



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:12 AM EDT

PDB ID : 2C6S / pdb_00002c6s
Title : human adenovirus penton base 2 12 chimera
Authors : Zubieta, C.; Blanchoin, L.; Cusack, S.
Deposited on : 2005-11-11
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

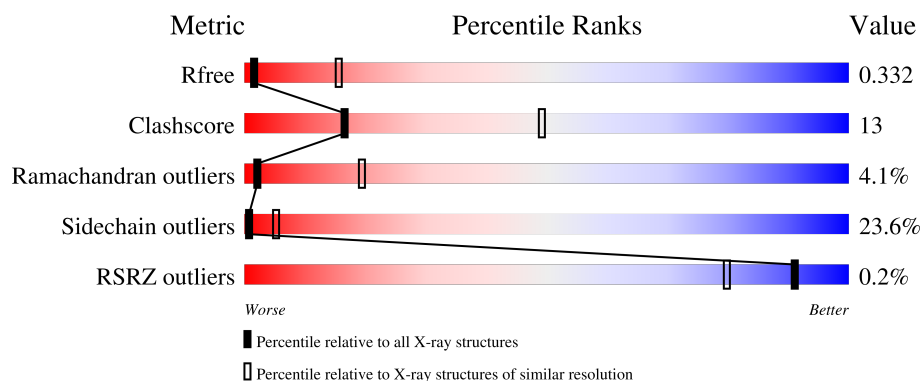
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	523	
1	B	523	
1	C	523	
1	D	523	
1	E	523	

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Mol	Chain	Length	Quality of chain
1	F	523	
1	G	523	
1	H	523	
1	I	523	
1	J	523	
1	K	523	
1	L	523	
1	M	523	
1	N	523	
1	O	523	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 53010 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 ADENOVIRUS 2,12 PENTON BASE CHIMERA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	B	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	C	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	D	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	E	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	F	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	G	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	H	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	I	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	J	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	K	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	L	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	M	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	N	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	O	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			

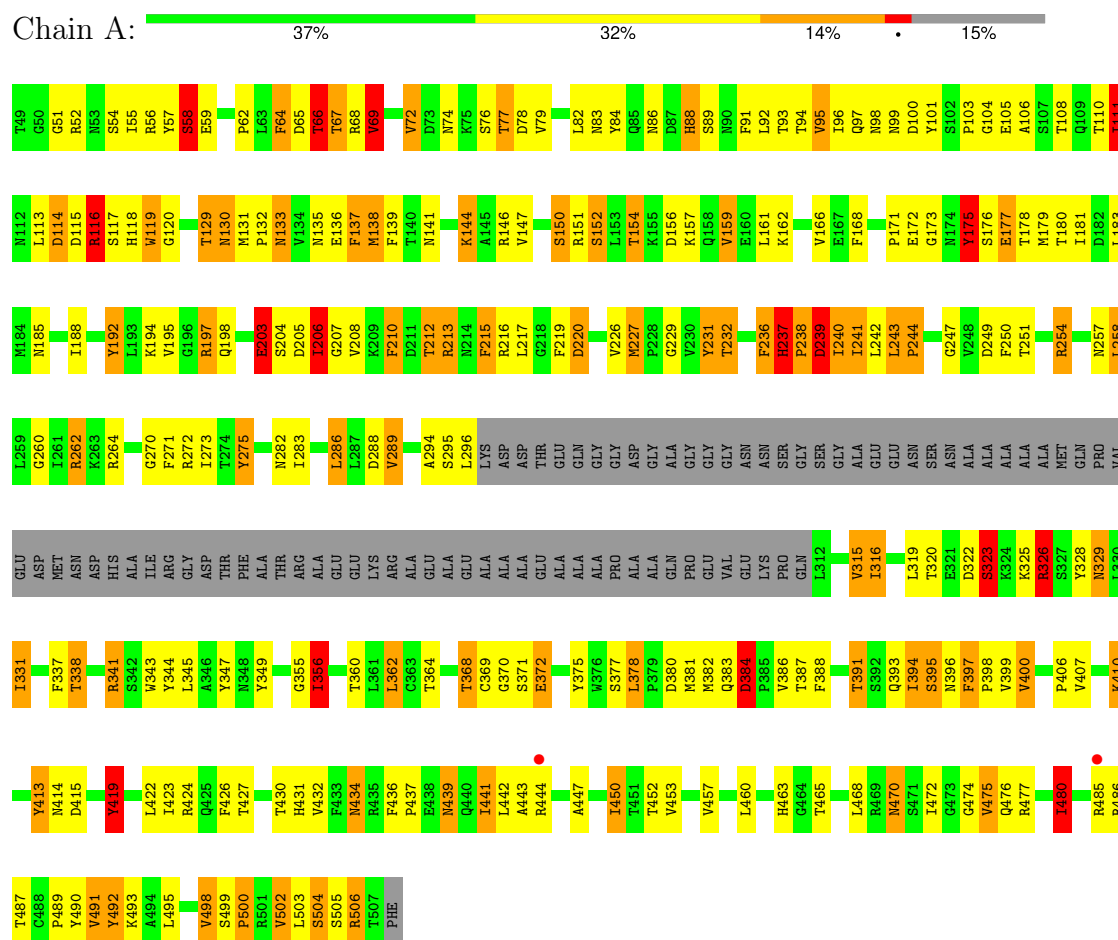
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	LEU	LYS	conflict	UNP P03276
B	312	LEU	LYS	conflict	UNP P03276
C	312	LEU	LYS	conflict	UNP P03276
D	312	LEU	LYS	conflict	UNP P03276
E	312	LEU	LYS	conflict	UNP P03276
F	312	LEU	LYS	conflict	UNP P03276
G	312	LEU	LYS	conflict	UNP P03276
H	312	LEU	LYS	conflict	UNP P03276
I	312	LEU	LYS	conflict	UNP P03276
J	312	LEU	LYS	conflict	UNP P03276
K	312	LEU	LYS	conflict	UNP P03276
L	312	LEU	LYS	conflict	UNP P03276
M	312	LEU	LYS	conflict	UNP P03276
N	312	LEU	LYS	conflict	UNP P03276
O	312	LEU	LYS	conflict	UNP P03276

