



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:56 PM GMT

PDB ID : 1RBA
Title : SUBSTITUTION OF ASP193 TO ASN AT THE ACTIVE SITE OF RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE RESULTS IN CONFORMATIONAL CHANGES
Authors : Schneider, G.; Soderlind, E.
Deposited on : 1991-11-18
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

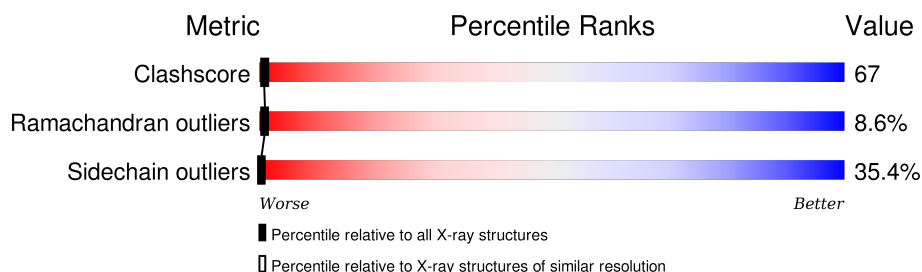
1 Overall quality at a glance

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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	466	
1	B	466	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6695 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 RUBISCO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3200	2029	566	590	15			
1	B	443	Total	C	N	O	S	0	0	0
			3385	2146	596	627	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASP	HIS	CONFLICT	UNP P04718
A	193	ASN	ASP	ENGINEERED MUTATION	UNP P04718
B	91	ASP	HIS	CONFLICT	UNP P04718
B	193	ASN	ASP	ENGINEERED MUTATION	UNP P04718

- Molecule 2 is water.

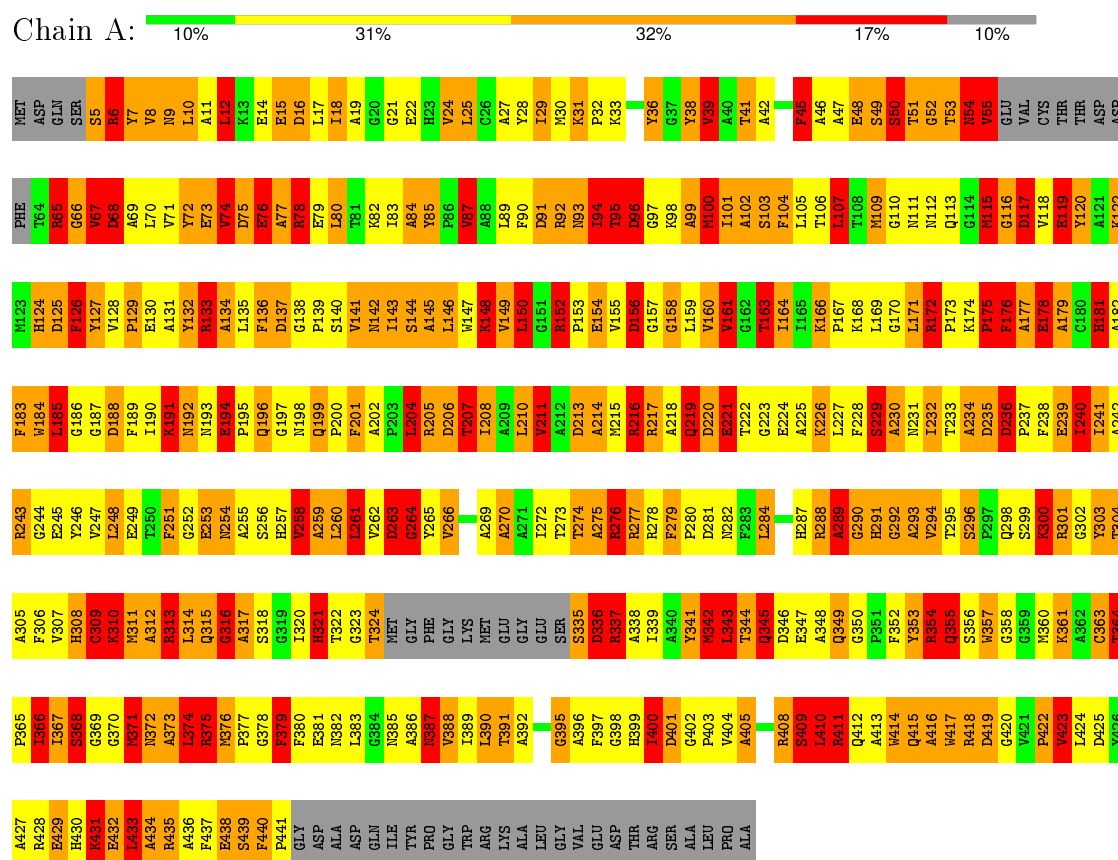
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	67	Total	O	0	0
			67	67		
2	B	43	Total	O	0	0
			43	43		

3 Residue-property plots

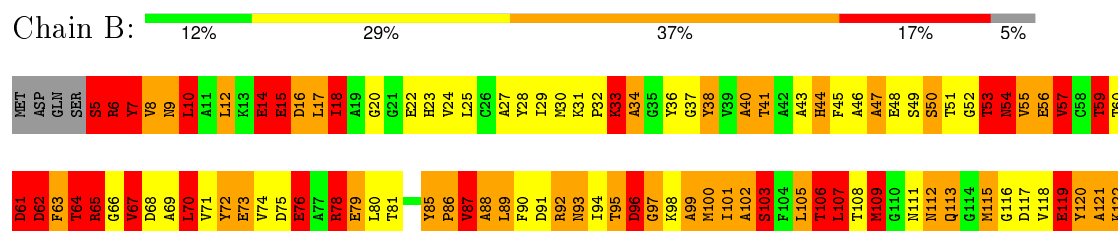
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: RUBISCO



• Molecule 1: RUBISCO



E429	H430	K431	E432	L433	A434	R435	A436	F437	E438	S439	F440	R441	G442	A443	A444	D445	Q446	I447	Y448	P449	G450	W451	R452	K453	A454	L455	G456	V457	GLU	ASP	THR	ARG	SER	ALA	LEU	PRO	ALA																						
S368	G369	G370	G371	N372	A373	I374	R375	R376	P377	G378	F379	F380	E381	N382	L383	G384	N385	A386	R387	V388	L389	L390		G393	G394	G395	A396	F397	G398	R399	L400	D401	G402	P403	V404	A405	G406	A407	R408	S409	L410	R411	Q412	A413	W414	Q415	A416	N417	R418	D419	G420	Y421	P422	V423	L424	D425	Y426	A427	R428
V307	H308	C309	K310	M311	A312	R313	L314	Q315	G316	A317		I320	R321	T322	G323	T324	MET	GLY	PHE	GLY	LYS	MET	GLU	GLY	GLU	SER	S335	D336	R337	A338	I339	A340	Y341	M342	I343	T344	Q345	D346	E347	A348	Q349	G350	P351	F352	Y353	R354	Q355	S356	W357	G358	G359	M360	K361	A362	C363	T364	P365	I366	I367
E245	I246	V247	L248	E249	T250	F251	G252	E253	N254	A255	S256	H257	V258	A259	L260	V262	D263	G264	V265	V266	A267	G268	A269		I272	T273		R276	R277	R278	F279	P280	D281	N282	F283	L284	H285	Y286	H287	R288	A289	G290	H291	G292	A293	V294	T295	S296	F297	S298	S299	K300	R301	G302	T303	T304	A305	F306	
F183	W184	L185	G186	G187	D188	F189	I190	K191	N192	N193	E194	P195	Q196		Q199	P200	P201	A202	P203	L204	R205	D206	T207	L208	A209	L210	V211	A212	D213	A214	N215	R216	R217	A218	Q219	D220	E221	T222	G223	E224	A225	R226	K227		A230	N231	I232	T233	L234	D235	D236	K237	F238	E239	I240	I241	A242	R243	G244
H123	H124	D125	F126	Y127	V128	P129	E130	A131	Y132	R133	A134	L135	F136	D137	G138	P139	S140	V141	N142	I143	S144	A145	L146	H147	K148	V149	L150	G151	R152	P153	E154	V155	D156	G157	G158	L159	V160	V161	G162	T163	I164	I165	K166	P167	K168	L169	G170	L171	R172	P173	K174	P175	F176	E177	E178	A179	C180	H181	A182

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.50Å 69.30Å 103.10Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.207 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6695	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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	1.60	21/3275 (0.6%)	3.37	475/4436 (10.7%)
1	B	1.51	21/3467 (0.6%)	3.32	453/4702 (9.6%)
All	All	1.55	42/6742 (0.6%)	3.35	928/9138 (10.2%)

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	1	3
1	B	0	2
All	All	1	5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	LYS	CD-CE	28.72	2.23	1.51
1	A	78	ARG	CA-CB	-25.14	0.98	1.53
1	B	190	ILE	C-N	21.16	1.82	1.34
1	B	278	ARG	CA-CB	-15.28	1.20	1.53
1	A	349	GLN	CA-CB	-14.30	1.22	1.53
1	A	191	LYS	CD-CE	10.78	1.78	1.51
1	A	150	LEU	CA-CB	-9.32	1.32	1.53
1	A	55	VAL	N-CA	-9.11	1.28	1.46
1	B	321	HIS	CB-CG	8.89	1.66	1.50
1	A	164	ILE	CA-CB	8.70	1.74	1.54
1	B	191	LYS	CD-CE	8.63	1.72	1.51
1	B	41	THR	CA-CB	8.32	1.75	1.53
1	A	5	SER	N-CA	-8.01	1.30	1.46
1	B	381	GLU	CG-CD	7.91	1.63	1.51
1	A	376	MET	CA-CB	7.77	1.71	1.53
1	A	176	PHE	CA-C	-7.55	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	323	GLY	C-N	-7.12	1.17	1.34
1	A	278	ARG	NE-CZ	7.02	1.42	1.33
1	B	10	LEU	N-CA	6.55	1.59	1.46
1	B	167	PRO	N-CD	-6.36	1.39	1.47
1	B	7	TYR	C-N	6.30	1.48	1.34
1	A	278	ARG	CD-NE	6.24	1.57	1.46
1	B	425	ASP	CB-CG	6.24	1.64	1.51
1	B	245	GLU	CD-OE2	-6.12	1.19	1.25
1	B	166	LYS	N-CA	-6.01	1.34	1.46
1	B	191	LYS	CB-CG	5.98	1.68	1.52
1	A	264	GLY	N-CA	-5.95	1.37	1.46
1	B	381	GLU	CD-OE1	5.94	1.32	1.25
1	A	66	GLY	N-CA	5.90	1.54	1.46
1	A	387	ASN	CB-CG	5.78	1.64	1.51
1	A	164	ILE	CA-C	5.77	1.68	1.52
1	A	176	PHE	C-N	-5.66	1.21	1.34
1	B	457	VAL	C-O	5.66	1.34	1.23
1	A	186	GLY	N-CA	5.65	1.54	1.46
1	A	278	ARG	CB-CG	5.63	1.67	1.52
1	A	216	ARG	CB-CG	-5.53	1.37	1.52
1	B	191	LYS	CG-CD	5.37	1.70	1.52
1	A	278	ARG	CG-CD	5.36	1.65	1.51
1	B	243	ARG	CG-CD	-5.29	1.38	1.51
1	B	133	ARG	CZ-NH2	5.29	1.40	1.33
1	B	76	GLU	CD-OE1	5.25	1.31	1.25
1	B	335	SER	CA-CB	5.22	1.60	1.52

