.44
1:C:391:ILE:HD13	1:C:392:LEU:HD21	1.99	0.44
1:A:109:THR:N	1:A:122:VAL:O	2.47	0.43
1:A:173:GLN:HG3	1:A:178:VAL:CG2	2.48	0.43
1:A:379:GLU:OE1	1:A:379:GLU:HA	2.16	0.43
1:A:398:ILE:O	1:A:402:GLN:HG3	2.18	0.43
1:A:445:LYS:H	1:A:445:LYS:HG3	1.19	0.43
1:B:13:LEU:CD2	1:B:58:PRO:HB2	2.48	0.43
1:B:205:LYS:HB2	1:B:205:LYS:HE2	1.67	0.43
1:B:453:LYS:O	1:B:455:ASP:N	2.51	0.43
1:C:159:ASP:O	1:C:160:ALA:C	2.60	0.43
1:A:66:ILE:O	1:A:66:ILE:HG22	2.18	0.43
1:A:152:GLN:O	1:A:169:GLY:HA2	2.18	0.43
1:A:186:VAL:HG12	1:A:187:ASP:N	2.32	0.43
1:A:356:ASN:OD1	1:A:389:LYS:N	2.50	0.43
1:B:476:LEU:O	1:B:480:LEU:HG	2.18	0.43
1:C:205:LYS:HE2	1:C:205:LYS:HB2	1.73	0.43
1:C:433:LEU:HD21	1:C:462:GLU:HB3	2.00	0.43
1:A:44:VAL:N	1:A:47:GLN:O	2.51	0.43
1:A:78:LYS:HB2	1:A:94:GLU:HB2	2.00	0.43
1:B:305:VAL:C	1:B:306:THR:CG2	2.91	0.43
1:B:429:LYS:HD2	1:B:458:GLU:OE1	2.18	0.43
1:C:305:VAL:C	1:C:306:THR:CG2	2.91	0.43
1:A:131:SER:C	1:A:133:GLU:H	2.26	0.43
1:B:54:ASP:O	1:B:56:ASN:N	2.51	0.43
1:B:441:GLN:HG2	1:B:441:GLN:H	1.63	0.43
1:B:475:ALA:HB3	1:B:492:PHE:CZ	2.51	0.43
1:C:398:ILE:HD13	1:C:430:TYR:CE2	2.54	0.43
1:A:433:LEU:CD1	1:A:463:LEU:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HG3	1:C:1:MET:N	2.33	0.43
1:B:117:ASN:HB2	1:B:132:MET:CG	2.47	0.43
1:B:428:ASN:HB2	1:B:429:LYS:H	1.41	0.43
1:C:192:GLN:HA	1:C:193:PRO:HD3	1.76	0.43
1:A:372:PHE:CZ	1:A:400:ARG:O	2.71	0.43
1:B:447:LEU:HD21	1:B:451:TRP:CH2	2.54	0.43
1:A:395:PRO:O	1:A:396:ASP:C	2.60	0.43
1:B:349:LEU:HD21	1:B:363:LEU:HB2	2.01	0.43
1:C:30:LEU:HD22	1:C:40:ILE:HG13	2.01	0.43
1:C:356:ASN:O	1:C:389:LYS:HE3	2.19	0.43
1:A:74:ASN:HD22	1:A:77:SER:N	2.09	0.43
1:A:407:GLN:HE22	1:A:408:PRO:HG2	1.83	0.43
1:A:460:SER:N	1:A:482:ALA:HB2	2.33	0.43
1:B:13:LEU:HD23	1:B:58:PRO:HB3	2.01	0.43
1:C:335:ILE:HD11	1:C:357:LEU:HD12	2.01	0.43
1:C:447:LEU:O	1:C:448:LEU:C	2.62	0.43
1:A:21:ASN:HA	1:A:22:PRO:HD3	1.85	0.43
1:A:129:HIS:CD2	1:A:141:MET:HG3	2.53	0.43
1:A:205:LYS:HE2	1:A:205:LYS:HB2	1.78	0.43
1:A:415:LEU:HD13	1:A:415:LEU:HA	1.62	0.43
1:C:128:TYR:O	1:C:129:HIS:HD2	2.01	0.43
1:C:250:VAL:HG22	1:C:252:PHE:CE1	2.53	0.43
1:C:390:GLY:O	1:C:391:ILE:C	2.62	0.43
1:C:398:ILE:CG2	1:C:414:LEU:HD11	2.41	0.43
1:B:4:ILE:O	1:B:4:ILE:HG23	2.18	0.42
1:C:164:TRP:O	1:C:165:LEU:HD23	2.19	0.42
1:A:283:HIS:ND1	1:A:295:MET:HG2	2.34	0.42
1:B:454:GLU:CB	1:B:456:LYS:CE	2.97	0.42
1:B:467:VAL:HG11	1:B:474:LEU:HB3	2.00	0.42
1:C:163:LYS:HD3	1:C:163:LYS:HA	1.86	0.42
1:C:427:LEU:HD13	1:C:435:LEU:HD12	2.01	0.42
1:B:484:VAL:HB	1:B:485:PRO:HD3	2.02	0.42
1:A:54:ASP:C	1:A:56:ASN:N	2.78	0.42
1:A:199:ALA:HB1	1:A:217:CYS:O	2.19	0.42
1:B:30:LEU:CD1	1:B:38:ILE:HG23	2.49	0.42
1:B:446:GLN:O	1:B:449:GLU:HB2	2.20	0.42
1:C:173:GLN:OE1	1:C:173:GLN:CA	2.37	0.42
1:C:464:GLY:HA3	1:C:479:TYR:CD2	2.54	0.42
1:B:181:MET:HE1	1:B:218:PHE:CD1	2.54	0.42
1:C:351:MET:HE3	1:C:351:MET:HB2	1.66	0.42