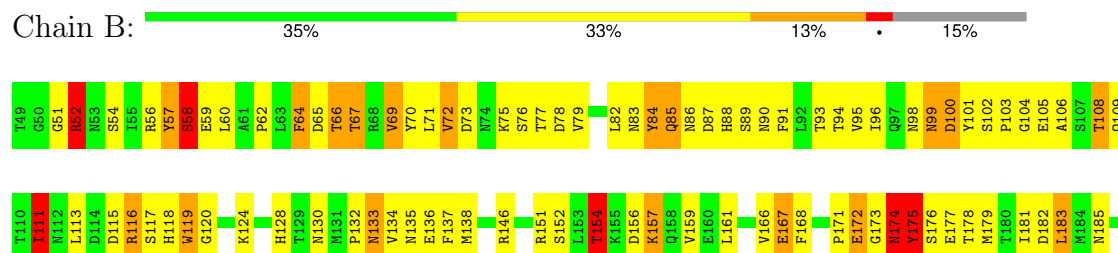
3 Residue-property plots

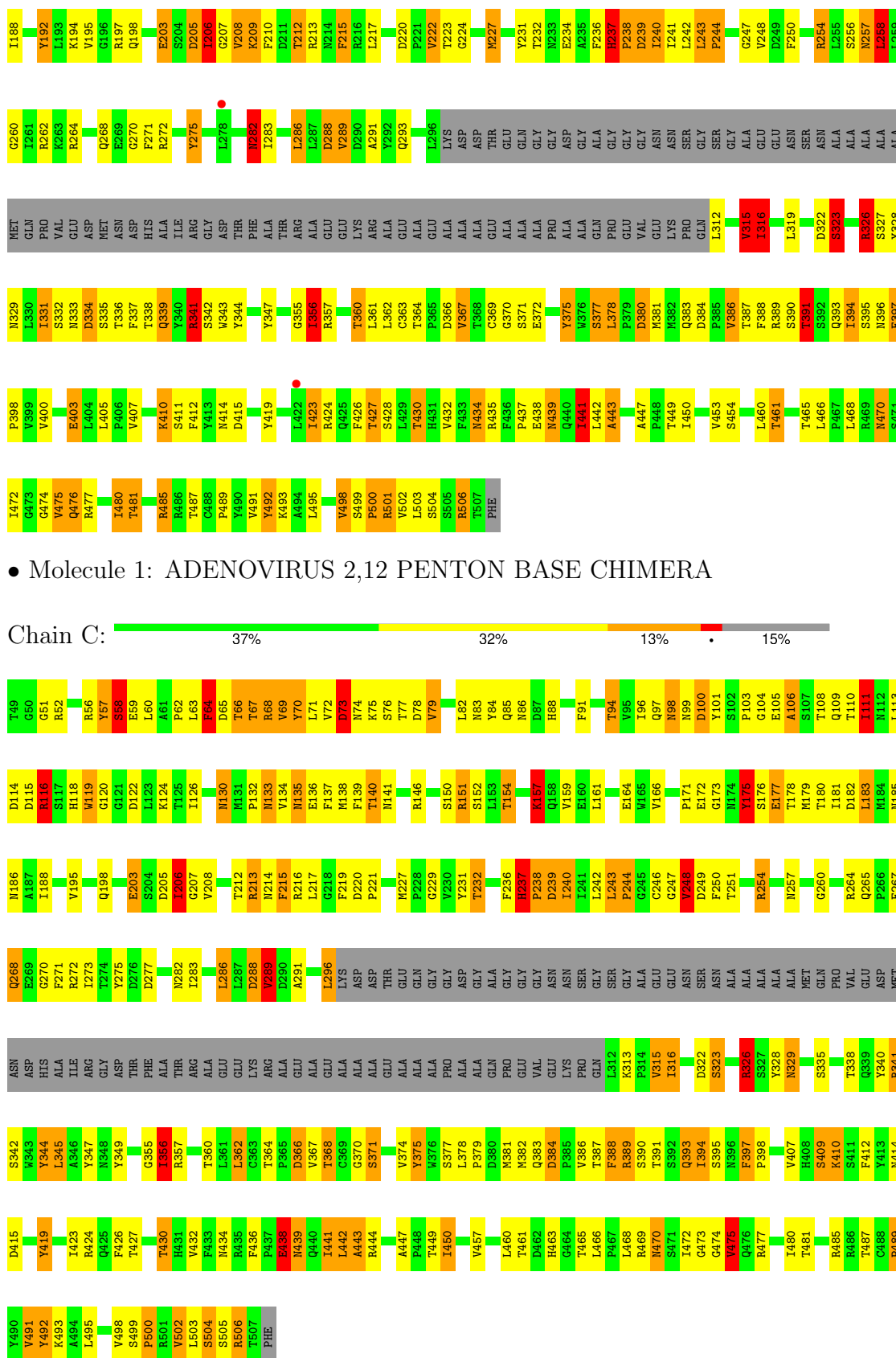
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

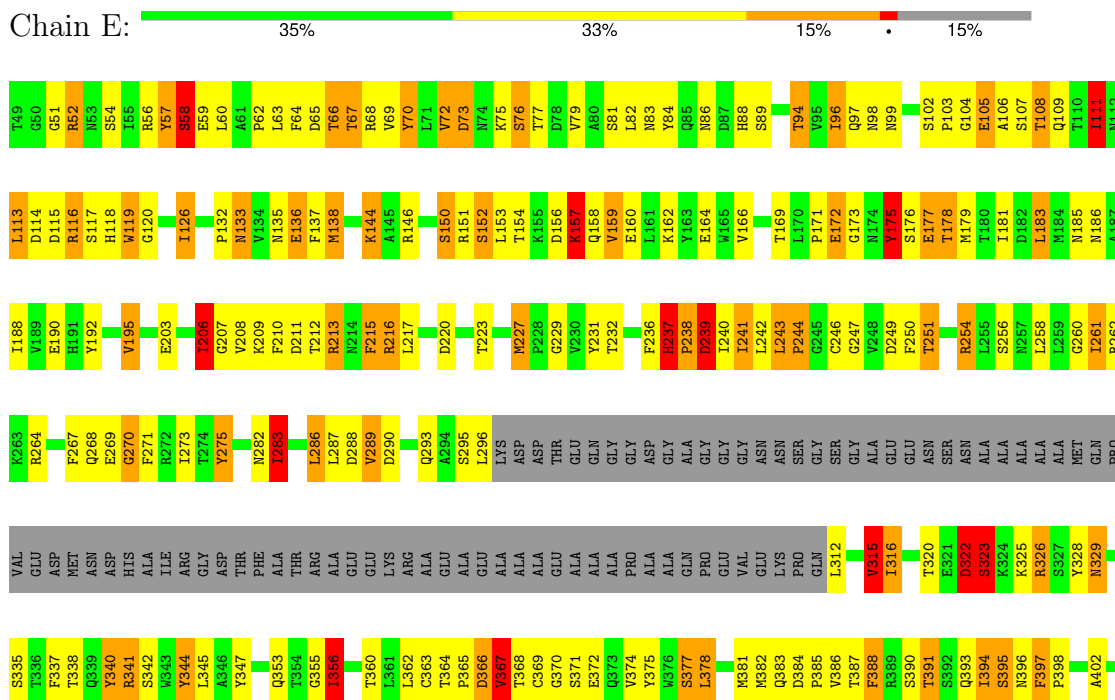
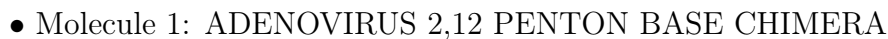
• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