All (928) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	ARG	CD-NE-CZ	30.43	166.20	123.60
1	A	435	ARG	CD-NE-CZ	28.34	163.27	123.60
1	B	133	ARG	NE-CZ-NH2	-27.72	106.44	120.30
1	B	92	ARG	CD-NE-CZ	27.45	162.03	123.60
1	B	441	PRO	C-N-CA	27.32	179.67	122.30
1	A	313	ARG	NE-CZ-NH2	25.95	133.28	120.30
1	B	313	ARG	NE-CZ-NH1	25.19	132.89	120.30
1	A	243	ARG	NE-CZ-NH1	25.10	132.85	120.30
1	A	172	ARG	NE-CZ-NH1	24.48	132.54	120.30
1	B	277	ARG	NE-CZ-NH1	24.26	132.43	120.30
1	A	401	ASP	CB-CG-OD1	21.30	137.47	118.30
1	A	263	ASP	C-N-CA	20.28	164.90	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	ARG	NE-CZ-NH2	-20.23	110.18	120.30
1	B	92	ARG	NE-CZ-NH1	19.03	129.82	120.30
1	A	276	ARG	NE-CZ-NH1	18.91	129.75	120.30
1	B	16	ASP	CB-CG-OD1	18.58	135.03	118.30
1	B	221	GLU	CA-CB-CG	17.94	152.86	113.40
1	A	313	ARG	NE-CZ-NH1	-17.62	111.49	120.30
1	A	216	ARG	CD-NE-CZ	17.37	147.91	123.60
1	B	205	ARG	NE-CZ-NH2	-17.30	111.65	120.30
1	B	303	TYR	CB-CG-CD1	17.30	131.38	121.00
1	B	253	GLU	CA-CB-CG	16.77	150.30	113.40
1	B	302	GLY	C-N-CA	16.28	162.41	121.70
1	B	278	ARG	CB-CA-C	16.28	142.95	110.40
1	A	172	ARG	NE-CZ-NH2	-16.05	112.28	120.30
1	A	276	ARG	CD-NE-CZ	15.42	145.19	123.60
1	A	314	LEU	CA-CB-CG	15.34	150.57	115.30
1	B	120	TYR	CB-CG-CD1	15.08	130.04	121.00
1	A	408	ARG	NE-CZ-NH2	-14.98	112.81	120.30
1	A	428	ARG	NE-CZ-NH2	-14.96	112.82	120.30
1	B	284	LEU	C-N-CA	14.96	159.10	121.70
1	A	68	ASP	CB-CG-OD1	14.91	131.72	118.30
1	B	243	ARG	NE-CZ-NH1	14.86	127.73	120.30
1	B	133	ARG	NE-CZ-NH1	14.70	127.65	120.30
1	A	236	ASP	CA-CB-CG	14.60	145.53	113.40
1	A	411	ARG	NE-CZ-NH1	14.46	127.53	120.30
1	A	117	ASP	CB-CG-OD1	-14.39	105.35	118.30
1	A	276	ARG	NE-CZ-NH2	-14.27	113.16	120.30
1	A	321	HIS	CA-CB-CG	14.12	137.61	113.60
1	B	7	TYR	C-N-CA	13.95	156.57	121.70
1	B	243	ARG	CA-CB-CG	13.94	144.07	113.40
1	A	401	ASP	CA-CB-CG	13.80	143.76	113.40
1	B	408	ARG	NE-CZ-NH2	-13.67	113.47	120.30
1	A	133	ARG	CD-NE-CZ	13.56	142.59	123.60
1	B	216	ARG	NE-CZ-NH2	13.51	127.05	120.30
1	B	429	GLU	CA-CB-CG	13.45	142.98	113.40
1	B	411	ARG	NE-CZ-NH2	-13.43	113.58	120.30
1	A	265	TYR	CB-CG-CD2	13.38	129.03	121.00
1	B	15	GLU	CA-CB-CG	13.34	142.74	113.40
1	B	276	ARG	NE-CZ-NH2	12.98	126.79	120.30
1	A	254	ASN	CA-CB-CG	12.93	141.85	113.40
1	B	346	ASP	CB-CG-OD1	-12.90	106.69	118.30
1	B	303	TYR	CB-CG-CD2	-12.88	113.27	121.00
1	A	347	GLU	N-CA-CB	12.76	133.57	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	B	443	ASP	CB-CG-OD1	-12.62	106.95	118.30
1	A	243	ARG	CD-NE-CZ	12.59	141.22	123.60
1	A	298	GLN	CG-CD-OE1	12.52	146.65	121.60
1	B	142	ASN	CA-CB-CG	12.52	140.94	113.40
1	B	57	VAL	CB-CA-C	12.48	135.12	111.40
1	A	96	ASP	CB-CG-OD1	12.47	129.52	118.30
1	A	133	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	A	152	ARG	NE-CZ-NH1	12.32	126.46	120.30
1	A	154	GLU	C-N-CA	12.30	152.44	121.70
1	A	53	THR	C-N-CA	12.11	151.98	121.70
1	A	135	LEU	CA-CB-CG	12.09	143.10	115.30
1	B	263	ASP	CA-CB-CG	12.07	139.95	113.40
1	A	6	ARG	CD-NE-CZ	12.02	140.43	123.60
1	B	120	TYR	CB-CG-CD2	-11.94	113.84	121.00
1	A	156	ASP	N-CA-CB	11.91	132.05	110.60
1	A	91	ASP	CA-CB-CG	11.89	139.55	113.40
1	A	75	ASP	CA-CB-CG	11.83	139.44	113.40
1	B	188	ASP	CA-CB-CG	11.83	139.43	113.40
1	A	403	PRO	C-N-CA	11.73	151.03	121.70
1	A	7	TYR	CB-CG-CD2	-11.72	113.97	121.00
1	A	145	ALA	CB-CA-C	11.66	127.59	110.10
1	A	127	TYR	CB-CG-CD1	11.66	128.00	121.00
1	B	216	ARG	NH1-CZ-NH2	-11.65	106.59	119.40
1	B	243	ARG	CG-CD-NE	11.64	136.25	111.80
1	A	217	ARG	NE-CZ-NH2	11.56	126.08	120.30
1	B	7	TYR	CA-CB-CG	-11.54	91.47	113.40
1	B	457	VAL	CB-CA-C	-11.52	89.50	111.40
1	B	452	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	A	278	ARG	NE-CZ-NH2	11.46	126.03	120.30
1	B	216	ARG	NE-CZ-NH1	11.42	126.01	120.30
1	B	303	TYR	N-CA-CB	11.40	131.12	110.60
1	A	189	PHE	CA-CB-CG	11.37	141.19	113.90
1	B	68	ASP	CB-CG-OD1	11.35	128.51	118.30
1	B	346	ASP	N-CA-CB	11.18	130.73	110.60
1	B	93	ASN	CA-CB-CG	11.18	137.99	113.40
1	A	187	GLY	C-N-CA	11.12	149.50	121.70
1	A	395	GLY	C-N-CA	11.08	149.39	121.70
1	B	265	TYR	CB-CG-CD2	11.04	127.62	121.00
1	B	5	SER	O-C-N	10.99	140.29	122.70
1	A	428	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	B	248	LEU	CA-CB-CG	10.94	140.47	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	ARG	NH1-CZ-NH2	-10.92	107.39	119.40
1	B	92	ARG	NH1-CZ-NH2	-10.86	107.45	119.40
1	A	109	MET	N-CA-CB	10.85	130.12	110.60
1	B	93	ASN	CB-CG-OD1	10.83	143.26	121.60
1	B	219	GLN	CA-CB-CG	10.73	137.01	113.40
1	B	443	ASP	C-N-CA	10.67	148.37	121.70
1	B	217	ARG	NE-CZ-NH1	10.65	125.62	120.30
1	B	243	ARG	CB-CG-CD	10.63	139.25	111.60
1	B	180	CYS	CA-CB-SG	10.59	133.07	114.00
1	A	100	MET	CA-CB-CG	10.58	131.29	113.30
1	B	195	PRO	C-N-CA	10.58	148.15	121.70
1	B	321	HIS	CA-CB-CG	10.54	131.52	113.60
1	A	343	LEU	CA-CB-CG	10.54	139.54	115.30
1	A	349	GLN	CB-CG-CD	10.51	138.92	111.60
1	B	354	ARG	NE-CZ-NH2	-10.46	115.07	120.30
1	B	192	ASN	CA-CB-CG	10.45	136.40	113.40
1	B	260	LEU	N-CA-CB	-10.44	89.52	110.40
1	B	117	ASP	CB-CG-OD2	-10.43	108.92	118.30
1	A	243	ARG	NH1-CZ-NH2	-10.42	107.94	119.40
1	A	387	ASN	CB-CA-C	10.41	131.22	110.40
1	A	127	TYR	CB-CG-CD2	-10.35	114.79	121.00
1	A	205	ARG	NE-CZ-NH1	-10.34	115.13	120.30
1	A	263	ASP	CB-CA-C	10.33	131.06	110.40
1	A	125	ASP	CB-CG-OD2	10.30	127.57	118.30
1	A	336	ASP	C-N-CA	10.29	147.43	121.70
1	B	18	ILE	CB-CG1-CD1	10.29	142.71	113.90
1	B	442	GLY	C-N-CA	10.29	147.41	121.70
1	A	194	GLU	O-C-N	-10.28	101.56	121.10
1	A	281	ASP	CB-CG-OD2	10.22	127.50	118.30
1	A	288	ARG	NE-CZ-NH2	10.21	125.40	120.30
1	A	349	GLN	N-CA-CB	10.18	128.91	110.60
1	A	373	ALA	C-N-CA	10.12	147.00	121.70
1	A	411	ARG	CD-NE-CZ	10.11	137.75	123.60
1	B	265	TYR	CB-CG-CD1	-10.10	114.94	121.00
1	A	28	TYR	CB-CG-CD2	10.03	127.02	121.00
1	A	161	VAL	O-C-N	10.03	140.24	123.20
1	A	298	GLN	CB-CG-CD	10.01	137.63	111.60
1	A	12	LEU	C-N-CA	10.01	146.73	121.70
1	A	354	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	B	137	ASP	CB-CG-OD2	9.95	127.25	118.30
1	B	360	MET	C-N-CA	9.94	146.54	121.70
1	B	220	ASP	CB-CG-OD1	9.91	127.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	ARG	CD-NE-CZ	9.88	137.44	123.60
1	B	260	LEU	CA-CB-CG	9.88	138.02	115.30
1	A	133	ARG	NH1-CZ-NH2	9.86	130.25	119.40
1	A	239	GLU	CG-CD-OE1	-9.86	98.59	118.30
1	B	117	ASP	CB-CG-OD1	9.77	127.09	118.30
1	B	172	ARG	CD-NE-CZ	9.77	137.28	123.60
1	A	68	ASP	CB-CG-OD2	-9.71	109.56	118.30
1	A	419	ASP	CB-CA-C	9.71	129.82	110.40
1	B	206	ASP	CB-CG-OD2	9.71	127.04	118.30
1	A	429	GLU	OE1-CD-OE2	-9.69	111.67	123.30
1	B	260	LEU	CB-CA-C	9.69	128.62	110.20
1	B	217	ARG	CD-NE-CZ	9.66	137.13	123.60
1	A	207	THR	N-CA-CB	9.66	128.66	110.30
1	A	176	PHE	N-CA-C	-9.63	85.00	111.00
1	B	371	MET	O-C-N	9.63	138.10	122.70
1	A	261	LEU	CA-CB-CG	9.61	137.40	115.30
1	B	425	ASP	CB-CA-C	9.61	129.62	110.40
1	B	445	ASP	CB-CG-OD1	9.58	126.92	118.30
1	A	263	ASP	CB-CG-OD2	9.57	126.91	118.30
1	A	172	ARG	CD-NE-CZ	9.56	136.99	123.60
1	A	315	GLN	CA-C-O	9.55	140.15	120.10
1	A	6	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	B	288	ARG	NE-CZ-NH1	-9.49	115.56	120.30
1	B	111	ASN	CB-CA-C	9.48	129.37	110.40
1	A	133	ARG	NE-CZ-NH1	-9.48	115.56	120.30
1	B	10	LEU	O-C-N	-9.47	107.54	122.70
1	B	205	ARG	NH1-CZ-NH2	9.46	129.80	119.40
1	B	278	ARG	NE-CZ-NH1	9.45	125.02	120.30
1	A	9	ASN	N-CA-CB	9.37	127.47	110.60
1	A	429	GLU	CB-CG-CD	9.35	139.44	114.20
1	A	401	ASP	OD1-CG-OD2	-9.32	105.60	123.30
1	A	148	LYS	N-CA-CB	-9.31	93.83	110.60
1	A	239	GLU	OE1-CD-OE2	9.30	134.46	123.30
1	B	401	ASP	CB-CG-OD2	9.30	126.67	118.30
1	B	284	LEU	CA-C-O	9.29	139.60	120.10
1	A	205	ARG	CD-NE-CZ	9.28	136.60	123.60
1	A	119	GLU	CA-CB-CG	9.28	133.82	113.40
1	B	188	ASP	CB-CA-C	-9.22	91.95	110.40
1	A	109	MET	CA-CB-CG	9.22	128.97	113.30
1	B	216	ARG	CB-CG-CD	9.22	135.57	111.60
1	B	340	ALA	N-CA-CB	-9.20	97.23	110.10
1	B	418	ARG	NE-CZ-NH1	9.19	124.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	ASP	OD1-CG-OD2	9.17	140.73	123.30
1	B	399	HIS	N-CA-CB	9.17	127.11	110.60
1	A	304	THR	N-CA-CB	9.13	127.65	110.30
1	A	260	LEU	CA-CB-CG	9.13	136.29	115.30
1	A	429	GLU	CA-CB-CG	9.12	133.46	113.40
1	B	322	THR	O-C-N	9.12	138.70	123.20
1	B	401	ASP	CB-CG-OD1	-9.12	110.09	118.30
1	A	161	VAL	CA-CB-CG1	-9.11	97.24	110.90
1	A	255	ALA	N-CA-CB	-9.07	97.41	110.10
1	A	163	THR	O-C-N	9.05	137.18	122.70
1	B	243	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	A	188	ASP	CA-C-N	9.03	137.07	117.20
1	A	375	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	A	75	ASP	N-CA-CB	9.02	126.83	110.60
1	B	194	GLU	CG-CD-OE2	9.00	136.29	118.30
1	A	221	GLU	N-CA-CB	8.95	126.71	110.60
1	A	28	TYR	CA-CB-CG	8.94	130.39	113.40
1	B	278	ARG	CA-CB-CG	8.94	133.06	113.40
1	A	84	ALA	C-N-CA	8.93	144.04	121.70
1	B	399	HIS	O-C-N	8.92	136.98	122.70
1	B	411	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	B	40	ALA	CB-CA-C	8.91	123.47	110.10
1	B	127	TYR	CB-CG-CD2	8.91	126.35	121.00
1	A	254	ASN	C-N-CA	8.91	143.97	121.70
1	B	146	LEU	CB-CA-C	8.91	127.12	110.20
1	B	428	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	206	ASP	CA-CB-CG	8.89	132.96	113.40
1	B	109	MET	CG-SD-CE	8.89	114.42	100.20
1	B	343	LEU	CA-CB-CG	8.89	135.74	115.30
1	B	91	ASP	CB-CG-OD2	8.87	126.28	118.30
1	A	51	THR	CA-CB-CG2	8.86	124.81	112.40
1	A	342	MET	CA-CB-CG	-8.80	98.34	113.30
1	B	136	PHE	CA-CB-CG	8.76	134.92	113.90
1	B	277	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	B	165	ILE	O-C-N	8.73	136.67	122.70
1	A	385	ASN	CA-CB-CG	8.72	132.58	113.40
1	A	75	ASP	CB-CG-OD2	8.71	126.14	118.30
1	A	216	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	361	LYS	CA-C-O	8.68	138.34	120.10
1	A	235	ASP	CB-CA-C	8.67	127.74	110.40
1	B	302	GLY	O-C-N	-8.61	108.92	122.70
1	A	188	ASP	CA-C-O	-8.60	102.03	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	ILE	CB-CA-C	8.57	128.74	111.60
1	A	68	ASP	CA-CB-CG	8.57	132.24	113.40
1	B	68	ASP	CB-CG-OD2	-8.56	110.59	118.30
1	B	152	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	B	400	ILE	CB-CA-C	8.55	128.69	111.60
1	B	54	ASN	C-N-CA	8.49	142.91	121.70
1	B	346	ASP	O-C-N	8.47	136.26	122.70
1	B	346	ASP	CA-CB-CG	8.47	132.04	113.40
1	B	430	HIS	CA-CB-CG	-8.46	99.21	113.60
1	B	246	TYR	CB-CG-CD2	-8.44	115.94	121.00
1	A	419	ASP	CB-CG-OD1	8.42	125.88	118.30
1	B	313	ARG	NH1-CZ-NH2	-8.42	110.14	119.40
1	A	45	PHE	CB-CA-C	8.38	127.17	110.40
1	B	130	GLU	CB-CG-CD	8.37	136.81	114.20
1	B	22	GLU	OE1-CD-OE2	8.37	133.34	123.30
1	A	236	ASP	CB-CG-OD1	8.32	125.79	118.30
1	B	231	ASN	OD1-CG-ND2	8.29	140.97	121.90
1	B	57	VAL	CA-CB-CG1	8.28	123.32	110.90
1	B	441	PRO	CA-N-CD	-8.26	99.94	111.50
1	A	387	ASN	N-CA-CB	-8.24	95.77	110.60
1	B	154	GLU	CG-CD-OE2	8.23	134.76	118.30
1	B	5	SER	CA-C-N	-8.22	99.11	117.20
1	A	310	LYS	N-CA-CB	8.22	125.39	110.60
1	A	78	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	336	ASP	CA-C-O	8.20	137.31	120.10
1	A	131	ALA	CB-CA-C	8.19	122.39	110.10
1	B	34	ALA	N-CA-CB	8.18	121.55	110.10
1	A	70	LEU	O-C-N	8.17	135.78	122.70
1	B	418	ARG	CD-NE-CZ	8.17	135.04	123.60
1	A	408	ARG	C-N-CA	8.16	142.11	121.70
1	B	249	GLU	C-N-CA	8.15	142.09	121.70
1	B	183	PHE	N-CA-CB	8.14	125.26	110.60
1	A	54	ASN	N-CA-CB	-8.14	95.95	110.60
1	B	342	MET	CB-CA-C	8.14	126.67	110.40
1	A	294	VAL	CA-CB-CG1	8.12	123.09	110.90
1	A	395	GLY	CA-C-O	8.11	135.19	120.60
1	B	102	ALA	N-CA-CB	8.11	121.45	110.10
1	B	429	GLU	CB-CG-CD	8.10	136.07	114.20
1	B	273	THR	CA-CB-CG2	8.08	123.71	112.40
1	B	452	ARG	CD-NE-CZ	8.06	134.89	123.60
1	B	384	GLY	C-N-CA	8.06	141.85	121.70
1	A	7	TYR	CB-CG-CD1	8.05	125.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	438	GLU	CA-CB-CG	8.04	131.08	113.40
1	B	141	VAL	N-CA-CB	8.03	129.17	111.50
1	A	396	ALA	N-CA-CB	-8.03	98.86	110.10
1	B	206	ASP	O-C-N	8.03	135.55	122.70
1	A	337	ARG	C-N-CA	8.02	141.76	121.70
1	B	263	ASP	CB-CG-OD1	8.02	125.52	118.30
1	B	276	ARG	CD-NE-CZ	-7.98	112.42	123.60
1	A	335	SER	O-C-N	-7.98	109.93	122.70
1	B	278	ARG	N-CA-CB	-7.98	96.23	110.60
1	A	6	ARG	N-CA-CB	7.94	124.90	110.60
1	B	95	THR	N-CA-CB	7.94	125.38	110.30
1	A	91	ASP	CB-CG-OD1	7.93	125.44	118.30
1	B	14	GLU	CB-CG-CD	7.93	135.60	114.20
1	B	412	GLN	CA-CB-CG	7.93	130.84	113.40
1	A	337	ARG	CA-C-O	7.92	136.74	120.10
1	B	259	ALA	CB-CA-C	7.92	121.98	110.10
1	B	119	GLU	CA-CB-CG	7.90	130.78	113.40
1	A	117	ASP	O-C-N	7.89	135.32	122.70
1	A	343	LEU	CB-CA-C	7.88	125.18	110.20
1	B	181	HIS	CA-CB-CG	7.87	126.98	113.60
1	B	219	GLN	C-N-CA	7.87	141.37	121.70
1	B	322	THR	CA-C-N	-7.85	100.51	116.20
1	B	442	GLY	CA-C-O	7.85	134.72	120.60
1	B	36	TYR	CA-CB-CG	7.84	128.29	113.40
1	A	276	ARG	CG-CD-NE	7.82	128.22	111.80
1	A	36	TYR	CB-CG-CD1	-7.82	116.31	121.00
1	B	7	TYR	O-C-N	-7.79	110.24	122.70
1	A	410	LEU	CB-CA-C	7.79	125.00	110.20
1	B	171	LEU	O-C-N	7.78	135.15	122.70
1	A	116	GLY	N-CA-C	-7.77	93.69	113.10
1	A	5	SER	N-CA-CB	-7.75	98.88	110.50
1	A	408	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	B	47	ALA	N-CA-CB	7.75	120.94	110.10
1	A	435	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	A	293	ALA	N-CA-CB	-7.72	99.29	110.10
1	A	298	GLN	O-C-N	7.72	135.06	122.70
1	A	137	ASP	CA-CB-CG	7.71	130.35	113.40
1	A	366	ILE	N-CA-C	-7.70	90.20	111.00
1	B	243	ARG	N-CA-CB	7.70	124.46	110.60
1	A	263	ASP	O-C-N	-7.70	110.12	123.20
1	B	160	VAL	CB-CA-C	7.69	126.01	111.40
1	B	241	ILE	CA-CB-CG2	7.68	126.26	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	TYR	CA-C-N	7.68	134.09	117.20
