



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:36 PM UTC

PDB ID : 1DXI / pdb_00001dxi
Title : STRUCTURE DETERMINATION OF GLUCOSE ISOMERASE FROM STREPTOMYCES MURINUS AT 2.6 ANGSTROMS RESOLUTION
Authors : Rasmussen, H.; La Cour, T.; Nyborg, J.; Schulein, M.
Deposited on : 1993-09-30
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

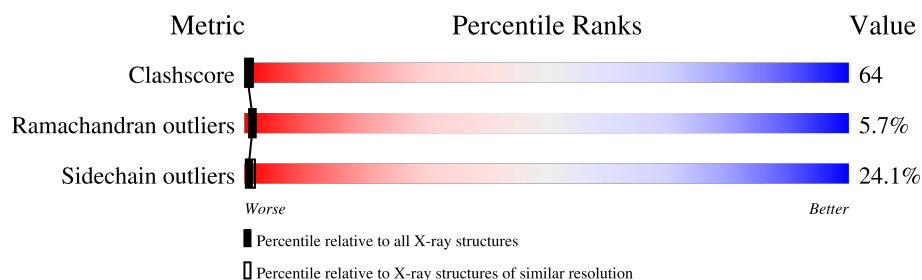
1 Overall quality at a glance

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	388	
1	B	388	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6054 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 D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3023	1908	536	570	9			
1	B	388	Total	C	N	O	S	0	0	0
			3023	1908	536	570	9			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is water.

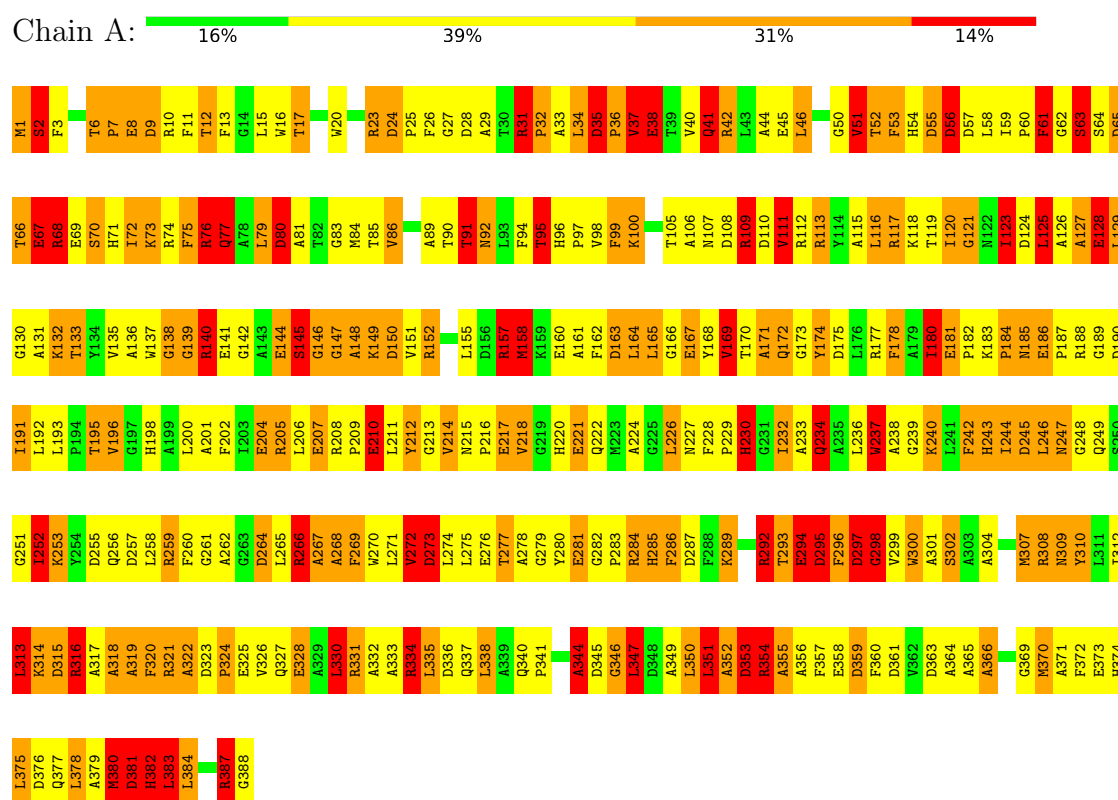
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	2	Total	O	0	0
			2	2		

3 Residue-property plots

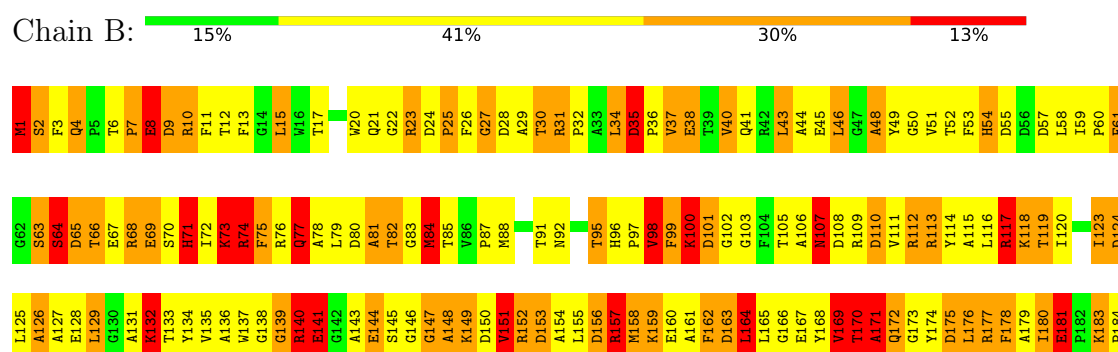
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: D-XYLOSE ISOMERASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.65Å 137.65Å 132.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6054	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.86	23/3097 (0.7%)	2.97	307/4198 (7.3%)
1	B	2.38	19/3097 (0.6%)	2.97	339/4198 (8.1%)
All	All	2.13	42/6194 (0.7%)	2.97	646/8396 (7.7%)

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	2	16
1	B	0	13
All	All	2	29

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	CA-CB	74.36	3.02	1.53
1	B	1	MET	N-CA	67.68	2.74	1.46
1	A	1	MET	N-CA	45.05	2.31	1.46
1	A	1	MET	C-O	36.95	1.97	1.23
1	B	382	HIS	N-CA	11.40	1.60	1.46
1	A	1	MET	CA-CB	-10.84	1.31	1.53
1	B	228	PHE	N-CA	9.90	1.53	1.46
1	A	381	ASP	N-CA	8.69	1.57	1.46
1	A	370	MET	C-O	8.02	1.33	1.23
1	B	381	ASP	C-O	7.91	1.34	1.23
1	A	347	LEU	N-CA	-7.88	1.36	1.46
1	B	1	MET	C-O	7.45	1.38	1.23
1	B	46	LEU	C-O	7.36	1.33	1.23
1	B	46	LEU	N-CA	7.30	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	381	ASP	N-CA	7.07	1.55	1.45
1	A	213	GLY	N-CA	6.89	1.55	1.45
1	A	346	GLY	CA-C	6.76	1.61	1.51
1	B	371	ALA	N-CA	6.65	1.54	1.46
1	B	280	TYR	N-CA	6.58	1.54	1.46
1	B	370	MET	N-CA	6.44	1.54	1.45
1	A	335	LEU	C-N	-6.26	1.25	1.33
1	B	353	ASP	CA-CB	-6.24	1.43	1.53
1	A	243	HIS	N-CA	6.18	1.53	1.46
1	A	212	TYR	C-O	6.12	1.31	1.24
1	B	297	ASP	C-N	-6.11	1.24	1.33
1	A	350	LEU	N-CA	-6.09	1.37	1.46
1	A	297	ASP	CA-CB	-6.05	1.45	1.53
1	A	139	GLY	N-CA	6.05	1.54	1.45
1	B	186	GLU	N-CA	5.99	1.54	1.46
1	A	387	ARG	N-CA	-5.96	1.38	1.46
1	B	370	MET	C-O	5.91	1.32	1.23
1	A	381	ASP	C-O	5.69	1.31	1.24
1	A	247	ASN	CA-CB	5.62	1.62	1.53
1	A	298	GLY	CA-C	5.57	1.59	1.51
1	B	71	HIS	N-CA	5.56	1.53	1.46
1	A	297	ASP	C-N	-5.34	1.25	1.33
1	A	91	THR	CA-CB	5.26	1.60	1.53
1	B	112	ARG	CD-NE	-5.24	1.39	1.46
1	A	352	ALA	N-CA	5.17	1.52	1.46
1	A	371	ALA	N-CA	5.12	1.52	1.46
1	B	316	ARG	NE-CZ	-5.12	1.27	1.33
1	A	147	GLY	N-CA	-5.11	1.38	1.45