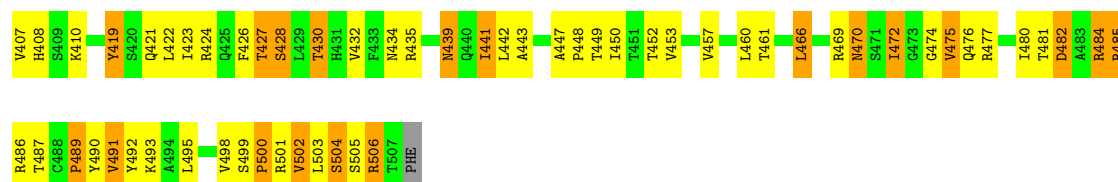


• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

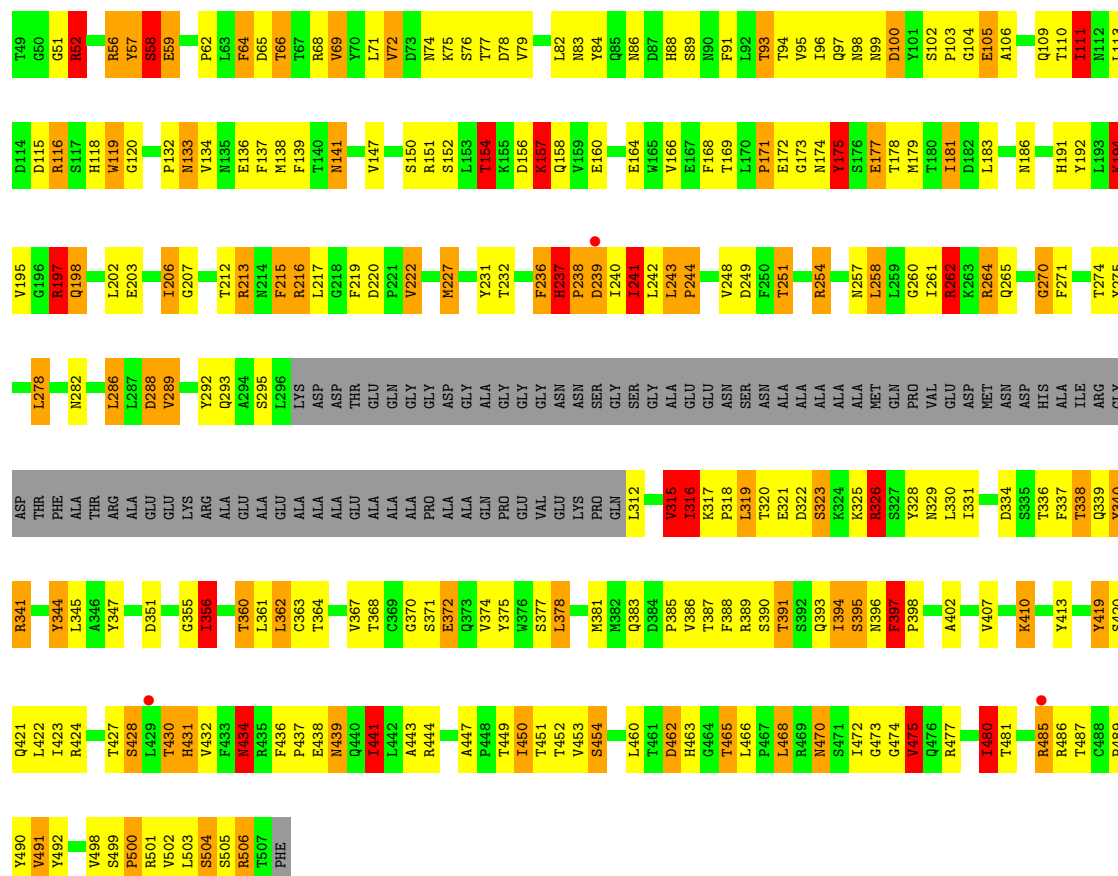




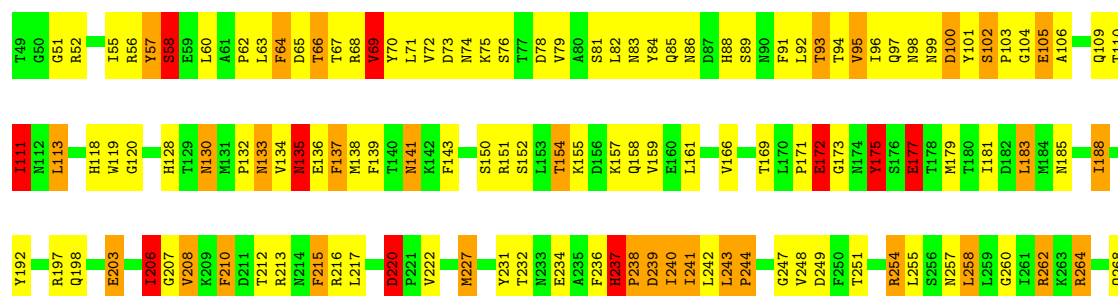


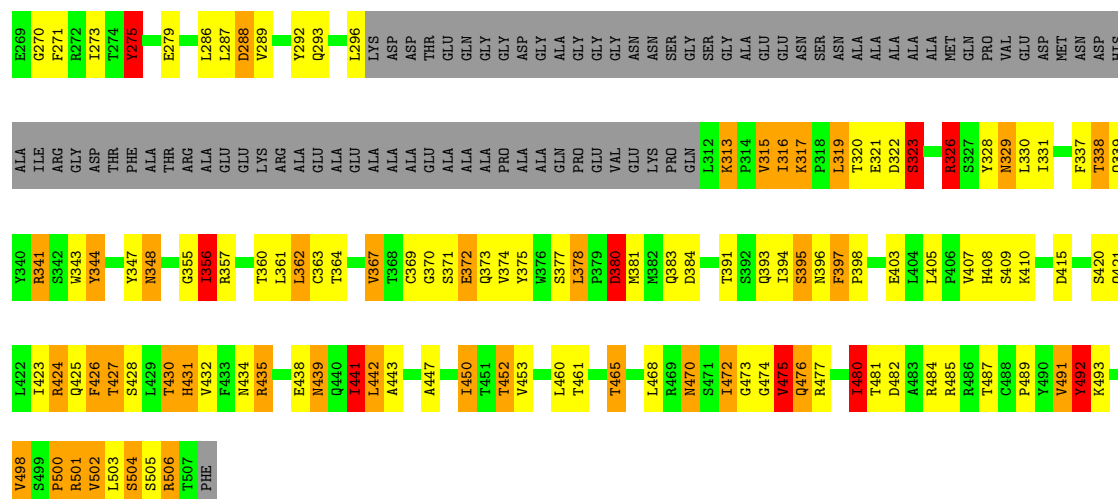


• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

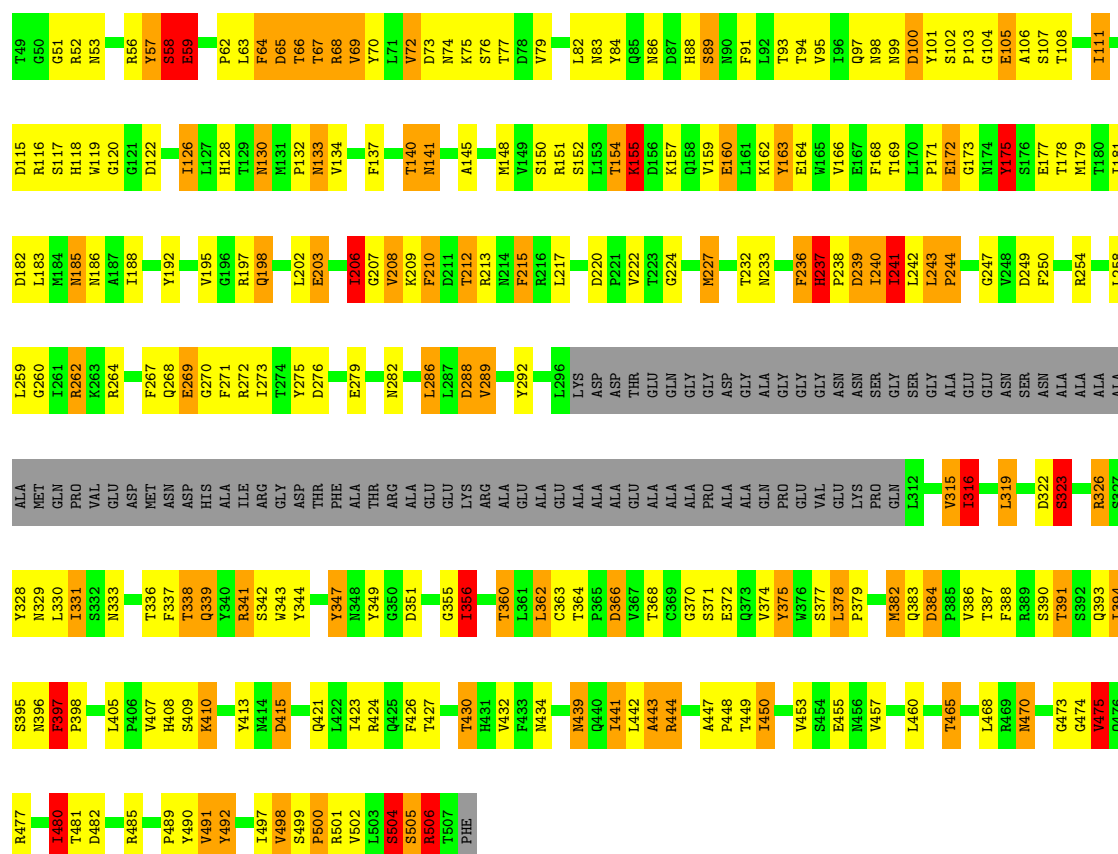


• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA



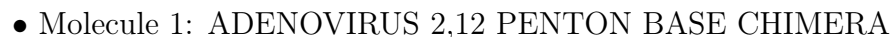


- Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

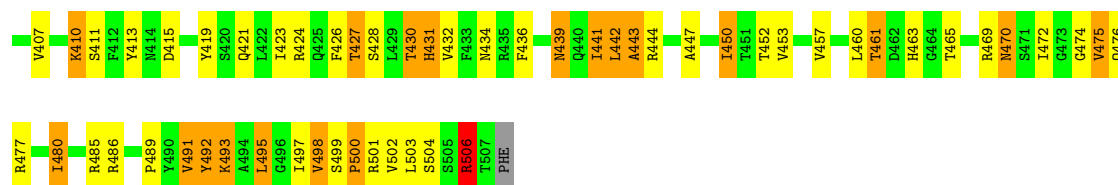


- Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA



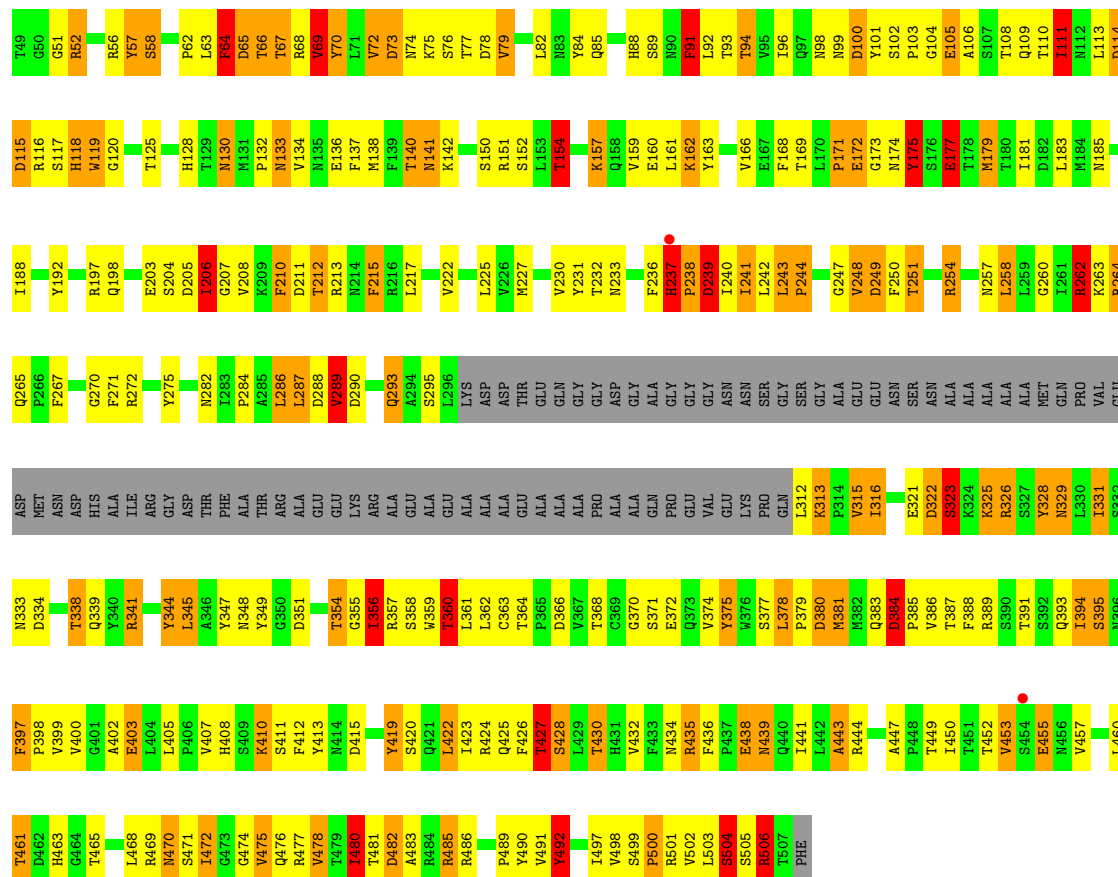


A	Y328	ALA	R254	L183	D114	T49		
	N329	ALA	L255	M184	D115	G50		
	L330	ALA	S256	N185	D116	G51		
	I331	GLN	N257	M186	R117	R52		
	D	D334	PRO	L258	A187	S117	N53	
		S335	VAL	G260	I188	H118	S54	
		T336	GLU	T261		I119	I95	
	F337	GLU	R262	Y192	G120	R56		
	T338	MET	K263	L193	K124	S58		
	ASP	ASN	R264	K194	T125	E59		
C	R341	ASP	Q268	R197	L126	P62		
	S342	HIS			L127	L63		
	W343	ALA			H128	F64		
	Y344	ILE	G270	Q198	T129	D65		
	L345	ARG	F271	V201	M130	T71		
	L346	GLY	R272	S204	P132	T66		
	Y347	ASP	T273	D205	M133	T67		
	D	D351	THR	T274	T206	V134	R68	
		G	G355	ALA	Y275	G207	N135	V69