1	B	321	HIS	O-C-N	7.67	134.98	122.70
1	B	226	LYS	CA-CB-CG	7.67	130.27	113.40
1	B	262	VAL	C-N-CA	7.67	140.86	121.70
1	A	303	TYR	CB-CG-CD1	7.66	125.60	121.00
1	A	85	TYR	CB-CG-CD2	7.65	125.59	121.00
1	A	157	GLY	N-CA-C	-7.65	93.98	113.10
1	A	255	ALA	C-N-CA	7.64	140.81	121.70
1	A	245	GLU	CG-CD-OE1	7.64	133.59	118.30
1	A	134	ALA	CB-CA-C	-7.62	98.67	110.10
1	B	95	THR	N-CA-C	-7.62	90.44	111.00
1	A	293	ALA	CB-CA-C	7.58	121.47	110.10
1	B	235	ASP	CB-CG-OD1	7.56	125.11	118.30
1	B	202	ALA	N-CA-CB	-7.56	99.51	110.10
1	B	221	GLU	CB-CG-CD	7.55	134.59	114.20
1	A	105	LEU	C-N-CA	7.55	140.57	121.70
1	A	306	PHE	C-N-CA	7.53	140.53	121.70
1	B	157	GLY	N-CA-C	-7.53	94.27	113.10
1	A	368	SER	N-CA-CB	-7.53	99.21	110.50
1	B	222	THR	N-CA-CB	7.53	124.60	110.30
1	A	409	SER	N-CA-CB	-7.53	99.21	110.50
1	B	136	PHE	C-N-CA	7.52	140.50	121.70
1	A	176	PHE	C-N-CA	7.50	140.46	121.70
1	B	66	GLY	CA-C-O	7.49	134.08	120.60
1	A	429	GLU	CG-CD-OE1	7.49	133.28	118.30
1	B	199	GLN	N-CA-CB	7.48	124.06	110.60
1	B	235	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	B	310	LYS	CA-CB-CG	7.47	129.83	113.40
1	B	360	MET	CA-C-O	7.47	135.78	120.10
1	B	7	TYR	N-CA-C	7.46	131.15	111.00
1	B	438	GLU	CG-CD-OE1	-7.45	103.40	118.30
1	A	133	ARG	N-CA-CB	7.45	124.01	110.60
1	B	186	GLY	C-N-CA	7.44	137.93	122.30
1	A	67	VAL	N-CA-CB	-7.44	95.14	111.50
1	A	199	GLN	N-CA-CB	7.43	123.97	110.60
1	B	264	GLY	CA-C-O	-7.43	107.23	120.60
1	A	270	ALA	N-CA-CB	7.42	120.49	110.10
1	B	188	ASP	N-CA-C	7.41	131.01	111.00
1	B	290	GLY	C-N-CA	7.41	140.22	121.70
1	A	337	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	263	ASP	CB-CG-OD1	-7.40	111.64	118.30
1	B	220	ASP	C-N-CA	7.40	140.20	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	SER	N-CA-CB	7.40	121.60	110.50
1	A	312	ALA	N-CA-CB	-7.38	99.76	110.10
1	A	296	SER	N-CA-CB	7.38	121.57	110.50
1	B	161	VAL	N-CA-CB	7.38	127.73	111.50
1	A	433	LEU	CA-C-N	7.37	133.42	117.20
1	B	322	THR	C-N-CA	7.37	137.77	122.30
1	A	85	TYR	CB-CA-C	-7.36	95.67	110.40
1	A	28	TYR	CB-CG-CD1	-7.35	116.59	121.00
1	B	260	LEU	C-N-CA	7.35	140.08	121.70
1	B	292	GLY	N-CA-C	-7.34	94.74	113.10
1	B	284	LEU	O-C-N	-7.31	111.01	122.70
1	A	403	PRO	O-C-N	-7.30	111.02	122.70
1	A	103	SER	C-N-CA	7.30	139.94	121.70
1	A	361	LYS	O-C-N	-7.28	111.05	122.70
1	A	264	GLY	N-CA-C	7.28	131.30	113.10
1	A	301	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	78	ARG	N-CA-CB	7.26	123.67	110.60
1	A	405	ALA	CB-CA-C	-7.25	99.23	110.10
1	A	371	MET	CB-CA-C	7.25	124.89	110.40
1	B	441	PRO	N-CA-CB	-7.24	94.62	103.30
1	B	425	ASP	N-CA-CB	-7.23	97.58	110.60
1	A	361	LYS	N-CA-CB	-7.23	97.58	110.60
1	B	379	PHE	CB-CG-CD2	-7.23	115.74	120.80
1	A	403	PRO	CA-C-O	7.22	137.53	120.20
1	B	38	TYR	CB-CG-CD1	-7.22	116.67	121.00
1	B	177	ALA	C-N-CA	7.22	139.75	121.70
1	A	379	PHE	CB-CG-CD2	-7.21	115.75	120.80
1	A	304	THR	CA-CB-CG2	7.20	122.48	112.40
1	B	345	GLN	CB-CG-CD	7.19	130.30	111.60
1	B	303	TYR	N-CA-C	-7.18	91.61	111.00
1	A	135	LEU	CB-CA-C	7.17	123.83	110.20
1	A	354	ARG	O-C-N	7.17	134.17	122.70
1	B	369	GLY	N-CA-C	7.17	131.03	113.10
1	B	16	ASP	CA-CB-CG	7.17	129.17	113.40
1	B	277	ARG	NH1-CZ-NH2	-7.16	111.52	119.40
1	A	361	LYS	C-N-CA	7.15	139.59	121.70
1	B	397	PHE	N-CA-CB	7.14	123.46	110.60
1	B	273	THR	OG1-CB-CG2	-7.13	93.59	110.00
1	A	251	PHE	O-C-N	-7.13	111.08	123.20
1	A	231	ASN	CB-CG-OD1	-7.12	107.36	121.60
1	B	87	VAL	CA-CB-CG2	7.11	121.57	110.90
1	B	246	TYR	CB-CG-CD1	7.08	125.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	LYS	CD-CE-NZ	7.08	127.98	111.70
1	B	78	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	132	TYR	CB-CG-CD2	7.04	125.22	121.00
1	A	432	GLU	N-CA-CB	-7.03	97.95	110.60
1	B	99	ALA	CB-CA-C	7.02	120.62	110.10
1	B	10	LEU	C-N-CA	7.01	139.24	121.70
1	A	156	ASP	CB-CA-C	-7.01	96.37	110.40
1	A	185	LEU	N-CA-C	-7.01	92.08	111.00
1	B	410	LEU	CA-CB-CG	7.01	131.42	115.30
1	B	15	GLU	CG-CD-OE2	-7.00	104.30	118.30
1	B	10	LEU	CA-C-N	6.97	132.54	117.20
1	B	185	LEU	CA-C-N	6.96	130.12	116.20
1	A	240	ILE	C-N-CA	6.95	139.06	121.70
1	A	420	GLY	C-N-CA	6.94	139.05	121.70
1	A	347	GLU	OE1-CD-OE2	-6.94	114.98	123.30
1	B	368	SER	CA-C-O	6.93	134.66	120.10
1	A	17	LEU	C-N-CA	6.93	139.02	121.70
1	A	344	THR	C-N-CA	6.93	139.01	121.70
1	B	143	ILE	O-C-N	-6.92	111.63	122.70
1	A	270	ALA	O-C-N	6.91	133.76	122.70
1	A	65	ARG	CD-NE-CZ	6.90	133.26	123.60
1	A	186	GLY	CA-C-O	-6.90	108.18	120.60
1	A	379	PHE	CB-CG-CD1	6.90	125.63	120.80
1	B	236	ASP	N-CA-CB	-6.90	98.18	110.60
1	A	368	SER	CA-C-O	6.90	134.58	120.10
1	A	78	ARG	C-N-CA	6.89	138.94	121.70
1	A	361	LYS	CD-CE-NZ	6.87	127.50	111.70
1	B	224	GLU	CG-CD-OE1	6.86	132.03	118.30
1	A	145	ALA	CA-C-O	6.84	134.46	120.10
1	B	216	ARG	CB-CA-C	6.84	124.07	110.40
1	A	164	ILE	CB-CA-C	6.83	125.27	111.60
1	A	289	ALA	N-CA-CB	6.82	119.65	110.10
1	B	190	ILE	CB-CG1-CD1	6.82	132.99	113.90
1	A	342	MET	CG-SD-CE	-6.81	89.30	100.20
1	B	96	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	54	ASN	CA-CB-CG	6.80	128.36	113.40
1	A	164	ILE	O-C-N	-6.80	111.82	122.70
1	B	102	ALA	CA-C-O	-6.80	105.83	120.10
1	B	293	ALA	C-N-CA	6.78	138.66	121.70
1	A	371	MET	CA-CB-CG	6.78	124.83	113.30
1	A	418	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	B	140	SER	N-CA-CB	6.78	120.67	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ALA	O-C-N	-6.78	111.86	122.70
1	B	163	THR	CA-C-N	-6.76	102.33	117.20
1	B	192	ASN	CB-CA-C	6.76	123.92	110.40
1	A	194	GLU	CA-C-N	6.74	135.98	117.10
1	B	16	ASP	OD1-CG-OD2	-6.74	110.49	123.30
1	A	6	ARG	NH1-CZ-NH2	-6.73	111.99	119.40
1	A	163	THR	CA-C-N	-6.73	102.39	117.20
1	B	162	GLY	CA-C-N	-6.73	102.39	117.20
1	A	367	ILE	CA-C-O	6.73	134.23	120.10
1	B	86	PRO	O-C-N	-6.72	111.94	122.70
1	A	178	GLU	O-C-N	6.72	133.44	122.70
1	A	24	VAL	CA-CB-CG2	6.71	120.97	110.90
1	A	296	SER	N-CA-C	-6.71	92.89	111.00
1	A	336	ASP	O-C-N	-6.71	111.97	122.70
1	B	192	ASN	N-CA-CB	6.70	122.66	110.60
1	B	137	ASP	CB-CG-OD1	-6.70	112.27	118.30
1	A	176	PHE	CA-C-N	6.69	131.92	117.20
1	A	181	HIS	O-C-N	6.69	133.40	122.70
1	A	221	GLU	CB-CA-C	-6.69	97.02	110.40
1	B	313	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	B	120	TYR	CG-CD2-CE2	6.68	126.65	121.30
1	A	414	TRP	C-N-CA	6.66	138.35	121.70
1	A	6	ARG	CA-CB-CG	6.65	128.04	113.40
1	A	50	SER	N-CA-CB	-6.65	100.52	110.50
1	B	276	ARG	NH1-CZ-NH2	-6.65	112.08	119.40
1	B	163	THR	O-C-N	6.65	133.34	122.70
1	B	217	ARG	CB-CG-CD	6.64	128.88	111.60
1	A	376	MET	CG-SD-CE	6.63	110.81	100.20
1	B	180	CYS	N-CA-CB	-6.62	98.68	110.60
1	B	216	ARG	C-N-CA	6.61	138.23	121.70
1	B	310	LYS	CB-CA-C	6.58	123.57	110.40
1	A	188	ASP	N-CA-C	6.58	128.75	111.00
1	B	136	PHE	CA-C-O	6.57	133.90	120.10
1	A	404	VAL	O-C-N	6.57	133.21	122.70
1	B	435	ARG	CD-NE-CZ	6.57	132.79	123.60
1	A	368	SER	C-N-CA	6.56	136.08	122.30
1	B	443	ASP	CA-C-O	6.56	133.88	120.10
1	B	154	GLU	C-N-CA	6.55	138.07	121.70
1	A	317	ALA	N-CA-C	-6.54	93.35	111.00
1	A	342	MET	CB-CG-SD	-6.54	92.79	112.40
1	B	230	ALA	C-N-CA	6.54	138.04	121.70
1	A	260	LEU	N-CA-CB	-6.53	97.33	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	ASN	N-CA-C	-6.53	93.37	111.00
1	A	253	GLU	CA-CB-CG	6.52	127.74	113.40
1	B	393	GLY	N-CA-C	-6.51	96.82	113.10
1	B	381	GLU	OE1-CD-OE2	-6.51	115.49	123.30
1	B	283	PHE	CA-CB-CG	6.51	129.52	113.90
1	A	87	VAL	CA-CB-CG1	6.50	120.66	110.90
1	B	162	GLY	CA-C-O	6.50	132.30	120.60
1	B	185	LEU	CB-CA-C	6.50	122.55	110.20
1	A	115	MET	CA-C-O	6.49	133.73	120.10
1	A	278	ARG	NH1-CZ-NH2	-6.49	112.26	119.40
1	B	260	LEU	O-C-N	-6.48	112.33	122.70
1	A	314	LEU	N-CA-CB	6.47	123.34	110.40
1	A	9	ASN	CA-CB-CG	-6.47	99.17	113.40
1	A	101	ILE	CA-CB-CG2	6.45	123.81	110.90
1	B	388	VAL	CA-CB-CG2	6.45	120.58	110.90
1	B	213	ASP	CB-CA-C	6.44	123.29	110.40
1	A	117	ASP	CB-CA-C	-6.43	97.53	110.40
1	B	346	ASP	N-CA-C	-6.43	93.63	111.00
1	B	408	ARG	NH1-CZ-NH2	6.43	126.48	119.40
1	B	394	GLY	N-CA-C	6.43	129.16	113.10
1	A	185	LEU	CB-CA-C	6.42	122.41	110.20
1	B	126	PHE	CA-CB-CG	6.41	129.29	113.90
1	B	346	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	251	PHE	CA-C-O	6.41	133.56	120.10
1	B	372	ASN	CB-CA-C	6.41	123.22	110.40
1	A	428	ARG	N-CA-CB	-6.40	99.08	110.60
1	A	298	GLN	CA-CB-CG	6.40	127.48	113.40
1	B	127	TYR	CB-CG-CD1	-6.40	117.16	121.00
1	B	179	ALA	CB-CA-C	6.38	119.67	110.10
1	A	8	VAL	CG1-CB-CG2	-6.37	100.71	110.90
1	A	65	ARG	NH1-CZ-NH2	-6.36	112.40	119.40
1	B	121	ALA	N-CA-CB	6.35	118.99	110.10
1	A	9	ASN	O-C-N	6.34	132.84	122.70
1	A	408	ARG	CA-C-O	6.34	133.41	120.10
1	A	11	ALA	N-CA-CB	6.32	118.95	110.10
1	A	213	ASP	CA-CB-CG	6.32	127.30	113.40
1	A	217	ARG	NH1-CZ-NH2	-6.31	112.45	119.40
1	A	315	GLN	N-CA-CB	-6.31	99.24	110.60
1	A	422	PRO	O-C-N	6.31	132.79	122.70
1	B	62	ASP	O-C-N	6.31	132.79	122.70
1	B	245	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	B	425	ASP	CB-CG-OD1	6.31	123.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	PHE	N-CA-CB	-6.30	99.25	110.60
1	A	303	TYR	CG-CD2-CE2	6.29	126.34	121.30
1	A	232	ILE	CA-C-O	-6.29	106.89	120.10
1	A	229	SER	CB-CA-C	-6.29	98.16	110.10
1	B	438	GLU	OE1-CD-OE2	6.28	130.84	123.30
1	B	263	ASP	OD1-CG-OD2	-6.28	111.37	123.30
1	A	48	GLU	CB-CG-CD	6.27	131.13	114.20
1	A	354	ARG	CA-C-O	-6.27	106.94	120.10
1	A	131	ALA	C-N-CA	6.27	137.37	121.70
1	B	258	VAL	CA-CB-CG2	6.26	120.29	110.90
1	B	28	TYR	CB-CA-C	-6.26	97.88	110.40
1	A	211	VAL	CG1-CB-CG2	-6.25	100.90	110.90
1	A	201	PHE	CB-CG-CD1	6.25	125.17	120.80
1	A	93	ASN	CB-CA-C	6.23	122.85	110.40
1	A	364	THR	N-CA-C	6.23	127.81	111.00
1	A	204	LEU	CB-CG-CD2	-6.22	100.43	111.00
1	A	355	GLN	CG-CD-NE2	6.22	131.62	116.70
1	B	223	GLY	N-CA-C	-6.21	97.58	113.10
1	B	262	VAL	CA-C-O	6.20	133.12	120.10
1	B	17	LEU	C-N-CA	6.20	137.20	121.70
1	B	120	TYR	CZ-CE2-CD2	-6.20	114.22	119.80
1	A	176	PHE	CB-CA-C	6.19	122.78	110.40
1	A	314	LEU	CB-CG-CD1	6.19	121.52	111.00
1	B	23	HIS	N-CA-CB	-6.19	99.46	110.60
1	A	54	ASN	O-C-N	6.18	132.59	122.70
1	B	445	ASP	CB-CA-C	6.18	122.76	110.40
1	A	25	LEU	CA-CB-CG	6.18	129.51	115.30
1	A	50	SER	N-CA-C	6.18	127.69	111.00
1	A	315	GLN	O-C-N	-6.18	112.70	123.20
1	A	316	GLY	O-C-N	6.18	132.58	122.70
1	A	143	ILE	CA-C-O	-6.17	107.14	120.10
1	B	204	LEU	O-C-N	6.17	132.57	122.70
1	A	245	GLU	CG-CD-OE2	-6.16	105.98	118.30
1	B	154	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	A	314	LEU	CB-CA-C	6.14	121.88	110.20
1	B	14	GLU	CA-CB-CG	6.14	126.90	113.40
1	A	90	PHE	CB-CG-CD1	6.13	125.09	120.80
1	A	152	ARG	O-C-N	6.12	132.74	121.10
1	B	57	VAL	O-C-N	6.12	132.50	122.70
1	B	64	THR	CB-CA-C	-6.12	95.06	111.60
1	B	130	GLU	CA-C-O	6.12	132.96	120.10
1	A	126	PHE	CA-CB-CG	6.12	128.59	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	B	309	CYS	N-CA-CB	-6.11	99.60	110.60
1	B	357	TRP	CB-CA-C	6.11	122.62	110.40
1	A	183	PHE	N-CA-CB	6.11	121.59	110.60
1	A	311	MET	C-N-CA	6.11	136.96	121.70
1	B	301	ARG	CB-CG-CD	6.11	127.48	111.60
1	A	361	LYS	N-CA-C	6.10	127.47	111.00
1	A	22	GLU	OE1-CD-OE2	6.09	130.61	123.30
1	A	181	HIS	CA-CB-CG	6.09	123.95	113.60
1	A	277	ARG	CB-CA-C	6.09	122.58	110.40
1	B	64	THR	N-CA-CB	6.09	121.87	110.30
1	A	17	LEU	CB-CA-C	6.09	121.77	110.20
1	A	142	ASN	CA-CB-CG	6.09	126.79	113.40
1	A	400	ILE	CA-C-O	-6.07	107.35	120.10
1	B	100	MET	CG-SD-CE	-6.07	90.49	100.20
1	A	161	VAL	CG1-CB-CG2	6.05	120.59	110.90
1	A	97	GLY	O-C-N	6.04	132.37	122.70
1	B	93	ASN	OD1-CG-ND2	-6.04	108.01	121.90
1	B	203	PRO	O-C-N	-6.04	113.04	122.70
1	A	185	LEU	CA-CB-CG	6.03	129.16	115.30
1	A	94	ILE	CB-CA-C	6.02	123.65	111.60
1	B	133	ARG	C-N-CA	6.01	136.74	121.70
1	A	311	MET	CA-CB-CG	6.01	123.52	113.30
1	A	263	ASP	CA-C-O	6.01	132.72	120.10
1	A	251	PHE	C-N-CA	6.00	134.91	122.30
1	A	423	VAL	N-CA-CB	-6.00	98.30	111.50
1	B	70	LEU	CA-C-O	-5.99	107.53	120.10
1	B	249	GLU	CA-C-O	5.98	132.67	120.10
1	B	418	ARG	CA-CB-CG	5.97	126.53	113.40
1	A	144	SER	N-CA-CB	5.97	119.45	110.50
1	B	448	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	A	98	LYS	CA-CB-CG	5.96	126.52	113.40
1	B	357	TRP	CA-C-O	5.96	132.62	120.10
1	A	107	LEU	CA-CB-CG	5.96	129.00	115.30
1	A	122	LYS	CB-CG-CD	5.95	127.08	111.60
1	A	85	TYR	CD1-CE1-CZ	-5.95	114.45	119.80
1	A	66	GLY	C-N-CA	5.93	136.54	121.70
1	A	160	VAL	N-CA-C	-5.93	94.98	111.00
1	A	100	MET	CG-SD-CE	5.92	109.67	100.20
1	B	161	VAL	CA-C-N	-5.92	104.36	116.20
1	A	223	GLY	C-N-CA	5.92	136.49	121.70
1	A	171	LEU	CB-CA-C	5.92	121.44	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	HIS	CB-CA-C	5.91	122.23	110.40
1	A	275	ALA	CB-CA-C	5.90	118.95	110.10
1	B	234	ALA	N-CA-CB	-5.90	101.84	110.10
1	B	301	ARG	CD-NE-CZ	-5.90	115.34	123.60
1	A	10	LEU	N-CA-C	-5.90	95.08	111.00
1	B	79	GLU	CA-CB-CG	5.89	126.37	113.40
1	A	156	ASP	CA-CB-CG	5.89	126.35	113.40
1	B	20	GLY	N-CA-C	-5.88	98.39	113.10
1	B	157	GLY	CA-C-O	-5.88	110.01	120.60
1	B	389	ILE	O-C-N	5.88	132.10	122.70
1	B	115	MET	CB-CG-SD	-5.87	94.78	112.40
1	A	222	THR	O-C-N	-5.87	113.22	123.20
1	B	389	ILE	CA-C-O	-5.87	107.78	120.10
1	A	94	ILE	CA-CB-CG1	5.86	122.14	111.00
1	B	216	ARG	N-CA-C	-5.86	95.17	111.00
1	B	446	GLN	C-N-CA	5.86	136.35	121.70
1	A	258	VAL	N-CA-CB	5.86	124.38	111.50
1	B	165	ILE	CA-C-N	-5.86	104.32	117.20
1	A	296	SER	CA-CB-OG	5.85	127.01	111.20
1	A	428	ARG	N-CA-C	5.85	126.79	111.00
1	A	129	PRO	O-C-N	-5.85	113.34	122.70
1	B	176	PHE	N-CA-CB	5.85	121.12	110.60
1	B	307	VAL	CA-CB-CG2	5.84	119.66	110.90
1	B	376	MET	CA-CB-CG	5.84	123.23	113.30