All (646) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ARG	CD-NE-CZ	36.79	175.90	124.40
1	A	146	GLY	CA-C-N	29.60	179.43	121.41
1	A	146	GLY	C-N-CA	29.60	179.43	121.41
1	A	349	ALA	CA-C-N	28.71	173.24	122.42
1	A	349	ALA	C-N-CA	28.71	173.24	122.42
1	A	346	GLY	CA-C-N	22.29	164.11	121.54
1	A	346	GLY	C-N-CA	22.29	164.11	121.54
1	A	335	LEU	CA-C-N	18.05	143.91	120.44
1	A	335	LEU	C-N-CA	18.05	143.91	120.44
1	B	294	GLU	CA-C-N	17.85	155.63	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	GLU	C-N-CA	17.85	155.63	121.54
1	B	347	LEU	N-CA-C	16.68	140.48	107.62
1	A	344	ALA	N-CA-C	16.05	133.69	109.62
1	B	328	GLU	CA-CB-CG	15.65	145.40	114.10
1	B	372	PHE	CA-CB-CG	15.21	129.01	113.80
1	A	63	SER	N-CA-CB	-14.90	88.36	110.87
1	B	316	ARG	CD-NE-CZ	14.89	145.24	124.40
1	A	146	GLY	O-C-N	-14.82	108.07	123.48
1	A	259	ARG	CA-CB-CG	14.23	142.57	114.10
1	A	149	LYS	CB-CG-CD	13.89	143.26	111.30
1	B	68	ARG	CD-NE-CZ	13.85	143.79	124.40
1	A	352	ALA	CA-C-N	13.41	147.15	121.54
1	A	352	ALA	C-N-CA	13.41	147.15	121.54
1	B	353	ASP	CA-CB-CG	13.26	125.86	112.60
1	B	68	ARG	NE-CZ-NH1	13.16	134.66	121.50
1	B	1	MET	N-CA-CB	-12.79	88.75	110.50
1	B	349	ALA	CA-C-N	12.66	144.81	121.52
1	B	349	ALA	C-N-CA	12.66	144.81	121.52
1	B	84	MET	CA-CB-CG	12.62	139.35	114.10
1	B	144	GLU	CB-CG-CD	12.57	133.97	112.60
1	B	382	HIS	CA-C-O	12.55	134.24	119.56
1	B	328	GLU	CB-CG-CD	11.96	132.94	112.60
1	A	109	ARG	CA-C-O	-11.89	107.79	120.63
1	B	37	VAL	CB-CA-C	11.86	128.59	112.22
1	A	63	SER	N-CA-C	-11.71	92.82	109.69
1	A	1	MET	CB-CA-C	11.65	132.23	110.10
1	B	361	ASP	CA-CB-CG	11.62	124.22	112.60
1	A	381	ASP	CA-C-O	-11.37	104.26	120.51
1	A	347	LEU	N-CA-C	11.20	134.65	110.80
1	A	146	GLY	CA-C-O	11.16	131.08	120.92
1	B	145	SER	O-C-N	11.10	137.35	122.59
1	B	316	ARG	NE-CZ-NH2	10.90	129.01	119.20
1	A	1	MET	CA-C-O	-10.79	102.45	120.80
1	B	257	ASP	CA-CB-CG	10.71	123.31	112.60
1	B	381	ASP	CA-C-N	-10.66	105.59	122.65
1	B	381	ASP	C-N-CA	-10.66	105.59	122.65
1	A	2	SER	CA-C-N	10.65	137.79	122.24
1	A	2	SER	C-N-CA	10.65	137.79	122.24
1	A	24	ASP	CA-CB-CG	10.64	123.24	112.60
1	B	186	GLU	CA-CB-CG	10.57	135.24	114.10
1	B	2	SER	N-CA-C	10.55	129.17	109.24
1	B	309	ASN	N-CA-C	10.32	122.61	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ARG	NE-CZ-NH1	10.30	131.80	121.50
1	A	152	ARG	CD-NE-CZ	10.16	138.63	124.40
1	A	336	ASP	N-CA-CB	-10.16	95.27	110.01
1	A	141	GLU	CA-CB-CG	10.12	134.34	114.10
1	B	9	ASP	CA-C-N	10.10	136.70	122.36
1	B	9	ASP	C-N-CA	10.10	136.70	122.36
1	A	289	LYS	O-C-N	10.04	130.32	121.39
1	B	1	MET	N-CA-C	9.95	138.84	111.00
1	A	149	LYS	CA-C-O	-9.93	108.09	120.20
1	B	110	ASP	N-CA-CB	9.81	126.89	110.41
1	A	167	GLU	N-CA-CB	9.79	124.26	110.07
1	B	384	LEU	CB-CA-C	9.76	135.08	111.65
1	A	167	GLU	CA-CB-CG	9.69	133.48	114.10
1	B	370	MET	CA-C-O	-9.69	111.22	121.87
1	B	382	HIS	CB-CA-C	9.62	126.83	110.56
1	B	177	ARG	CA-C-O	9.61	131.51	120.75
1	B	157	ARG	CA-CB-CG	9.54	133.19	114.10
1	A	384	LEU	CB-CA-C	9.44	124.67	111.74
1	B	268	ALA	CA-C-N	9.42	132.69	120.44
1	B	268	ALA	C-N-CA	9.42	132.69	120.44
1	B	298	GLY	N-CA-C	-9.27	91.22	113.18
1	A	230	HIS	CA-C-N	9.25	130.25	119.98
1	A	230	HIS	C-N-CA	9.25	130.25	119.98
1	A	1	MET	O-C-N	9.25	137.80	123.00
1	B	117	ARG	O-C-N	9.19	131.65	122.09
1	A	245	ASP	CA-CB-CG	9.12	121.72	112.60
1	B	224	ALA	CA-C-O	9.09	130.68	119.95
1	B	144	GLU	CA-CB-CG	9.03	132.15	114.10
1	B	46	LEU	O-C-N	-9.02	112.57	122.85
1	B	153	ASP	N-CA-C	-8.99	101.43	111.14
1	A	67	GLU	N-CA-C	-8.98	101.47	111.07
1	A	366	ALA	O-C-N	8.91	132.31	122.15
1	B	172	GLN	OE1-CD-NE2	-8.86	113.74	122.60
1	A	296	PHE	CA-C-O	-8.84	111.72	121.00
1	A	38	GLU	N-CA-CB	8.81	122.84	110.07
1	B	363	ASP	CA-C-O	-8.80	110.15	120.10
1	A	308	ARG	CD-NE-CZ	8.77	136.67	124.40
1	B	308	ARG	NE-CZ-NH2	8.71	127.04	119.20
1	A	387	ARG	N-CA-C	8.71	129.34	110.80
1	B	222	GLN	CB-CG-CD	8.70	127.39	112.60
1	B	338	LEU	CA-C-O	8.69	129.96	119.97
1	B	350	LEU	N-CA-C	-8.68	101.53	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	ASP	N-CA-CB	8.67	124.01	109.87
1	A	128	GLU	CA-CB-CG	8.65	131.40	114.10
1	A	3	PHE	N-CA-CB	-8.64	100.41	110.35
1	B	38	GLU	CB-CG-CD	8.62	127.26	112.60
1	A	226	LEU	CB-CA-C	8.61	127.55	110.42
1	A	123	ILE	O-C-N	8.59	130.53	121.94
1	B	34	LEU	CA-C-O	-8.56	111.49	121.16
1	A	297	ASP	CA-C-N	8.55	138.17	121.41
1	A	297	ASP	C-N-CA	8.55	138.17	121.41
1	B	266	ARG	NE-CZ-NH2	-8.55	111.51	119.20
1	B	143	ALA	CA-C-O	8.52	131.97	120.47
1	A	298	GLY	N-CA-C	-8.44	93.17	113.18
1	B	344	ALA	CA-C-N	8.43	137.65	121.54
1	B	344	ALA	C-N-CA	8.43	137.65	121.54
1	A	3	PHE	N-CA-C	8.42	121.26	110.65
1	B	289	LYS	CB-CG-CD	8.40	130.63	111.30
1	A	53	PHE	CA-C-O	8.40	130.28	121.38
1	B	145	SER	CA-C-O	-8.36	108.55	120.51
1	B	163	ASP	CA-CB-CG	8.30	120.90	112.60
1	A	382	HIS	N-CA-CB	8.28	124.48	110.49
1	A	281	GLU	CA-CB-CG	8.27	130.63	114.10
1	B	381	ASP	N-CA-C	-8.25	99.96	110.19
1	B	181	GLU	CB-CG-CD	8.23	126.59	112.60
1	B	38	GLU	O-C-N	-8.22	113.60	122.07
1	B	348	ASP	N-CA-C	-8.18	100.04	111.81
1	B	2	SER	CA-C-N	8.15	136.07	121.97
1	B	2	SER	C-N-CA	8.15	136.07	121.97
1	A	61	PHE	N-CA-CB	8.13	124.23	110.49
1	A	145	SER	CA-C-N	8.10	130.22	122.36
1	A	145	SER	C-N-CA	8.10	130.22	122.36
1	B	381	ASP	CA-C-O	-8.06	113.55	122.01
1	A	304	ALA	N-CA-C	-8.03	101.61	111.40
1	B	77	GLN	CB-CG-CD	8.03	126.24	112.60
1	A	277	THR	CA-CB-OG1	-8.01	97.58	109.60
1	B	175	ASP	CB-CA-C	8.01	123.47	111.06
1	B	380	MET	N-CA-C	-7.99	103.13	113.12
1	B	110	ASP	CA-CB-CG	7.99	120.59	112.60
1	A	302	SER	N-CA-CB	7.98	121.58	110.01
1	B	242	PHE	CA-CB-CG	7.94	121.74	113.80
1	A	243	HIS	CA-CB-CG	7.92	121.72	113.80
1	B	46	LEU	N-CA-C	-7.92	99.86	110.55
1	B	157	ARG	N-CA-CB	7.90	121.47	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	ASP	CA-CB-CG	7.88	120.48	112.60
1	A	381	ASP	N-CA-C	-7.88	94.02	110.80
1	A	297	ASP	CA-CB-CG	7.87	120.47	112.60
1	B	35	ASP	CB-CA-C	7.81	120.72	109.08
1	B	255	ASP	CB-CA-C	7.80	121.39	110.16
1	A	340	GLN	O-C-N	7.75	128.95	121.66
1	A	110	ASP	N-CA-CB	7.75	122.62	110.46
1	B	75	PHE	CA-CB-CG	7.74	121.54	113.80
1	B	157	ARG	CA-C-O	-7.74	112.69	120.82
1	B	221	GLU	CA-C-O	7.72	128.87	119.38
1	B	358	GLU	CB-CG-CD	7.68	125.66	112.60
1	A	24	ASP	CB-CA-C	7.65	125.24	110.17
1	B	68	ARG	NE-CZ-NH2	-7.63	112.33	119.20
1	A	46	LEU	CB-CA-C	7.62	124.73	110.63
1	B	290	PRO	N-CA-C	-7.60	101.43	110.70
1	A	111	VAL	N-CA-C	-7.58	102.74	111.00
1	A	268	ALA	CA-C-O	-7.53	112.49	120.63
1	A	65	ASP	CB-CA-C	7.52	124.79	109.67
1	A	9	ASP	CB-CA-C	7.49	124.26	110.11
1	A	174	TYR	CA-C-O	7.48	129.48	121.55
1	B	341	PRO	CA-C-N	7.48	130.16	120.44
1	B	341	PRO	C-N-CA	7.48	130.16	120.44
1	B	34	LEU	N-CA-C	-7.48	98.06	109.95
1	A	67	GLU	CA-C-O	-7.47	112.97	120.82
1	A	140	ARG	NE-CZ-NH1	7.46	128.96	121.50
1	A	334	ARG	CB-CG-CD	7.44	128.41	111.30
1	A	244	ILE	CA-C-O	-7.41	113.89	121.67
1	B	385	GLY	CA-C-N	7.41	135.70	121.54
1	B	385	GLY	C-N-CA	7.41	135.70	121.54
1	A	186	GLU	CA-CB-CG	7.41	128.91	114.10
1	B	350	LEU	O-C-N	7.38	132.84	122.36
1	B	215	ASN	O-C-N	7.37	127.44	121.17
1	B	368	ARG	CB-CA-C	7.37	121.31	110.26
1	B	386	ALA	O-C-N	7.36	132.37	122.59
1	B	116	LEU	CA-C-O	7.34	128.26	120.70
1	B	191	ILE	O-C-N	7.34	131.78	122.61
1	B	169	VAL	CB-CA-C	7.34	121.27	111.88
1	A	149	LYS	CA-CB-CG	7.33	128.77	114.10
1	B	144	GLU	N-CA-C	-7.33	103.28	111.71
1	B	118	LYS	CA-C-N	7.32	130.68	120.29
1	B	118	LYS	C-N-CA	7.32	130.68	120.29
1	A	100	LYS	CA-CB-CG	7.31	128.73	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	ASN	OD1-CG-ND2	7.31	129.91	122.60
1	A	221	GLU	CA-C-O	7.31	128.15	119.60
1	A	344	ALA	N-CA-CB	-7.30	101.63	110.53
1	A	51	VAL	CA-C-O	-7.29	112.74	120.76
1	A	255	ASP	CA-C-O	-7.29	111.95	120.62
1	B	363	ASP	N-CA-CB	7.29	121.44	110.22
1	B	266	ARG	NE-CZ-NH1	7.24	128.74	121.50
1	B	245	ASP	CA-C-O	7.23	128.00	120.40
1	A	55	ASP	CA-CB-CG	7.22	119.82	112.60
1	B	98	VAL	CB-CA-C	-7.20	99.48	111.29
1	A	56	ASP	CA-CB-CG	7.18	119.78	112.60
1	B	61	PHE	CA-CB-CG	7.17	120.97	113.80
1	B	124	ASP	CA-CB-CG	7.16	119.76	112.60
1	B	124	ASP	O-C-N	7.16	129.74	122.08
1	A	380	MET	CB-CA-C	7.15	124.65	110.42
1	A	382	HIS	CA-CB-CG	7.14	120.94	113.80
1	A	95	THR	CA-CB-OG1	-7.13	98.90	109.60
1	B	287	ASP	CA-CB-CG	7.12	119.72	112.60
1	B	8	GLU	O-C-N	7.10	132.03	122.59
1	A	205	ARG	O-C-N	7.10	130.57	122.20
1	A	246	LEU	CB-CA-C	7.08	121.50	109.53
1	B	99	PHE	CA-C-N	7.08	135.06	121.54
1	B	99	PHE	C-N-CA	7.08	135.06	121.54
1	B	64	SER	N-CA-CB	7.08	122.45	110.49
1	B	353	ASP	CB-CA-C	7.04	122.63	110.45
1	A	140	ARG	CB-CA-C	7.03	122.45	110.56
1	A	334	ARG	CD-NE-CZ	7.02	134.22	124.40
1	B	297	ASP	N-CA-C	-7.01	98.52	109.25
1	B	313	LEU	O-C-N	7.01	129.55	122.12
1	A	310	TYR	N-CA-C	-7.01	103.57	111.14
1	A	75	PHE	CA-C-N	7.00	129.66	120.28
1	A	75	PHE	C-N-CA	7.00	129.66	120.28
1	A	330	LEU	CB-CA-C	7.00	124.67	110.38
1	B	51	VAL	O-C-N	-7.00	115.48	122.76
1	A	369	GLY	N-CA-C	-6.97	100.70	111.64
1	B	84	MET	O-C-N	6.96	130.83	122.96
1	A	214	VAL	N-CA-C	6.96	118.83	108.46
1	B	38	GLU	CB-CA-C	6.95	121.78	110.88
1	A	141	GLU	CB-CG-CD	6.94	124.40	112.60
1	B	218	VAL	N-CA-CB	6.94	117.90	110.62
1	B	249	GLN	O-C-N	-6.92	115.51	123.33
1	B	74	ARG	CD-NE-CZ	6.92	134.08	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	LYS	CA-C-O	-6.91	114.20	119.59
1	B	334	ARG	NE-CZ-NH1	-6.91	114.59	121.50
1	A	333	ALA	CA-C-N	6.89	132.56	122.63
1	A	333	ALA	C-N-CA	6.89	132.56	122.63
1	B	245	ASP	CA-C-N	6.89	131.94	122.77
1	B	245	ASP	C-N-CA	6.89	131.94	122.77
1	B	374	HIS	N-CA-CB	6.89	120.33	110.13
1	A	355	ALA	CA-C-O	6.89	126.72	119.14
1	B	264	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	157	ARG	NH1-CZ-NH2	-6.86	110.38	119.30
1	A	292	ARG	CG-CD-NE	6.84	127.04	112.00
1	B	143	ALA	CB-CA-C	6.83	120.93	111.23
1	B	383	LEU	CB-CA-C	6.82	124.00	110.42
1	A	8	GLU	CB-CG-CD	6.82	124.19	112.60
1	A	242	PHE	CA-CB-CG	6.80	120.61	113.80
1	A	152	ARG	NE-CZ-NH1	6.79	128.29	121.50
1	B	147	GLY	O-C-N	-6.79	113.87	122.70
1	A	212	TYR	O-C-N	-6.79	113.56	122.59
1	A	261	GLY	CA-C-N	6.78	130.99	120.75
1	A	261	GLY	C-N-CA	6.78	130.99	120.75
1	A	370	MET	CA-C-N	-6.78	108.58	121.54
1	A	370	MET	C-N-CA	-6.78	108.58	121.54
1	B	226	LEU	CB-CA-C	6.76	120.96	109.80
1	B	295	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	296	PHE	CA-C-N	-6.76	113.46	122.85
1	A	296	PHE	C-N-CA	-6.76	113.46	122.85
1	A	53	PHE	N-CA-C	6.74	118.44	108.60
1	A	330	LEU	N-CA-C	-6.73	103.75	112.23
1	B	329	ALA	O-C-N	6.72	131.53	122.59
1	B	145	SER	N-CA-CB	6.72	121.85	110.49
1	B	353	ASP	N-CA-CB	6.71	120.87	110.46
1	A	380	MET	CA-C-O	-6.71	110.92	120.51
1	A	351	LEU	CA-C-O	-6.69	110.94	120.51
1	B	370	MET	O-C-N	-6.69	114.92	122.75
1	B	194	PRO	N-CA-C	6.69	122.88	114.92
1	A	344	ALA	O-C-N	-6.68	114.36	122.71
1	B	140	ARG	CA-C-O	6.67	127.46	119.59
1	B	344	ALA	N-CA-C	6.66	119.80	109.60
1	B	266	ARG	CD-NE-CZ	6.66	133.72	124.40
1	B	204	GLU	CA-C-N	6.65	133.43	121.92
1	B	204	GLU	C-N-CA	6.65	133.43	121.92
1	B	177	ARG	O-C-N	-6.65	116.51	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	ALA	CA-C-O	6.65	127.81	120.63
1	B	31	ARG	CA-C-O	-6.64	114.51	120.56
1	A	163	ASP	N-CA-C	-6.64	103.86	112.23
1	B	206	LEU	N-CA-CB	-6.64	100.61	110.17
1	B	383	LEU	CA-C-N	-6.64	111.84	122.53
1	B	383	LEU	C-N-CA	-6.64	111.84	122.53
1	B	268	ALA	O-C-N	6.64	129.26	122.09
1	B	128	GLU	CA-CB-CG	6.63	127.35	114.10
1	A	92	ASN	CA-C-O	-6.62	112.81	120.49
1	B	84	MET	N-CA-CB	6.61	120.33	110.29
1	A	330	LEU	CA-CB-CG	6.59	139.37	116.30
1	B	346	GLY	CA-C-N	-6.58	113.40	123.14
1	B	346	GLY	C-N-CA	-6.58	113.40	123.14
1	A	3	PHE	CA-C-N	6.57	129.59	120.65
1	A	3	PHE	C-N-CA	6.57	129.59	120.65
1	A	172	GLN	CA-C-O	-6.57	113.55	120.58
1	B	370	MET	N-CA-CB	-6.57	100.87	110.26
1	A	217	GLU	CB-CG-CD	6.56	123.75	112.60
1	B	153	ASP	CA-CB-CG	6.56	119.16	112.60
1	B	316	ARG	NH1-CZ-NH2	-6.52	110.83	119.30
1	B	247	ASN	CA-C-O	-6.51	114.15	121.25
1	B	23	ARG	CD-NE-CZ	6.51	133.51	124.40
1	A	297	ASP	N-CA-CB	6.50	121.11	110.39
1	A	294	GLU	CA-CB-CG	6.49	127.08	114.10
1	A	285	HIS	O-C-N	6.48	130.62	123.04
1	A	9	ASP	N-CA-C	-6.47	103.46	112.45
1	B	3	PHE	CB-CA-C	6.47	117.75	109.80
1	B	316	ARG	NE-CZ-NH1	-6.47	115.03	121.50
1	A	99	PHE	CA-C-N	6.46	131.51	120.72
1	A	99	PHE	C-N-CA	6.46	131.51	120.72
1	B	301	ALA	CA-C-O	6.46	127.60	120.82
1	B	315	ASP	O-C-N	6.46	131.01	122.30
1	A	77	GLN	N-CA-CB	-6.45	100.61	110.16
1	A	180	ILE	N-CA-CB	6.44	118.23	110.31
1	B	188	ARG	CD-NE-CZ	-6.44	115.39	124.40
1	A	165	LEU	CB-CA-C	6.43	120.87	110.96
1	B	27	GLY	CA-C-N	6.42	131.03	120.94
1	B	27	GLY	C-N-CA	6.42	131.03	120.94
1	B	66	THR	O-C-N	6.42	128.71	122.03
1	B	69	GLU	N-CA-CB	6.41	120.22	110.28
1	A	292	ARG	CA-CB-CG	6.40	126.90	114.10
1	B	30	THR	CA-CB-CG2	6.40	121.38	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ALA	O-C-N	6.40	128.74	122.09
1	B	172	GLN	CB-CG-CD	6.39	123.47	112.60
1	B	117	ARG	NE-CZ-NH2	-6.39	113.45	119.20
1	B	224	ALA	CB-CA-C	6.38	121.30	111.02
1	A	220	HIS	CA-CB-CG	6.36	120.16	113.80
1	A	129	LEU	CB-CA-C	6.36	121.06	109.99
1	A	42	ARG	CD-NE-CZ	6.35	133.29	124.40
1	A	383	LEU	CA-C-N	-6.34	112.98	122.24
1	A	383	LEU	C-N-CA	-6.34	112.98	122.24
1	B	157	ARG	O-C-N	6.34	128.60	122.07
1	B	382	HIS	N-CA-C	-6.32	105.15	112.92
1	B	123	ILE	N-CA-C	-6.31	104.36	110.42
1	B	176	LEU	O-C-N	6.31	129.90	121.83
1	B	124	ASP	N-CA-CB	6.31	119.41	109.82
1	B	147	GLY	CA-C-N	6.30	133.79	122.38
1	B	147	GLY	C-N-CA	6.30	133.79	122.38
1	B	82	THR	CA-CB-OG1	-6.30	100.15	109.60
1	B	289	LYS	O-C-N	6.30	128.35	121.23
1	B	190	ASP	O-C-N	6.29	131.33	123.28
1	A	247	ASN	N-CA-CB	-6.28	101.02	111.57
1	B	174	TYR	CA-C-N	-6.28	113.16	122.83
1	B	174	TYR	C-N-CA	-6.28	113.16	122.83
1	A	266	ARG	CA-C-N	-6.26	112.30	120.44
1	A	266	ARG	C-N-CA	-6.26	112.30	120.44
1	A	139	GLY	N-CA-C	-6.25	98.36	113.18
1	B	31	ARG	O-C-N	6.25	127.75	121.56
1	A	61	PHE	CA-C-O	-6.24	111.59	120.51
1	A	31	ARG	NE-CZ-NH2	-6.23	113.59	119.20
1	A	178	PHE	CB-CA-C	6.23	122.15	109.76
1	B	31	ARG	CB-CA-C	-6.21	103.19	110.76
1	A	41	GLN	OE1-CD-NE2	6.19	128.79	122.60
1	B	383	LEU	N-CA-CB	-6.18	100.05	110.49
1	A	37	VAL	CA-C-N	-6.18	112.04	120.44
1	A	37	VAL	C-N-CA	-6.18	112.04	120.44
1	A	125	LEU	O-C-N	6.17	128.45	122.03
1	B	316	ARG	CA-C-O	-6.16	114.02	120.55
1	A	378	LEU	N-CA-C	-6.14	104.50	111.07
1	B	235	ALA	CA-C-O	-6.14	114.31	121.07
1	B	201	ALA	CB-CA-C	6.14	121.29	110.85
1	B	165	LEU	CA-C-N	6.14	128.02	120.22
1	B	165	LEU	C-N-CA	6.14	128.02	120.22
1	A	150	ASP	N-CA-CB	6.14	119.76	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	THR	N-CA-C	-6.14	100.01	109.52
1	A	214	VAL	N-CA-CB	-6.13	101.38	111.44
1	B	196	VAL	CB-CA-C	6.13	120.42	112.14
1	B	354	ARG	CD-NE-CZ	6.12	132.97	124.40
1	A	380	MET	N-CA-C	-6.12	97.77	110.80
1	B	175	ASP	CA-CB-CG	-6.12	106.48	112.60
1	A	177	ARG	NE-CZ-NH1	6.12	127.62	121.50
1	A	269	PHE	CA-CB-CG	6.11	119.91	113.80
1	B	84	MET	CB-CA-C	-6.10	98.23	109.46
1	B	169	VAL	N-CA-CB	6.10	117.28	110.51
1	B	382	HIS	O-C-N	-6.09	115.03	122.34
1	A	316	ARG	NE-CZ-NH2	-6.09	113.72	119.20
1	A	308	ARG	N-CA-C	-6.09	104.56	112.23
1	A	259	ARG	CD-NE-CZ	6.08	132.92	124.40
1	A	79	LEU	CB-CA-C	6.08	122.52	110.42
1	B	9	ASP	N-CA-C	-6.08	105.51	113.17
1	B	54	HIS	N-CA-C	-6.08	101.53	110.52
1	B	40	VAL	N-CA-CB	-6.08	103.77	110.51
1	B	4	GLN	OE1-CD-NE2	6.05	128.65	122.60
1	B	180	ILE	O-C-N	6.05	129.60	122.83
1	B	380	MET	CB-CA-C	6.05	119.54	109.56
1	A	382	HIS	CA-C-N	6.03	133.06	121.54
1	A	382	HIS	C-N-CA	6.03	133.06	121.54
1	B	37	VAL	N-CA-C	-6.03	104.63	110.72
1	B	15	LEU	N-CA-CB	-6.02	100.63	110.14
1	A	67	GLU	N-CA-CB	5.99	118.70	110.01
1	A	185	ASN	CA-CB-CG	-5.99	106.61	112.60
1	B	46	LEU	CA-C-O	-5.98	114.75	121.81
1	B	151	VAL	CA-C-O	-5.98	112.43	119.85
1	A	340	GLN	CB-CG-CD	5.97	122.76	112.60
1	B	308	ARG	CA-C-N	5.97	128.77	120.29
1	B	308	ARG	C-N-CA	5.97	128.77	120.29
1	A	211	LEU	CA-C-O	-5.97	112.21	119.43
1	B	303	ALA	CA-C-N	5.97	130.83	120.68
1	B	303	ALA	C-N-CA	5.97	130.83	120.68
1	B	344	ALA	CA-C-O	5.96	128.72	121.98
1	A	1	MET	CG-SD-CE	5.94	113.97	100.90
1	A	300	TRP	CB-CA-C	5.93	120.64	110.79
1	B	132	LYS	CG-CD-CE	5.93	124.94	111.30
1	B	171	ALA	CA-C-O	-5.93	112.03	120.51
1	A	204	GLU	CA-CB-CG	5.93	125.96	114.10
1	B	298	GLY	O-C-N	5.93	130.41	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	LEU	N-CA-C	-5.91	104.75	113.61
1	B	292	ARG	CD-NE-CZ	5.91	132.67	124.40
1	A	257	ASP	CB-CA-C	5.91	119.66	111.63
1	A	162	PHE	O-C-N	5.90	129.13	122.22
1	B	224	ALA	N-CA-C	-5.89	105.41	112.59
1	B	71	HIS	N-CA-C	-5.88	98.28	110.80
1	A	298	GLY	O-C-N	5.88	130.34	122.70
1	A	148	ALA	N-CA-C	5.87	118.63	111.82
1	A	365	ALA	CA-C-N	5.85	128.60	120.29
1	A	365	ALA	C-N-CA	5.85	128.60	120.29
1	B	311	LEU	CB-CA-C	5.85	121.41	110.70
1	B	157	ARG	NE-CZ-NH1	5.85	127.35	121.50
1	B	196	VAL	N-CA-C	-5.84	104.66	110.62
1	B	146	GLY	CA-C-O	-5.84	110.41	120.57
1	B	357	PHE	CA-C-N	5.84	128.03	120.44
1	B	357	PHE	C-N-CA	5.84	128.03	120.44
1	A	3	PHE	CB-CA-C	-5.82	103.77	111.74
1	A	73	LYS	O-C-N	5.81	128.06	122.07
1	A	212	TYR	N-CA-C	5.81	123.17	110.80
1	A	66	THR	CA-C-N	-5.80	112.89	120.44
1	A	66	THR	C-N-CA	-5.80	112.89	120.44
1	B	107	ASN	CA-CB-CG	-5.80	106.80	112.60
1	B	293	THR	N-CA-C	-5.80	106.04	113.23
1	B	150	ASP	CA-C-O	-5.80	114.05	120.60
1	A	293	THR	CA-C-N	5.79	131.33	122.93
1	A	293	THR	C-N-CA	5.79	131.33	122.93
1	A	109	ARG	CD-NE-CZ	-5.79	116.29	124.40
1	A	292	ARG	NE-CZ-NH1	5.79	127.29	121.50
1	B	340	GLN	OE1-CD-NE2	5.79	128.39	122.60
1	A	296	PHE	CB-CA-C	5.79	119.87	110.96
1	B	286	PHE	N-CA-C	5.79	117.95	108.52
1	B	240	LYS	N-CA-C	5.78	121.05	113.30
1	A	297	ASP	N-CA-C	-5.78	97.00	107.75
1	A	251	GLY	N-CA-C	5.78	117.93	112.04
1	A	149	LYS	CB-CA-C	-5.77	101.25	110.14
1	B	266	ARG	O-C-N	5.77	128.73	122.15
1	A	317	ALA	CA-C-N	5.77	127.94	120.44
1	A	317	ALA	C-N-CA	5.77	127.94	120.44
1	B	222	GLN	OE1-CD-NE2	-5.77	116.83	122.60
1	B	281	GLU	CA-C-O	5.77	125.39	119.05
1	A	286	PHE	CA-C-O	5.77	127.07	120.84
1	A	50	GLY	O-C-N	5.76	130.19	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ARG	CA-CB-CG	5.76	125.62	114.10
1	A	349	ALA	CB-CA-C	5.76	121.02	112.03
1	B	162	PHE	O-C-N	5.76	129.72	122.23
1	B	227	ASN	CB-CA-C	-5.76	101.62	110.26
1	A	240	LYS	N-CA-C	5.75	119.61	112.59
1	B	46	LEU	CB-CA-C	5.75	121.19	109.76
1	A	40	VAL	CA-C-N	5.74	127.91	120.44
1	A	40	VAL	C-N-CA	5.74	127.91	120.44
1	B	208	ARG	CB-CA-C	5.74	120.04	110.97
1	B	368	ARG	CA-C-O	5.74	127.24	120.58
1	B	131	ALA	N-CA-C	-5.74	102.96	110.53
1	B	244	ILE	CA-C-N	5.73	131.44	123.07
1	B	244	ILE	C-N-CA	5.73	131.44	123.07
1	A	324	PRO	N-CA-C	-5.73	105.22	113.75
1	B	374	HIS	CA-C-O	-5.73	114.42	120.55
1	A	76	ARG	NE-CZ-NH1	5.72	127.22	121.50
1	A	322	ALA	CB-CA-C	5.72	121.80	110.42
1	A	158	MET	CA-C-N	5.72	127.87	120.44
1	A	158	MET	C-N-CA	5.72	127.87	120.44
1	A	144	GLU	O-C-N	5.71	129.98	122.33
1	B	256	GLN	N-CA-C	-5.71	105.09	112.68
1	B	296	PHE	N-CA-CB	5.71	120.13	110.49
1	B	342	THR	CA-CB-OG1	-5.70	101.05	109.60
1	B	81	ALA	N-CA-C	-5.69	104.28	111.11
1	B	291	PRO	CA-C-O	5.69	127.80	121.43
1	B	230	HIS	CA-CB-CG	5.68	119.48	113.80
1	A	377	GLN	CA-C-N	5.67	127.82	120.44
1	A	377	GLN	C-N-CA	5.67	127.82	120.44
1	A	319	ALA	CA-C-O	-5.67	113.45	119.97
1	A	267	ALA	CB-CA-C	5.67	119.78	110.88
1	A	127	ALA	CA-C-O	-5.67	114.39	121.02
1	A	77	GLN	CA-C-O	5.67	126.42	120.42
1	A	334	ARG	CA-CB-CG	5.67	125.44	114.10
1	B	176	LEU	CA-C-N	5.67	134.56	121.87
1	B	176	LEU	C-N-CA	5.67	134.56	121.87
1	B	100	LYS	CA-C-O	5.66	128.61	120.51
1	B	117	ARG	CA-C-O	-5.65	114.85	120.90
1	A	167	GLU	CA-C-O	-5.65	114.88	120.70
1	A	169	VAL	N-CA-C	-5.65	104.86	110.62
1	B	166	GLY	CA-C-O	5.65	126.51	120.30
1	A	281	GLU	N-CA-CB	5.64	118.94	110.53
1	A	247	ASN	CB-CA-C	-5.64	100.80	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ILE	CA-C-O	-5.64	113.73	120.78
1	B	131	ALA	CA-C-O	-5.64	115.33	121.87
1	B	227	ASN	CA-C-O	-5.64	114.04	120.58
1	A	167	GLU	O-C-N	5.63	128.17	122.09
1	B	111	VAL	N-CA-C	-5.62	103.90	111.44
1	A	363	ASP	CB-CA-C	5.62	120.40	110.85
1	A	375	LEU	CA-C-O	5.61	126.42	119.97
1	B	259	ARG	CA-C-O	-5.60	115.71	121.87
1	A	180	ILE	CA-CB-CG1	5.60	119.91	110.40
1	B	190	ASP	CA-CB-CG	-5.59	107.01	112.60
1	B	184	PRO	O-C-N	-5.59	115.86	122.17
1	B	128	GLU	CB-CA-C	-5.58	99.63	110.46
1	B	214	VAL	CA-C-N	5.58	128.66	122.74
1	B	214	VAL	C-N-CA	5.58	128.66	122.74
1	B	305	GLY	N-CA-C	-5.58	106.04	112.73
1	B	180	ILE	CA-C-O	-5.57	114.17	120.74
1	A	289	LYS	CB-CA-C	-5.56	101.91	109.42
1	B	382	HIS	N-CA-CB	-5.56	102.44	110.56
1	B	101	ASP	O-C-N	5.56	130.46	123.12
1	A	324	PRO	O-C-N	-5.55	115.86	122.24
1	A	340	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	A	224	ALA	N-CA-C	-5.55	106.55	113.38
1	B	382	HIS	CA-C-N	5.55	132.13	121.54
1	B	382	HIS	C-N-CA	5.55	132.13	121.54
1	B	77	GLN	CA-C-N	5.54	129.97	120.71
1	B	77	GLN	C-N-CA	5.54	129.97	120.71
1	A	354	ARG	CA-C-O	-5.54	112.59	120.51
1	B	43	LEU	N-CA-C	-5.53	105.66	112.90
1	A	72	ILE	CA-C-O	-5.53	115.31	121.17
1	B	340	GLN	N-CA-CB	5.53	116.72	110.03
1	A	80	ASP	CA-C-O	-5.52	114.56	121.02
1	A	331	ARG	O-C-N	5.52	128.05	122.09
1	A	377	GLN	OE1-CD-NE2	5.52	128.12	122.60
1	A	121	GLY	N-CA-C	-5.51	105.97	112.64
1	A	359	ASP	CA-C-O	-5.51	113.04	120.15
1	A	177	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	A	370	MET	N-CA-C	-5.50	102.14	110.28
1	B	44	ALA	CA-C-N	5.50	128.09	120.29
1	B	44	ALA	C-N-CA	5.50	128.09	120.29
1	B	351	LEU	N-CA-C	-5.48	104.99	110.97
1	B	340	GLN	CB-CG-CD	-5.48	103.29	112.60
1	B	310	TYR	CA-C-O	5.47	126.24	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	SER	O-C-N	5.46	129.86	122.59
1	B	208	ARG	CA-C-N	5.46	124.98	119.19
1	B	208	ARG	C-N-CA	5.46	124.98	119.19
1	A	76	ARG	CD-NE-CZ	5.46	132.05	124.40
1	A	302	SER	O-C-N	5.46	127.70	122.07
1	B	99	PHE	CB-CA-C	5.46	120.48	110.11
1	B	148	ALA	CB-CA-C	-5.45	100.20	110.01
1	B	192	LEU	CA-CB-CG	5.45	135.38	116.30
1	B	140	ARG	CB-CA-C	5.45	119.92	110.72
1	B	227	ASN	O-C-N	5.44	129.82	122.96
1	A	313	LEU	N-CA-C	-5.43	105.44	111.36
1	A	272	VAL	CA-CB-CG2	5.43	119.63	110.40
1	A	220	HIS	N-CA-CB	5.43	118.58	110.22
1	A	35	ASP	CA-C-N	5.42	126.61	119.84
1	A	35	ASP	C-N-CA	5.42	126.61	119.84
1	B	354	ARG	O-C-N	5.41	130.24	122.13
1	A	35	ASP	CB-CA-C	5.40	116.88	108.61
1	A	195	THR	CA-C-N	5.39	127.55	120.60
1	A	195	THR	C-N-CA	5.39	127.55	120.60
1	A	381	ASP	CA-C-N	-5.39	111.25	121.54
1	A	381	ASP	C-N-CA	-5.39	111.25	121.54
1	A	181	GLU	N-CA-CB	5.38	118.78	110.12
1	A	230	HIS	O-C-N	5.38	128.29	122.11
1	A	314	LYS	O-C-N	5.37	127.67	122.09
1	B	170	THR	CA-C-N	5.36	131.78	121.54
1	B	170	THR	C-N-CA	5.36	131.78	121.54
1	A	237	TRP	N-CA-C	-5.35	99.39	110.80
1	B	141	GLU	N-CA-CB	-5.34	103.36	110.57
1	B	164	LEU	CA-C-O	-5.34	114.83	120.55
1	B	261	GLY	N-CA-C	-5.34	108.33	114.69
1	A	6	THR	CA-C-O	5.34	125.78	120.28
1	B	342	THR	O-C-N	5.34	127.57	122.07
1	A	266	ARG	CD-NE-CZ	5.33	131.87	124.40
1	A	243	HIS	CA-C-O	-5.33	115.53	121.23
1	B	126	ALA	CA-C-O	-5.33	115.20	120.90
1	B	48	ALA	N-CA-CB	5.32	117.67	110.38
1	B	73	LYS	N-CA-CB	5.32	117.78	110.07
1	B	349	ALA	CA-C-O	5.32	128.75	121.89
1	A	32	PRO	N-CA-C	-5.32	102.93	111.38
1	A	214	VAL	O-C-N	-5.32	117.41	123.10
1	A	116	LEU	CB-CA-C	5.31	119.30	110.90
1	A	338	LEU	CA-C-O	5.31	126.10	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	GLU	N-CA-C	5.31	117.33	107.99
1	A	217	GLU	CG-CD-OE2	-5.30	106.21	118.40
1	B	250	SER	O-C-N	-5.29	116.08	122.65
1	A	247	ASN	N-CA-C	5.29	116.18	108.14
1	A	289	LYS	CA-C-O	-5.29	114.30	119.69
1	A	33	ALA	N-CA-C	-5.28	102.04	109.96
1	B	208	ARG	CA-C-O	5.28	126.93	120.54
1	A	81	ALA	O-C-N	5.27	129.60	122.59
1	B	235	ALA	O-C-N	5.26	127.71	122.08
1	B	305	GLY	CA-C-O	5.26	126.17	120.75
1	A	67	GLU	CA-CB-CG	5.26	124.62	114.10
1	B	66	THR	N-CA-CB	5.26	117.59	109.91
1	B	227	ASN	N-CA-CB	5.26	117.81	109.71
1	A	346	GLY	N-CA-C	-5.25	100.73	113.18
1	B	378	LEU	N-CA-C	-5.25	105.47	111.14
1	B	207	GLU	CA-C-N	-5.25	115.74	123.30
1	B	207	GLU	C-N-CA	-5.25	115.74	123.30
1	A	189	GLY	O-C-N	5.24	129.52	122.70
1	B	84	MET	CA-C-O	-5.24	115.44	121.47
1	A	66	THR	OG1-CB-CG2	5.24	119.78	109.30
1	B	123	ILE	O-C-N	5.23	127.04	121.91
1	B	152	ARG	NH1-CZ-NH2	5.23	126.10	119.30
1	B	251	GLY	CA-C-O	-5.22	115.92	122.61
1	B	129	LEU	CB-CA-C	5.22	119.41	110.01
1	B	178	PHE	CA-C-O	5.22	127.88	121.72
1	B	214	VAL	N-CA-CB	-5.21	102.84	112.43
1	B	52	THR	CB-CA-C	5.21	120.47	109.79
1	A	373	GLU	N-CA-C	5.21	117.70	111.71
1	A	57	ASP	CA-C-O	5.21	126.02	120.24
1	B	335	LEU	N-CA-C	-5.20	106.89	113.18
1	B	381	ASP	O-C-N	-5.20	115.39	122.36
1	B	1	MET	CA-CB-CG	-5.20	103.70	114.10
1	A	313	LEU	CB-CA-C	5.20	119.68	110.85
1	B	374	HIS	N-CA-C	-5.20	105.06	111.40
1	B	181	GLU	CG-CD-OE1	5.19	130.34	118.40
1	A	318	ALA	CA-C-O	5.18	126.26	120.82
1	A	234	GLN	CA-CB-CG	5.18	124.46	114.10
1	A	62	GLY	N-CA-C	-5.18	100.91	113.18
1	B	15	LEU	CA-C-O	5.17	126.00	120.20
1	B	222	GLN	CA-C-N	5.17	128.87	120.60
1	B	222	GLN	C-N-CA	5.17	128.87	120.60
1	A	86	VAL	CA-C-N	5.16	125.24	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	VAL	C-N-CA	5.16	125.24	119.87
1	A	139	GLY	O-C-N	5.16	129.41	122.70
1	A	210	GLU	CG-CD-OE1	-5.16	106.54	118.40
1	A	309	ASN	CB-CA-C	5.15	120.55	110.67
1	B	222	GLN	CB-CA-C	5.15	119.60	110.85
1	A	354	ARG	CD-NE-CZ	-5.14	117.20	124.40
1	A	384	LEU	N-CA-CB	-5.14	104.44	110.35
1	B	185	ASN	CA-C-O	-5.14	115.58	120.56
1	B	156	ASP	N-CA-C	-5.13	105.38	111.69
1	A	175	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	206	LEU	CA-C-N	5.12	131.36	122.56
1	A	206	LEU	C-N-CA	5.12	131.36	122.56
1	A	328	GLU	CA-CB-CG	5.12	124.33	114.10
1	A	320	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	37	VAL	N-CA-C	-5.11	105.41	110.62
1	A	352	ALA	N-CA-CB	5.11	117.65	109.28
1	A	332	ALA	CA-C-O	-5.10	115.05	121.02
1	A	73	LYS	CB-CA-C	-5.10	102.88	110.88
1	B	100	LYS	CA-C-N	5.09	130.09	122.86
1	B	100	LYS	C-N-CA	5.09	130.09	122.86
1	A	68	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	B	368	ARG	CB-CG-CD	5.08	122.99	111.30
1	A	172	GLN	CB-CG-CD	-5.08	103.97	112.60
1	A	224	ALA	CA-C-O	5.07	124.93	119.15
1	A	375	LEU	N-CA-C	-5.07	105.94	111.82
1	A	273	ASP	CA-C-O	5.06	127.74	120.51
1	B	284	ARG	NE-CZ-NH1	5.06	126.56	121.50
1	B	363	ASP	O-C-N	5.05	128.13	122.22
1	A	286	PHE	CA-C-N	-5.05	115.29	122.41
1	A	286	PHE	C-N-CA	-5.05	115.29	122.41
1	B	124	ASP	CA-C-O	-5.04	115.52	121.07
1	A	226	LEU	O-C-N	-5.04	115.89	122.59
1	B	183	LYS	CA-C-N	5.04	124.21	118.97
1	B	183	LYS	C-N-CA	5.04	124.21	118.97
1	B	110	ASP	N-CA-C	-5.04	107.08	113.18
1	B	348	ASP	CA-C-N	-5.04	114.28	123.34
1	B	348	ASP	C-N-CA	-5.04	114.28	123.34
1	A	316	ARG	CA-CB-CG	-5.03	104.03	114.10
1	A	264	ASP	CA-C-N	-5.03	114.01	120.65
1	A	264	ASP	C-N-CA	-5.03	114.01	120.65
1	A	376	ASP	CA-CB-CG	-5.01	107.58	112.60
1	A	109	ARG	N-CA-C	5.01	117.39	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	VAL	CB-CA-C	5.01	119.51	111.29
1	B	116	LEU	CB-CA-C	5.01	118.81	110.90
1	A	31	ARG	CD-NE-CZ	5.01	131.41	124.40
1	A	34	LEU	CB-CA-C	5.01	118.07	109.51
1	B	269	PHE	O-C-N	5.01	127.23	122.07
1	B	388	GLY	CA-C-O	-5.01	105.98	121.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	347	LEU	CA
1	A	382	HIS	CA