			G356	THR	N282	V208	E136	L71
E	L356	ARG	L286	K209	F137	V72		
	T360	ALA		F210	M138	D73		
	L361	GLU		D211	F139	W74		
	L362	GLU	L287	T212	T140	K75		
	G	G367	LVS	V289	R213	S76	T77	
		T	T368	ARG	D290	N214	K142	D78
			T369	GLU	A291	T215	F143	D78
	G370	ALA	S295	R216	K144	V79		
	S371	GLU	L296	L217	S150	L82		
	F	Y374	ALA	LVS	D220	R151	N83	
Y375		ALA	ASP	V226	S152	Y84		
Y376		GLU	ASP		L153	Q85		
L376		ALA	THR	M227	T154	N86		
S377		ALA	GLU	V230	K155	D87		
L378		ALA	GLN		R157	H88		
L379		PRO	GLY		K157	S89		
F379		ALA	ASP	T232	Q158	N90		
G		M	M382	ALA	N233	V159	F91	
			Q383	GLN	E234	E160	L92	
	L384		GLN	A235	T93	T93		
	L385	PRO	GLY	F236	V166	T94		
	L386	GLU	GLY	R237	E167	V95		
	L387	VAL	GLY	P238	F168	I96		
	T387	GLU	ASN	D239	T169	Q87		
	F388	LVS	ASN	T240	L170	N98		
	R389	PRO	SER	T241	P171	N99		
	S390	GLN	SER	L242	E172	D100		
H	T391	L312	L243	G173	Y101	I109		
	S392	R315	GLY	N174	S102			
	Q393	I316	GLY	Y175	P103			
	L394	S395	ALA	G247	S176	G104		
	N396	ASN	ASN	V248	E177	E105		
	F397	S323	SER	D249	T178	A106		
	T398	ASN	ASN	F250	M179	I109		
	Y399	R326	ALA	T251	T180			
	Y400	S327	ALA	H252	L181	R192		



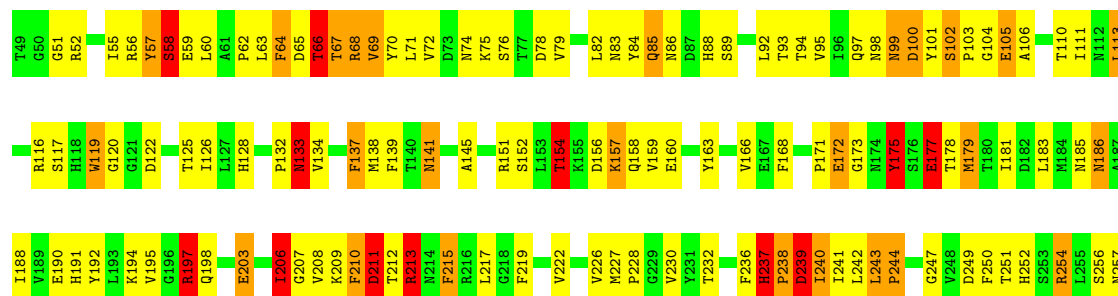
• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