1	B	443	ASP	OD1-CG-OD2	5.83	134.39	123.30
1	B	207	THR	CA-CB-OG1	-5.83	96.76	109.00
1	B	347	GLU	N-CA-CB	5.83	121.10	110.60
1	A	76	GLU	CG-CD-OE1	-5.82	106.66	118.30
1	A	298	GLN	CG-CD-NE2	-5.82	102.72	116.70
1	B	68	ASP	CB-CA-C	-5.82	98.75	110.40
1	B	341	TYR	CA-C-N	-5.82	104.39	117.20
1	A	152	ARG	NH1-CZ-NH2	-5.81	113.00	119.40
1	A	255	ALA	O-C-N	-5.81	113.40	122.70
1	B	109	MET	CA-CB-CG	5.81	123.18	113.30
1	B	168	LYS	CA-CB-CG	5.80	126.16	113.40
1	A	208	ILE	CB-CG1-CD1	5.80	130.14	113.90
1	A	277	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	B	273	THR	CB-CA-C	5.79	127.23	111.60
1	A	10	LEU	CB-CA-C	5.78	121.18	110.20
1	A	29	ILE	C-N-CA	5.78	136.14	121.70
1	A	125	ASP	CA-C-O	-5.78	107.97	120.10
1	A	38	TYR	N-CA-CB	5.77	120.99	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	ARG	CD-NE-CZ	-5.77	115.52	123.60
1	A	303	TYR	N-CA-CB	5.77	120.98	110.60
1	A	221	GLU	CA-CB-CG	5.76	126.08	113.40
1	B	347	GLU	OE1-CD-OE2	-5.76	116.38	123.30
1	B	88	ALA	N-CA-CB	-5.76	102.04	110.10
1	A	78	ARG	CA-CB-CG	5.75	126.06	113.40
1	B	224	GLU	CB-CG-CD	5.75	129.74	114.20
1	B	91	ASP	CB-CA-C	5.75	121.89	110.40
1	A	418	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	235	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	433	LEU	O-C-N	-5.73	113.53	122.70
1	B	288	ARG	N-CA-C	-5.71	95.58	111.00
1	B	272	ILE	CA-CB-CG2	5.70	122.31	110.90
1	B	184	TRP	N-CA-CB	5.70	120.86	110.60
1	A	12	LEU	CB-CA-C	5.70	121.03	110.20
1	A	207	THR	O-C-N	5.70	131.81	122.70
1	B	443	ASP	N-CA-C	-5.70	95.62	111.00
1	A	143	ILE	CA-C-N	5.69	129.72	117.20
1	B	38	TYR	CA-CB-CG	-5.69	102.59	113.40
1	A	185	LEU	CA-C-O	-5.68	108.17	120.10
1	B	324	THR	CA-CB-CG2	5.68	120.35	112.40
1	B	238	PHE	CA-C-O	-5.67	108.18	120.10
1	A	391	THR	N-CA-C	-5.67	95.70	111.00
1	A	120	TYR	CB-CG-CD2	5.67	124.40	121.00
1	B	179	ALA	C-N-CA	5.66	135.86	121.70
1	B	249	GLU	O-C-N	-5.66	113.65	122.70
1	A	236	ASP	N-CA-C	-5.65	95.73	111.00
1	A	120	TYR	CA-CB-CG	5.65	124.14	113.40
1	A	99	ALA	CA-C-O	-5.65	108.24	120.10
1	A	344	THR	CA-CB-OG1	-5.64	97.15	109.00
1	A	366	ILE	N-CA-CB	5.64	123.78	110.80
1	A	93	ASN	O-C-N	-5.64	113.67	122.70
1	B	194	GLU	CG-CD-OE1	-5.64	107.02	118.30
1	A	368	SER	CA-C-N	-5.64	104.93	116.20
1	B	91	ASP	N-CA-CB	-5.64	100.45	110.60
1	B	157	GLY	O-C-N	5.63	132.78	123.20
1	B	267	ALA	N-CA-CB	5.63	117.98	110.10
1	A	189	PHE	C-N-CA	-5.63	107.64	121.70
1	A	254	ASN	O-C-N	-5.62	113.71	122.70
1	A	367	ILE	CA-C-N	-5.62	104.83	117.20
1	A	418	ARG	NH1-CZ-NH2	5.62	125.58	119.40
1	B	446	GLN	CB-CG-CD	5.62	126.21	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	VAL	C-N-CA	5.62	135.74	121.70
1	A	145	ALA	C-N-CA	5.61	135.72	121.70
1	A	158	GLY	N-CA-C	5.61	127.11	113.10
1	A	301	ARG	N-CA-C	5.60	126.12	111.00
1	B	251	PHE	CB-CA-C	5.60	121.59	110.40
1	A	246	TYR	CZ-CE2-CD2	5.59	124.83	119.80
1	B	240	ILE	CA-CB-CG2	5.59	122.07	110.90
1	A	223	GLY	CA-C-O	5.58	130.65	120.60
1	A	265	TYR	CD1-CG-CD2	-5.58	111.77	117.90
1	B	133	ARG	NH1-CZ-NH2	5.57	125.53	119.40
1	B	141	VAL	CA-CB-CG2	5.57	119.26	110.90
1	A	48	GLU	CA-C-O	5.57	131.80	120.10
1	B	20	GLY	C-N-CA	5.57	133.99	122.30
1	B	36	TYR	CB-CG-CD1	5.56	124.34	121.00
1	B	14	GLU	OE1-CD-OE2	-5.56	116.62	123.30
1	B	85	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	B	310	LYS	CB-CG-CD	5.56	126.05	111.60
1	A	176	PHE	CA-CB-CG	-5.56	100.56	113.90
1	A	289	ALA	CA-C-N	-5.56	105.08	116.20
1	A	116	GLY	O-C-N	5.55	131.59	122.70
1	B	132	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	A	15	GLU	CG-CD-OE2	-5.55	107.21	118.30
1	B	209	ALA	CB-CA-C	5.55	118.42	110.10
1	A	160	VAL	CB-CA-C	5.54	121.93	111.40
1	B	97	GLY	CA-C-O	5.54	130.58	120.60
1	A	353	TYR	O-C-N	5.54	131.57	122.70
1	B	353	TYR	N-CA-CB	-5.54	100.62	110.60
1	A	265	TYR	N-CA-CB	5.54	120.57	110.60
1	A	231	ASN	CA-C-O	5.53	131.72	120.10
1	B	431	LYS	CB-CA-C	-5.53	99.34	110.40
1	A	410	LEU	CB-CG-CD2	-5.52	101.61	111.00
1	B	195	PRO	O-C-N	-5.52	113.86	122.70
1	A	22	GLU	C-N-CA	5.52	135.50	121.70
1	A	210	LEU	CB-CG-CD1	5.52	120.39	111.00
1	B	294	VAL	O-C-N	-5.52	113.88	122.70
1	B	194	GLU	OE1-CD-OE2	-5.51	116.68	123.30
1	B	217	ARG	C-N-CA	5.50	135.46	121.70
1	B	435	ARG	CA-CB-CG	-5.50	101.30	113.40
1	A	93	ASN	CA-C-O	5.50	131.64	120.10
1	A	16	ASP	CB-CA-C	5.49	121.38	110.40
1	B	341	TYR	CA-C-O	5.49	131.63	120.10
1	A	230	ALA	CA-C-O	5.49	131.62	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	A	210	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	A	72	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	A	133	ARG	CA-C-N	5.47	129.24	117.20
1	A	348	ALA	CB-CA-C	5.47	118.30	110.10
1	A	431	LYS	N-CA-C	5.47	125.76	111.00
1	A	197	GLY	CA-C-O	5.46	130.43	120.60
1	A	72	TYR	CB-CG-CD2	5.46	124.27	121.00
1	A	15	GLU	CB-CA-C	-5.45	99.49	110.40
1	A	288	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	B	194	GLU	CA-CB-CG	5.45	125.39	113.40
1	B	203	PRO	CA-C-O	5.43	133.24	120.20
1	B	362	ALA	CA-C-O	5.43	131.51	120.10
1	A	269	ALA	CB-CA-C	5.43	118.24	110.10
1	A	92	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	53	THR	C-N-CA	5.42	135.26	121.70
1	A	177	ALA	CB-CA-C	5.42	118.23	110.10
1	B	23	HIS	N-CA-C	5.42	125.64	111.00
1	A	179	ALA	CA-C-O	-5.42	108.72	120.10
1	A	226	LYS	CA-CB-CG	5.41	125.31	113.40
1	A	337	ARG	O-C-N	-5.41	114.04	122.70
1	A	120	TYR	N-CA-CB	-5.41	100.86	110.60
1	A	284	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	300	LYS	CB-CG-CD	5.41	125.65	111.60
1	B	395	GLY	C-N-CA	5.41	135.21	121.70
1	A	258	VAL	CA-C-N	-5.40	105.33	117.20
1	B	269	ALA	CB-CA-C	5.40	118.19	110.10
1	A	317	ALA	CA-C-O	-5.39	108.77	120.10
1	A	73	GLU	OE1-CD-OE2	5.39	129.77	123.30
1	B	348	ALA	C-N-CA	5.39	135.17	121.70
1	A	353	TYR	CB-CG-CD1	5.39	124.23	121.00
1	B	350	GLY	N-CA-C	-5.38	99.65	113.10
1	B	205	ARG	CB-CA-C	-5.38	99.64	110.40
1	A	117	ASP	OD1-CG-OD2	5.38	133.51	123.30
1	B	354	ARG	O-C-N	5.37	131.29	122.70
1	A	309	CYS	C-N-CA	5.37	135.12	121.70
1	B	80	LEU	N-CA-C	5.36	125.48	111.00
1	B	80	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	A	352	PHE	CA-CB-CG	5.36	126.75	113.90
1	B	404	VAL	CA-CB-CG1	5.36	118.93	110.90
1	B	363	CYS	N-CA-C	-5.35	96.55	111.00
1	A	253	GLU	CG-CD-OE1	5.35	129.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	ARG	CB-CG-CD	5.35	125.50	111.60
1	B	213	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	B	130	GLU	CA-C-N	-5.34	105.44	117.20
1	A	349	GLN	CA-CB-CG	5.34	125.15	113.40
1	B	354	ARG	CA-C-O	-5.34	108.89	120.10
1	B	386	ALA	C-N-CA	5.34	135.04	121.70
1	A	19	ALA	N-CA-CB	5.33	117.57	110.10
1	B	455	LEU	CA-C-N	-5.33	105.54	116.20
1	A	115	MET	C-N-CA	5.33	133.48	122.30
1	B	47	ALA	O-C-N	5.33	131.22	122.70
1	B	105	LEU	O-C-N	5.33	131.22	122.70
1	A	346	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	69	ALA	CA-C-O	-5.32	108.93	120.10
1	B	156	ASP	N-CA-CB	5.32	120.17	110.60
1	B	285	HIS	CA-CB-CG	-5.32	104.56	113.60
1	A	411	ARG	O-C-N	5.32	131.21	122.70
1	A	303	TYR	CA-CB-CG	5.31	123.48	113.40
1	A	236	ASP	CB-CA-C	5.31	121.01	110.40
1	B	103	SER	N-CA-CB	5.31	118.46	110.50
1	A	336	ASP	N-CA-CB	-5.30	101.05	110.60
1	B	263	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	357	TRP	CB-CA-C	5.30	121.00	110.40
1	A	70	LEU	CB-CA-C	-5.30	100.14	110.20
1	A	78	ARG	O-C-N	-5.30	114.23	122.70
1	A	236	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	91	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	A	8	VAL	CA-C-O	5.29	131.21	120.10
1	A	259	ALA	N-CA-CB	-5.29	102.69	110.10
1	B	254	ASN	N-CA-C	5.29	125.29	111.00
1	A	95	THR	C-N-CA	5.29	134.93	121.70
1	B	382	ASN	O-C-N	-5.29	114.24	122.70
1	A	201	PHE	CA-CB-CG	5.29	126.59	113.90
1	B	106	THR	C-N-CA	5.29	134.91	121.70
1	B	211	VAL	N-CA-C	-5.28	96.73	111.00
1	B	421	VAL	CG1-CB-CG2	-5.28	102.45	110.90
1	B	127	TYR	C-N-CA	5.28	134.89	121.70
1	A	347	GLU	CA-CB-CG	5.28	125.01	113.40
1	A	225	ALA	CA-C-O	5.27	131.17	120.10
1	A	73	GLU	CA-CB-CG	5.26	124.98	113.40
1	B	15	GLU	OE1-CD-OE2	5.26	129.62	123.30
1	A	300	LYS	CB-CA-C	5.26	120.92	110.40
1	B	447	ILE	CB-CA-C	-5.26	101.08	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	THR	CA-C-O	5.26	131.14	120.10
1	B	150	LEU	C-N-CA	5.26	133.34	122.30
1	A	161	VAL	N-CA-CB	5.25	123.05	111.50
1	A	175	PRO	N-CA-C	5.25	125.75	112.10
1	B	64	THR	O-C-N	5.25	131.10	122.70
1	B	217	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
1	B	313	ARG	N-CA-CB	5.25	120.05	110.60
1	A	298	GLN	N-CA-CB	5.25	120.05	110.60
1	B	282	ASN	CA-C-O	-5.25	109.08	120.10
1	A	204	LEU	CB-CA-C	5.24	120.16	110.20
1	B	239	GLU	CA-CB-CG	5.24	124.93	113.40
1	A	76	GLU	OE1-CD-OE2	5.24	129.59	123.30
1	A	346	ASP	C-N-CA	5.24	134.80	121.70
1	B	43	ALA	CA-C-O	5.24	131.10	120.10
1	B	193	ASN	O-C-N	-5.24	114.32	122.70
1	B	160	VAL	CA-CB-CG2	5.24	118.76	110.90
1	A	70	LEU	CA-C-O	-5.23	109.12	120.10
1	B	260	LEU	CA-C-O	5.23	131.09	120.10
1	B	107	LEU	CA-CB-CG	5.23	127.32	115.30
1	B	120	TYR	C-N-CA	5.23	134.76	121.70
1	B	313	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	135	LEU	O-C-N	-5.22	114.35	122.70
1	A	48	GLU	C-N-CA	5.22	134.75	121.70
1	B	6	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	B	215	MET	O-C-N	5.22	131.05	122.70
1	A	75	ASP	CA-C-O	-5.21	109.15	120.10
1	B	278	ARG	CD-NE-CZ	5.21	130.90	123.60
1	B	204	LEU	N-CA-CB	5.21	120.82	110.40
1	A	49	SER	O-C-N	5.20	131.02	122.70
1	A	375	ARG	CD-NE-CZ	5.20	130.88	123.60
1	B	61	ASP	O-C-N	5.20	131.01	122.70
1	B	320	ILE	N-CA-CB	-5.20	98.85	110.80
1	B	76	GLU	O-C-N	5.19	131.01	122.70
1	A	77	ALA	N-CA-CB	-5.19	102.84	110.10
1	B	320	ILE	CA-CB-CG1	5.18	120.84	111.00
1	B	72	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	B	357	TRP	CA-CB-CG	5.17	123.52	113.70
1	A	261	LEU	CB-CG-CD1	5.17	119.78	111.00
1	B	62	ASP	CA-C-N	-5.17	105.83	117.20
1	B	133	ARG	CA-C-O	5.16	130.94	120.10
1	B	427	ALA	C-N-CA	5.16	134.60	121.70
1	B	236	ASP	CB-CG-OD1	-5.16	113.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	SER	N-CA-CB	5.16	118.23	110.50
1	B	146	LEU	N-CA-C	-5.15	97.08	111.00
1	A	360	MET	CA-CB-CG	-5.15	104.54	113.30
1	B	277	ARG	CA-CB-CG	5.15	124.73	113.40
1	B	428	ARG	NH1-CZ-NH2	-5.15	113.73	119.40
1	B	262	VAL	N-CA-CB	5.15	122.83	111.50
1	A	352	PHE	CB-CG-CD2	-5.15	117.20	120.80
1	A	308	HIS	CA-CB-CG	5.15	122.35	113.60
1	B	418	ARG	N-CA-C	-5.14	97.12	111.00
1	B	278	ARG	NH1-CZ-NH2	-5.13	113.75	119.40
1	B	27	ALA	CB-CA-C	5.13	117.80	110.10
1	A	301	ARG	C-N-CA	5.13	133.07	122.30
1	B	201	PHE	CA-CB-CG	5.13	126.21	113.90
1	A	11	ALA	CB-CA-C	-5.13	102.41	110.10
1	B	167	PRO	N-CD-CG	-5.13	95.51	103.20
1	B	321	HIS	CA-C-N	-5.13	105.92	117.20
1	B	371	MET	CA-CB-CG	-5.12	104.59	113.30
1	A	65	ARG	CG-CD-NE	5.12	122.56	111.80
1	B	211	VAL	N-CA-CB	5.12	122.76	111.50
1	B	199	GLN	N-CA-C	-5.12	97.18	111.00
1	A	236	ASP	N-CA-CB	5.11	119.80	110.60
1	A	239	GLU	C-N-CA	5.11	134.48	121.70
1	A	432	GLU	OE1-CD-OE2	-5.11	117.16	123.30
1	B	164	ILE	CB-CA-C	-5.11	101.37	111.60
1	A	39	VAL	O-C-N	5.11	130.88	122.70
1	A	269	ALA	N-CA-CB	-5.11	102.95	110.10
1	B	33	LYS	N-CA-CB	5.11	119.80	110.60
1	B	263	ASP	CB-CA-C	5.11	120.62	110.40
1	B	231	ASN	CB-CG-ND2	-5.11	104.45	116.70
1	B	366	ILE	CA-CB-CG1	5.11	120.70	111.00
1	A	397	PHE	CB-CG-CD1	5.10	124.37	120.80
1	A	74	VAL	CA-C-N	-5.10	105.98	117.20
1	B	61	ASP	CA-C-N	-5.10	105.99	117.20
1	B	366	ILE	CB-CA-C	5.10	121.79	111.60
1	A	73	GLU	CG-CD-OE2	-5.10	108.11	118.30
1	A	337	ARG	N-CA-CB	5.10	119.77	110.60
1	A	234	ALA	N-CA-CB	-5.09	102.97	110.10
1	B	288	ARG	CA-C-O	-5.09	109.41	120.10
1	A	245	GLU	C-N-CA	5.09	134.42	121.70
1	B	136	PHE	O-C-N	-5.08	114.57	122.70
1	B	151	GLY	C-N-CA	5.08	134.41	121.70
1	A	374	LEU	N-CA-CB	-5.08	100.24	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	PRO	C-N-CA	-5.08	109.00	121.70
1	A	347	GLU	CG-CD-OE1	5.07	128.45	118.30
1	B	399	HIS	CB-CA-C	-5.07	100.25	110.40
1	A	249	GLU	OE1-CD-OE2	5.07	129.38	123.30
1	B	112	ASN	N-CA-CB	-5.07	101.48	110.60
1	B	310	LYS	CA-C-N	-5.06	106.06	117.20
1	B	69	ALA	N-CA-CB	5.06	117.18	110.10
1	B	420	GLY	O-C-N	-5.05	114.61	122.70
1	A	132	TYR	CG-CD1-CE1	5.05	125.34	121.30
1	A	161	VAL	C-N-CA	-5.04	111.71	122.30
1	A	234	ALA	C-N-CA	-5.04	109.09	121.70
1	B	63	PHE	CB-CA-C	5.04	120.49	110.40
1	B	245	GLU	CG-CD-OE2	5.04	128.39	118.30
1	A	303	TYR	CZ-CE2-CD2	-5.04	115.27	119.80
1	B	288	ARG	N-CA-CB	5.04	119.66	110.60
1	A	225	ALA	CB-CA-C	5.03	117.65	110.10
1	B	306	PHE	CZ-CE2-CD2	-5.03	114.06	120.10
1	B	448	TYR	CB-CG-CD2	5.02	124.01	121.00
1	A	290	GLY	N-CA-C	-5.02	100.56	113.10
1	A	348	ALA	C-N-CA	5.02	134.24	121.70
1	A	422	PRO	CA-C-N	-5.01	106.17	117.20
1	A	219	GLN	N-CA-CB	5.01	119.62	110.60
1	A	176	PHE	CA-C-O	-5.01	109.58	120.10
1	A	196	GLN	CA-CB-CG	5.01	124.42	113.40
1	B	408	ARG	CB-CA-C	5.01	120.42	110.40
1	A	341	TYR	CB-CA-C	5.01	120.42	110.40
1	B	457	VAL	CA-CB-CG2	5.01	118.41	110.90
1	A	278	ARG	CG-CD-NE	5.01	122.31	111.80
1	A	435	ARG	CA-C-O	-5.01	109.58	120.10
1	B	241	ILE	O-C-N	-5.01	114.69	122.70
1	A	265	TYR	CG-CD1-CE1	5.00	125.30	121.30
1	B	315	GLN	CG-CD-OE1	-5.00	111.59	121.60
1	B	278	ARG	CB-CG-CD	5.00	124.61	111.60
1	B	286	TYR	N-CA-CB	-5.00	101.60	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	349	GLN	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	GLU	Mainchain
1	A	354	ARG	Sidechain
1	A	433	LEU	Mainchain
1	B	288	ARG	Sidechain
1	B	301	ARG	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	3200	0	3097	469	2
1	B	3385	0	3266	459	2
2	A	67	0	0	3	0
2	B	43	0	0	1	0
All	All	6695	0	6363	871	3