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Sidechain
1	A	117	ARG	Sidechain
1	A	157	ARG	Sidechain
1	A	297	ASP	Mainchain
1	A	298	GLY	Mainchain
1	A	316	ARG	Sidechain
1	A	334	ARG	Sidechain
1	A	344	ALA	Mainchain
1	A	354	ARG	Sidechain
1	A	380	MET	Mainchain
1	A	381	ASP	Mainchain
1	A	382	HIS	Mainchain
1	A	51	VAL	Mainchain
1	A	61	PHE	Mainchain
1	A	67	GLU	Mainchain
1	A	76	ARG	Sidechain
1	B	113	ARG	Sidechain
1	B	117	ARG	Sidechain
1	B	140	ARG	Sidechain
1	B	157	ARG	Sidechain
1	B	175	ASP	Sidechain
1	B	177	ARG	Sidechain
1	B	196	VAL	Mainchain
1	B	298	GLY	Mainchain
1	B	316	ARG	Sidechain
1	B	380	MET	Mainchain

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Mol	Chain	Res	Type	Group
1	B	71	HIS	Mainchain
1	B	74	ARG	Sidechain
1	B	98	VAL	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	3023	0	2890	409	31
1	B	3023	0	2894	410	32
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	6054	0	5784	760	34

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 64.