1:C:410:GLN:OE1	1:C:410:GLN:CA	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LYS:NZ	1:B:143:ASP:CG	2.78	0.42
1:B:309:HIS:CD2	1:B:312:THR:OG1	2.62	0.42
1:A:163:LYS:O	1:A:186:VAL:HB	2.19	0.42
1:B:185:SER:HB3	1:B:188:ARG:HG2	2.01	0.42
1:B:484:VAL:HB	1:B:485:PRO:CD	2.50	0.42
1:C:37:PHE:HA	1:C:53:ILE:O	2.19	0.42
1:C:407:GLN:HA	1:C:408:PRO:HD2	1.44	0.42
1:A:117:ASN:HB2	1:A:132:MET:CG	2.46	0.42
1:B:301:GLU:HG3	1:B:321:LYS:HE2	1.99	0.42
1:B:368:PHE:O	1:B:369:ASN:C	2.63	0.42
1:C:343:GLN:O	1:C:344:ASN:HB2	2.19	0.42
1:C:440:LEU:HD11	1:C:467:VAL:CG2	2.48	0.42
1:A:461:GLU:CG	1:A:484:VAL:HG11	2.49	0.42
1:B:205:LYS:NZ	1:B:210:ALA:O	2.49	0.42
1:B:475:ALA:CB	1:B:492:PHE:HZ	2.33	0.42
1:C:197:HIS:HD2	1:C:221:ARG:N	2.14	0.42
1:A:140:LYS:NZ	1:A:143:ASP:CG	2.78	0.42
1:B:163:LYS:O	1:B:186:VAL:HB	2.19	0.42
1:B:181:MET:HE1	1:B:218:PHE:CG	2.55	0.42
1:B:398:ILE:HD11	1:B:431:GLU:HG2	2.02	0.42
1:B:475:ALA:O	1:B:478:VAL:HG23	2.19	0.42
1:C:216:PHE:HD2	1:C:231:ILE:CD1	2.25	0.42
1:C:261:PRO:HB3	1:C:275:LEU:HD11	2.01	0.42
1:C:374:GLN:CG	1:C:375:GLY:N	2.80	0.42
1:C:442:GLN:CD	1:C:444:ARG:NH1	2.78	0.42
1:C:450:LYS:O	1:C:454:GLU:CG	2.62	0.42
1:A:176:ARG:CD	1:A:177:VAL:HG23	2.50	0.41
1:A:197:HIS:HB3	1:A:261:PRO:HB2	2.01	0.41
1:B:116:LEU:HD22	1:B:116:LEU:N	2.30	0.41
1:B:236:PRO:O	1:B:237:PRO:C	2.61	0.41
1:B:342:LEU:O	1:B:343:GLN:C	2.63	0.41
1:B:371:LEU:HD13	1:B:379:GLU:HG3	2.02	0.41
1:B:454:GLU:O	1:B:456:LYS:HE3	2.19	0.41
1:C:421:LEU:N	1:C:421:LEU:HD23	2.35	0.41
1:C:486:ASN:O	1:C:487:LYS:HG2	2.19	0.41
1:A:459:CYS:C	1:A:482:ALA:HB2	2.45	0.41
1:C:349:LEU:HD22	1:C:364:PHE:CE2	2.54	0.41
1:C:368:PHE:CD2	1:C:400:ARG:NH2	2.85	0.41
1:C:422:LEU:HD23	1:C:422:LEU:HA	1.69	0.41
1:C:464:GLY:HA3	1:C:479:TYR:CE2	2.55	0.41
1:C:472:PRO:O	1:C:474:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:HIS:NE2	1:A:326:SER:CB	2.79	0.41
1:B:356:ASN:CG	1:B:356:ASN:O	2.62	0.41
1:B:442:GLN:HE21	1:B:442:GLN:HB2	1.48	0.41
1:C:3:GLN:O	1:C:4:ILE:HB	2.20	0.41
1:A:164:TRP:CZ2	1:A:234:GLY:CA	3.04	0.41
1:A:388:PRO:C	1:A:389:LYS:HG2	2.44	0.41
1:B:265:GLN:HG3	1:B:315:ILE:HG13	2.03	0.41
1:C:476:LEU:HD23	1:C:477:SER:N	2.35	0.41
1:A:43:LYS:HA	1:A:47:GLN:O	2.21	0.41
1:A:221:ARG:HD2	1:A:259:ASP:O	2.21	0.41
1:B:379:GLU:OE1	1:B:379:GLU:HA	2.20	0.41
1:B:421:LEU:CB	1:B:427:LEU:HD11	2.49	0.41
1:C:181:MET:HE1	1:C:218:PHE:CD1	2.55	0.41
1:C:218:PHE:CZ	1:C:229:HIS:CD2	3.08	0.41
1:A:301:GLU:HG3	1:A:321:LYS:HE2	2.02	0.41
1:A:421:LEU:HB3	1:A:427:LEU:CD2	2.49	0.41
1:B:54:ASP:C	1:B:56:ASN:N	2.76	0.41
1:B:363:LEU:HD23	1:B:366:ARG:NH1	2.36	0.41
1:A:349:LEU:HD22	1:A:364:PHE:CE2	2.55	0.41
1:B:91:PHE:CZ	1:B:96:LYS:C	2.99	0.41
1:B:309:HIS:CD2	1:B:312:THR:HG23	2.55	0.41
1:B:447:LEU:HD11	1:B:451:TRP:CZ2	2.55	0.41
1:C:401:PHE:HB3	1:C:414:LEU:HD12	2.03	0.41
1:A:144:ARG:HD3	1:A:167:LEU:CD2	2.50	0.41
1:A:354:ARG:NE	1:A:355:ASN:OD1	2.44	0.41
1:A:398:ILE:HG23	1:A:414:LEU:HD11	2.01	0.41