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 67.

All (871) 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:41:THR:CA	1:B:41:THR:CB	1.75	1.61
1:A:164:ILE:CA	1:A:164:ILE:CB	1.74	1.60
1:A:335:SER:HB3	1:A:338:ALA:CB	1.21	1.56
1:A:191:LYS:CD	1:A:191:LYS:CE	1.78	1.56
1:B:190:ILE:C	1:B:191:LYS:N	1.82	1.32
1:A:335:SER:CB	1:A:338:ALA:HB2	1.59	1.32
1:A:335:SER:CB	1:A:338:ALA:CB	2.16	1.22
1:B:166:LYS:HD3	1:B:167:PRO:HA	1.21	1.17
1:B:346:ASP:HB3	1:B:357:TRP:HB2	1.25	1.17
1:A:361:LYS:CE	1:A:361:LYS:CD	2.23	1.16
1:B:457:VAL:O	1:B:457:VAL:HG13	1.30	1.10
1:B:32:PRO:HB3	1:B:41:THR:HG21	1.34	1.10
1:A:309:CYS:HB3	1:A:320:ILE:HD13	1.34	1.07
1:A:156:ASP:HB3	1:A:387:ASN:ND2	1.72	1.03
1:B:323:GLY:O	1:B:324:THR:HB	1.25	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLY:C	1:B:64:THR:HG22	1.79	1.03
1:A:156:ASP:HB3	1:A:387:ASN:HD22	1.18	1.03
1:A:335:SER:HB3	1:A:338:ALA:HB1	1.40	1.02
1:A:439:SER:C	1:A:440:PHE:N	2.16	0.99
1:B:56:GLU:O	1:B:57:VAL:CB	2.09	0.99
1:B:187:GLY:HA2	1:B:411:ARG:HH22	1.28	0.99
1:A:376:MET:SD	1:A:380:PHE:CZ	2.56	0.99
1:B:323:GLY:O	1:B:324:THR:CB	2.10	0.98
1:B:346:ASP:CB	1:B:357:TRP:HB2	1.92	0.98
1:B:14:GLU:HB2	1:B:72:TYR:HE1	1.27	0.97
1:B:457:VAL:O	1:B:457:VAL:CG1	2.01	0.97
1:A:439:SER:C	1:A:440:PHE:CA	2.33	0.97
1:A:169:LEU:O	1:B:51:THR:HG23	1.65	0.96
1:B:56:GLU:O	1:B:57:VAL:HB	1.16	0.95
1:B:38:TYR:HE2	1:B:74:VAL:HG13	1.31	0.94
1:B:59:THR:CG2	1:B:64:THR:HG23	1.98	0.94
1:A:14:GLU:HG2	1:A:18:ILE:HD12	1.50	0.94
1:B:7:TYR:OH	1:B:51:THR:HB	1.68	0.93
1:A:170:GLY:CA	1:B:64:THR:HG22	1.98	0.93
1:A:355:GLN:HE21	1:A:356:SER:N	1.65	0.93
1:B:128:VAL:HG23	1:B:355:GLN:HE22	1.32	0.93
1:A:324:THR:HG21	1:A:336:ASP:HB3	1.52	0.92
1:B:12:LEU:HD12	1:B:17:LEU:HD11	1.49	0.91
1:A:372:ASN:ND2	1:A:375:ARG:HE	1.67	0.91
1:A:439:SER:C	1:A:440:PHE:HA	1.91	0.90
1:A:390:LEU:HD23	1:A:392:ALA:HB2	1.51	0.90
1:A:229:SER:HA	1:A:259:ALA:HB3	1.53	0.90
1:A:166:LYS:HE3	1:B:54:ASN:HB2	1.54	0.89
1:A:164:ILE:HG12	1:A:392:ALA:O	1.72	0.89
1:A:355:GLN:NE2	1:A:356:SER:H	1.69	0.89
1:A:116:GLY:O	1:A:117:ASP:HB2	1.70	0.89
1:A:433:LEU:HD12	1:A:436:ALA:HB3	1.56	0.88
1:B:38:TYR:CE2	1:B:74:VAL:HG13	2.08	0.87
1:A:379:PHE:HE1	1:A:383:LEU:HD22	1.38	0.87
1:B:38:TYR:CE2	1:B:74:VAL:CG1	2.58	0.86
1:B:456:GLY:O	1:B:457:VAL:HB	1.73	0.85
1:A:170:GLY:HA3	1:B:64:THR:HG22	1.58	0.85
1:B:59:THR:HG21	1:B:64:THR:HG23	1.59	0.84
1:B:377:PRO:HG3	1:B:423:VAL:HG21	1.59	0.84
1:B:421:VAL:HG12	1:B:426:TYR:HB2	1.60	0.84
1:B:261:LEU:HA	1:B:285:HIS:HB3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ILE:HD12	1:B:390:LEU:HD12	1.60	0.83
1:A:173:PRO:HA	1:A:207:THR:HG23	1.59	0.83
1:B:312:ALA:HA	1:B:315:GLN:HG2	1.62	0.82
1:A:171:LEU:CD2	1:A:176:PHE:HB2	2.09	0.82
1:B:163:THR:HB	1:B:183:PHE:CD1	2.15	0.82
1:B:452:ARG:HB2	1:B:453:LYS:HD2	1.59	0.82
1:A:142:ASN:ND2	1:A:361:LYS:CE	2.42	0.82
1:B:87:VAL:HG11	1:B:132:TYR:HB2	1.62	0.82
1:B:454:ALA:O	1:B:455:LEU:HB2	1.80	0.82
1:A:126:PHE:CZ	1:A:310:LYS:HD3	2.14	0.81
1:A:8:VAL:HG21	1:A:39:VAL:HG13	1.61	0.81
1:B:301:ARG:HB2	1:B:301:ARG:NH1	1.96	0.81
1:A:365:PRO:HD2	1:A:388:VAL:HG12	1.62	0.81
1:A:113:GLN:O	1:B:292:GLY:HA3	1.79	0.81
1:A:160:VAL:HG12	1:A:389:ILE:HG23	1.63	0.81
1:A:142:ASN:ND2	1:A:361:LYS:HE2	1.97	0.80
1:A:232:ILE:HG12	1:A:260:LEU:HD22	1.61	0.80
1:A:355:GLN:HE21	1:A:356:SER:H	0.85	0.80
1:B:38:TYR:CD2	1:B:74:VAL:HG11	2.16	0.80
1:A:296:SER:HB3	1:B:301:ARG:NH2	1.97	0.80
1:A:427:ALA:O	1:A:434:ALA:HB2	1.83	0.79
1:B:255:ALA:HA	1:B:258:VAL:HG22	1.62	0.79
1:A:324:THR:CG2	1:A:336:ASP:HB3	2.13	0.79
1:B:418:ARG:O	1:B:419:ASP:HB2	1.83	0.79
1:A:295:THR:CG2	1:A:305:ALA:HB2	2.13	0.79
1:B:169:LEU:HD11	1:B:195:PRO:HB2	1.65	0.79
1:A:208:ILE:HA	1:A:211:VAL:HG12	1.63	0.79
1:B:14:GLU:HB2	1:B:72:TYR:CE1	2.17	0.78
1:A:374:LEU:HD11	1:A:437:PHE:HA	1.64	0.78
1:A:172:ARG:HB2	1:A:175:PRO:HG2	1.64	0.78
1:B:194:GLU:HG2	1:B:287:HIS:HE1	1.46	0.78
1:A:92:ARG:HG3	1:A:93:ASN:H	1.47	0.78
1:B:59:THR:HG22	1:B:64:THR:HG23	1.66	0.78
1:B:52:GLY:C	1:B:54:ASN:H	1.85	0.77
1:A:164:ILE:CB	1:A:164:ILE:N	2.47	0.77
1:A:75:ASP:OD1	1:A:78:ARG:HB2	1.84	0.77
1:B:298:GLN:NE2	1:B:298:GLN:HA	1.98	0.77
1:B:309:CYS:HB3	1:B:343:LEU:HD11	1.66	0.77
1:B:371:MET:CE	1:B:376:MET:HA	2.15	0.77
1:B:187:GLY:HA2	1:B:411:ARG:NH2	2.00	0.76
1:B:294:VAL:HG13	1:B:302:GLY:HA2	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:VAL:HG13	1:B:390:LEU:HD23	1.67	0.75
1:B:89:LEU:H	1:B:89:LEU:HD12	1.52	0.75
1:B:371:MET:HE2	1:B:376:MET:HA	1.67	0.75
1:A:284:LEU:HD12	1:A:317:ALA:HA	1.69	0.75
1:B:177:ALA:O	1:B:180:CYS:HB3	1.86	0.75
1:A:6:ARG:NH2	1:A:53:THR:OG1	2.19	0.75
1:A:400:ILE:HD12	1:A:435:ARG:HB3	1.69	0.75
1:B:148:LYS:HG3	1:B:154:GLU:HG2	1.69	0.75
1:A:216:ARG:HH21	1:A:254:ASN:ND2	1.84	0.74
1:A:192:ASN:ND2	1:A:196:GLN:HB2	2.02	0.74
1:A:390:LEU:CD2	1:A:392:ALA:HB2	2.17	0.74
1:A:53:THR:N	1:B:166:LYS:HD2	2.02	0.74
1:A:142:ASN:HD21	1:A:361:LYS:HE2	1.51	0.74
1:A:266:VAL:HG21	1:B:106:THR:HG23	1.69	0.74
1:A:335:SER:HB3	1:A:338:ALA:HB2	0.75	0.74
1:B:414:TRP:O	1:B:417:TRP:HB3	1.87	0.74
1:A:237:PRO:O	1:A:241:ILE:HD12	1.88	0.73
1:A:163:THR:HB	1:A:183:PHE:CE1	2.23	0.73
1:B:292:GLY:O	1:B:294:VAL:N	2.21	0.73
1:B:366:ILE:HB	1:B:389:ILE:HB	1.71	0.73
1:B:38:TYR:CD2	1:B:74:VAL:CG1	2.72	0.73
1:A:93:ASN:ND2	1:B:239:GLU:HG2	2.03	0.73
1:A:9:ASN:HB3	1:A:12:LEU:HD22	1.69	0.73
1:A:7:TYR:CE1	1:A:68:ASP:HB3	2.24	0.73
1:B:10:LEU:HD23	1:B:73:GLU:HA	1.71	0.73
1:B:232:ILE:HG12	1:B:240:ILE:HD12	1.70	0.73
1:A:379:PHE:CE1	1:A:383:LEU:HD22	2.24	0.72
1:A:24:VAL:HG23	1:A:87:VAL:HG23	1.71	0.72
1:B:8:VAL:HG22	1:B:71:VAL:HB	1.70	0.72
1:B:128:VAL:HG23	1:B:355:GLN:NE2	2.04	0.72
1:B:38:TYR:HD2	1:B:74:VAL:HG11	1.52	0.72
1:A:270:ALA:HA	1:B:235:ASP:O	1.89	0.72
1:A:54:ASN:O	1:A:55:VAL:HB	1.88	0.72
1:A:166:LYS:HZ1	1:B:52:GLY:HA3	1.55	0.72
1:B:346:ASP:HB3	1:B:357:TRP:CB	2.13	0.72
1:B:71:VAL:HG11	1:B:74:VAL:CG2	2.20	0.72
1:A:378:GLY:O	1:A:382:ASN:HB2	1.90	0.72
1:A:170:GLY:C	1:B:64:THR:CG2	2.58	0.71
1:A:94:ILE:HG23	1:B:239:GLU:OE2	1.90	0.71
1:A:171:LEU:HD21	1:A:176:PHE:HB2	1.72	0.71
1:A:163:THR:HB	1:A:183:PHE:CZ	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:THR:CG2	1:B:64:THR:CG2	2.67	0.71
1:B:215:MET:SD	1:B:251:PHE:HE2	2.13	0.71
1:B:164:ILE:HG13	1:B:164:ILE:O	1.90	0.71
1:B:130:GLU:CG	1:B:131:ALA:H	2.02	0.71
1:A:172:ARG:O	1:A:175:PRO:HB2	1.90	0.71
1:A:192:ASN:HD21	1:A:196:GLN:CB	2.03	0.70
1:B:172:ARG:HB3	1:B:173:PRO:HD2	1.72	0.70
1:A:106:THR:HG22	1:A:107:LEU:HD12	1.72	0.70
1:B:173:PRO:HD3	1:B:202:ALA:HA	1.72	0.70
1:A:372:ASN:OD1	1:A:375:ARG:HG2	1.91	0.70
1:A:195:PRO:O	1:A:199:GLN:NE2	2.24	0.70
1:B:163:THR:HB	1:B:183:PHE:CE1	2.26	0.70
1:A:433:LEU:O	1:A:434:ALA:C	2.29	0.70
1:B:24:VAL:HG13	1:B:127:TYR:O	1.92	0.70
1:A:109:MET:CE	1:A:303:TYR:HB3	2.21	0.70
1:A:303:TYR:HB2	1:A:307:VAL:HG11	1.74	0.70
1:B:6:ARG:HB3	1:B:7:TYR:CD2	2.27	0.69
1:B:166:LYS:CD	1:B:167:PRO:HA	2.11	0.69
1:B:422:PRO:O	1:B:424:LEU:N	2.26	0.69
1:B:216:ARG:NH2	1:B:254:ASN:HB2	2.07	0.69
1:B:234:ALA:HB3	1:B:240:ILE:HG22	1.75	0.69
1:A:294:VAL:HG22	1:A:302:GLY:HA3	1.74	0.69
1:B:159:LEU:HD11	1:B:390:LEU:HB3	1.74	0.69
1:A:31:LYS:O	1:A:119:GLU:HB2	1.93	0.69
1:A:198:ASN:HA	1:A:204:LEU:H	1.57	0.69
1:A:171:LEU:HD12	1:B:59:THR:OG1	1.93	0.69
1:A:6:ARG:NH2	1:A:51:THR:HG22	2.08	0.69
1:B:424:LEU:HD21	1:B:448:TYR:HB3	1.75	0.68
1:A:372:ASN:CG	1:A:375:ARG:HE	1.96	0.68
1:A:185:LEU:HD12	1:A:221:GLU:HG2	1.75	0.68
1:B:418:ARG:HH11	1:B:418:ARG:HG2	1.57	0.68
1:B:95:THR:O	1:B:96:ASP:HB2	1.92	0.68
1:A:53:THR:H	1:B:166:LYS:HD2	1.59	0.68
1:A:142:ASN:ND2	1:A:361:LYS:NZ	2.42	0.68
1:A:401:ASP:HB3	1:A:405:ALA:HB2	1.75	0.68
1:B:103:SER:O	1:B:107:LEU:HB2	1.94	0.68
1:B:312:ALA:O	1:B:317:ALA:HB3	1.94	0.68
1:A:433:LEU:HD12	1:A:433:LEU:O	1.92	0.68
1:A:184:TRP:CH2	1:A:228:PHE:HB2	2.29	0.68
1:A:243:ARG:O	1:A:247:VAL:HG23	1.93	0.67
1:A:100:MET:HE1	1:B:233:THR:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:NZ	1:B:52:GLY:HA3	2.09	0.67
1:A:372:ASN:ND2	1:A:375:ARG:NE	2.41	0.67
1:A:65:ARG:C	1:A:67:VAL:H	1.98	0.67
1:A:91:ASP:OD1	1:B:243:ARG:NH2	2.26	0.67
1:B:172:ARG:CB	1:B:173:PRO:HD2	2.24	0.67
1:A:115:MET:HE2	1:A:118:VAL:HG23	1.75	0.67
1:A:290:GLY:O	1:A:291:HIS:C	2.32	0.67
1:A:440:PHE:O	1:A:440:PHE:CD1	2.47	0.67
1:A:173:PRO:CA	1:A:207:THR:HG23	2.23	0.67
1:B:51:THR:HG21	1:B:64:THR:O	1.95	0.67
1:A:164:ILE:CA	1:A:164:ILE:CG2	2.71	0.67
1:A:372:ASN:HA	1:A:395:GLY:HA2	1.75	0.67
1:A:294:VAL:CG2	1:A:302:GLY:HA3	2.24	0.67
1:B:78:ARG:HG3	1:B:78:ARG:O	1.95	0.67
1:A:339:ILE:O	1:A:343:LEU:HB3	1.94	0.66
1:A:274:THR:HB	1:B:237:PRO:CG	2.25	0.66
1:A:172:ARG:HH22	1:B:62:ASP:CB	2.08	0.66
1:B:183:PHE:HD1	1:B:190:ILE:HD11	1.59	0.66
1:A:263:ASP:O	1:A:266:VAL:HG23	1.96	0.66
1:B:8:VAL:CG1	1:B:9:ASN:N	2.59	0.66
1:A:377:PRO:HA	1:A:380:PHE:HB2	1.78	0.66
1:A:170:GLY:O	1:B:64:THR:HG22	1.95	0.66
1:B:32:PRO:HB3	1:B:41:THR:CG2	2.19	0.66
1:A:30:MET:HE1	1:A:42:ALA:HA	1.76	0.66
1:A:8:VAL:HG21	1:A:39:VAL:CG1	2.26	0.66
1:A:288:ARG:O	1:A:289:ALA:CB	2.42	0.66
1:A:46:ALA:HB1	1:A:69:ALA:O	1.95	0.66
1:A:128:VAL:CG2	1:A:132:TYR:HD2	2.07	0.66
1:A:110:GLY:O	1:A:113:GLN:HB2	1.95	0.66
1:B:194:GLU:HG2	1:B:287:HIS:CE1	2.29	0.66
1:B:408:ARG:HG2	1:B:432:GLU:HG2	1.78	0.66
1:A:433:LEU:CD1	1:A:436:ALA:HB3	2.24	0.66
1:A:228:PHE:CE2	1:A:230:ALA:HB2	2.31	0.66
1:A:238:PHE:CE2	1:B:278:ARG:HD3	2.31	0.66
1:B:379:PHE:O	1:B:383:LEU:HB3	1.95	0.66
1:A:33:LYS:O	1:A:36:TYR:HB2	1.94	0.65
1:B:452:ARG:HB2	1:B:453:LYS:CD	2.26	0.65
1:A:169:LEU:HD11	1:A:195:PRO:HB2	1.78	0.65
1:A:8:VAL:HG22	1:A:71:VAL:HB	1.77	0.65
1:A:435:ARG:HA	1:A:438:GLU:HB3	1.78	0.65
1:B:128:VAL:HG12	1:B:132:TYR:CD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:HG23	1:A:87:VAL:CG2	2.25	0.65
1:B:322:THR:CG2	1:B:323:GLY:N	2.58	0.65
1:A:109:MET:HE1	1:A:303:TYR:HB3	1.77	0.65
1:A:270:ALA:O	1:A:274:THR:HG22	1.96	0.65
1:A:293:ALA:HB2	1:B:113:GLN:HG2	1.78	0.65
1:B:425:ASP:HA	1:B:428:ARG:HB2	1.79	0.65
1:A:371:MET:SD	1:A:376:MET:HG3	2.37	0.64
1:B:130:GLU:HG2	1:B:131:ALA:H	1.60	0.64
1:A:232:ILE:CG1	1:A:260:LEU:HD22	2.26	0.64
1:B:374:LEU:O	1:B:448:TYR:HE2	1.80	0.64
1:B:255:ALA:HA	1:B:258:VAL:CG2	2.27	0.64
1:A:274:THR:HB	1:B:237:PRO:HG3	1.79	0.64
1:A:21:GLY:HA2	1:A:129:PRO:HB2	1.79	0.64
1:A:139:PRO:HG2	1:A:361:LYS:HB3	1.79	0.64
1:A:364:THR:HG22	1:A:388:VAL:HA	1.80	0.64
1:A:75:ASP:HB3	1:A:80:LEU:HD23	1.80	0.64
1:B:217:ARG:O	1:B:221:GLU:HG2	1.97	0.64
1:B:254:ASN:HB3	1:B:257:HIS:CD2	2.32	0.64
1:B:59:THR:HG22	1:B:64:THR:CG2	2.28	0.64
1:B:261:LEU:HG	1:B:285:HIS:CD2	2.33	0.64
1:B:442:GLY:HA2	1:B:445:ASP:N	2.12	0.64
1:A:32:PRO:HG3	1:A:41:THR:HG21	1.78	0.64
1:B:215:MET:O	1:B:219:GLN:HG2	1.98	0.64
1:B:12:LEU:HD11	1:B:17:LEU:HD21	1.80	0.64
1:A:92:ARG:CD	1:A:99:ALA:HA	2.28	0.64
1:A:262:VAL:HG12	1:A:264:GLY:HA2	1.80	0.63
1:B:427:ALA:O	1:B:434:ALA:HB2	1.98	0.63
1:B:86:PRO:O	1:B:89:LEU:HD12	1.98	0.63
1:B:418:ARG:O	1:B:419:ASP:CB	2.46	0.63
1:A:414:TRP:O	1:A:417:TRP:HB3	1.98	0.63
1:B:59:THR:HG21	1:B:64:THR:CG2	2.29	0.63
1:A:372:ASN:HD22	1:A:440:PHE:HE1	1.46	0.63
1:A:192:ASN:HD21	1:A:196:GLN:HB2	1.63	0.63
1:A:273:THR:HG21	1:B:236:ASP:HB2	1.81	0.63
1:B:421:VAL:CG1	1:B:426:TYR:HB2	2.27	0.63
1:B:71:VAL:HG11	1:B:74:VAL:HG23	1.79	0.63
1:B:6:ARG:CD	1:B:7:TYR:H	2.11	0.63
1:B:166:LYS:HD3	1:B:167:PRO:CA	2.14	0.63
1:A:303:TYR:HB2	1:A:307:VAL:CG1	2.29	0.63
1:B:8:VAL:HG13	1:B:9:ASN:N	2.14	0.63
1:A:9:ASN:O	1:A:12:LEU:HB3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ARG:HB2	1:B:301:ARG:HH11	1.64	0.62
1:B:139:PRO:HD3	1:B:313:ARG:O	1.97	0.62
1:A:76:GLU:O	1:A:79:GLU:HG3	1.98	0.62
1:A:429:GLU:HB3	1:A:430:HIS:ND1	2.14	0.62
1:A:173:PRO:HA	1:A:207:THR:CG2	2.29	0.62
1:A:122:LYS:NZ	1:A:296:SER:O	2.32	0.62
1:A:14:GLU:O	1:A:18:ILE:HB	1.99	0.62
1:B:357:TRP:O	1:B:359:GLY:N	2.32	0.62
1:B:355:GLN:HG3	1:B:356:SER:N	2.14	0.62
1:A:171:LEU:HD21	1:A:176:PHE:CA	2.30	0.62
1:A:199:GLN:HB3	1:A:200:PRO:HD2	1.81	0.62
1:B:371:MET:HB3	1:B:390:LEU:HD11	1.80	0.62
1:A:122:LYS:HB2	1:A:300:LYS:O	2.00	0.62
1:B:41:THR:N	1:B:41:THR:CB	2.61	0.62
1:B:192:ASN:ND2	1:B:231:ASN:HB2	2.15	0.62
1:B:454:ALA:O	1:B:455:LEU:CB	2.48	0.62
1:A:192:ASN:ND2	1:A:196:GLN:CB	2.63	0.62
1:A:415:GLN:O	1:A:419:ASP:HB2	2.00	0.62
1:B:396:ALA:HA	1:B:406:GLY:HA3	1.82	0.62
1:A:398:GLY:O	1:A:440:PHE:HD2	1.81	0.62
1:B:294:VAL:HG13	1:B:302:GLY:CA	2.30	0.61
1:A:100:MET:HE2	1:B:234:ALA:HA	1.82	0.61
1:B:232:ILE:O	1:B:240:ILE:HB	1.99	0.61
1:B:233:THR:OG1	1:B:262:VAL:HA	1.99	0.61
1:A:145:ALA:HA	1:A:148:LYS:HD3	1.82	0.61
1:B:218:ALA:HA	1:B:221:GLU:HG2	1.81	0.61