All (760) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ARG:HD2	1:B:382:HIS:CD2	1.36	1.55
1:A:345:ASP:HB3	1:A:347:LEU:CD2	1.44	1.48
1:A:316:ARG:NE	1:A:382:HIS:NE2	1.74	1.31
1:A:381:ASP:HB2	1:A:383:LEU:O	1.26	1.30
1:A:316:ARG:HB3	1:A:382:HIS:CD2	1.69	1.26
1:A:70:SER:O	1:A:74:ARG:HG3	1.37	1.22
1:A:382:HIS:O	1:A:383:LEU:HD23	1.39	1.21
1:A:345:ASP:CB	1:A:347:LEU:HD22	1.68	1.21
1:A:8:GLU:HA	1:A:10:ARG:NH1	1.59	1.18
1:B:316:ARG:CD	1:B:382:HIS:HD2	1.58	1.16
1:B:316:ARG:CD	1:B:382:HIS:CD2	2.29	1.16
1:A:316:ARG:CD	1:A:382:HIS:NE2	2.08	1.15
1:A:382:HIS:C	1:A:383:LEU:HD23	1.72	1.15
1:A:73:LYS:HE2	1:A:74:ARG:HE	1.12	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ASP:HB2	1:B:383:LEU:HD11	1.18	1.12
1:B:347:LEU:CD1	1:B:349:ALA:HB3	1.80	1.11
1:A:320:PHE:HA	1:A:383:LEU:HD22	1.32	1.09
1:B:323:ASP:CB	1:B:383:LEU:HD11	1.84	1.08
1:A:1:MET:C	1:A:1:MET:O	1.97	1.08
1:A:73:LYS:CE	1:A:74:ARG:HE	1.65	1.08
1:B:323:ASP:OD2	1:B:383:LEU:HD13	1.54	1.06
1:B:347:LEU:HD11	1:B:349:ALA:HB3	1.37	1.05
1:A:382:HIS:CD2	1:A:388:GLY:HA2	1.93	1.04
1:B:96:HIS:HB3	1:B:98:VAL:HG23	1.36	1.04
1:A:316:ARG:CG	1:A:382:HIS:NE2	2.21	1.03
1:A:387:ARG:HG3	1:A:388:GLY:H	1.20	1.03
1:A:316:ARG:NE	1:A:382:HIS:CE1	2.27	1.02
1:A:132:LYS:CG	1:A:133:THR:HG23	1.91	1.00
1:A:345:ASP:HB3	1:A:347:LEU:HD22	1.01	1.00
1:B:149:LYS:HE2	1:B:154:ALA:HB2	1.38	1.00
1:B:316:ARG:HB3	1:B:382:HIS:CD2	1.96	1.00
1:B:347:LEU:HD13	1:B:349:ALA:CA	1.93	0.98
1:A:316:ARG:HB3	1:A:382:HIS:NE2	1.78	0.98
1:B:25:PRO:HB2	1:B:26:PHE:CD1	1.97	0.98
1:B:183:LYS:HZ1	1:B:186:GLU:HG3	1.27	0.98
1:B:319:ALA:O	1:B:383:LEU:HG	1.63	0.98
1:B:149:LYS:HZ3	1:B:149:LYS:HB3	1.25	0.98
1:B:310:TYR:O	1:B:314:LYS:HB2	1.64	0.97
1:B:350:LEU:H	1:B:350:LEU:HD23	1.30	0.97
1:A:132:LYS:HG2	1:A:133:THR:HG23	1.45	0.96
1:A:92:ASN:HD21	1:A:95:THR:HG23	1.29	0.96
1:A:316:ARG:CB	1:A:382:HIS:NE2	2.31	0.94
1:A:345:ASP:CB	1:A:347:LEU:CD2	2.37	0.94
1:A:1:MET:N	1:A:1:MET:CA	2.31	0.93
1:A:370:MET:HE3	1:B:101:ASP:OD2	1.67	0.92
1:B:347:LEU:CD2	1:B:349:ALA:HB3	1.99	0.92
1:B:229:PRO:HA	1:B:232:ILE:HD11	1.47	0.92
1:A:316:ARG:CB	1:A:382:HIS:CD2	2.52	0.92
1:B:115:ALA:O	1:B:119:THR:HG23	1.68	0.92
1:A:25:PRO:HG2	1:A:26:PHE:CD1	2.04	0.92
1:A:259:ARG:O	1:A:262:ALA:HB3	1.67	0.92
1:B:61:PHE:CZ	1:B:96:HIS:HD2	1.86	0.92
1:B:61:PHE:CZ	1:B:96:HIS:CD2	2.58	0.92
1:A:2:SER:HA	1:A:308:ARG:NH2	1.85	0.92
1:A:113:ARG:NH1	1:B:342:THR:O	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ARG:HG3	1:A:388:GLY:N	1.81	0.91
1:A:92:ASN:HD21	1:A:95:THR:CG2	1.83	0.91
1:A:316:ARG:HE	1:A:382:HIS:CE1	1.86	0.91
1:A:218:VAL:O	1:A:222:GLN:HG3	1.71	0.90
1:A:8:GLU:HA	1:A:10:ARG:HH11	1.32	0.89
1:A:72:ILE:O	1:A:76:ARG:HG3	1.72	0.89
1:B:323:ASP:HB2	1:B:383:LEU:CD1	2.01	0.89
1:B:115:ALA:O	1:B:119:THR:CG2	2.21	0.89
1:A:42:ARG:O	1:A:46:LEU:HD13	1.72	0.88
1:A:382:HIS:CD2	1:A:388:GLY:CA	2.56	0.88
1:A:73:LYS:HE2	1:A:74:ARG:NE	1.87	0.88
1:A:345:ASP:HB3	1:A:347:LEU:HD23	1.55	0.87
1:B:347:LEU:CD1	1:B:349:ALA:CB	2.52	0.87
1:B:374:HIS:NE2	1:B:378:LEU:HD11	1.89	0.87
1:B:25:PRO:HB2	1:B:26:PHE:CE1	2.10	0.87
1:A:378:LEU:O	1:A:381:ASP:O	1.92	0.87
1:B:232:ILE:CD1	1:B:274:LEU:HD23	2.05	0.86
1:A:190:ASP:CG	1:B:227:ASN:HD22	1.83	0.86
1:B:96:HIS:CB	1:B:98:VAL:HG23	2.06	0.86
1:A:341:PRO:HA	1:B:157:ARG:NH2	1.91	0.85
1:A:96:HIS:HD2	1:A:98:VAL:H	1.23	0.85
1:B:382:HIS:HB3	1:B:387:ARG:O	1.76	0.85
1:A:13:PHE:HE2	1:A:307:MET:HE3	1.40	0.84
1:A:155:LEU:HD21	1:B:234:GLN:HG3	1.59	0.84
1:B:320:PHE:HA	1:B:383:LEU:CD2	2.08	0.83
1:A:68:ARG:NH2	1:A:125:LEU:HD22	1.93	0.83
1:B:6:THR:O	1:B:8:GLU:N	2.12	0.83
1:B:387:ARG:HG3	1:B:388:GLY:H	1.43	0.83
1:A:330:LEU:HD12	1:A:335:LEU:CD1	2.08	0.83
1:A:354:ARG:HA	1:A:358:GLU:OE1	1.77	0.83
1:B:316:ARG:HD2	1:B:382:HIS:NE2	1.94	0.82
1:B:347:LEU:HD11	1:B:349:ALA:CB	2.08	0.82
1:A:320:PHE:HA	1:A:383:LEU:CD2	2.09	0.82
1:A:338:LEU:O	1:B:157:ARG:HD3	1.80	0.81
1:B:99:PHE:HE1	1:B:115:ALA:HB2	1.45	0.81
1:B:196:VAL:HG23	1:B:221:GLU:OE1	1.78	0.81
1:B:323:ASP:OD2	1:B:383:LEU:CD1	2.27	0.81
1:B:149:LYS:CE	1:B:154:ALA:HB2	2.09	0.81
1:B:164:LEU:HD12	1:B:167:GLU:OE1	1.79	0.81
1:B:66:THR:HG23	1:B:67:GLU:N	1.96	0.81
1:A:12:THR:HG21	1:A:52:THR:HG22	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASP:O	1:A:69:GLU:HG2	1.81	0.80
1:A:195:THR:OG1	1:A:198:HIS:HD2	1.63	0.80
1:A:42:ARG:HG3	1:A:46:LEU:HD13	1.63	0.80
1:A:73:LYS:HG3	1:A:74:ARG:N	1.94	0.80
1:A:96:HIS:CD2	1:A:98:VAL:HG12	2.16	0.80
1:B:96:HIS:CG	1:B:98:VAL:CG2	2.64	0.80
1:B:268:ALA:O	1:B:272:VAL:HG23	1.80	0.80
1:A:117:ARG:NH1	1:B:350:LEU:O	2.15	0.80
1:A:345:ASP:CA	1:A:347:LEU:HD22	2.12	0.80
1:A:190:ASP:CG	1:B:227:ASN:ND2	2.41	0.79
1:B:229:PRO:HA	1:B:232:ILE:CD1	2.13	0.79
1:A:96:HIS:CD2	1:A:98:VAL:H	2.01	0.79
1:A:353:ASP:OD2	1:A:356:ALA:HB2	1.82	0.79
1:A:8:GLU:HA	1:A:10:ARG:HH12	1.45	0.79
1:B:320:PHE:HA	1:B:383:LEU:HD23	1.65	0.79
1:B:149:LYS:CE	1:B:154:ALA:CB	2.62	0.78
1:B:36:PRO:O	1:B:40:VAL:HG23	1.84	0.78
1:B:381:ASP:OD2	1:B:384:LEU:CD2	2.31	0.78
1:A:132:LYS:HG3	1:A:133:THR:CG2	2.12	0.78
1:B:232:ILE:HD12	1:B:274:LEU:HD23	1.66	0.78
1:B:347:LEU:HD21	1:B:349:ALA:HB3	1.64	0.78
1:A:382:HIS:C	1:A:383:LEU:CD2	2.57	0.78
1:A:94:PHE:O	1:A:140:ARG:HD2	1.84	0.77
1:A:382:HIS:HD2	1:A:388:GLY:HA2	1.46	0.77
1:B:66:THR:HG23	1:B:67:GLU:H	1.49	0.77
1:B:292:ARG:HG3	1:B:292:ARG:HH11	1.49	0.77
1:B:323:ASP:CG	1:B:383:LEU:CD1	2.58	0.77
1:A:25:PRO:HG2	1:A:26:PHE:HD1	1.50	0.76
1:A:230:HIS:O	1:A:233:ALA:HB3	1.85	0.76
1:B:323:ASP:CG	1:B:383:LEU:HD11	2.10	0.76
1:B:382:HIS:HB3	1:B:387:ARG:C	2.10	0.76
1:A:354:ARG:O	1:A:359:ASP:N	2.18	0.76
1:B:64:SER:O	1:B:67:GLU:N	2.18	0.76
1:B:77:GLN:O	1:B:81:ALA:HB2	1.85	0.76
1:A:132:LYS:HZ3	1:A:133:THR:CG2	2.00	0.75
1:B:96:HIS:CG	1:B:98:VAL:HG23	2.22	0.75
1:A:370:MET:CE	1:B:101:ASP:OD2	2.34	0.75
1:A:92:ASN:ND2	1:A:95:THR:HG23	2.00	0.75
1:B:323:ASP:HB3	1:B:326:VAL:HB	1.67	0.75
1:A:132:LYS:HG3	1:A:133:THR:HG23	1.67	0.74
1:A:338:LEU:HD22	1:B:107:ASN:HD21	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ALA:O	1:B:306:CYS:HB2	1.87	0.74
1:B:347:LEU:HD13	1:B:349:ALA:C	2.12	0.74
1:B:97:PRO:O	1:B:100:LYS:HG3	1.88	0.74
1:A:9:ASP:O	1:A:10:ARG:HB2	1.86	0.74
1:B:316:ARG:CB	1:B:382:HIS:CD2	2.70	0.74
1:A:341:PRO:HB2	1:A:344:ALA:HB2	1.70	0.74
1:B:348:ASP:OD1	1:B:351:LEU:CD2	2.36	0.74
1:A:44:ALA:N	1:A:84:MET:HE1	2.03	0.73
1:B:149:LYS:HE2	1:B:154:ALA:CB	2.13	0.73
1:A:142:GLY:HA3	1:A:190:ASP:O	1.89	0.73
1:B:183:LYS:NZ	1:B:186:GLU:HG3	2.04	0.73
1:A:296:PHE:O	1:A:299:VAL:HB	1.89	0.73
1:B:30:THR:HG23	1:B:292:ARG:NH1	2.03	0.73
1:B:153:ASP:O	1:B:156:ASP:HB2	1.88	0.72
1:B:124:ASP:O	1:B:127:ALA:HB3	1.89	0.72
1:A:357:PHE:HB2	1:B:117:ARG:HG2	1.72	0.72
1:A:354:ARG:NH1	1:A:359:ASP:OD2	2.22	0.72
1:B:64:SER:OG	1:B:67:GLU:HG3	1.89	0.71
1:A:59:ILE:HG21	1:A:68:ARG:HG2	1.71	0.71
1:B:159:LYS:HG2	1:B:206:LEU:HD12	1.73	0.71
1:A:167:GLU:O	1:A:171:ALA:N	2.21	0.71
1:A:217:GLU:OE1	1:A:247:ASN:ND2	2.24	0.71
1:A:232:ILE:HD11	1:A:274:LEU:HG	1.71	0.71
1:B:64:SER:HB2	1:B:66:THR:HG22	1.71	0.71
1:B:232:ILE:HD12	1:B:274:LEU:CD2	2.20	0.71
1:B:316:ARG:CB	1:B:382:HIS:HD2	2.02	0.71
1:A:151:VAL:HG13	1:B:233:ALA:CB	2.21	0.70
1:B:347:LEU:CD1	1:B:349:ALA:CA	2.69	0.70
1:A:150:ASP:OD1	1:A:152:ARG:NH1	2.24	0.70
1:B:194:PRO:HD2	1:B:198:HIS:CG	2.25	0.70
1:B:203:ILE:HA	1:B:206:LEU:HD22	1.72	0.70
1:A:124:ASP:OD1	1:A:168:TYR:OH	2.06	0.70
1:A:272:VAL:HG13	1:A:310:TYR:CZ	2.25	0.70
1:B:316:ARG:CG	1:B:382:HIS:HD2	2.03	0.70
1:B:387:ARG:CG	1:B:388:GLY:H	2.02	0.70
1:B:336:ASP:O	1:B:340:GLN:NE2	2.25	0.70
1:A:132:LYS:NZ	1:A:133:THR:HG23	2.07	0.70
1:B:24:ASP:HB2	1:B:25:PRO:HD2	1.73	0.69
1:B:64:SER:CB	1:B:67:GLU:HG3	2.22	0.69
1:A:319:ALA:O	1:A:383:LEU:HD13	1.92	0.69
1:B:348:ASP:OD1	1:B:351:LEU:HD21	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:HD2	1:B:342:THR:O	1.92	0.69
1:A:13:PHE:CE2	1:A:307:MET:HE3	2.25	0.69
1:A:42:ARG:HG3	1:A:46:LEU:CD1	2.22	0.69
1:B:151:VAL:O	1:B:155:LEU:HB2	1.92	0.69
1:B:363:ASP:HA	1:B:366:ALA:CB	2.23	0.69
1:B:269:PHE:CE1	1:B:317:ALA:HB2	2.27	0.68
1:A:2:SER:HA	1:A:308:ARG:HH22	1.56	0.68
1:A:25:PRO:HG2	1:A:26:PHE:CE1	2.28	0.68
1:A:139:GLY:O	1:A:188:ARG:HG2	1.94	0.68
1:B:347:LEU:CD2	1:B:349:ALA:CB	2.70	0.68
1:A:1:MET:C	1:A:2:SER:OG	2.36	0.68
1:A:107:ASN:O	1:B:334:ARG:HB3	1.94	0.68
1:A:195:THR:OG1	1:A:198:HIS:CD2	2.47	0.68
1:A:52:THR:HG21	1:A:285:HIS:CD2	2.28	0.68
1:A:381:ASP:O	1:A:383:LEU:N	2.27	0.68
1:A:325:GLU:OE1	1:A:384:LEU:HD12	1.93	0.68
1:A:132:LYS:HZ3	1:A:133:THR:HG23	1.59	0.67
1:A:135:VAL:HG12	1:A:136:ALA:N	2.07	0.67
1:B:220:HIS:O	1:B:223:MET:HB2	1.94	0.67
1:B:21:GLN:HB3	1:B:29:ALA:HB1	1.76	0.67
1:A:372:PHE:CE1	1:B:148:ALA:HB1	2.29	0.67
1:B:92:ASN:OD1	1:B:95:THR:HG23	1.94	0.67
1:B:362:VAL:CG1	1:B:363:ASP:N	2.57	0.67
1:A:96:HIS:HD2	1:A:98:VAL:HG12	1.57	0.67
1:B:195:THR:OG1	1:B:198:HIS:ND1	2.24	0.67
1:B:266:ARG:HH12	1:B:376:ASP:CG	2.02	0.67
1:B:183:LYS:HE2	1:B:185:ASN:O	1.95	0.66
1:A:99:PHE:CE1	1:A:115:ALA:HB2	2.30	0.66
1:B:144:GLU:HB3	1:B:188:ARG:HH21	1.60	0.66
1:A:100:LYS:NZ	1:B:368:ARG:O	2.28	0.66
1:A:151:VAL:HG13	1:B:233:ALA:HB3	1.78	0.66
1:A:53:PHE:O	1:A:90:THR:HG22	1.96	0.66
1:A:73:LYS:HG3	1:A:74:ARG:HG2	1.77	0.66
1:A:249:GLN:NE2	1:A:253:LYS:HG2	2.11	0.66
1:B:159:LYS:NZ	1:B:163:ASP:OD2	2.28	0.66
1:A:119:THR:HG22	1:A:123:ILE:HD12	1.78	0.66
1:B:109:ARG:O	1:B:113:ARG:HG3	1.96	0.66
1:B:191:ILE:HG22	1:B:192:LEU:O	1.94	0.66
1:B:1:MET:O	1:B:2:SER:OG	2.14	0.65
1:A:356:ALA:O	1:B:114:TYR:HA	1.95	0.65
1:A:79:LEU:O	1:A:83:GLY:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASP:O	1:A:277:THR:N	2.17	0.65
1:B:149:LYS:HB3	1:B:149:LYS:NZ	1.96	0.65
1:B:181:GLU:OE2	1:B:220:HIS:CE1	2.49	0.65
1:B:208:ARG:HB2	1:B:210:GLU:OE2	1.96	0.65
1:A:1:MET:O	1:A:2:SER:OG	2.14	0.65
1:A:135:VAL:CG1	1:A:136:ALA:N	2.58	0.65
1:B:363:ASP:HA	1:B:366:ALA:HB3	1.79	0.65
1:A:132:LYS:CG	1:A:133:THR:CG2	2.68	0.65
1:A:168:TYR:CE1	1:A:172:GLN:HG3	2.31	0.64
1:B:244:ILE:O	1:B:285:HIS:HB3	1.98	0.64
1:B:350:LEU:H	1:B:350:LEU:CD2	2.06	0.64
1:B:123:ILE:HG23	1:B:176:LEU:HD13	1.78	0.64
1:B:387:ARG:HG3	1:B:388:GLY:N	2.13	0.64
1:A:44:ALA:CA	1:A:84:MET:HE1	2.28	0.64
1:A:381:ASP:C	1:A:383:LEU:N	2.55	0.64
1:B:149:LYS:HE3	1:B:154:ALA:CB	2.27	0.64
1:B:137:TRP:HD1	1:B:181:GLU:O	1.81	0.64
1:A:312:ILE:O	1:A:316:ARG:HG3	1.98	0.64
1:A:272:VAL:HG12	1:A:276:GLU:HG2	1.80	0.63
1:A:265:LEU:O	1:A:268:ALA:HB3	1.98	0.63
1:B:347:LEU:CG	1:B:349:ALA:HB3	2.27	0.63
1:B:382:HIS:CB	1:B:387:ARG:O	2.46	0.63
1:B:6:THR:OG1	1:B:8:GLU:HG2	1.98	0.63
1:B:324:PRO:HA	1:B:327:GLN:NE2	2.13	0.63
1:A:11:PHE:HB3	1:A:307:MET:HE2	1.79	0.63
1:B:30:THR:CG2	1:B:292:ARG:NH1	2.61	0.63
1:A:169:VAL:O	1:A:172:GLN:O	2.16	0.63
1:A:325:GLU:OE1	1:A:384:LEU:CD1	2.47	0.62
1:A:387:ARG:CG	1:A:388:GLY:N	2.61	0.62
1:B:157:ARG:NH2	1:B:160:GLU:OE1	2.31	0.62
1:B:66:THR:CG2	1:B:67:GLU:H	2.11	0.62
1:B:308:ARG:HG3	1:B:312:ILE:HD11	1.80	0.62