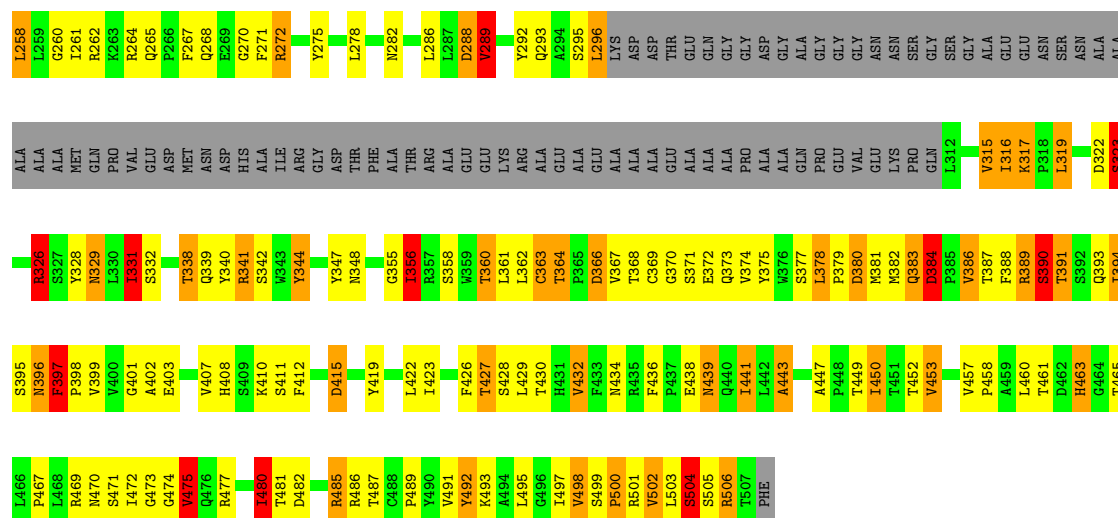
Chain K: 32% 33% 16% 15%



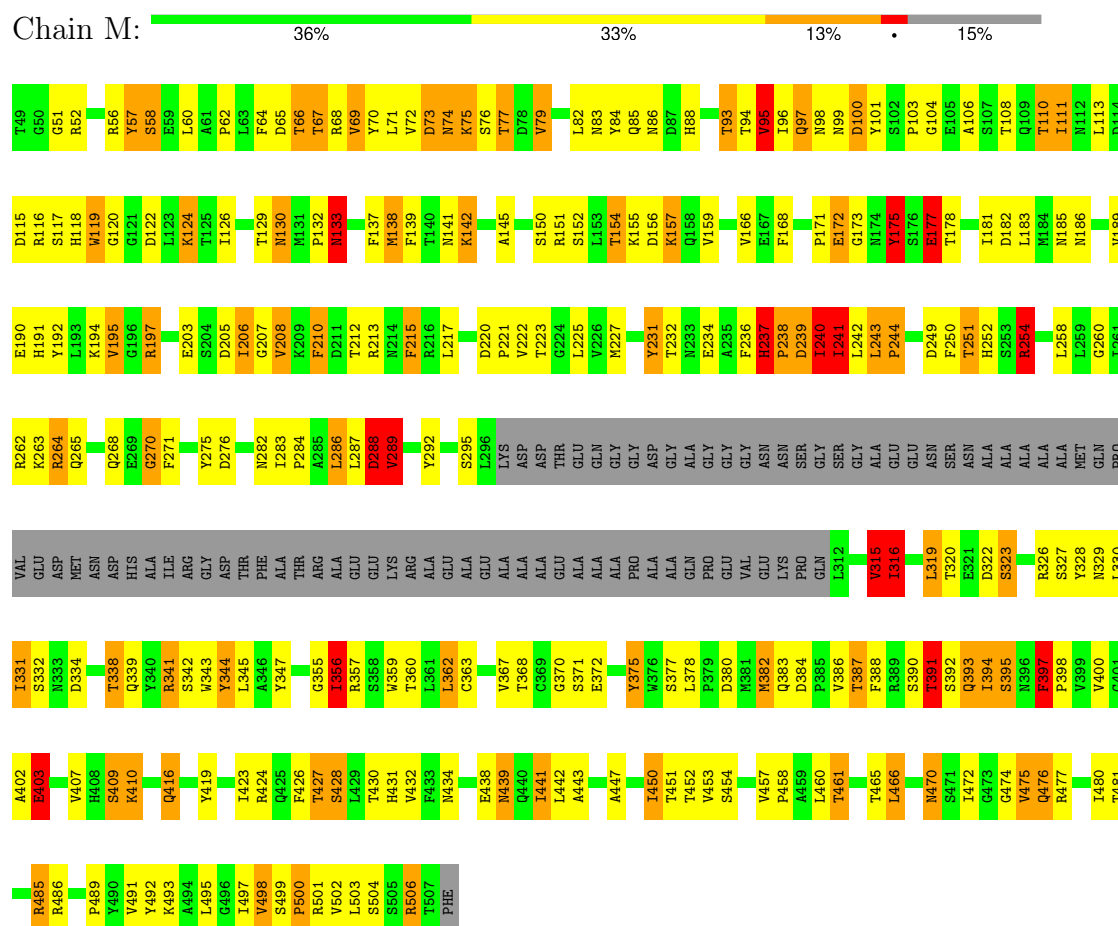
• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

Chain L: 33% 35% 12% 15%