1:A:171:LEU:HD21	1:A:176:PHE:CB	2.30	0.61
1:B:59:THR:HG23	1:B:60:THR:H	1.66	0.61
1:A:148:LYS:HB3	1:A:154:GLU:HG2	1.81	0.61
1:A:342:MET:HE2	1:A:349:GLN:O	2.01	0.61
1:A:141:VAL:HG22	1:A:145:ALA:CB	2.30	0.61
1:B:443:ASP:O	1:B:447:ILE:HD12	2.00	0.61
1:A:295:THR:HG22	1:A:305:ALA:HB2	1.82	0.61
1:B:216:ARG:O	1:B:220:ASP:HB2	2.01	0.61
1:B:457:VAL:O	1:B:457:VAL:HG22	2.01	0.61
1:A:226:LYS:O	1:A:257:HIS:HB3	2.00	0.61
1:B:99:ALA:HB2	1:B:135:LEU:HB2	1.83	0.61
1:B:102:ALA:O	1:B:106:THR:OG1	2.19	0.61
1:B:160:VAL:HG22	1:B:389:ILE:HG23	1.83	0.61
1:A:216:ARG:HH21	1:A:254:ASN:HD21	1.48	0.61
1:B:412:GLN:HB3	1:B:426:TYR:HE2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PRO:HD3	1:A:313:ARG:O	2.00	0.61
1:A:295:THR:HG21	1:A:305:ALA:HB2	1.82	0.61
1:A:427:ALA:HB2	1:A:437:PHE:CE1	2.34	0.61
1:A:276:ARG:O	1:A:280:PRO:HB3	2.01	0.60
1:B:204:LEU:HG	1:B:208:ILE:HD13	1.83	0.60
1:A:292:GLY:O	1:B:301:ARG:NH2	2.33	0.60
1:A:198:ASN:HB2	1:A:204:LEU:HD23	1.84	0.60
1:A:244:GLY:HA3	1:A:279:PHE:CZ	2.36	0.60
1:B:438:GLU:HG3	1:B:451:TRP:HH2	1.67	0.60
1:A:230:ALA:O	1:A:232:ILE:HG23	2.02	0.60
1:A:171:LEU:HD21	1:A:176:PHE:N	2.16	0.60
1:A:398:GLY:O	1:A:440:PHE:CD2	2.55	0.60
1:A:440:PHE:O	1:A:440:PHE:HD1	1.84	0.60
1:A:439:SER:HG	1:A:440:PHE:N	1.99	0.60
1:A:215:MET:HE3	1:A:251:PHE:HE2	1.67	0.60
1:A:429:GLU:HB3	1:A:430:HIS:CE1	2.36	0.60
1:A:229:SER:HB3	1:A:261:LEU:HD23	1.82	0.59
1:A:21:GLY:HA2	1:A:129:PRO:CB	2.32	0.59
1:A:418:ARG:NH1	1:A:419:ASP:OD1	2.35	0.59
1:B:407:ALA:HA	1:B:410:LEU:HB2	1.82	0.59
1:B:412:GLN:OE1	1:B:432:GLU:HB2	2.02	0.59
1:B:119:GLU:HG3	1:B:120:TYR:CD2	2.37	0.59
1:A:372:ASN:HA	1:A:395:GLY:CA	2.32	0.59
1:B:215:MET:SD	1:B:251:PHE:CE2	2.95	0.59
1:A:310:LYS:HG2	1:A:310:LYS:O	2.02	0.59
1:A:164:ILE:HG21	1:A:391:THR:O	2.03	0.59
1:B:190:ILE:C	1:B:191:LYS:CA	2.70	0.59
1:A:183:PHE:O	1:A:183:PHE:CD1	2.56	0.59
1:A:126:PHE:CE2	1:A:310:LYS:HD3	2.38	0.59
1:A:170:GLY:O	1:B:64:THR:CG2	2.50	0.58
1:B:321:HIS:HA	1:B:366:ILE:O	2.03	0.58
1:A:401:ASP:HB2	1:A:435:ARG:HH21	1.68	0.58
1:A:273:THR:O	1:A:277:ARG:HG2	2.03	0.58
1:B:32:PRO:CB	1:B:41:THR:HG21	2.22	0.58
1:B:86:PRO:O	1:B:89:LEU:CD1	2.51	0.58
1:B:25:LEU:HD22	1:B:72:TYR:CE2	2.38	0.58
1:B:128:VAL:HG12	1:B:132:TYR:HD2	1.68	0.58
1:B:254:ASN:HB3	1:B:257:HIS:HD2	1.66	0.58
1:A:364:THR:CG2	1:A:388:VAL:HA	2.33	0.58
1:A:276:ARG:HD3	1:A:316:GLY:O	2.04	0.58
1:A:173:PRO:CB	1:A:207:THR:HG23	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:MET:CE	1:A:251:PHE:HE2	2.16	0.58
1:A:45:PHE:HD1	1:A:83:ILE:HD11	1.68	0.58
1:A:335:SER:CA	1:A:338:ALA:HB2	2.30	0.58
1:B:248:LEU:HD12	1:B:258:VAL:HG23	1.86	0.58
1:A:156:ASP:CB	1:A:387:ASN:HD22	2.05	0.58
1:A:234:ALA:HB3	1:A:240:ILE:HG12	1.86	0.58
1:B:85:TYR:CZ	1:B:108:THR:HG22	2.38	0.58
1:B:128:VAL:HB	1:B:133:ARG:HB2	1.84	0.58
1:A:143:ILE:O	1:A:143:ILE:HG12	2.04	0.58
1:A:184:TRP:O	1:A:226:LYS:HE2	2.04	0.58
1:A:234:ALA:O	1:A:240:ILE:HD11	2.05	0.57
1:B:261:LEU:HG	1:B:285:HIS:HD2	1.68	0.57
1:B:71:VAL:CG1	1:B:74:VAL:HG23	2.35	0.57
1:A:205:ARG:NH1	1:B:94:ILE:HB	2.19	0.57
1:A:103:SER:HA	1:A:106:THR:HB	1.85	0.57
1:B:219:GLN:OE1	1:B:254:ASN:ND2	2.38	0.57
1:B:179:ALA:O	1:B:182:ALA:HB3	2.04	0.57
1:A:307:VAL:O	1:A:311:MET:HB2	2.04	0.57
1:A:50:SER:OG	1:A:89:LEU:HD21	2.05	0.57
1:A:423:VAL:HG12	1:A:437:PHE:CZ	2.39	0.57
1:A:92:ARG:HD3	1:A:99:ALA:HA	1.86	0.57
1:B:367:ILE:HD12	1:B:390:LEU:CD1	2.31	0.57
1:A:39:VAL:O	1:A:42:ALA:HB3	2.05	0.57
1:A:288:ARG:O	1:A:289:ALA:HB3	2.03	0.57
1:B:41:THR:CG2	1:B:41:THR:CA	2.77	0.57
1:A:53:THR:H	1:B:166:LYS:CD	2.18	0.57
1:B:364:THR:HG22	1:B:366:ILE:HG22	1.87	0.56
1:B:161:VAL:HG23	1:B:411:ARG:CZ	2.35	0.56
1:A:39:VAL:HA	1:A:42:ALA:HB3	1.87	0.56
1:B:176:PHE:O	1:B:177:ALA:C	2.44	0.56
1:B:120:TYR:HA	1:B:301:ARG:CD	2.36	0.56
1:A:372:ASN:HB2	1:A:440:PHE:CZ	2.41	0.56
1:B:194:GLU:O	1:B:263:ASP:OD2	2.23	0.56
1:B:211:VAL:O	1:B:212:ALA:C	2.43	0.56
1:B:165:ILE:HD13	1:B:179:ALA:HB1	1.87	0.56
1:B:365:PRO:HB2	1:B:388:VAL:HG12	1.87	0.56
1:A:172:ARG:HH22	1:B:62:ASP:CG	2.07	0.56
1:A:144:SER:O	1:A:148:LYS:HG2	2.05	0.56
1:A:260:LEU:HD13	1:A:275:ALA:HB1	1.87	0.56
1:B:105:LEU:HD23	1:B:109:MET:HE3	1.87	0.56
1:A:75:ASP:O	1:A:77:ALA:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PRO:HG3	1:A:41:THR:CG2	2.36	0.56
1:A:211:VAL:HG22	1:A:251:PHE:CZ	2.41	0.56
1:A:140:SER:OG	1:A:276:ARG:NH1	2.38	0.56
1:A:109:MET:O	1:B:290:GLY:HA3	2.05	0.56
1:A:39:VAL:HG23	1:A:74:VAL:HG21	1.88	0.56
1:A:184:TRP:HH2	1:A:228:PHE:HB2	1.68	0.56
1:A:139:PRO:HG2	1:A:361:LYS:CB	2.36	0.56
1:B:120:TYR:HA	1:B:301:ARG:HG3	1.88	0.56
1:B:427:ALA:HB2	1:B:433:LEU:HG	1.88	0.56
1:B:231:ASN:HD22	1:B:261:LEU:HB3	1.71	0.55
1:A:364:THR:O	1:A:366:ILE:HD13	2.06	0.55
1:A:95:THR:OG1	1:B:239:GLU:OE1	2.18	0.55
1:A:423:VAL:HG12	1:A:437:PHE:HZ	1.71	0.55
1:A:92:ARG:HD2	1:A:99:ALA:HA	1.88	0.55
1:A:338:ALA:O	1:A:342:MET:HB2	2.06	0.55
1:B:14:GLU:CB	1:B:72:TYR:HE1	2.10	0.55
1:A:349:GLN:HA	1:A:354:ARG:HA	1.88	0.55
1:B:376:MET:N	1:B:377:PRO:HD2	2.21	0.55
1:A:296:SER:CB	1:B:301:ARG:NH2	2.69	0.55
1:A:400:ILE:HG21	1:A:435:ARG:HH12	1.72	0.55
1:A:337:ARG:O	1:A:337:ARG:HD3	2.06	0.55
1:B:192:ASN:HD21	1:B:231:ASN:N	2.04	0.55
1:A:33:LYS:HA	1:A:119:GLU:OE2	2.07	0.55
1:A:374:LEU:HD11	1:A:437:PHE:CA	2.34	0.55
1:A:184:TRP:CD1	1:A:190:ILE:HD13	2.42	0.55
1:A:248:LEU:HD22	1:A:282:ASN:ND2	2.22	0.55
1:B:269:ALA:O	1:B:273:THR:OG1	2.25	0.55
1:B:59:THR:C	1:B:61:ASP:H	2.09	0.55
1:A:192:ASN:HD21	1:A:196:GLN:HB3	1.72	0.55
1:A:411:ARG:O	1:A:414:TRP:HB3	2.07	0.55
1:B:81:THR:HG22	1:B:81:THR:O	2.07	0.55
1:A:113:GLN:HE22	1:A:301:ARG:HD2	1.72	0.54
1:B:162:GLY:O	1:B:183:PHE:CE1	2.60	0.54
1:A:173:PRO:HB3	1:A:207:THR:HG23	1.88	0.54
1:A:31:LYS:HG3	1:A:79:GLU:OE2	2.08	0.54
1:A:185:LEU:CD1	1:A:221:GLU:HG2	2.37	0.54
1:B:425:ASP:O	1:B:428:ARG:HB2	2.07	0.54
1:B:183:PHE:CD1	1:B:190:ILE:HD11	2.41	0.54
1:A:69:ALA:HA	1:A:85:TYR:HA	1.88	0.54
1:A:184:TRP:NE1	1:A:190:ILE:HD13	2.22	0.54
1:A:199:GLN:CB	1:A:200:PRO:HD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:HB3	1:A:120:TYR:CD2	2.43	0.54
1:A:371:MET:CE	1:A:379:PHE:HD2	2.21	0.54
1:B:98:LYS:HB3	1:B:135:LEU:O	2.08	0.54
1:A:405:ALA:O	1:A:409:SER:HB2	2.08	0.54
1:B:128:VAL:O	1:B:129:PRO:O	2.25	0.54
1:A:263:ASP:HA	1:A:287:HIS:HB3	1.90	0.54
1:A:122:LYS:HD2	1:A:303:TYR:O	2.08	0.54
1:A:310:LYS:NZ	1:A:355:GLN:HG3	2.23	0.53
1:B:186:GLY:O	1:B:407:ALA:HB3	2.08	0.53
1:A:301:ARG:HH11	1:A:301:ARG:HG3	1.73	0.53
1:A:376:MET:SD	1:A:380:PHE:HZ	2.26	0.53
1:A:439:SER:O	1:A:440:PHE:HA	2.06	0.53
1:B:310:LYS:NZ	1:B:355:GLN:NE2	2.56	0.53
1:A:216:ARG:NH2	1:A:254:ASN:ND2	2.56	0.53
1:A:239:GLU:O	1:A:242:ALA:HB3	2.07	0.53
1:B:322:THR:HG23	1:B:323:GLY:N	2.23	0.53
1:B:436:ALA:O	1:B:439:SER:HB2	2.09	0.53
1:B:128:VAL:HG21	1:B:314:LEU:HD11	1.91	0.53
1:B:248:LEU:HD12	1:B:258:VAL:CG2	2.38	0.53
1:A:272:ILE:HG13	1:A:284:LEU:HD11	1.90	0.53
1:A:168:LYS:HD2	1:A:194:GLU:OE2	2.08	0.53
1:B:320:ILE:N	1:B:366:ILE:HD13	2.24	0.53
1:B:444:ALA:O	1:B:451:TRP:HD1	1.91	0.53
1:A:211:VAL:O	1:A:214:ALA:HB3	2.08	0.53
1:B:93:ASN:HB2	1:B:96:ASP:HB3	1.90	0.53
1:B:45:PHE:HA	1:B:115:MET:CE	2.39	0.53
1:B:7:TYR:CD2	1:B:7:TYR:N	2.76	0.53
1:A:205:ARG:CZ	1:B:94:ILE:HD12	2.38	0.53
1:A:21:GLY:CA	1:A:129:PRO:HB2	2.39	0.53
1:A:148:LYS:HG3	1:A:149:VAL:N	2.24	0.53
1:A:213:ASP:O	1:A:214:ALA:C	2.47	0.53
1:A:122:LYS:HE3	1:A:304:THR:HG22	1.90	0.52
1:A:145:ALA:O	1:A:146:LEU:HD23	2.10	0.52
1:A:386:ALA:N	1:A:387:ASN:OD1	2.39	0.52
1:B:128:VAL:CG2	1:B:355:GLN:HE22	2.13	0.52
1:B:442:GLY:HA3	1:B:445:ASP:HB2	1.91	0.52
1:B:65:ARG:O	1:B:65:ARG:HG3	2.09	0.52
1:B:409:SER:HA	1:B:412:GLN:CG	2.40	0.52
1:B:122:LYS:HZ2	1:B:302:GLY:CA	2.22	0.52
1:A:401:ASP:HB3	1:A:405:ALA:CB	2.40	0.52
1:A:427:ALA:HB1	1:A:434:ALA:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:CA	1:A:164:ILE:HB	2.17	0.52
1:B:139:PRO:HA	1:B:316:GLY:O	2.09	0.52
1:A:145:ALA:HA	1:A:148:LYS:CD	2.39	0.52
1:B:139:PRO:HG3	1:B:317:ALA:O	2.09	0.52
1:B:292:GLY:O	1:B:293:ALA:C	2.48	0.52
1:A:211:VAL:HG22	1:A:251:PHE:HZ	1.75	0.52
1:B:194:GLU:HB3	1:B:287:HIS:ND1	2.23	0.52
1:A:378:GLY:O	1:A:382:ASN:CB	2.58	0.52
1:A:30:MET:CE	1:A:42:ALA:HA	2.39	0.52
1:A:128:VAL:HG13	1:A:133:ARG:HB3	1.92	0.52
1:B:231:ASN:HA	1:B:261:LEU:O	2.10	0.52
1:B:147:TRP:HE3	1:B:154:GLU:HA	1.75	0.52
1:A:172:ARG:HH22	1:B:62:ASP:HB3	1.75	0.51
1:A:361:LYS:CE	1:A:361:LYS:CG	2.87	0.51
1:A:38:TYR:O	1:A:39:VAL:C	2.49	0.51
1:B:173:PRO:HD3	1:B:202:ALA:CA	2.40	0.51
1:B:335:SER:HB2	1:B:351:PRO:CG	2.40	0.51
1:B:335:SER:HB2	1:B:351:PRO:HG3	1.93	0.51
1:A:301:ARG:HG3	1:A:301:ARG:NH1	2.25	0.51
1:B:407:ALA:HA	1:B:410:LEU:HD22	1.92	0.51
1:B:349:GLN:OE1	1:B:350:GLY:O	2.29	0.51
1:B:6:ARG:HD2	1:B:7:TYR:H	1.75	0.51
1:A:49:SER:O	1:A:107:LEU:HB3	2.10	0.51
1:B:9:ASN:HB2	1:B:70:LEU:HB2	1.92	0.51
1:A:168:LYS:N	1:B:51:THR:O	2.35	0.51
1:B:192:ASN:HD21	1:B:231:ASN:HB2	1.76	0.51
1:B:324:THR:HA	1:B:379:PHE:HE2	1.75	0.51
1:A:372:ASN:HD21	1:A:375:ARG:NE	2.06	0.51
1:A:14:GLU:HG2	1:A:18:ILE:CD1	2.32	0.51
1:B:308:HIS:O	1:B:311:MET:HB3	2.10	0.51
1:B:126:PHE:CE1	1:B:310:LYS:HG3	2.46	0.51
1:B:232:ILE:HG12	1:B:240:ILE:CD1	2.39	0.51
1:B:32:PRO:O	1:B:33:LYS:C	2.49	0.51
1:B:276:ARG:HD2	1:B:316:GLY:HA3	1.92	0.51
1:A:277:ARG:HD2	1:B:236:ASP:CG	2.31	0.51
1:B:139:PRO:O	1:B:361:LYS:HD2	2.11	0.51
1:A:71:VAL:HA	1:A:82:LYS:O	2.11	0.51
1:B:122:LYS:HZ2	1:B:302:GLY:HA3	1.76	0.51
1:A:167:PRO:HD2	1:B:59:THR:HB	1.93	0.51
1:A:128:VAL:CG2	1:A:132:TYR:CD2	2.92	0.51
1:B:49:SER:HB3	1:B:85:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:TRP:CD1	1:B:226:LYS:HG3	2.46	0.51
1:A:159:LEU:HD13	1:A:380:PHE:CZ	2.46	0.50
1:A:184:TRP:CZ2	1:A:228:PHE:HB2	2.46	0.50
1:A:110:GLY:O	1:B:290:GLY:HA2	2.12	0.50
1:A:335:SER:O	1:A:338:ALA:HB3	2.11	0.50
1:A:410:LEU:O	1:A:413:ALA:HB3	2.11	0.50
1:B:241:ILE:HG13	1:B:242:ALA:N	2.26	0.50
1:B:307:VAL:O	1:B:311:MET:HB2	2.11	0.50
1:B:418:ARG:NH1	1:B:418:ARG:HG2	2.20	0.50
1:A:376:MET:O	1:A:379:PHE:N	2.35	0.50
1:A:435:ARG:O	1:A:439:SER:N	2.43	0.50
1:B:404:VAL:HG23	1:B:408:ARG:NH2	2.26	0.50
1:B:207:THR:O	1:B:211:VAL:HG13	2.11	0.50
1:A:367:ILE:HG22	1:A:390:LEU:HD12	1.94	0.50
1:A:310:LYS:HG3	1:A:357:TRP:CH2	2.47	0.50
1:B:403:PRO:O	1:B:406:GLY:N	2.42	0.50
1:B:49:SER:HB3	1:B:85:TYR:HE1	1.76	0.50
1:B:46:ALA:O	1:B:50:SER:OG	2.21	0.50
1:A:372:ASN:ND2	1:A:440:PHE:CE1	2.80	0.50
1:A:141:VAL:HG22	1:A:145:ALA:HB1	1.94	0.50
1:A:27:ALA:HB2	1:A:353:TYR:OH	2.11	0.50
1:B:130:GLU:O	1:B:131:ALA:C	2.50	0.49
1:A:161:VAL:HG12	1:A:390:LEU:HB3	1.93	0.49
1:A:308:HIS:O	1:A:312:ALA:HB2	2.11	0.49
1:B:14:GLU:CB	1:B:72:TYR:CE1	2.90	0.49
1:A:15:GLU:O	1:A:18:ILE:HG22	2.12	0.49
1:B:247:VAL:O	1:B:251:PHE:HB2	2.12	0.49
1:A:408:ARG:O	1:A:412:GLN:CD	2.50	0.49
1:B:54:ASN:O	1:B:55:VAL:HG23	2.12	0.49
1:B:93:ASN:ND2	1:B:96:ASP:OD2	2.37	0.49
1:B:393:GLY:HA2	1:B:397:PHE:CD1	2.47	0.49
1:B:208:ILE:HG22	1:B:250:THR:HG21	1.95	0.49
1:B:436:ALA:O	1:B:439:SER:N	2.42	0.49
1:A:309:CYS:HB3	1:A:320:ILE:HG21	1.94	0.49
1:B:252:GLY:O	1:B:254:ASN:N	2.45	0.49
1:A:422:PRO:O	1:A:425:ASP:HB2	2.13	0.49
1:B:163:THR:HG22	1:B:190:ILE:HG13	1.93	0.49
1:A:116:GLY:O	1:A:117:ASP:CB	2.54	0.49
1:A:128:VAL:HG22	1:A:132:TYR:HD2	1.75	0.49
1:B:400:ILE:HD13	1:B:438:GLU:O	2.13	0.49
1:A:372:ASN:ND2	1:A:375:ARG:HH21	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:LEU:HG	1:B:433:LEU:O	2.12	0.49
1:A:416:ALA:O	1:A:417:TRP:C	2.51	0.49
1:B:37:GLY:O	1:B:38:TYR:C	2.51	0.49
1:B:409:SER:HA	1:B:412:GLN:HG3	1.94	0.49
1:B:126:PHE:CZ	1:B:310:LYS:HG3	2.47	0.49
1:A:94:ILE:HD13	1:B:243:ARG:HA	1.94	0.49
1:A:139:PRO:HD3	1:A:316:GLY:HA2	1.95	0.49
1:A:323:GLY:HA3	1:A:368:SER:OG	2.13	0.49
1:A:341:TYR:O	1:A:345:GLN:HG3	2.13	0.49
1:B:266:VAL:HG13	1:B:289:ALA:HB3	1.94	0.49
1:A:169:LEU:HD21	1:A:195:PRO:HG2	1.94	0.48
1:B:379:PHE:CE1	1:B:383:LEU:HD22	2.47	0.48
1:B:194:GLU:HB3	1:B:287:HIS:CE1	2.48	0.48
1:B:241:ILE:HA	1:B:279:PHE:CZ	2.48	0.48
1:A:133:ARG:HG2	1:A:134:ALA:N	2.24	0.48
1:B:371:MET:HE3	1:B:376:MET:HA	1.94	0.48
1:A:6:ARG:NH2	1:A:51:THR:CG2	2.76	0.48
1:B:8:VAL:HG13	1:B:9:ASN:H	1.78	0.48
1:B:216:ARG:HH11	1:B:216:ARG:HG3	1.77	0.48
1:A:112:ASN:HA	1:A:115:MET:HG3	1.95	0.48
1:B:252:GLY:O	1:B:253:GLU:C	2.52	0.48
1:B:398:GLY:HA3	1:B:440:PHE:HZ	1.78	0.48
1:A:168:LYS:NZ	1:B:48:GLU:HG3	2.28	0.48
1:B:29:ILE:HB	1:B:124:HIS:CD2	2.49	0.48
1:B:239:GLU:OE2	1:B:243:ARG:HD2	2.13	0.48
1:A:166:LYS:HA	1:A:167:PRO:C	2.34	0.48
1:B:89:LEU:HD12	1:B:89:LEU:N	2.21	0.48
1:A:371:MET:O	1:A:395:GLY:HA3	2.13	0.48
1:A:238:PHE:HE2	1:B:278:ARG:HD3	1.78	0.48
1:B:338:ALA:O	1:B:341:TYR:HB2	2.14	0.48
1:B:415:GLN:O	1:B:416:ALA:C	2.51	0.48