1:A:444:ARG:NH1	1:A:444:ARG:CG	2.84	0.41
1:B:21:ASN:HA	1:B:22:PRO:HD3	1.85	0.41
1:B:349:LEU:HD21	1:B:363:LEU:CB	2.51	0.41
1:B:351:MET:HE2	1:B:351:MET:HB2	1.56	0.41
1:C:24:ASN:ND2	1:C:42:GLU:CG	2.71	0.41
1:C:243:PHE:CD2	1:C:243:PHE:C	2.98	0.41
1:A:111:TRP:HA	1:A:120:ALA:O	2.21	0.41
1:A:133:GLU:OE2	1:A:133:GLU:HA	2.20	0.41
1:A:376:ASN:ND2	1:A:379:GLU:HB2	2.36	0.41
1:A:469:SER:HB2	1:A:470:VAL:H	1.74	0.41
1:B:301:GLU:CG	1:B:321:LYS:HE2	2.51	0.41
1:B:305:VAL:C	1:B:306:THR:HG23	2.46	0.41
1:B:356:ASN:HA	1:B:388:PRO:HB3	2.03	0.41
1:B:441:GLN:C	1:B:443:GLY:H	2.29	0.41
1:B:445:LYS:O	1:B:446:GLN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ILE:HG22	1:C:25:ILE:O	2.21	0.41
1:C:74:ASN:HD22	1:C:77:SER:N	2.08	0.41
1:C:205:LYS:O	1:C:205:LYS:HG3	2.17	0.41
1:C:468:LYS:NZ	1:C:479:TYR:CE1	2.89	0.41
1:C:474:LEU:O	1:C:478:VAL:HG23	2.21	0.41
1:A:192:GLN:HA	1:A:193:PRO:HD3	1.76	0.41
1:A:227:LYS:HD3	1:A:249:ASP:HB3	2.03	0.41
1:B:69:ASP:HB2	1:B:83:LYS:O	2.21	0.41
1:B:404:VAL:HA	1:B:405:PRO:HD3	1.73	0.41
1:B:452:LEU:O	1:B:455:ASP:HA	2.21	0.41
1:C:218:PHE:CE2	1:C:229:HIS:HB2	2.55	0.41
1:C:244:PRO:O	1:C:245:LYS:C	2.64	0.41
1:C:371:LEU:HB3	1:C:376:ASN:HB3	2.01	0.41
1:C:447:LEU:HD23	1:C:451:TRP:HZ2	1.80	0.41
1:A:261:PRO:HB3	1:A:275:LEU:HD11	2.02	0.40
1:B:63:ARG:C	1:B:64:ARG:HG2	2.46	0.40
1:B:83:LYS:HZ2	1:B:83:LYS:HG2	1.75	0.40
1:B:170:ILE:HG22	1:B:179:GLY:HA2	2.04	0.40
1:B:205:LYS:HD3	1:B:209:ASN:O	2.21	0.40
1:C:86:LYS:HE2	1:C:106:ASP:HA	2.01	0.40
1:A:176:ARG:HG2	1:A:177:VAL:N	2.33	0.40
1:B:66:ILE:HG21	1:B:82:LEU:HD22	2.03	0.40
1:B:353:VAL:O	1:B:354:ARG:C	2.64	0.40
1:B:423:ASP:O	1:B:424:GLN:C	2.65	0.40
1:B:439:VAL:CG1	1:B:444:ARG:HB2	2.43	0.40
1:B:478:VAL:O	1:B:482:ALA:N	2.54	0.40
1:C:18:LEU:HD23	1:C:18:LEU:HA	1.98	0.40
1:C:65:PRO:O	1:C:66:ILE:CG1	2.69	0.40
1:A:205:LYS:NZ	1:A:210:ALA:O	2.52	0.40
1:A:400:ARG:HD2	1:A:400:ARG:HA	1.83	0.40
1:B:95:MET:O	1:B:97:SER:N	2.54	0.40
1:B:173:GLN:O	1:B:174:GLN:C	2.63	0.40
1:B:410:GLN:HB3	1:B:411:THR:H	1.77	0.40
1:B:454:GLU:HB2	1:B:456:LYS:HE3	2.03	0.40
1:C:257:GLN:H	1:C:257:GLN:HG2	1.70	0.40
1:C:433:LEU:HG	1:C:437:ARG:HH12	1.86	0.40
1:A:4:ILE:HG23	1:A:337:TYR:HB2	2.03	0.40
1:A:197:HIS:HD2	1:A:221:ARG:N	2.15	0.40
1:A:476:LEU:CD2	1:C:170:ILE:HD12	2.48	0.40
1:B:4:ILE:HG12	1:B:333:ASN:HB3	2.04	0.40
1:B:173:GLN:HG3	1:B:178:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:LEU:HA	1:B:415:LEU:HD13	1.65	0.40
1:C:351:MET:O	1:C:352:ALA:C	2.65	0.40
1:C:364:PHE:O	1:C:366:ARG:N	2.54	0.40
1:C:422:LEU:HD23	1:C:427:LEU:CD1	2.51	0.40
1:A:14:GLN:HE21	1:A:14:GLN:C	2.29	0.40
1:A:66:ILE:HG21	1:A:82:LEU:HD22	2.04	0.40
1:A:273:VAL:HB	1:A:285:TYR:HB2	2.04	0.40
1:C:21:ASN:HA	1:C:22:PRO:HD3	1.90	0.40
1:C:206:MET:SD	1:C:243:PHE:HB2	2.61	0.40
1:C:342:LEU:O	1:C:343:GLN:O	2.40	0.40
1:C:413:PRO:CD	1:C:416:GLN:HE21	2.33	0.40
1:C:422:LEU:HD23	1:C:427:LEU:HD11	2.02	0.40