1:B:105:THR:OG1	1:B:141:GLU:HG3	2.00	0.62
1:A:345:ASP:H	1:A:347:LEU:HB2	1.65	0.62
1:B:21:GLN:HB3	1:B:31:ARG:O	1.99	0.62
1:A:372:PHE:CD1	1:B:148:ALA:HB1	2.34	0.62
1:B:31:ARG:NH2	1:B:291:PRO:O	2.33	0.61
1:B:381:ASP:OD2	1:B:384:LEU:HD23	2.00	0.61
1:B:266:ARG:NH1	1:B:376:ASP:OD1	2.33	0.61
1:A:12:THR:CG2	1:A:52:THR:HG22	2.31	0.61
1:A:59:ILE:CD1	1:A:71:HIS:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LEU:O	1:B:384:LEU:CG	2.49	0.61
1:A:319:ALA:O	1:A:383:LEU:CD1	2.49	0.61
1:B:96:HIS:CD2	1:B:98:VAL:CG2	2.84	0.61
1:B:12:THR:CG2	1:B:49:TYR:HD1	2.14	0.60
1:B:66:THR:CG2	1:B:67:GLU:N	2.63	0.60
1:A:380:MET:O	1:A:382:HIS:N	2.35	0.60
1:A:15:LEU:HD23	1:A:51:VAL:CG1	2.30	0.60
1:B:99:PHE:CE1	1:B:115:ALA:HB2	2.31	0.60
1:B:323:ASP:CB	1:B:383:LEU:CD1	2.67	0.60
1:A:260:PHE:HE1	1:A:313:LEU:CD1	2.14	0.60
1:B:30:THR:HG21	1:B:292:ARG:O	2.02	0.60
1:A:35:ASP:OD2	1:A:37:VAL:CG2	2.50	0.60
1:B:11:PHE:HZ	1:B:311:LEU:HD13	1.65	0.60
1:A:59:ILE:HD12	1:A:71:HIS:HB2	1.83	0.60
1:A:119:THR:HG22	1:A:123:ILE:CD1	2.31	0.60
1:B:208:ARG:CB	1:B:210:GLU:OE2	2.50	0.60
1:B:362:VAL:HG12	1:B:363:ASP:H	1.66	0.60
1:A:17:THR:HG21	1:A:286:PHE:O	2.02	0.59
1:A:140:ARG:HA	1:A:188:ARG:HD3	1.84	0.59
1:B:324:PRO:HA	1:B:327:GLN:HE21	1.67	0.59
1:A:35:ASP:OD2	1:A:37:VAL:HG23	2.03	0.59
1:B:382:HIS:O	1:B:383:LEU:HB2	2.02	0.59
1:A:1:MET:C	1:A:2:SER:HG	2.11	0.59
1:A:58:LEU:HD11	1:A:75:PHE:CD1	2.37	0.59
1:A:172:GLN:O	1:A:174:TYR:N	2.35	0.59
1:A:190:ASP:OD1	1:B:227:ASN:ND2	2.35	0.59
1:A:381:ASP:C	1:A:383:LEU:H	2.10	0.59
1:A:354:ARG:O	1:A:359:ASP:HB2	2.02	0.59
1:A:280:TYR:CZ	1:A:282:GLY:HA3	2.37	0.59
1:A:35:ASP:O	1:A:38:GLU:N	2.36	0.59
1:B:12:THR:HG22	1:B:49:TYR:HD1	1.66	0.59
1:B:346:GLY:O	1:B:347:LEU:HD23	2.01	0.59
1:B:354:ARG:C	1:B:356:ALA:H	2.11	0.59
1:B:92:ASN:OD1	1:B:95:THR:CG2	2.51	0.59
1:B:106:ALA:O	1:B:112:ARG:HD3	2.03	0.59
1:A:191:ILE:HG22	1:A:192:LEU:O	2.03	0.58
1:B:217:GLU:OE2	1:B:220:HIS:NE2	2.37	0.58
1:A:269:PHE:HE1	1:A:270:TRP:CZ3	2.20	0.58
1:A:338:LEU:HB2	1:B:107:ASN:ND2	2.19	0.58
1:B:70:SER:HA	1:B:73:LYS:HG3	1.85	0.58
1:A:8:GLU:CA	1:A:10:ARG:HH11	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:VAL:HG21	1:A:247:ASN:O	2.03	0.58
1:B:21:GLN:HG2	1:B:31:ARG:O	2.03	0.58
1:B:149:LYS:HE3	1:B:154:ALA:HB1	1.86	0.58
1:B:348:ASP:OD1	1:B:351:LEU:HD23	2.02	0.58
1:B:383:LEU:O	1:B:384:LEU:HG	2.04	0.58
1:B:363:ASP:O	1:B:366:ALA:HB3	2.03	0.57
1:A:125:LEU:HD12	1:A:129:LEU:HD13	1.86	0.57
1:A:337:GLN:NE2	1:B:109:ARG:H	2.02	0.57
1:A:380:MET:O	1:A:381:ASP:C	2.47	0.57
1:A:366:ALA:HB1	1:B:97:PRO:HB2	1.85	0.57
1:B:25:PRO:CB	1:B:26:PHE:CD1	2.81	0.57
1:A:233:ALA:CB	1:B:151:VAL:HG22	2.34	0.57
1:A:264:ASP:HB3	1:A:267:ALA:HB3	1.86	0.57
1:A:99:PHE:HE1	1:A:115:ALA:HB2	1.69	0.57
1:A:326:VAL:HG22	1:A:378:LEU:HD13	1.87	0.57
1:B:326:VAL:HG21	1:B:383:LEU:CD2	2.34	0.57
1:B:387:ARG:CB	1:B:387:ARG:HH11	2.17	0.57
1:A:2:SER:HA	1:A:308:ARG:HH21	1.67	0.57
1:B:354:ARG:HG3	1:B:354:ARG:HH11	1.70	0.57
1:A:151:VAL:HG11	1:B:230:HIS:HA	1.87	0.57
1:A:207:GLU:O	1:A:208:ARG:HG3	2.05	0.57
1:A:214:VAL:O	1:A:216:PRO:HD3	2.05	0.57
1:A:116:LEU:CD2	1:A:165:LEU:HD13	2.35	0.56
1:B:217:GLU:OE2	1:B:220:HIS:CD2	2.58	0.56
1:B:347:LEU:HD21	1:B:349:ALA:CB	2.33	0.56
1:A:316:ARG:CG	1:A:382:HIS:CE1	2.89	0.56
1:B:370:MET:HG3	1:B:372:PHE:CE2	2.40	0.56
1:B:228:PHE:HB3	1:B:229:PRO:HD3	1.86	0.56
1:B:194:PRO:HD2	1:B:198:HIS:CB	2.34	0.56
1:A:73:LYS:HE3	1:A:74:ARG:HE	1.62	0.56
1:A:361:ASP:CG	1:A:364:ALA:HB2	2.30	0.56
1:A:44:ALA:HB2	1:A:84:MET:HE2	1.87	0.56
1:A:218:VAL:HG22	1:A:247:ASN:CB	2.35	0.56
1:B:63:SER:O	1:B:65:ASP:N	2.38	0.56
1:B:138:GLY:O	1:B:140:ARG:N	2.38	0.56
1:B:324:PRO:O	1:B:325:GLU:C	2.50	0.55
1:A:246:LEU:HB2	1:A:286:PHE:CD1	2.41	0.55
1:A:183:LYS:HG2	1:A:184:PRO:HD2	1.89	0.55
1:A:320:PHE:HE2	1:A:321:ARG:HH21	1.53	0.55
1:A:330:LEU:HD12	1:A:335:LEU:HD12	1.85	0.55
1:A:381:ASP:O	1:A:382:HIS:C	2.50	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TRP:CD2	1:A:289:LYS:HG2	2.41	0.55
1:B:158:MET:HG2	1:B:202:PHE:CZ	2.42	0.55
1:B:137:TRP:HZ2	1:B:183:LYS:HD3	1.72	0.55
1:A:233:ALA:HB1	1:B:151:VAL:HG22	1.88	0.55
1:A:312:ILE:CG2	1:A:316:ARG:HD2	2.36	0.55
1:A:67:GLU:O	1:A:68:ARG:C	2.49	0.55
1:A:346:GLY:H	1:A:347:LEU:CB	2.20	0.55
1:A:106:ALA:O	1:A:112:ARG:HD3	2.06	0.55
1:B:185:ASN:HD22	1:B:186:GLU:N	2.05	0.55
1:A:309:ASN:O	1:A:313:LEU:HG	2.07	0.55
1:A:338:LEU:HD11	1:B:154:ALA:HA	1.88	0.55
1:B:316:ARG:HB3	1:B:382:HIS:HD2	1.48	0.55
1:A:204:GLU:HG3	1:B:204:GLU:HG3	1.88	0.55
1:A:319:ALA:HB1	1:A:383:LEU:HD11	1.89	0.55
1:B:256:GLN:O	1:B:257:ASP:HB2	2.05	0.55
1:A:326:VAL:O	1:A:330:LEU:HD22	2.07	0.54
1:B:158:MET:HG3	1:B:162:PHE:HE2	1.72	0.54
1:B:308:ARG:O	1:B:312:ILE:HG13	2.07	0.54
1:B:362:VAL:HG12	1:B:363:ASP:N	2.22	0.54
1:B:308:ARG:CG	1:B:312:ILE:HD11	2.36	0.54
1:B:323:ASP:CG	1:B:383:LEU:HD13	2.24	0.54
1:A:185:ASN:HA	1:A:191:ILE:HG13	1.88	0.54
1:A:260:PHE:CE1	1:A:313:LEU:CD1	2.90	0.54
1:B:61:PHE:CE2	1:B:96:HIS:CD2	2.95	0.54
1:B:123:ILE:HG23	1:B:176:LEU:CD1	2.36	0.54
1:A:218:VAL:HG22	1:A:247:ASN:HB3	1.90	0.54
1:A:351:LEU:HD21	1:B:120:ILE:HG21	1.89	0.54
1:A:387:ARG:CG	1:A:388:GLY:H	2.07	0.54
1:A:284:ARG:HG2	1:A:310:TYR:CE2	2.43	0.54
1:A:272:VAL:HG21	1:A:313:LEU:HB2	1.90	0.54
1:B:25:PRO:CB	1:B:26:PHE:CE1	2.86	0.54
1:B:181:GLU:HB2	1:B:215:ASN:O	2.08	0.54
1:B:20:TRP:O	1:B:31:ARG:NH1	2.41	0.54
1:B:134:TYR:O	1:B:178:PHE:HA	2.08	0.54
1:A:180:ILE:O	1:A:182:PRO:HD3	2.08	0.54
1:A:319:ALA:C	1:A:383:LEU:HD11	2.33	0.54
1:A:341:PRO:CB	1:A:344:ALA:HB2	2.38	0.54
1:B:296:PHE:O	1:B:299:VAL:HB	2.08	0.54
1:A:354:ARG:NH2	1:A:358:GLU:HB3	2.23	0.53
1:A:357:PHE:CD1	1:B:117:ARG:HB3	2.43	0.53
1:A:387:ARG:NH1	1:A:387:ARG:HG2	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:PHE:CE2	1:B:96:HIS:HD2	2.23	0.53
1:B:381:ASP:OD2	1:B:384:LEU:HD21	2.06	0.53
1:A:32:PRO:HD2	1:A:296:PHE:CZ	2.43	0.53
1:A:52:THR:CG2	1:A:285:HIS:CD2	2.91	0.53
1:A:6:THR:O	1:A:8:GLU:N	2.42	0.53
1:A:146:GLY:HA2	1:A:148:ALA:H	1.72	0.53
1:B:179:ALA:HA	1:B:213:GLY:O	2.08	0.53
1:A:249:GLN:HE21	1:A:253:LYS:HG2	1.72	0.53
1:B:323:ASP:HB2	1:B:383:LEU:HD21	1.89	0.53
1:A:111:VAL:O	1:A:112:ARG:C	2.52	0.53
1:B:15:LEU:HD22	1:B:53:PHE:HB2	1.89	0.53
1:B:380:MET:O	1:B:387:ARG:HD2	2.08	0.53
1:A:178:PHE:O	1:A:212:TYR:O	2.27	0.53
1:A:357:PHE:CE1	1:B:118:LYS:HA	2.44	0.53
1:A:387:ARG:HG2	1:A:387:ARG:HH11	1.74	0.53
1:B:336:ASP:OD1	1:B:337:GLN:N	2.42	0.53
1:A:54:HIS:HA	1:A:90:THR:O	2.09	0.53
1:B:320:PHE:O	1:B:326:VAL:HG11	2.07	0.53
1:B:159:LYS:HE2	1:B:205:ARG:O	2.09	0.53
1:A:259:ARG:O	1:A:262:ALA:CB	2.48	0.53
1:B:87:PRO:O	1:B:132:LYS:N	2.37	0.53
1:B:158:MET:HG3	1:B:162:PHE:CE2	2.44	0.53
1:B:347:LEU:HD13	1:B:349:ALA:N	2.23	0.53
1:A:20:TRP:CG	1:A:289:LYS:HG2	2.44	0.53
1:A:73:LYS:HG3	1:A:74:ARG:CG	2.39	0.53
1:A:341:PRO:HA	1:B:157:ARG:HH22	1.70	0.53
1:B:78:ALA:HA	1:B:81:ALA:HB3	1.89	0.53
1:B:236:LEU:HD13	1:B:278:ALA:CB	2.38	0.52
1:A:77:GLN:O	1:A:80:ASP:OD1	2.27	0.52
1:A:319:ALA:CB	1:A:383:LEU:HD11	2.39	0.52
1:B:354:ARG:O	1:B:359:ASP:HB2	2.09	0.52
1:A:183:LYS:HE2	1:A:185:ASN:O	2.08	0.52
1:A:35:ASP:OD1	1:A:36:PRO:HD2	2.09	0.52
1:A:272:VAL:HG13	1:A:310:TYR:CE1	2.43	0.52
1:A:346:GLY:H	1:A:347:LEU:HB2	1.74	0.52
1:A:355:ALA:O	1:A:360:PHE:HB2	2.10	0.52
1:A:137:TRP:HB2	1:A:181:GLU:HB3	1.92	0.52
1:B:350:LEU:HA	1:B:353:ASP:OD1	2.09	0.52
1:A:132:LYS:HZ3	1:A:133:THR:HG21	1.74	0.52
1:B:244:ILE:HG12	1:B:246:LEU:HD13	1.91	0.52
1:B:320:PHE:CE1	1:B:379:ALA:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:HG3	1:A:133:THR:HG22	1.90	0.52
1:B:96:HIS:ND1	1:B:97:PRO:HD2	2.24	0.52
1:A:232:ILE:HG13	1:A:274:LEU:CD2	2.40	0.52
1:A:326:VAL:HG12	1:A:330:LEU:CD2	2.40	0.52
1:B:24:ASP:O	1:B:25:PRO:C	2.53	0.51
1:B:382:HIS:CG	1:B:387:ARG:O	2.64	0.51
1:B:132:LYS:HE2	1:B:133:THR:N	2.26	0.51
1:A:228:PHE:O	1:A:232:ILE:HG23	2.10	0.51
1:B:194:PRO:HG2	1:B:198:HIS:CE1	2.45	0.51
1:A:23:ARG:HG2	1:A:29:ALA:HB2	1.93	0.51
1:B:92:ASN:O	1:B:118:LYS:HE2	2.11	0.51
1:B:370:MET:HB3	1:B:372:PHE:CD2	2.46	0.51
1:B:181:GLU:OE2	1:B:220:HIS:HE1	1.94	0.51
1:B:228:PHE:O	1:B:229:PRO:C	2.54	0.51
1:B:64:SER:HB2	1:B:67:GLU:HG3	1.93	0.50
1:B:115:ALA:O	1:B:119:THR:HG22	2.07	0.50
1:A:209:PRO:O	1:A:240:LYS:NZ	2.44	0.50
1:A:272:VAL:O	1:A:276:GLU:N	2.37	0.50
1:B:96:HIS:O	1:B:97:PRO:C	2.54	0.50
1:A:234:GLN:HG2	1:B:155:LEU:HD21	1.93	0.50
1:A:11:PHE:CB	1:A:307:MET:HE2	2.42	0.50
1:A:105:THR:HG23	1:A:158:MET:HE3	1.93	0.50
1:B:1:MET:N	1:B:1:MET:CA	2.74	0.50
1:B:79:LEU:O	1:B:83:GLY:N	2.44	0.50
1:B:125:LEU:O	1:B:126:ALA:C	2.55	0.50
1:B:276:GLU:HG3	1:B:314:LYS:HG2	1.93	0.50
1:A:15:LEU:HD21	1:A:51:VAL:HG11	1.94	0.50
1:A:91:THR:HG21	1:A:119:THR:HA	1.93	0.50
1:A:320:PHE:CA	1:A:383:LEU:CD2	2.88	0.50
1:B:226:LEU:HD12	1:B:227:ASN:H	1.75	0.50
1:A:12:THR:CG2	1:A:52:THR:CG2	2.89	0.50
1:A:312:ILE:HG23	1:A:316:ARG:HD2	1.94	0.50
1:B:347:LEU:HD22	1:B:349:ALA:N	2.27	0.50
1:A:284:ARG:HD3	1:A:310:TYR:CZ	2.47	0.50
1:A:321:ARG:O	1:A:322:ALA:HB2	2.12	0.50
1:B:228:PHE:HB3	1:B:229:PRO:CD	2.42	0.50
1:A:15:LEU:CD2	1:A:51:VAL:HG11	2.41	0.50
1:A:140:ARG:HH21	1:A:187:PRO:CB	2.24	0.50
1:A:227:ASN:HD22	1:B:190:ASP:CG	2.20	0.50
1:A:238:ALA:O	1:A:240:LYS:HG2	2.11	0.50
1:A:272:VAL:CG1	1:A:310:TYR:CE1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:GLY:O	1:B:299:VAL:C	2.55	0.49
1:A:116:LEU:O	1:A:120:ILE:HD12	2.12	0.49
1:A:316:ARG:HG2	1:A:382:HIS:CE1	2.47	0.49
1:A:140:ARG:HH21	1:A:187:PRO:HB3	1.78	0.49
1:B:11:PHE:CZ	1:B:311:LEU:HD13	2.47	0.49
1:A:73:LYS:HE2	1:A:74:ARG:CG	2.42	0.49
1:A:309:ASN:O	1:A:313:LEU:CG	2.60	0.49
1:B:20:TRP:CH2	1:B:22:GLY:HA2	2.47	0.49
1:B:48:ALA:HB3	1:B:84:MET:HE1	1.93	0.49
1:B:330:LEU:HD12	1:B:335:LEU:HD13	1.95	0.49
1:A:45:GLU:OE1	1:A:46:LEU:HD12	2.12	0.49
1:A:201:ALA:HB2	1:B:201:ALA:HB2	1.95	0.49
1:B:183:LYS:O	1:B:191:ILE:HB	2.13	0.49
1:A:108:ASP:OD1	1:B:370:MET:HE1	2.12	0.49
1:A:232:ILE:HG12	1:A:271:LEU:CD1	2.42	0.49
1:B:308:ARG:O	1:B:312:ILE:CG1	2.61	0.49
1:A:184:PRO:O	1:A:191:ILE:HB	2.12	0.48
1:A:37:VAL:O	1:A:41:GLN:HB2	2.12	0.48
1:A:323:ASP:OD1	1:A:325:GLU:N	2.46	0.48
1:B:170:THR:HG21	1:B:208:ARG:NH2	2.27	0.48
1:B:309:ASN:O	1:B:313:LEU:HG	2.13	0.48
1:B:354:ARG:C	1:B:356:ALA:N	2.71	0.48
1:A:15:LEU:CD2	1:A:51:VAL:CG1	2.91	0.48
1:A:309:ASN:O	1:A:313:LEU:HD12	2.13	0.48
1:A:370:MET:HE1	1:B:107:ASN:HB2	1.96	0.48
1:A:73:LYS:HE2	1:A:74:ARG:HG2	1.95	0.48
1:A:73:LYS:HG3	1:A:74:ARG:H	1.74	0.48
1:A:338:LEU:HD22	1:B:107:ASN:ND2	2.23	0.48
1:A:357:PHE:HE1	1:B:118:LYS:HA	1.78	0.48
1:B:137:TRP:HE1	1:B:183:LYS:HB2	1.78	0.48
1:B:330:LEU:HD13	1:B:375:LEU:HD11	1.95	0.48
1:A:370:MET:HB3	1:A:372:PHE:CE2	2.49	0.48
1:A:35:ASP:OD1	1:A:36:PRO:N	2.47	0.48
1:A:68:ARG:HH21	1:A:125:LEU:HD22	1.71	0.48
1:A:309:ASN:O	1:A:313:LEU:CD1	2.62	0.48
1:B:15:LEU:HD22	1:B:53:PHE:CB	2.43	0.48
1:B:21:GLN:CB	1:B:31:ARG:O	2.61	0.48
1:B:159:LYS:CE	1:B:205:ARG:O	2.61	0.48
1:B:181:GLU:HB2	1:B:215:ASN:HD22	1.79	0.48