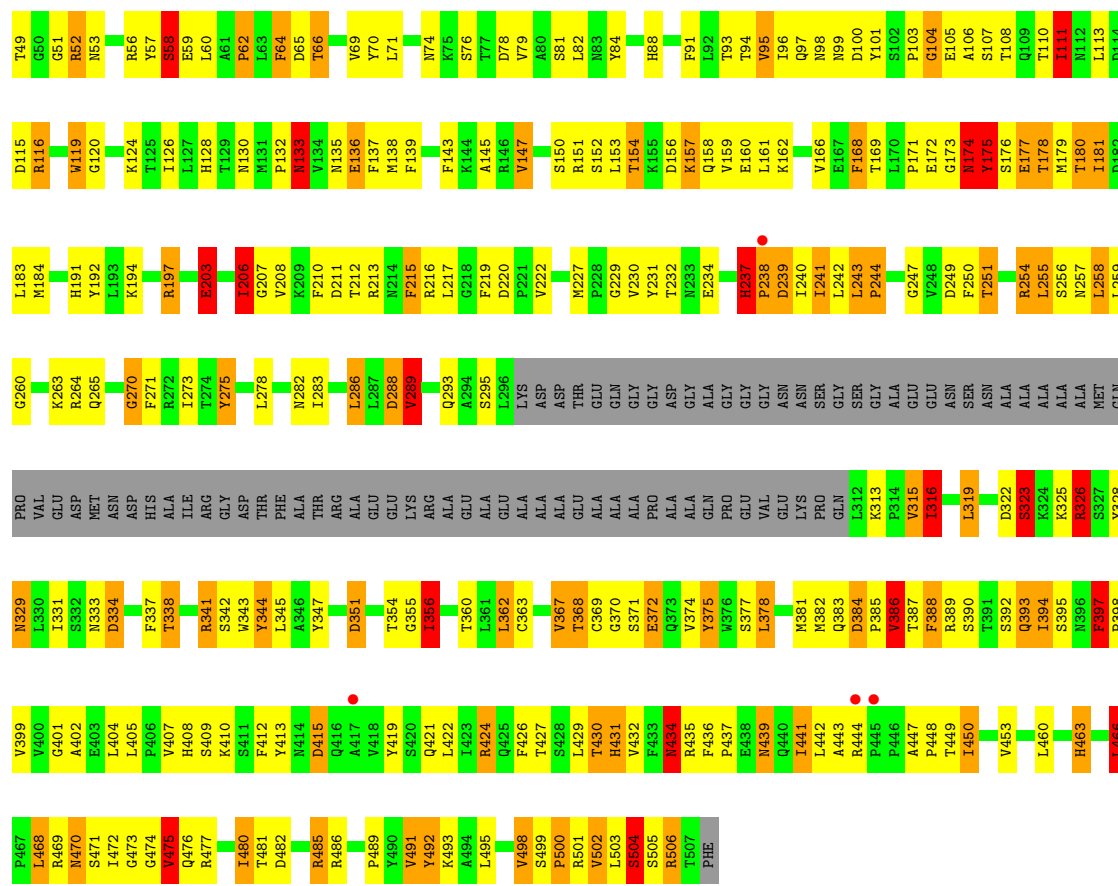


• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA



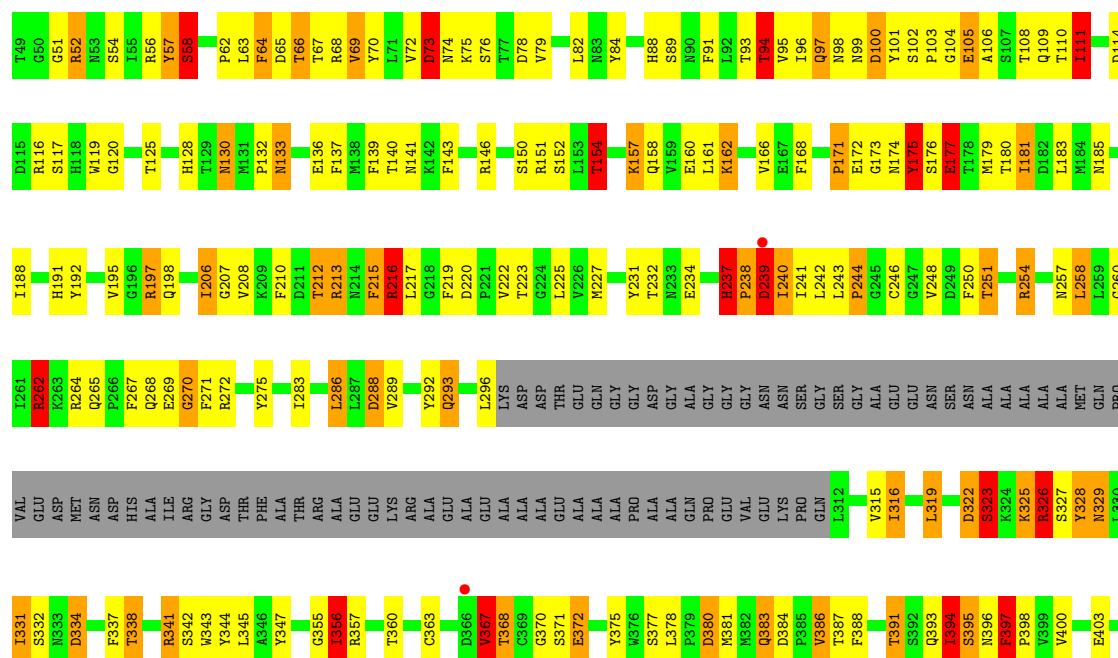
• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