All (1) 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:B:188:ARG:NH2	1:B:441:GLN:NE2[2_654]	2.10	0.10

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	485/494 (98%)	433 (89%)	36 (7%)	16 (3%)	3	5
1	B	491/494 (99%)	435 (89%)	39 (8%)	17 (4%)	3	4
1	C	485/494 (98%)	418 (86%)	43 (9%)	24 (5%)	1	2
All	All	1461/1482 (99%)	1286 (88%)	118 (8%)	57 (4%)	2	3

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	LYS
1	A	470	VAL
1	B	96	LYS
1	B	189	LYS
1	B	257	GLN
1	C	57	ASP
1	C	96	LYS
1	C	173	GLN
1	C	189	LYS
1	C	257	GLN
1	C	486	ASN
1	A	55	MET
1	A	96	LYS
1	A	223	GLN
1	A	257	GLN
1	B	57	ASP
1	B	374	GLN
1	B	377	TYR
1	B	410	GLN
1	B	428	ASN
1	B	459	CYS
1	C	136	SER
1	C	467	VAL
1	C	473	THR
1	A	112	LYS
1	A	469	SER
1	B	66	ILE
1	B	112	LYS
1	B	442	GLN
1	C	55	MET
1	C	112	LYS
1	C	362	GLU
1	C	408	PRO
1	C	418	PHE
1	C	462	GLU
1	A	100	LYS
1	A	408	PRO
1	A	443	GLY
1	B	55	MET
1	B	136	SER
1	C	102	HIS
1	C	472	PRO
1	A	57	ASP