1:B:347:LEU:HD22	1:B:349:ALA:CB	2.44	0.47
1:A:59:ILE:CD1	1:A:71:HIS:CB	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:O	1:A:129:LEU:HD12	2.14	0.47
1:B:103:GLY:O	1:B:112:ARG:HG2	2.13	0.47
1:A:44:ALA:HB2	1:A:84:MET:CE	2.43	0.47
1:A:248:GLY:O	1:A:258:LEU:HB2	2.14	0.47
1:A:229:PRO:O	1:A:230:HIS:C	2.58	0.47
1:A:232:ILE:HG13	1:A:274:LEU:HD21	1.96	0.47
1:A:357:PHE:HD1	1:B:117:ARG:HB3	1.80	0.47
1:A:56:ASP:CG	1:A:118:LYS:HZ1	2.23	0.47
1:A:97:PRO:O	1:A:100:LYS:HB2	2.14	0.47
1:B:228:PHE:O	1:B:231:GLY:N	2.45	0.47
1:A:24:ASP:OD1	1:A:27:GLY:N	2.47	0.47
1:A:35:ASP:OD1	1:A:36:PRO:CD	2.63	0.47
1:A:51:VAL:N	1:A:85:THR:O	2.45	0.47
1:A:135:VAL:CG1	1:A:136:ALA:H	2.27	0.47
1:A:148:ALA:HB1	1:B:372:PHE:CE1	2.49	0.47
1:A:269:PHE:HE1	1:A:270:TRP:CH2	2.32	0.47
1:A:297:ASP:OD1	1:A:301:ALA:N	2.47	0.47
1:B:13:PHE:HB2	1:B:43:LEU:HD13	1.96	0.47
1:B:64:SER:O	1:B:66:THR:N	2.48	0.47
1:B:88:MET:HA	1:B:133:THR:O	2.14	0.47
1:B:325:GLU:O	1:B:328:GLU:HB3	2.15	0.47
1:B:380:MET:C	1:B:381:ASP:O	2.56	0.47
1:A:89:ALA:HB3	1:A:126:ALA:HB2	1.97	0.47
1:A:316:ARG:HB3	1:A:382:HIS:CE1	2.46	0.47
1:A:387:ARG:CG	1:A:387:ARG:HH11	2.27	0.47
1:B:1:MET:C	1:B:2:SER:OG	2.58	0.47
1:B:28:ASP:O	1:B:29:ALA:C	2.55	0.47
1:B:354:ARG:HH11	1:B:354:ARG:CG	2.27	0.47
1:A:379:ALA:O	1:A:380:MET:HG2	2.15	0.47
1:A:166:GLY:O	1:A:170:THR:HG23	2.15	0.47
1:A:323:ASP:O	1:A:324:PRO:C	2.56	0.47
1:B:323:ASP:CB	1:B:383:LEU:HD21	2.43	0.47
1:A:319:ALA:C	1:A:383:LEU:CD1	2.89	0.46
1:A:374:HIS:O	1:A:378:LEU:HG	2.15	0.46
1:A:260:PHE:HE1	1:A:313:LEU:HD12	1.79	0.46
1:B:110:ASP:OD1	1:B:110:ASP:O	2.33	0.46
1:A:237:TRP:H	1:A:239:GLY:H	1.63	0.46
1:B:64:SER:OG	1:B:67:GLU:CG	2.60	0.46
1:B:271:LEU:O	1:B:274:LEU:HB3	2.16	0.46
1:B:326:VAL:HG21	1:B:383:LEU:HD22	1.97	0.46
1:A:75:PHE:CE2	1:A:79:LEU:HD21	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:O	1:A:192:LEU:C	2.56	0.46
1:A:259:ARG:HG3	1:A:302:SER:O	2.16	0.46
1:A:337:GLN:HE21	1:B:109:ARG:H	1.62	0.46
1:B:21:GLN:CG	1:B:31:ARG:O	2.63	0.46
1:B:135:VAL:CG1	1:B:136:ALA:N	2.79	0.46
1:A:31:ARG:NH2	1:A:294:GLU:O	2.43	0.46
1:A:53:PHE:O	1:A:90:THR:CG2	2.64	0.46
1:A:272:VAL:O	1:A:273:ASP:C	2.58	0.46
1:A:106:ALA:C	1:A:108:ASP:H	2.24	0.46
1:A:337:GLN:O	1:B:112:ARG:NH1	2.45	0.46
1:A:351:LEU:O	1:A:352:ALA:C	2.53	0.46
1:B:36:PRO:O	1:B:40:VAL:CG2	2.59	0.46
1:A:105:THR:CG2	1:A:158:MET:HE3	2.46	0.46
1:B:370:MET:HB3	1:B:372:PHE:CE2	2.50	0.46
1:A:328:GLU:O	1:A:331:ARG:HB2	2.16	0.46
1:B:46:LEU:O	1:B:48:ALA:N	2.49	0.46
1:A:315:ASP:O	1:A:318:ALA:HB3	2.16	0.46
1:B:218:VAL:HG13	1:B:246:LEU:HA	1.98	0.46
1:B:316:ARG:HB3	1:B:382:HIS:CG	2.45	0.46
1:B:332:ALA:O	1:B:334:ARG:NH1	2.48	0.46
1:A:35:ASP:OD1	1:A:37:VAL:HG22	2.15	0.45
1:A:168:TYR:CZ	1:A:172:GLN:HG3	2.51	0.45
1:A:178:PHE:HB2	1:A:212:TYR:CD2	2.51	0.45
1:B:54:HIS:O	1:B:55:ASP:C	2.58	0.45
1:B:132:LYS:CE	1:B:133:THR:OG1	2.63	0.45
1:B:363:ASP:HA	1:B:366:ALA:HB2	1.96	0.45
1:A:109:ARG:NH1	1:A:113:ARG:CZ	2.80	0.45
1:A:296:PHE:O	1:A:300:TRP:CD1	2.69	0.45
1:B:295:ASP:O	1:B:299:VAL:HG23	2.15	0.45
1:A:264:ASP:CG	1:A:267:ALA:HB2	2.41	0.45
1:A:117:ARG:HD3	1:B:350:LEU:O	2.17	0.45
1:B:10:ARG:HB3	1:B:283:PRO:HA	1.99	0.45
1:A:227:ASN:O	1:A:230:HIS:HB2	2.16	0.45
1:A:382:HIS:HD2	1:A:388:GLY:CA	2.15	0.45
1:B:226:LEU:HD13	1:B:226:LEU:HA	1.88	0.45
1:A:86:VAL:O	1:A:131:ALA:HA	2.17	0.45
1:A:294:GLU:HB3	1:A:298:GLY:HA3	1.99	0.45
1:A:345:ASP:N	1:A:347:LEU:HB2	2.31	0.45
1:B:35:ASP:O	1:B:38:GLU:N	2.50	0.45
1:B:132:LYS:HE3	1:B:133:THR:OG1	2.16	0.45
1:B:382:HIS:O	1:B:383:LEU:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:MET:HB3	1:A:372:PHE:CD2	2.51	0.45
1:B:135:VAL:HG22	1:B:179:ALA:HB3	1.97	0.45
1:B:250:SER:N	1:B:256:GLN:OE1	2.41	0.45
1:A:53:PHE:HD1	1:A:54:HIS:O	2.00	0.45
1:A:244:ILE:HD13	1:A:275:LEU:HD11	1.99	0.45
1:A:361:ASP:O	1:A:364:ALA:HB3	2.17	0.45
1:A:60:PRO:O	1:A:61:PHE:C	2.60	0.45
1:B:64:SER:HB2	1:B:66:THR:CG2	2.45	0.45
1:A:94:PHE:CB	1:A:140:ARG:HG3	2.47	0.45
1:A:132:LYS:HE2	1:A:283:PRO:HD3	1.99	0.45
1:B:144:GLU:HB2	1:B:188:ARG:HE	1.81	0.45
1:B:319:ALA:C	1:B:383:LEU:HG	2.38	0.45
1:A:109:ARG:NH1	1:A:113:ARG:CD	2.80	0.44
1:A:157:ARG:HD2	1:B:338:LEU:O	2.18	0.44
1:A:205:ARG:HD3	1:A:205:ARG:HA	1.85	0.44
1:B:179:ALA:HB1	1:B:215:ASN:HB2	1.99	0.44
1:B:259:ARG:O	1:B:262:ALA:HB3	2.17	0.44
1:B:384:LEU:O	1:B:385:GLY:C	2.61	0.44
1:A:334:ARG:NH1	1:B:108:ASP:OD2	2.50	0.44
1:A:158:MET:HG2	1:A:202:PHE:CZ	2.52	0.44
1:B:21:GLN:HG2	1:B:32:PRO:C	2.42	0.44
1:B:236:LEU:HD13	1:B:278:ALA:HB1	1.99	0.44
1:B:73:LYS:O	1:B:74:ARG:C	2.61	0.44
1:B:198:HIS:O	1:B:199:ALA:C	2.60	0.44
1:A:60:PRO:HG2	1:A:63:SER:OG	2.18	0.44
1:A:128:GLU:C	1:A:129:LEU:HD12	2.43	0.44
1:A:237:TRP:CG	1:B:155:LEU:HD23	2.52	0.44
1:A:354:ARG:O	1:A:359:ASP:CB	2.65	0.44
1:B:78:ALA:O	1:B:82:THR:OG1	2.31	0.44
1:B:107:ASN:HD22	1:B:107:ASN:HA	1.27	0.44
1:A:59:ILE:HA	1:A:60:PRO:HD2	1.73	0.44
1:B:22:GLY:O	1:B:292:ARG:NE	2.51	0.44
1:B:383:LEU:O	1:B:384:LEU:HD23	2.18	0.44
1:A:196:VAL:O	1:A:200:LEU:HG	2.17	0.44
1:A:382:HIS:HB3	1:A:388:GLY:HA3	1.99	0.44
1:B:305:GLY:O	1:B:306:CYS:C	2.61	0.44
1:A:354:ARG:HB3	1:A:358:GLU:HB2	2.00	0.44
1:B:54:HIS:HB2	1:B:57:ASP:OD2	2.18	0.44
1:B:137:TRP:HE1	1:B:183:LYS:CB	2.31	0.44
1:A:28:ASP:O	1:A:292:ARG:NH2	2.49	0.44
1:B:294:GLU:OE1	1:B:294:GLU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ASP:C	1:B:350:LEU:HD23	2.43	0.44
1:A:46:LEU:HD21	1:A:300:TRP:HE3	1.81	0.43
1:A:113:ARG:HH12	1:B:343:ALA:HA	1.83	0.43
1:A:217:GLU:O	1:A:228:PHE:CE1	2.71	0.43
1:A:245:ASP:OD1	1:A:285:HIS:ND1	2.33	0.43
1:B:137:TRP:CZ2	1:B:183:LYS:HD3	2.50	0.43
1:B:59:ILE:HA	1:B:60:PRO:HD2	1.70	0.43
1:B:72:ILE:H	1:B:72:ILE:HG13	1.71	0.43
1:B:180:ILE:O	1:B:214:VAL:HA	2.19	0.43
1:B:195:THR:HA	1:B:221:GLU:OE2	2.17	0.43
1:A:120:ILE:O	1:A:121:GLY:C	2.61	0.43
1:B:60:PRO:HD2	1:B:71:HIS:CD2	2.53	0.43
1:B:345:ASP:C	1:B:347:LEU:N	2.75	0.43
1:A:157:ARG:CD	1:B:338:LEU:O	2.65	0.43
1:A:144:GLU:CD	1:A:188:ARG:HH21	2.22	0.43
1:A:326:VAL:HG12	1:A:330:LEU:HD22	2.00	0.43
1:B:22:GLY:O	1:B:292:ARG:HD2	2.18	0.43
1:B:222:GLN:O	1:B:225:GLY:HA2	2.18	0.43
1:A:109:ARG:HH11	1:A:113:ARG:CD	2.32	0.43
1:A:215:ASN:OD1	1:A:243:HIS:ND1	2.52	0.43
1:A:316:ARG:CZ	1:A:382:HIS:CE1	2.97	0.43
1:A:356:ALA:HB3	1:B:117:ARG:HH21	1.82	0.43
1:B:159:LYS:NZ	1:B:206:LEU:HA	2.34	0.43
1:B:188:ARG:O	1:B:189:GLY:C	2.61	0.43
1:B:298:GLY:O	1:B:301:ALA:HB3	2.19	0.43
1:B:374:HIS:NE2	1:B:378:LEU:CD1	2.73	0.43
1:A:322:ALA:O	1:A:324:PRO:HD3	2.19	0.43
1:B:64:SER:C	1:B:66:THR:N	2.75	0.43
1:A:125:LEU:O	1:A:128:GLU:N	2.52	0.43
1:A:148:ALA:CB	1:B:372:PHE:CD1	3.01	0.43
1:A:382:HIS:CD2	1:A:388:GLY:HA3	2.52	0.43
1:B:169:VAL:O	1:B:170:THR:C	2.62	0.43
1:B:283:PRO:O	1:B:285:HIS:N	2.51	0.43
1:B:383:LEU:HD22	1:B:383:LEU:HA	1.67	0.43
1:A:59:ILE:HD11	1:A:72:ILE:HG13	2.00	0.43
1:A:85:THR:OG1	1:A:86:VAL:N	2.52	0.43
1:A:297:ASP:CG	1:A:300:TRP:HB2	2.44	0.43
1:B:307:MET:O	1:B:311:LEU:HB2	2.19	0.43
1:B:327:GLN:HE21	1:B:327:GLN:HB2	1.71	0.43
1:A:361:ASP:OD1	1:A:364:ALA:N	2.43	0.42
1:B:50:GLY:CA	1:B:85:THR:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLY:O	1:B:201:ALA:N	2.45	0.42
1:B:300:TRP:O	1:B:303:ALA:HB3	2.19	0.42
1:B:381:ASP:HB2	1:B:384:LEU:HD23	2.00	0.42
1:A:360:PHE:CE2	1:B:114:TYR:HB2	2.53	0.42
1:B:24:ASP:OD1	1:B:27:GLY:N	2.51	0.42
1:B:26:PHE:CD1	1:B:26:PHE:N	2.87	0.42
1:B:134:TYR:HB2	1:B:176:LEU:HD22	2.02	0.42
1:A:214:VAL:N	1:A:240:LYS:O	2.45	0.42
1:A:266:ARG:O	1:A:267:ALA:C	2.60	0.42
1:A:274:LEU:O	1:A:278:ALA:CB	2.68	0.42
1:B:168:TYR:O	1:B:169:VAL:C	2.61	0.42
1:B:323:ASP:HB2	1:B:383:LEU:CD2	2.49	0.42
1:B:345:ASP:C	1:B:347:LEU:H	2.27	0.42
1:A:139:GLY:O	1:A:187:PRO:HD2	2.20	0.42
1:A:312:ILE:HG22	1:A:316:ARG:HD2	2.01	0.42
1:B:4:GLN:O	1:B:6:THR:HG23	2.19	0.42
1:B:349:ALA:N	1:B:350:LEU:HD23	2.34	0.42
1:A:160:GLU:O	1:A:164:LEU:HB2	2.20	0.42
1:B:277:THR:C	1:B:279:GLY:H	2.26	0.42
1:A:84:MET:HG3	1:A:85:THR:H	1.84	0.42
1:A:217:GLU:OE2	1:A:287:ASP:OD2	2.38	0.42
1:A:346:GLY:N	1:A:347:LEU:HD13	2.34	0.42
1:B:264:ASP:OD1	1:B:267:ALA:CB	2.67	0.42
1:B:13:PHE:HB2	1:B:43:LEU:CD1	2.49	0.42
1:B:203:ILE:HG23	1:B:212:TYR:HB2	2.00	0.42
1:A:184:PRO:HB3	1:B:226:LEU:HD21	2.01	0.42
1:A:210:GLU:CD	1:A:210:GLU:H	2.27	0.42
1:A:212:TYR:O	1:A:242:PHE:CE2	2.72	0.42
1:A:316:ARG:HG3	1:A:316:ARG:H	1.59	0.42
1:A:387:ARG:CG	1:A:387:ARG:NH1	2.83	0.42
1:B:30:THR:HG23	1:B:292:ARG:CZ	2.50	0.42
1:B:347:LEU:CD1	1:B:349:ALA:C	2.89	0.42
1:B:96:HIS:CG	1:B:98:VAL:HG22	2.51	0.42
1:B:137:TRP:CH2	1:B:139:GLY:HA2	2.55	0.42
1:A:320:PHE:CA	1:A:383:LEU:HD22	2.23	0.42
1:B:350:LEU:HG	1:B:351:LEU:N	2.35	0.42
1:A:193:LEU:HD11	1:A:202:PHE:CD2	2.55	0.41
1:B:171:ALA:C	1:B:173:GLY:H	2.28	0.41
1:A:16:TRP:CE3	1:A:54:HIS:HD2	2.39	0.41
1:A:148:ALA:HB1	1:B:372:PHE:CD1	2.55	0.41
1:A:382:HIS:CG	1:A:388:GLY:CA	3.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:MET:O	1:B:161:ALA:HB3	2.20	0.41
1:B:158:MET:CG	1:B:202:PHE:CZ	3.03	0.41
1:A:130:GLY:O	1:A:131:ALA:C	2.63	0.41
1:A:218:VAL:HG13	1:A:247:ASN:HB2	2.01	0.41
1:B:135:VAL:HG12	1:B:136:ALA:N	2.36	0.41
1:B:208:ARG:HB3	1:B:210:GLU:OE2	2.19	0.41
1:B:266:ARG:NH2	1:B:380:MET:HB2	2.35	0.41
1:A:97:PRO:C	1:A:99:PHE:N	2.78	0.41
1:A:124:ASP:O	1:A:127:ALA:HB3	2.19	0.41
1:A:163:ASP:HA	1:A:208:ARG:HH12	1.84	0.41
1:A:198:HIS:CD2	1:A:198:HIS:H	2.39	0.41
1:A:338:LEU:HD22	1:B:149:LYS:HG2	2.01	0.41
1:B:64:SER:O	1:B:65:ASP:C	2.64	0.41
1:B:387:ARG:CG	1:B:387:ARG:HH11	2.33	0.41
1:A:357:PHE:HB2	1:B:117:ARG:CG	2.46	0.41
1:B:144:GLU:H	1:B:188:ARG:NH2	2.19	0.41
1:B:350:LEU:CD2	1:B:351:LEU:HD23	2.51	0.41
1:A:188:ARG:HE	1:A:188:ARG:HA	1.86	0.41
1:B:50:GLY:HA3	1:B:85:THR:O	2.21	0.41
1:A:137:TRP:CD2	1:A:138:GLY:O	2.74	0.41
1:A:236:LEU:O	1:B:152:ARG:HG2	2.20	0.41
1:B:43:LEU:O	1:B:46:LEU:O	2.38	0.41
1:B:96:HIS:CD2	1:B:98:VAL:HG21	2.55	0.41
1:B:144:GLU:H	1:B:188:ARG:HH21	1.67	0.41
1:B:193:LEU:HD11	1:B:202:PHE:CD2	2.56	0.41
1:B:270:TRP:CE3	1:B:270:TRP:HA	2.56	0.41
1:B:336:ASP:O	1:B:339:ALA:HB3	2.20	0.41
1:B:350:LEU:HD21	1:B:351:LEU:CD2	2.51	0.41
1:B:159:LYS:NZ	1:B:205:ARG:O	2.50	0.41
1:A:212:TYR:C	1:A:242:PHE:CE2	2.99	0.40
1:A:310:TYR:O	1:A:314:LYS:N	2.50	0.40
1:A:338:LEU:CD2	1:B:149:LYS:HG2	2.51	0.40
1:B:103:GLY:H	1:B:141:GLU:CD	2.29	0.40
1:B:350:LEU:HD21	1:B:351:LEU:HD23	2.02	0.40
1:A:295:ASP:O	1:A:299:VAL:HG23	2.21	0.40
1:B:6:THR:HA	1:B:7:PRO:HD2	1.90	0.40
1:B:208:ARG:O	1:B:211:LEU:HB2	2.21	0.40
1:B:217:GLU:O	1:B:218:VAL:C	2.63	0.40
1:A:109:ARG:NH1	1:A:113:ARG:NE	2.70	0.40
1:A:116:LEU:HD11	1:A:161:ALA:HA	2.04	0.40
1:A:227:ASN:HB2	1:B:190:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ARG:HD3	1:A:302:SER:HB2	2.02	0.40
1:B:185:ASN:O	1:B:186:GLU:HB3	2.21	0.40
1:A:79:LEU:HD22	1:A:86:VAL:HG23	2.03	0.40
1:A:140:ARG:HA	1:A:188:ARG:CD	2.51	0.40
1:A:279:GLY:O	1:A:280:TYR:C	2.64	0.40
1:B:24:ASP:HB2	1:B:25:PRO:CD	2.47	0.40
1:B:110:ASP:HA	1:B:113:ARG:HB2	2.04	0.40
1:B:170:THR:HG22	1:B:171:ALA:N	2.35	0.40