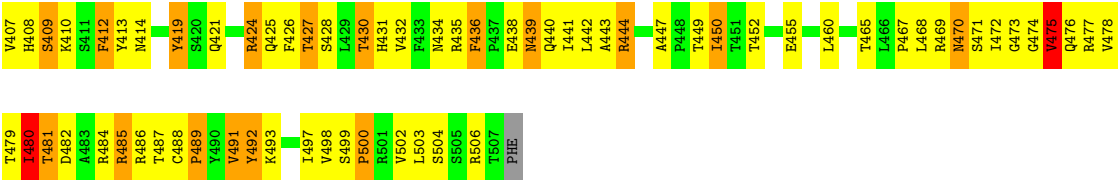




• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

Chain O: 35% 34% 12% 15%





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	266.50Å 292.90Å 307.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.60 15.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-3.60) 88.0 (15.00-3.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.275 , 0.340 0.277 , 0.332	Depositor DCC
R_{free} test set	3041 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	131.0	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	53010	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.12	15/3617 (0.4%)	1.29	18/4926 (0.4%)
1	B	1.28	25/3617 (0.7%)	1.36	25/4926 (0.5%)
1	C	1.25	19/3617 (0.5%)	1.32	20/4926 (0.4%)
1	D	1.14	11/3617 (0.3%)	1.33	19/4926 (0.4%)
1	E	1.18	21/3617 (0.6%)	1.32	17/4926 (0.3%)
1	F	1.25	23/3617 (0.6%)	1.34	23/4926 (0.5%)
1	G	1.28	21/3617 (0.6%)	1.33	25/4926 (0.5%)
1	H	1.15	12/3617 (0.3%)	1.30	15/4926 (0.3%)
1	I	1.10	7/3617 (0.2%)	1.32	19/4926 (0.4%)
1	J	1.16	22/3617 (0.6%)	1.31	21/4926 (0.4%)
1	K	1.23	23/3617 (0.6%)	1.34	18/4926 (0.4%)
1	L	1.14	17/3617 (0.5%)	1.33	21/4926 (0.4%)
1	M	1.30	31/3617 (0.9%)	1.37	23/4926 (0.5%)
1	N	1.18	16/3617 (0.4%)	1.34	27/4926 (0.5%)
1	O	1.33	34/3617 (0.9%)	1.38	25/4926 (0.5%)
All	All	1.21	297/54255 (0.5%)	1.33	316/73890 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	109
1	B	0	105
1	C	0	111
1	D	0	107
1	E	0	103
1	F	0	108
1	G	0	113
1	H	0	114
1	I	0	115
1	J	0	112

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	119
1	L	0	115
1	M	0	105
1	N	0	116
1	O	0	115
All	All	0	1667