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Mol	Chain	Res	Type
1	A	66	ILE
1	B	100	LYS
1	B	102	HIS
1	C	66	ILE
1	C	100	LYS
1	C	343	GLN
1	C	391	ILE
1	C	403	SER
1	C	405	PRO
1	C	463	LEU
1	A	102	HIS
1	A	136	SER
1	A	483	ASN
1	B	438	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/422 (46%)	145 (74%)	51 (26%)	0	1
1	B	341/422 (81%)	266 (78%)	75 (22%)	1	2
1	C	416/422 (99%)	309 (74%)	107 (26%)	0	1
All	All	953/1266 (75%)	720 (76%)	233 (24%)	1	1

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	30	LEU
1	A	49	GLN
1	A	67	SER
1	A	78	LYS
1	A	96	LYS
1	A	97	SER
1	A	105	THR

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Mol	Chain	Res	Type
1	A	106	ASP
1	A	109	THR
1	A	133	GLU
1	A	135	GLU
1	A	136	SER
1	A	154	ILE
1	A	165	LEU
1	A	176	ARG
1	A	177	VAL
1	A	188	ARG
1	A	189	LYS
1	A	191	SER
1	A	194	ILE
1	A	205	LYS
1	A	206	MET
1	A	221	ARG
1	A	366	ARG
1	A	389	LYS
1	A	391	ILE
1	A	396	ASP
1	A	407	GLN
1	A	410	GLN
1	A	415	LEU
1	A	424	GLN
1	A	426	GLN
1	A	428	ASN
1	A	433	LEU
1	A	435	LEU
1	A	439	VAL
1	A	441	GLN
1	A	444	ARG
1	A	445	LYS
1	A	448	LEU
1	A	450	LYS
1	A	456	LYS
1	A	458	GLU
1	A	460	SER
1	A	461	GLU
1	A	466	LEU
1	A	470	VAL
1	A	474	LEU
1	A	477	SER

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Mol	Chain	Res	Type
1	A	480	LEU
1	B	43	LYS
1	B	46	GLU
1	B	47	GLN
1	B	49	GLN
1	B	59	SER
1	B	62	ILE
1	B	63	ARG
1	B	67	SER
1	B	83	LYS
1	B	86	LYS
1	B	89	GLN
1	B	96	LYS
1	B	97	SER
1	B	105	THR
1	B	106	ASP
1	B	109	THR
1	B	112	LYS
1	B	123	THR
1	B	125	ASN
1	B	128	TYR
1	B	133	GLU
1	B	135	GLU
1	B	136	SER
1	B	144	ARG
1	B	158	THR
1	B	163	LYS
1	B	165	LEU
1	B	170	ILE
1	B	171	SER
1	B	206	MET
1	B	214	THR
1	B	231	ILE
1	B	233	VAL
1	B	235	THR
1	B	245	LYS
1	B	249	ASP
1	B	250	VAL
1	B	257	GLN
1	B	262	VAL
1	B	268	GLU
1	B	282	ILE