1:B:6:ARG:HG3	1:B:53:THR:HG21	1.96	0.48
1:A:128:VAL:HG12	1:A:355:GLN:OE1	2.13	0.48
1:B:364:THR:O	1:B:366:ILE:HG23	2.14	0.48
1:B:29:ILE:O	1:B:122:LYS:N	2.46	0.48
1:A:301:ARG:HH21	1:B:296:SER:CB	2.26	0.48
1:A:369:GLY:O	1:A:371:MET:N	2.43	0.48
1:A:182:ALA:HA	1:A:185:LEU:HD22	1.94	0.48
1:A:303:TYR:CE1	1:A:308:HIS:HB2	2.48	0.47
1:B:30:MET:HG2	1:B:118:VAL:HG13	1.95	0.47
1:B:128:VAL:C	1:B:129:PRO:O	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:PRO:CD	1:B:59:THR:HB	2.44	0.47
1:B:404:VAL:CG2	1:B:408:ARG:HH21	2.26	0.47
1:B:140:SER:O	1:B:361:LYS:HE3	2.14	0.47
1:A:159:LEU:HD13	1:A:380:PHE:HZ	1.79	0.47
1:A:237:PRO:HA	1:A:240:ILE:HB	1.97	0.47
1:B:143:ILE:O	1:B:144:SER:C	2.53	0.47
1:B:283:PHE:HE1	1:B:285:HIS:ND1	2.12	0.47
1:B:298:GLN:HE21	1:B:298:GLN:HA	1.75	0.47
1:A:141:VAL:HG22	1:A:145:ALA:HB3	1.95	0.47
1:A:163:THR:CB	1:A:183:PHE:CZ	2.96	0.47
1:A:45:PHE:CD1	1:A:83:ILE:HD11	2.48	0.47
1:B:306:PHE:HB2	1:B:335:SER:O	2.13	0.47
1:A:208:ILE:CG2	1:A:247:VAL:HG13	2.44	0.47
1:A:106:THR:O	1:A:110:GLY:HA3	2.14	0.47
1:A:273:THR:CG2	1:B:236:ASP:HB2	2.43	0.47
1:B:199:GLN:HB3	1:B:200:PRO:CD	2.44	0.47
1:B:241:ILE:O	1:B:245:GLU:N	2.47	0.47
1:B:205:ARG:HB3	1:B:246:TYR:CZ	2.49	0.47
1:B:41:THR:CA	1:B:41:THR:HB	2.19	0.47
1:B:29:ILE:O	1:B:121:ALA:HA	2.15	0.47
1:B:189:PHE:O	1:B:190:ILE:HD12	2.15	0.47
1:A:295:THR:HG23	1:A:305:ALA:N	2.29	0.47
1:A:365:PRO:CD	1:A:388:VAL:HG12	2.41	0.47
1:B:120:TYR:HB2	1:B:300:LYS:O	2.15	0.47
1:B:244:GLY:O	1:B:248:LEU:HD22	2.14	0.47
1:A:238:PHE:HA	1:A:241:ILE:HB	1.96	0.47
1:A:313:ARG:HB3	1:A:363:CYS:HB3	1.97	0.47
1:A:376:MET:SD	1:A:380:PHE:CE2	3.08	0.47
1:A:92:ARG:HG3	1:A:93:ASN:N	2.23	0.47
1:A:310:LYS:HG3	1:A:357:TRP:HH2	1.80	0.47
1:B:366:ILE:HG21	1:B:389:ILE:HD12	1.95	0.47
1:A:72:TYR:CE1	1:A:84:ALA:HB2	2.49	0.47
1:A:194:GLU:HG2	1:A:287:HIS:HE1	1.80	0.47
1:A:349:GLN:HG2	1:A:350:GLY:N	2.30	0.47
1:A:167:PRO:CG	1:B:59:THR:HB	2.44	0.46
1:A:342:MET:SD	1:A:357:TRP:HZ2	2.38	0.46
1:B:161:VAL:HG11	1:B:410:LEU:HD23	1.97	0.46
1:B:449:PRO:O	1:B:450:GLY:C	2.53	0.46
1:A:104:PHE:CD1	1:A:104:PHE:C	2.89	0.46
1:B:264:GLY:HA3	1:B:272:ILE:HD11	1.96	0.46
1:A:181:HIS:O	1:A:185:LEU:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:VAL:CG2	1:B:212:ALA:N	2.78	0.46
1:B:393:GLY:HA2	1:B:397:PHE:CE1	2.50	0.46
1:A:181:HIS:HA	1:A:184:TRP:HB2	1.97	0.46
1:A:204:LEU:HD21	1:A:243:ARG:HG2	1.98	0.46
1:A:164:ILE:CA	1:A:164:ILE:CG1	2.83	0.46
1:B:357:TRP:O	1:B:360:MET:N	2.48	0.46
1:B:78:ARG:O	1:B:78:ARG:CG	2.62	0.46
1:B:165:ILE:CD1	1:B:171:LEU:HD11	2.46	0.46
1:B:55:VAL:HG22	2:B:495:HOH:O	2.14	0.46
1:A:119:GLU:O	1:A:301:ARG:NH1	2.49	0.46
1:A:208:ILE:HG21	1:A:247:VAL:HG13	1.97	0.46
1:A:262:VAL:HG11	1:A:272:ILE:HD12	1.98	0.46
1:A:125:ASP:OD2	1:A:353:TYR:HD2	1.99	0.46
1:B:209:ALA:HB2	1:B:246:TYR:OH	2.16	0.46
1:A:194:GLU:O	1:A:263:ASP:OD2	2.33	0.46
1:B:184:TRP:CG	1:B:226:LYS:HG3	2.51	0.46
1:A:172:ARG:CB	1:A:175:PRO:HG2	2.40	0.46
1:B:323:GLY:N	1:B:367:ILE:HG22	2.31	0.46
1:B:426:TYR:O	1:B:430:HIS:NE2	2.48	0.46
1:B:204:LEU:O	1:B:208:ILE:HB	2.16	0.46
1:B:380:PHE:CE2	1:B:414:TRP:HB2	2.51	0.46
1:A:322:THR:HB	1:A:365:PRO:HB3	1.97	0.46
1:A:39:VAL:CG2	1:A:74:VAL:HG21	2.45	0.46
1:B:258:VAL:O	1:B:282:ASN:OD1	2.34	0.46
1:A:164:ILE:HA	1:A:164:ILE:CB	2.18	0.46
1:A:183:PHE:HD1	1:A:190:ILE:HD11	1.80	0.46
1:B:148:LYS:HG3	1:B:154:GLU:CG	2.43	0.46
1:B:399:HIS:HB2	1:B:406:GLY:HA2	1.98	0.45
1:A:150:LEU:HD11	1:A:227:LEU:CD1	2.46	0.45
1:B:239:GLU:OE2	1:B:243:ARG:NE	2.45	0.45
1:B:31:LYS:O	1:B:119:GLU:HB3	2.16	0.45
1:B:401:ASP:OD2	1:B:435:ARG:HD3	2.16	0.45
1:A:170:GLY:HA2	1:B:67:VAL:HG11	1.97	0.45
1:B:163:THR:HG23	1:B:164:ILE:N	2.31	0.45
1:B:380:PHE:HE2	1:B:414:TRP:HB2	1.81	0.45
1:B:37:GLY:O	1:B:40:ALA:N	2.49	0.45
1:A:218:ALA:O	1:A:221:GLU:N	2.49	0.45
1:B:93:ASN:O	1:B:97:GLY:HA2	2.16	0.45
1:A:164:ILE:CG2	1:A:164:ILE:N	2.80	0.45
1:B:15:GLU:HA	1:B:18:ILE:HB	1.99	0.45
1:B:304:THR:O	1:B:307:VAL:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ILE:CD1	1:A:260:LEU:HD22	2.46	0.45
1:B:453:LYS:HD2	1:B:453:LYS:N	2.32	0.45
1:A:291:HIS:O	1:A:293:ALA:N	2.49	0.45
1:B:47:ALA:O	1:B:52:GLY:HA2	2.17	0.45
1:B:444:ALA:O	1:B:451:TRP:CD1	2.70	0.45
1:A:147:TRP:CH2	1:A:156:ASP:HA	2.52	0.45
1:A:95:THR:HB	1:A:96:ASP:H	1.61	0.45
1:B:143:ILE:HG22	1:B:364:THR:OG1	2.15	0.45
1:A:150:LEU:HD11	1:A:227:LEU:HD11	1.99	0.45
1:A:228:PHE:O	1:A:258:VAL:HG12	2.16	0.45
1:B:232:ILE:HD13	1:B:262:VAL:CG1	2.46	0.45
1:B:44:HIS:O	1:B:47:ALA:N	2.35	0.45
1:B:217:ARG:O	1:B:221:GLU:CG	2.63	0.45
1:B:365:PRO:HG2	1:B:388:VAL:HG12	1.98	0.45
1:B:349:GLN:HA	1:B:354:ARG:HA	1.97	0.45
1:B:223:GLY:O	1:B:224:GLU:HG3	2.17	0.45
1:B:183:PHE:HD2	1:B:403:PRO:HB3	1.81	0.45
1:A:291:HIS:O	1:A:294:VAL:HG12	2.17	0.45
1:A:412:GLN:HA	1:A:415:GLN:HB2	1.98	0.45
1:B:216:ARG:HH22	1:B:254:ASN:HB2	1.82	0.44
1:A:127:TYR:HB2	1:A:353:TYR:HB3	1.99	0.44
1:B:101:ILE:HG23	1:B:105:LEU:CD1	2.47	0.44
1:A:383:LEU:O	1:A:383:LEU:HG	2.17	0.44
1:A:402:GLY:O	1:A:405:ALA:N	2.50	0.44
1:A:291:HIS:NE2	2:A:486:HOH:O	2.36	0.44
1:A:219:GLN:HB3	1:A:224:GLU:O	2.16	0.44
1:B:374:LEU:O	1:B:448:TYR:CE2	2.66	0.44
1:B:346:ASP:HA	1:B:357:TRP:HB2	1.98	0.44
1:A:142:ASN:CG	1:A:361:LYS:NZ	2.70	0.44
1:A:106:THR:HG21	1:B:195:PRO:HA	2.00	0.44
1:A:292:GLY:HA2	1:A:295:THR:O	2.18	0.44
1:A:94:ILE:HD13	1:A:94:ILE:HG21	1.75	0.44
1:B:75:ASP:OD2	1:B:78:ARG:NH1	2.50	0.44
1:B:6:ARG:HB3	1:B:7:TYR:CE2	2.53	0.44
1:B:416:ALA:HB2	1:B:426:TYR:CD2	2.52	0.44
1:A:309:CYS:HA	1:A:312:ALA:CB	2.47	0.44
1:A:146:LEU:HD22	1:A:227:LEU:HD22	2.00	0.44
1:B:130:GLU:HG2	1:B:130:GLU:H	1.18	0.44
1:A:159:LEU:HD22	1:A:380:PHE:CZ	2.53	0.44
1:A:229:SER:CB	1:A:261:LEU:HD23	2.45	0.44
1:B:172:ARG:CB	1:B:173:PRO:CD	2.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:PRO:HG2	1:B:388:VAL:CG1	2.48	0.44
1:B:142:ASN:HB2	1:B:144:SER:H	1.82	0.44
1:A:440:PHE:HA	1:A:441:PRO:HD3	1.88	0.44
1:A:101:ILE:HG12	1:A:136:PHE:CE1	2.52	0.44
1:A:303:TYR:CD1	1:A:308:HIS:HB2	2.53	0.44
1:A:364:THR:HA	1:A:365:PRO:HD3	1.82	0.44
1:A:184:TRP:CD1	1:A:226:LYS:HB3	2.52	0.44
1:B:239:GLU:O	1:B:243:ARG:HD2	2.17	0.44
1:A:89:LEU:O	1:B:199:GLN:NE2	2.41	0.44
1:A:310:LYS:HE2	1:A:342:MET:HE3	1.99	0.44
1:A:400:ILE:HG13	1:A:439:SER:HB3	1.99	0.44
1:A:324:THR:C	2:A:518:HOH:O	2.56	0.44
1:A:184:TRP:CE2	1:A:226:LYS:HB3	2.53	0.44
1:B:262:VAL:O	1:B:287:HIS:N	2.46	0.44
1:A:241:ILE:HG22	1:A:242:ALA:N	2.33	0.44
1:B:165:ILE:HD11	1:B:171:LEU:HD11	1.99	0.44
1:A:174:LYS:N	1:A:175:PRO:HD2	2.33	0.43
1:B:285:HIS:CE1	1:B:366:ILE:HD12	2.53	0.43
1:B:376:MET:O	1:B:379:PHE:HB3	2.18	0.43
1:B:166:LYS:HA	1:B:167:PRO:HA	1.58	0.43
1:A:147:TRP:CZ3	1:A:156:ASP:HA	2.53	0.43
1:B:75:ASP:HB3	1:B:78:ARG:HB3	2.00	0.43
1:B:337:ARG:O	1:B:337:ARG:HG2	2.18	0.43
1:B:44:HIS:C	1:B:44:HIS:ND1	2.69	0.43
1:A:103:SER:HA	1:A:106:THR:CB	2.47	0.43
1:A:156:ASP:CB	1:A:387:ASN:ND2	2.63	0.43
1:A:379:PHE:O	1:A:380:PHE:C	2.56	0.43
1:A:400:ILE:CG2	1:A:435:ARG:HH12	2.30	0.43
1:A:227:LEU:HD23	1:A:257:HIS:HA	1.99	0.43
1:B:241:ILE:O	1:B:245:GLU:HB2	2.18	0.43
1:A:194:GLU:HG2	1:A:287:HIS:CE1	2.53	0.43
1:B:421:VAL:HA	1:B:422:PRO:HD3	1.91	0.43
1:A:119:GLU:O	1:A:120:TYR:HB3	2.18	0.43
1:B:172:ARG:HA	1:B:202:ALA:HB2	2.00	0.43
1:A:125:ASP:HB3	1:A:353:TYR:CE2	2.53	0.43
1:B:376:MET:SD	1:B:380:PHE:CE2	3.11	0.43
1:B:310:LYS:HZ2	1:B:355:GLN:NE2	2.16	0.43
1:A:208:ILE:HA	1:A:211:VAL:CG1	2.43	0.43
1:B:404:VAL:HG23	1:B:408:ARG:HH21	1.83	0.43
1:A:233:THR:OG1	1:A:262:VAL:HA	2.18	0.43
1:A:272:ILE:HG21	1:A:315:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:TRP:CE3	1:B:154:GLU:HA	2.53	0.43
1:B:101:ILE:HG12	1:B:136:PHE:CE1	2.54	0.43
1:A:335:SER:C	1:A:338:ALA:HB3	2.38	0.43
1:A:184:TRP:O	1:A:226:LYS:CE	2.66	0.43
1:B:313:ARG:HD3	1:B:357:TRP:CZ3	2.54	0.43
1:B:121:ALA:O	1:B:301:ARG:HA	2.19	0.43
1:A:176:PHE:O	1:A:179:ALA:N	2.52	0.43
1:B:448:TYR:HA	1:B:449:PRO:HD2	1.69	0.43
1:A:6:ARG:HH21	1:A:51:THR:HG22	1.82	0.43
1:A:387:ASN:OD1	1:A:387:ASN:N	2.52	0.43
1:A:399:HIS:ND1	1:A:400:ILE:N	2.67	0.43
1:B:146:LEU:O	1:B:147:TRP:C	2.57	0.43
1:A:127:TYR:O	1:A:129:PRO:HD3	2.18	0.43
1:A:100:MET:CE	1:B:233:THR:O	2.65	0.43
1:B:408:ARG:O	1:B:412:GLN:HG2	2.18	0.43
1:B:386:ALA:HB2	1:B:417:TRP:CZ3	2.54	0.43
1:A:173:PRO:HG3	1:A:202:ALA:HA	1.99	0.43
1:A:216:ARG:O	1:A:220:ASP:OD1	2.37	0.43
1:A:410:LEU:O	1:A:411:ARG:C	2.57	0.43
1:A:244:GLY:HA3	1:A:279:PHE:CE2	2.54	0.43
1:B:174:LYS:O	1:B:175:PRO:C	2.56	0.43
1:A:109:MET:HB3	1:A:113:GLN:HG3	2.01	0.42
1:A:320:ILE:HG12	1:A:321:HIS:H	1.85	0.42
1:A:272:ILE:HG21	1:A:315:GLN:CG	2.48	0.42
1:B:118:VAL:HG12	1:B:119:GLU:N	2.34	0.42
1:A:324:THR:HG21	1:A:336:ASP:CB	2.37	0.42
1:B:440:PHE:HA	1:B:441:PRO:HD2	1.65	0.42
1:A:7:TYR:CE2	1:A:47:ALA:HB2	2.54	0.42
1:A:152:ARG:HB3	1:A:153:PRO:HD2	2.02	0.42
1:A:320:ILE:O	1:A:366:ILE:HG12	2.19	0.42
1:B:24:VAL:HG21	1:B:90:PHE:CE2	2.54	0.42
1:B:126:PHE:CE1	1:B:307:VAL:HG13	2.55	0.42
1:B:288:ARG:HD3	1:B:288:ARG:HH11	1.60	0.42
1:B:452:ARG:O	1:B:456:GLY:O	2.36	0.42
1:A:109:MET:HE2	1:A:303:TYR:HB3	2.00	0.42
1:B:181:HIS:HA	1:B:184:TRP:HE3	1.85	0.42
1:B:5:SER:O	1:B:6:ARG:HB2	2.20	0.42
1:B:366:ILE:CG2	1:B:389:ILE:HD12	2.49	0.42
1:B:14:GLU:HG3	1:B:72:TYR:OH	2.20	0.42
1:A:101:ILE:O	1:A:102:ALA:C	2.57	0.42
1:A:52:GLY:HA3	1:B:166:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:CB	1:A:363:CYS:HB3	2.49	0.42
1:B:127:TYR:HE1	1:B:355:GLN:HA	1.85	0.42
1:B:306:PHE:HA	1:B:339:ILE:CD1	2.50	0.42
1:B:336:ASP:HA	1:B:339:ILE:HG13	2.01	0.42
1:B:431:LYS:O	1:B:432:GLU:C	2.57	0.42
1:B:71:VAL:CG1	1:B:74:VAL:CG2	2.94	0.42
1:A:184:TRP:O	1:A:226:LYS:NZ	2.48	0.42
1:A:128:VAL:HG13	1:A:133:ARG:CB	2.49	0.42
1:B:161:VAL:HG23	1:B:411:ARG:NH2	2.34	0.42
1:B:409:SER:HA	1:B:412:GLN:HG2	2.02	0.42
1:A:122:LYS:HB3	1:A:124:HIS:HE1	1.85	0.42
1:A:73:GLU:HB3	1:A:82:LYS:HD3	2.02	0.42
1:A:408:ARG:O	1:A:412:GLN:NE2	2.53	0.42
1:B:365:PRO:CB	1:B:388:VAL:HG12	2.50	0.42
1:B:393:GLY:O	1:B:397:PHE:HD1	2.03	0.42
1:B:152:ARG:HA	1:B:153:PRO:HD2	1.82	0.42
1:A:296:SER:CB	1:B:301:ARG:HH21	2.33	0.41
1:B:298:GLN:OE1	1:B:300:LYS:HD2	2.20	0.41
1:B:9:ASN:O	1:B:12:LEU:HB2	2.20	0.41
1:A:248:LEU:HD23	1:A:258:VAL:HG21	2.00	0.41
1:B:94:ILE:HG13	1:B:95:THR:N	2.34	0.41
1:B:96:ASP:OD2	1:B:98:LYS:HB2	2.20	0.41
1:B:160:VAL:HG23	1:B:189:PHE:HB2	2.02	0.41
1:B:90:PHE:CD1	1:B:107:LEU:HD13	2.55	0.41
1:A:12:LEU:HD23	1:A:12:LEU:O	2.20	0.41
1:A:379:PHE:C	1:A:379:PHE:CD1	2.93	0.41
1:B:193:ASN:O	1:B:196:GLN:HB2	2.20	0.41
1:B:7:TYR:HH	1:B:51:THR:HB	1.76	0.41
1:B:444:ALA:HA	1:B:448:TYR:HB2	2.02	0.41
1:A:400:ILE:HB	1:A:435:ARG:CZ	2.50	0.41
1:B:216:ARG:CG	1:B:216:ARG:NH1	2.82	0.41
1:B:147:TRP:O	1:B:148:LYS:C	2.58	0.41
1:A:199:GLN:HB3	1:A:200:PRO:CD	2.48	0.41
1:B:306:PHE:CE1	1:B:342:MET:HG2	2.55	0.41
1:B:122:LYS:HZ2	1:B:302:GLY:N	2.18	0.41
1:B:30:MET:C	1:B:30:MET:SD	2.99	0.41
1:A:371:MET:CG	1:A:376:MET:HG3	2.51	0.41
1:A:401:ASP:CB	1:A:405:ALA:HB2	2.44	0.41
1:B:70:LEU:H	1:B:70:LEU:HD12	1.85	0.41
1:A:92:ARG:CG	1:A:93:ASN:N	2.83	0.41
1:A:335:SER:CB	1:A:338:ALA:HB1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:MET:CE	1:A:251:PHE:CE2	3.01	0.41
1:B:33:LYS:HE2	1:B:116:GLY:O	2.20	0.41
1:A:106:THR:CG2	1:A:107:LEU:HD12	2.46	0.41
1:A:113:GLN:HA	1:A:113:GLN:NE2	2.34	0.41
1:A:318:SER:O	1:A:363:CYS:HA	2.21	0.41
1:A:295:THR:CG2	1:A:305:ALA:CB	2.94	0.41
1:B:355:GLN:HG3	1:B:356:SER:H	1.83	0.41
1:A:274:THR:HB	1:B:237:PRO:CD	2.51	0.41
1:B:443:ASP:O	1:B:447:ILE:HB	2.20	0.41
1:A:177:ALA:O	1:A:178:GLU:C	2.59	0.41
1:B:41:THR:O	1:B:44:HIS:HB3	2.20	0.41
1:B:403:PRO:HB2	1:B:404:VAL:H	1.51	0.41
1:B:291:HIS:O	1:B:292:GLY:C	2.57	0.41
1:A:237:PRO:O	1:A:241:ILE:CD1	2.63	0.41
2:A:502:HOH:O	1:B:235:ASP:HB2	2.21	0.41
1:B:78:ARG:HH11	1:B:78:ARG:CB	2.34	0.41
1:A:236:ASP:OD2	1:B:277:ARG:NH1	2.54	0.41
1:A:299:SER:HB2	1:B:301:ARG:HH22	1.87	0.40
1:A:371:MET:HE1	1:A:379:PHE:HD2	1.84	0.40
1:A:127:TYR:HB2	1:A:353:TYR:CB	2.52	0.40
1:B:199:GLN:HB3	1:B:200:PRO:HD2	2.02	0.40
1:B:67:VAL:O	1:B:89:LEU:HG	2.21	0.40
1:B:186:GLY:HA3	1:B:404:VAL:O	2.21	0.40
1:A:51:THR:O	1:A:53:THR:N	2.54	0.40
1:B:212:ALA:O	1:B:216:ARG:NH1	2.54	0.40
1:B:243:ARG:O	1:B:247:VAL:HG23	2.21	0.40
1:A:381:GLU:OE1	1:A:381:GLU:HA	2.21	0.40
1:B:400:ILE:HD13	1:B:439:SER:HA	2.03	0.40
1:B:146:LEU:HD23	1:B:227:LEU:HD13	2.03	0.40
1:B:403:PRO:O	1:B:404:VAL:C	2.60	0.40
1:A:30:MET:O	1:A:79:GLU:O	2.39	0.40
1:A:181:HIS:CD2	1:A:217:ARG:NH1	2.89	0.40
1:A:175:PRO:O	1:A:176:PHE:O	2.39	0.40
1:A:309:CYS:CB	1:A:320:ILE:HG21	2.51	0.40
1:B:301:ARG:CB	1:B:301:ARG:NH1	2.77	0.40
1:B:125:ASP:HB2	1:B:351:PRO:HB2	2.03	0.40