All (34) 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:345:ASP:CB	1:B:35:ASP:N[3_555]	0.82	1.38
1:A:345:ASP:CG	1:B:35:ASP:N[3_555]	0.86	1.34
1:A:345:ASP:CG	1:B:35:ASP:CA[3_555]	0.90	1.30
1:A:345:ASP:OD1	1:B:35:ASP:C[3_555]	1.12	1.08
1:A:345:ASP:OD1	1:B:35:ASP:O[3_555]	1.33	0.87
1:A:345:ASP:OD2	1:B:35:ASP:CA[3_555]	1.34	0.86
1:B:308:ARG:NH1	1:B:381:ASP:OD2[7_555]	1.49	0.71
1:A:345:ASP:C	1:B:35:ASP:CB[3_555]	1.53	0.67
1:A:345:ASP:OD1	1:B:35:ASP:CA[3_555]	1.56	0.64
1:A:345:ASP:CG	1:B:34:LEU:C[3_555]	1.60	0.60
1:A:345:ASP:CB	1:B:34:LEU:C[3_555]	1.65	0.55
1:A:345:ASP:OD1	1:B:35:ASP:N[3_555]	1.65	0.55
1:A:346:GLY:N	1:B:35:ASP:CB[3_555]	1.68	0.52
1:A:345:ASP:O	1:B:35:ASP:OD2[3_555]	1.75	0.45
1:A:346:GLY:CA	1:B:35:ASP:OD2[3_555]	1.75	0.45
1:A:345:ASP:CG	1:B:35:ASP:C[3_555]	1.82	0.38
1:B:308:ARG:NH1	1:B:381:ASP:CG[7_555]	1.89	0.31
1:A:345:ASP:CA	1:B:35:ASP:N[3_555]	1.94	0.26
1:A:345:ASP:OD2	1:B:35:ASP:N[3_555]	1.94	0.26
1:A:345:ASP:CB	1:B:35:ASP:CA[3_555]	1.96	0.24
1:A:345:ASP:O	1:B:35:ASP:CG[3_555]	1.97	0.23
1:A:292:ARG:NH1	1:B:140:ARG:NH1[7_555]	1.99	0.21
1:A:345:ASP:OD2	1:B:34:LEU:O[3_555]	1.99	0.21
1:A:346:GLY:N	1:B:35:ASP:CG[3_555]	2.03	0.17
1:A:345:ASP:O	1:B:35:ASP:CB[3_555]	2.04	0.16
1:A:346:GLY:CA	1:B:35:ASP:CG[3_555]	2.04	0.16
1:A:140:ARG:NH2	1:B:24:ASP:OD2[7_555]	2.13	0.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:THR:O	1:A:370:MET:N[7_555]	2.13	0.07
1:A:345:ASP:OD2	1:B:34:LEU:C[3_555]	2.13	0.07
1:A:345:ASP:CG	1:B:34:LEU:O[3_555]	2.13	0.07
1:B:308:ARG:NH1	1:B:381:ASP:OD1[7_555]	2.13	0.07
1:A:316:ARG:NH2	1:A:387:ARG:N[7_555]	2.14	0.06
1:A:345:ASP:C	1:B:35:ASP:CG[3_555]	2.15	0.05
1:A:346:GLY:CA	1:B:74:ARG:NH1[3_555]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/388 (100%)	309 (80%)	53 (14%)	24 (6%)	1	1
1	B	386/388 (100%)	312 (81%)	54 (14%)	20 (5%)	1	2
All	All	772/776 (100%)	621 (80%)	107 (14%)	44 (6%)	1	1