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Mol	Chain	Res	Type
1	B	283	HIS
1	B	284	LEU
1	B	288	GLU
1	B	326	SER
1	B	342	LEU
1	B	351	MET
1	B	366	ARG
1	B	374	GLN
1	B	379	GLU
1	B	391	ILE
1	B	400	ARG
1	B	404	VAL
1	B	412	SER
1	B	415	LEU
1	B	424	GLN
1	B	426	GLN
1	B	428	ASN
1	B	429	LYS
1	B	433	LEU
1	B	435	LEU
1	B	442	GLN
1	B	445	LYS
1	B	448	LEU
1	B	450	LYS
1	B	456	LYS
1	B	457	LEU
1	B	461	GLU
1	B	466	LEU
1	B	471	ASP
1	B	473	THR
1	B	474	LEU
1	B	478	VAL
1	B	481	ARG
1	B	487	LYS
1	C	1	MET
1	C	3	GLN
1	C	16	GLN
1	C	20	ILE
1	C	29	THR
1	C	30	LEU
1	C	36	LYS
1	C	43	LYS

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Mol	Chain	Res	Type
1	C	46	GLU
1	C	47	GLN
1	C	49	GLN
1	C	59	SER
1	C	62	ILE
1	C	67	SER
1	C	78	LYS
1	C	83	LYS
1	C	86	LYS
1	C	89	GLN
1	C	96	LYS
1	C	97	SER
1	C	105	THR
1	C	106	ASP
1	C	109	THR
1	C	112	LYS
1	C	123	THR
1	C	125	ASN
1	C	128	TYR
1	C	133	GLU
1	C	135	GLU
1	C	136	SER
1	C	144	ARG
1	C	147	SER
1	C	154	ILE
1	C	158	THR
1	C	163	LYS
1	C	165	LEU
1	C	170	ILE
1	C	173	GLN
1	C	176	ARG
1	C	177	VAL
1	C	188	ARG
1	C	189	LYS
1	C	191	SER
1	C	194	ILE
1	C	205	LYS
1	C	206	MET
1	C	214	THR
1	C	231	ILE
1	C	233	VAL
1	C	245	LYS

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Mol	Chain	Res	Type
1	C	249	ASP
1	C	250	VAL
1	C	257	GLN
1	C	262	VAL
1	C	268	GLU
1	C	282	ILE
1	C	283	HIS
1	C	284	LEU
1	C	288	GLU
1	C	303	ILE
1	C	326	SER
1	C	342	LEU
1	C	347	LEU
1	C	350	ARG
1	C	351	MET
1	C	353	VAL
1	C	361	GLU
1	C	363	LEU
1	C	364	PHE
1	C	367	LYS
1	C	369	ASN
1	C	371	LEU
1	C	372	PHE
1	C	378	SER
1	C	383	VAL
1	C	386	ASN
1	C	391	ILE
1	C	401	PHE
1	C	410	GLN
1	C	411	THR
1	C	421	LEU
1	C	427	LEU
1	C	429	LYS
1	C	431	GLU
1	C	433	LEU
1	C	435	LEU
1	C	437	ARG
1	C	442	GLN
1	C	444	ARG
1	C	447	LEU
1	C	448	LEU
1	C	450	LYS

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Mol	Chain	Res	Type
1	C	452	LEU
1	C	453	LYS
1	C	454	GLU
1	C	456	LYS
1	C	460	SER
1	C	461	GLU
1	C	462	GLU
1	C	466	LEU
1	C	468	LYS
1	C	473	THR
1	C	474	LEU
1	C	476	LEU
1	C	477	SER
1	C	479	TYR
1	C	484	VAL

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

Mol	Chain	Res	Type
1	A	24	ASN
1	A	74	ASN
1	A	203	GLN
1	A	376	ASN
1	A	402	GLN
1	A	407	GLN
1	A	410	GLN
1	A	424	GLN
1	B	60	ASN
1	B	209	ASN
1	B	257	GLN
1	B	309	HIS
1	B	374	GLN
1	B	376	ASN
1	B	424	GLN
1	B	426	GLN
1	B	441	GLN
1	B	442	GLN
1	B	490	GLN
1	C	21	ASN
1	C	24	ASN
1	C	60	ASN
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	89	GLN
1	C	174	GLN
1	C	197	HIS
1	C	203	GLN
1	C	209	ASN
1	C	229	HIS
1	C	257	GLN
1	C	309	HIS
1	C	374	GLN
1	C	376	ASN
1	C	386	ASN
1	C	402	GLN
1	C	407	GLN
1	C	416	GLN
1	C	441	GLN
1	C	486	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	222:GLY	C	223:GLN	N	1.16
1	A	174:GLN	C	175:ASN	N	1.15

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.