All (3) 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:419:ASP:OD1	1:B:60:THR:O[2_646]	1.73	0.47
1:A:358:GLY:O	1:A:431:LYS:CB[2_646]	1.97	0.23
1:B:172:ARG:NH1	1:B:419:ASP:OD1[2_745]	2.17	0.03

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	411/466 (88%)	303 (74%)	71 (17%)	37 (9%)	1	1
1	B	439/466 (94%)	328 (75%)	75 (17%)	36 (8%)	1	1
All	All	850/932 (91%)	631 (74%)	146 (17%)	73 (9%)	1	1

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	A	95	THR
1	A	130	GLU
1	A	155	VAL
1	A	188	ASP
1	A	207	THR
1	A	289	ALA
1	A	292	GLY
1	A	345	GLN
1	A	370	GLY
1	A	417	TRP
1	A	423	VAL
1	B	6	ARG
1	B	7	TYR
1	B	8	VAL
1	B	10	LEU
1	B	34	ALA
1	B	55	VAL

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Mol	Chain	Res	Type
1	B	57	VAL
1	B	59	THR
1	B	63	PHE
1	B	88	ALA
1	B	96	ASP
1	B	129	PRO
1	B	155	VAL
1	B	253	GLU
1	B	293	ALA
1	B	347	GLU
1	B	358	GLY
1	B	423	VAL
1	B	441	PRO
1	B	454	ALA
1	B	455	LEU
1	A	52	GLY
1	A	54	ASN
1	A	66	GLY
1	A	102	ALA
1	A	115	MET
1	A	117	ASP
1	A	138	GLY
1	A	158	GLY
1	A	252	GLY
1	A	264	GLY
1	A	310	LYS
1	A	373	ALA
1	A	434	ALA
1	B	54	ASN
1	B	177	ALA
1	B	302	GLY
1	B	404	VAL
1	B	419	ASP
1	B	450	GLY
1	A	104	PHE
1	A	156	ASP
1	A	176	PHE
1	A	291	HIS
1	A	316	GLY
1	A	415	GLN
1	B	131	ALA
1	B	340	ALA

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Mol	Chain	Res	Type
1	B	403	PRO
1	A	39	VAL
1	A	146	LEU
1	A	416	ALA
1	B	112	ASN
1	A	214	ALA
1	B	76	GLU
1	B	194	GLU
1	B	290	GLY
1	A	206	ASP
1	B	339	ILE
1	B	252	GLY
1	A	388	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/354 (90%)	206 (65%)	111 (35%)	0	0
1	B	335/354 (95%)	215 (64%)	120 (36%)	0	0
All	All	652/708 (92%)	421 (65%)	231 (35%)	0	0

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	6	ARG
1	A	10	LEU
1	A	12	LEU
1	A	16	ASP
1	A	18	ILE
1	A	25	LEU
1	A	29	ILE
1	A	31	LYS
1	A	41	THR

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Mol	Chain	Res	Type
1	A	45	PHE
1	A	48	GLU
1	A	50	SER
1	A	55	VAL
1	A	65	ARG
1	A	67	VAL
1	A	68	ASP
1	A	74	VAL
1	A	78	ARG
1	A	80	LEU
1	A	87	VAL
1	A	94	ILE
1	A	95	THR
1	A	96	ASP
1	A	100	MET
1	A	107	LEU
1	A	111	ASN
1	A	117	ASP
1	A	119	GLU
1	A	124	HIS
1	A	126	PHE
1	A	133	ARG
1	A	136	PHE
1	A	137	ASP
1	A	141	VAL
1	A	148	LYS
1	A	149	VAL
1	A	150	LEU
1	A	152	ARG
1	A	156	ASP
1	A	161	VAL
1	A	163	THR
1	A	166	LYS
1	A	172	ARG
1	A	175	PRO
1	A	178	GLU
1	A	181	HIS
1	A	184	TRP
1	A	185	LEU
1	A	191	LYS
1	A	192	ASN
1	A	193	ASN

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Mol	Chain	Res	Type
1	A	194	GLU
1	A	201	PHE
1	A	204	LEU
1	A	207	THR
1	A	210	LEU
1	A	211	VAL
1	A	216	ARG
1	A	219	GLN
1	A	220	ASP
1	A	221	GLU
1	A	229	SER
1	A	235	ASP
1	A	236	ASP
1	A	240	ILE
1	A	241	ILE
1	A	248	LEU
1	A	253	GLU
1	A	256	SER
1	A	258	VAL
1	A	261	LEU
1	A	263	ASP
1	A	266	VAL
1	A	274	THR
1	A	276	ARG
1	A	279	PHE
1	A	300	LYS
1	A	309	CYS
1	A	310	LYS
1	A	313	ARG
1	A	314	LEU
1	A	321	HIS
1	A	324	THR
1	A	336	ASP
1	A	337	ARG
1	A	342	MET
1	A	343	LEU
1	A	344	THR
1	A	345	GLN
1	A	355	GLN
1	A	363	CYS
1	A	364	THR
1	A	366	ILE

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Mol	Chain	Res	Type
1	A	368	SER
1	A	371	MET
1	A	372	ASN
1	A	374	LEU
1	A	375	ARG
1	A	379	PHE
1	A	387	ASN
1	A	390	LEU
1	A	400	ILE
1	A	409	SER
1	A	410	LEU
1	A	411	ARG
1	A	424	LEU
1	A	431	LYS
1	A	432	GLU
1	A	438	GLU
1	A	440	PHE
1	B	5	SER
1	B	6	ARG
1	B	9	ASN
1	B	12	LEU
1	B	14	GLU
1	B	15	GLU
1	B	16	ASP
1	B	18	ILE
1	B	33	LYS
1	B	44	HIS
1	B	50	SER
1	B	53	THR
1	B	56	GLU
1	B	57	VAL
1	B	59	THR
1	B	61	ASP
1	B	62	ASP
1	B	64	THR
1	B	65	ARG
1	B	67	VAL
1	B	70	LEU
1	B	73	GLU
1	B	76	GLU
1	B	78	ARG
1	B	79	GLU

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Mol	Chain	Res	Type
1	B	87	VAL
1	B	89	LEU
1	B	92	ARG
1	B	100	MET
1	B	101	ILE
1	B	103	SER
1	B	106	THR
1	B	107	LEU
1	B	109	MET
1	B	113	GLN
1	B	119	GLU
1	B	122	LYS
1	B	128	VAL
1	B	130	GLU
1	B	144	SER
1	B	148	LYS
1	B	154	GLU
1	B	155	VAL
1	B	161	VAL
1	B	163	THR
1	B	165	ILE
1	B	166	LYS
1	B	168	LYS
1	B	174	LYS
1	B	181	HIS
1	B	184	TRP
1	B	185	LEU
1	B	192	ASN
1	B	194	GLU
1	B	201	PHE
1	B	204	LEU
1	B	205	ARG
1	B	208	ILE
1	B	213	ASP
1	B	216	ARG
1	B	219	GLN
1	B	222	THR
1	B	226	LYS
1	B	232	ILE
1	B	240	ILE
1	B	241	ILE
1	B	248	LEU

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Mol	Chain	Res	Type
1	B	250	THR
1	B	251	PHE
1	B	258	VAL
1	B	260	LEU
1	B	261	LEU
1	B	272	ILE
1	B	273	THR
1	B	278	ARG
1	B	281	ASP
1	B	284	LEU
1	B	286	TYR
1	B	288	ARG
1	B	298	GLN
1	B	300	LYS
1	B	301	ARG
1	B	320	ILE
1	B	321	HIS
1	B	322	THR
1	B	324	THR
1	B	337	ARG
1	B	343	LEU
1	B	345	GLN
1	B	346	ASP
1	B	347	GLU
1	B	351	PRO
1	B	354	ARG
1	B	355	GLN
1	B	356	SER
1	B	366	ILE
1	B	367	ILE
1	B	372	ASN
1	B	374	LEU
1	B	375	ARG
1	B	376	MET
1	B	382	ASN
1	B	388	VAL
1	B	390	LEU
1	B	397	PHE
1	B	400	ILE
1	B	409	SER
1	B	410	LEU
1	B	411	ARG

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Mol	Chain	Res	Type
1	B	412	GLN
1	B	414	TRP
1	B	418	ARG
1	B	429	GLU
1	B	431	LYS
1	B	439	SER
1	B	441	PRO
1	B	443	ASP
1	B	453	LYS
1	B	455	LEU
1	B	457	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	111	ASN
1	A	113	GLN
1	A	124	HIS
1	A	142	ASN
1	A	192	ASN
1	A	193	ASN
1	A	196	GLN
1	A	254	ASN
1	A	257	HIS
1	A	282	ASN
1	A	315	GLN
1	A	321	HIS
1	A	355	GLN
1	A	415	GLN
1	B	44	HIS
1	B	112	ASN
1	B	192	ASN
1	B	231	ASN
1	B	254	ASN
1	B	282	ASN
1	B	287	HIS
1	B	345	GLN
1	B	349	GLN
1	B	355	GLN

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 carbohydrates 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 [i](#)

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.