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	PHE
1	A	186	GLU
1	A	347	LEU
1	A	351	LEU
1	A	387	ARG
1	B	7	PRO
1	B	8	GLU
1	B	102	GLY
1	B	295	ASP
1	B	345	ASP
1	B	383	LEU
1	B	386	ALA
1	A	138	GLY

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Mol	Chain	Res	Type
1	A	173	GLY
1	A	237	TRP
1	A	353	ASP
1	A	382	HIS
1	B	65	ASP
1	B	139	GLY
1	B	329	ALA
1	A	17	THR
1	A	23	ARG
1	A	147	GLY
1	A	184	PRO
1	A	354	ARG
1	A	380	MET
1	A	383	LEU
1	B	76	ARG
1	B	171	ALA
1	B	252	ILE
1	A	56	ASP
1	A	68	ARG
1	A	252	ILE
1	B	17	THR
1	B	75	PHE
1	B	147	GLY
1	B	172	GLN
1	A	2	SER
1	B	25	PRO
1	A	7	PRO
1	A	145	SER
1	A	298	GLY
1	B	64	SER
1	B	186	GLU

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/297 (100%)	225 (76%)	72 (24%)	1	1
1	B	297/297 (100%)	226 (76%)	71 (24%)	1	1
All	All	594/594 (100%)	451 (76%)	143 (24%)	1	1

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	12	THR
1	A	31	ARG
1	A	34	LEU
1	A	35	ASP
1	A	36	PRO
1	A	37	VAL
1	A	38	GLU
1	A	41	GLN
1	A	52	THR
1	A	55	ASP
1	A	63	SER
1	A	64	SER
1	A	66	THR
1	A	70	SER
1	A	77	GLN
1	A	80	ASP
1	A	91	THR
1	A	95	THR
1	A	109	ARG
1	A	111	VAL
1	A	120	ILE
1	A	123	ILE
1	A	125	LEU
1	A	128	GLU
1	A	132	LYS
1	A	133	THR
1	A	140	ARG
1	A	145	SER
1	A	149	LYS
1	A	157	ARG
1	A	158	MET

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Mol	Chain	Res	Type
1	A	164	LEU
1	A	169	VAL
1	A	180	ILE
1	A	191	ILE
1	A	196	VAL
1	A	207	GLU
1	A	210	GLU
1	A	218	VAL
1	A	221	GLU
1	A	226	LEU
1	A	230	HIS
1	A	232	ILE
1	A	234	GLN
1	A	252	ILE
1	A	253	LYS
1	A	256	GLN
1	A	266	ARG
1	A	272	VAL
1	A	273	ASP
1	A	281	GLU
1	A	284	ARG
1	A	292	ARG
1	A	294	GLU
1	A	295	ASP
1	A	307	MET
1	A	313	LEU
1	A	315	ASP
1	A	321	ARG
1	A	327	GLN
1	A	330	LEU
1	A	334	ARG
1	A	347	LEU
1	A	350	LEU
1	A	353	ASP
1	A	375	LEU
1	A	380	MET
1	A	381	ASP
1	A	382	HIS
1	A	383	LEU
1	A	387	ARG
1	B	1	MET
1	B	9	ASP

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Mol	Chain	Res	Type
1	B	10	ARG
1	B	23	ARG
1	B	35	ASP
1	B	37	VAL
1	B	41	GLN
1	B	45	GLU
1	B	58	LEU
1	B	63	SER
1	B	64	SER
1	B	68	ARG
1	B	69	GLU
1	B	71	HIS
1	B	73	LYS
1	B	74	ARG
1	B	77	GLN
1	B	80	ASP
1	B	84	MET
1	B	91	THR
1	B	95	THR
1	B	98	VAL
1	B	100	LYS
1	B	107	ASN
1	B	117	ARG
1	B	119	THR
1	B	129	LEU
1	B	132	LYS
1	B	141	GLU
1	B	149	LYS
1	B	151	VAL
1	B	158	MET
1	B	159	LYS
1	B	164	LEU
1	B	169	VAL
1	B	170	THR
1	B	181	GLU
1	B	186	GLU
1	B	206	LEU
1	B	208	ARG
1	B	214	VAL
1	B	218	VAL
1	B	221	GLU
1	B	222	GLN

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Mol	Chain	Res	Type
1	B	226	LEU
1	B	227	ASN
1	B	232	ILE
1	B	246	LEU
1	B	265	LEU
1	B	266	ARG
1	B	292	ARG
1	B	293	THR
1	B	311	LEU
1	B	312	ILE
1	B	314	LYS
1	B	325	GLU
1	B	328	GLU
1	B	330	LEU
1	B	335	LEU
1	B	340	GLN
1	B	347	LEU
1	B	354	ARG
1	B	362	VAL
1	B	363	ASP
1	B	368	ARG
1	B	370	MET
1	B	375	LEU
1	B	381	ASP
1	B	382	HIS
1	B	383	LEU
1	B	387	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	54	HIS
1	A	77	GLN
1	A	96	HIS
1	A	172	GLN
1	A	198	HIS
1	A	337	GLN
1	A	377	GLN
1	B	4	GLN
1	B	21	GLN
1	B	71	HIS

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Mol	Chain	Res	Type
1	B	96	HIS
1	B	107	ASN
1	B	185	ASN
1	B	220	HIS
1	B	227	ASN
1	B	230	HIS
1	B	309	ASN
1	B	327	GLN
1	B	382	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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.