All (297) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	220	ASP	CG-OD2	22.53	1.68	1.25
1	C	157	LYS	CE-NZ	19.25	2.07	1.49
1	F	326	ARG	CZ-NH1	17.57	1.57	1.32
1	O	372	GLU	CD-OE1	16.91	1.57	1.25
1	F	194	LYS	CE-NZ	16.47	1.98	1.49
1	C	157	LYS	CD-CE	16.23	2.01	1.52
1	A	372	GLU	CD-OE2	16.15	1.56	1.25
1	H	366	ASP	CG-OD2	14.45	1.52	1.25
1	B	146	ARG	CZ-NH1	13.62	1.51	1.32
1	B	424	ARG	CZ-NH1	13.56	1.51	1.32
1	G	317	LYS	CD-CE	13.48	1.92	1.52
1	O	421	GLN	CD-NE2	13.47	1.61	1.33
1	M	416	GLN	CD-OE1	13.44	1.49	1.23
1	F	100	ASP	CG-OD2	13.16	1.50	1.25
1	M	124	LYS	CD-CE	13.16	1.92	1.52
1	I	366	ASP	CG-OD2	13.04	1.50	1.25
1	D	324	LYS	CE-NZ	12.84	1.87	1.49
1	C	130	ASN	CG-OD1	12.63	1.47	1.23
1	K	290	ASP	CG-OD2	12.57	1.49	1.25
1	H	421	GLN	CD-NE2	12.35	1.59	1.33
1	J	100	ASP	CG-OD2	12.26	1.48	1.25
1	M	142	LYS	CD-CE	12.20	1.89	1.52
1	K	313	LYS	CG-CD	12.18	1.89	1.52
1	L	366	ASP	CG-OD2	12.14	1.48	1.25
1	B	424	ARG	CZ-NH2	12.04	1.49	1.33
1	E	216	ARG	CZ-NH1	11.61	1.49	1.32
1	E	144	LYS	CE-NZ	11.59	1.84	1.49
1	E	366	ASP	CG-OD2	11.43	1.47	1.25
1	G	421	GLN	CD-NE2	11.38	1.57	1.33
1	O	216	ARG	CZ-NH1	11.36	1.48	1.32
1	F	194	LYS	CD-CE	11.34	1.86	1.52
1	B	167	GLU	CD-OE1	11.31	1.46	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	403	GLU	CD-OE2	11.26	1.46	1.25
1	O	431	HIS	CG-CD2	11.24	1.48	1.35
1	M	142	LYS	CE-NZ	11.23	1.83	1.49
1	N	372	GLU	CD-OE2	11.21	1.46	1.25
1	G	100	ASP	CG-OD2	11.12	1.46	1.25
1	G	339	GLN	CD-OE1	11.12	1.44	1.23
1	K	325	LYS	CE-NZ	10.97	1.82	1.49
1	G	313	LYS	CG-CD	10.83	1.84	1.52
1	O	431	HIS	CE1-NE2	10.56	1.43	1.32
1	M	124	LYS	CG-CD	10.55	1.84	1.52
1	A	144	LYS	CE-NZ	10.48	1.80	1.49
1	N	100	ASP	CG-OD2	10.34	1.45	1.25
1	C	157	LYS	CG-CD	10.28	1.83	1.52
1	C	366	ASP	CG-OD2	10.24	1.44	1.25
1	B	282	ASN	CG-ND2	10.20	1.54	1.33
1	O	325	LYS	CD-CE	10.18	1.82	1.52
1	L	317	LYS	CD-CE	10.17	1.82	1.52
1	N	421	GLN	CD-OE1	10.10	1.42	1.23
1	M	124	LYS	CE-NZ	9.87	1.78	1.49
1	M	416	GLN	CD-NE2	9.85	1.53	1.33
1	K	366	ASP	CG-OD2	9.83	1.44	1.25
1	O	424	ARG	CZ-NH1	9.79	1.46	1.32
1	N	421	GLN	CD-NE2	9.76	1.53	1.33
1	M	424	ARG	CZ-NH1	9.73	1.46	1.32
1	B	167	GLU	CG-CD	9.67	1.76	1.52
1	N	326	ARG	CZ-NH2	9.65	1.46	1.33
1	E	157	LYS	CD-CE	9.51	1.80	1.52
1	O	403	GLU	CD-OE1	9.42	1.43	1.25
1	F	174	ASN	CG-OD1	9.41	1.41	1.23
1	J	124	LYS	CD-CE	9.29	1.80	1.52
1	C	384	ASP	CG-OD2	9.29	1.43	1.25
1	N	316	ILE	CA-CB	9.26	1.67	1.54
1	C	393	GLN	CD-OE1	9.07	1.40	1.23
1	O	216	ARG	CD-NE	8.97	1.58	1.46
1	E	190	GLU	CD-OE1	8.94	1.42	1.25
1	O	220	ASP	CG-OD2	8.93	1.42	1.25
1	K	399	VAL	CA-CB	8.87	1.64	1.54
1	M	424	ARG	CD-NE	8.85	1.58	1.46
1	M	339	GLN	CD-OE1	8.77	1.40	1.23
1	O	455	GLU	CD-OE1	8.75	1.42	1.25
1	L	203	GLU	CD-OE2	8.72	1.42	1.25
1	H	316	ILE	CA-CB	8.69	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	GLN	CD-NE2	8.60	1.51	1.33
1	K	290	ASP	CG-OD1	8.55	1.41	1.25
1	J	124	LYS	CG-CD	8.54	1.78	1.52
1	G	316	ILE	CA-CB	8.51	1.66	1.54
1	G	425	GLN	CD-NE2	8.45	1.50	1.33
1	G	421	GLN	CD-OE1	8.44	1.39	1.23
1	O	425	GLN	CG-CD	8.41	1.73	1.52
1	O	162	LYS	CD-CE	8.39	1.77	1.52
1	B	414	ASN	CG-ND2	8.34	1.50	1.33
1	M	289	VAL	CA-CB	8.29	1.63	1.54
1	F	197	ARG	CZ-NH2	8.23	1.44	1.33
1	F	197	ARG	CZ-NH1	8.20	1.44	1.32
1	K	435	ARG	CZ-NH1	8.09	1.44	1.32
1	O	269	GLU	CD-OE2	8.03	1.40	1.25
1	J	142	LYS	CD-CE	8.01	1.76	1.52
1	K	422	LEU	CG-CD1	7.89	1.78	1.52
1	B	67	THR	CA-CB	7.82	1.64	1.53
1	J	423	ILE	CA-CB	7.79	1.63	1.54
1	O	158	GLN	CD-OE1	7.74	1.38	1.23
1	A	316	ILE	CA-CB	7.70	1.65	1.54
1	G	331	ILE	CA-CB	7.70	1.62	1.54
1	N	326	ARG	CZ-NH1	7.68	1.43	1.32
1	B	339	GLN	CD-NE2	7.68	1.49	1.33
1	J	289	VAL	CA-CB	7.64	1.62	1.54
1	A	146	ARG	CZ-NH1	7.61	1.43	1.32
1	B	341	ARG	CZ-NH1	7.61	1.43	1.32
1	H	339	GLN	CD-OE1	7.61	1.38	1.23
1	F	203	GLU	CD-OE2	7.58	1.39	1.25
1	B	424	ARG	NE-CZ	7.54	1.41	1.33
1	M	74	ASN	CG-ND2	7.47	1.49	1.33
1	M	423	ILE	CA-CB	7.45	1.63	1.54
1	C	94	THR	CA-CB	7.42	1.62	1.53
1	B	366	ASP	CG-OD2	7.38	1.39	1.25
1	O	425	GLN	CD-NE2	7.32	1.48	1.33
1	M	100	ASP	CG-OD1	7.32	1.39	1.25
1	G	66	THR	CA-CB	7.26	1.65	1.53
1	F	462	ASP	CG-OD2	7.26	1.39	1.25
1	A	289	VAL	CA-CB	7.25	1.61	1.54
1	J	421	GLN	CD-NE2	7.23	1.48	1.33
1	N	263	LYS	CD-CE	7.21	1.74	1.52
1	B	154	THR	CA-CB	7.19	1.64	1.53
1	G	424	ARG	CZ-NH1	7.19	1.42	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	422	LEU	CG-CD2	7.18	1.76	1.52
1	F	339	GLN	CD-NE2	7.14	1.48	1.33
1	O	326	ARG	CZ-NH1	7.08	1.42	1.32
1	I	480	ILE	CA-CB	7.05	1.61	1.53
1	L	386	VAL	CA-CB	-7.02	1.47	1.54
1	B	174	ASN	CG-OD1	6.99	1.36	1.23
1	H	289	VAL	CA-CB	6.97	1.61	1.54
1	D	394	ILE	CA-CB	6.95	1.64	1.54
1	D	94	THR	CA-CB	6.90	1.61	1.53
1	O	431	HIS	CG-ND1	6.85	1.45	1.38
1	K	94	THR	CA-CB	6.82	1.61	1.53
1	E	96	ILE	CA-CB	-6.79	1.45	1.53
1	K	423	ILE	CA-CB	6.79	1.62	1.54
1	J	154	THR	CA-CB	6.79	1.63	1.53
1	J	387	THR	CA-CB	6.79	1.65	1.53
1	F	154	THR	CA-CB	6.78	1.63	1.53
1	K	313	LYS	CB-CG	6.76	1.72	1.52
1	B	315	VAL	CA-CB	6.76	1.63	1.54
1	G	465	THR	CA-CB	6.75	1.62	1.53
1	M	288	ASP	CG-OD2	6.74	1.38	1.25
1	M	195	VAL	CA-CB	6.72	1.63	1.54
1	F	289	VAL	CA-CB	6.71	1.61	1.54
1	I	364	THR	CA-CB	6.71	1.63	1.53
1	J	331	ILE	CA-CB	6.68	1.63	1.54
1	C	289	VAL	CA-CB	6.67	1.61	1.54
1	K	315	VAL	CA-CB	6.63	1.63	1.54
1	H	155	LYS	CE-NZ	6.63	1.69	1.49
1	B	391	THR	CA-CB	6.60	1.63	1.53
1	E	195	VAL	CA-CB	6.60	1.63	1.54
1	E	108	THR	CA-CB	6.56	1.63	1.53
1	M	154	THR	CA-CB	6.56	1.63	1.53
1	C	316	ILE	CA-CB	6.55	1.63	1.54
1	K	263	LYS	CD-CE	6.52	1.72	1.52
1	O	424	ARG	NE-CZ	6.51	1.40	1.33
1	C	77	THR	CA-CB	6.48	1.63	1.53
1	H	360	THR	CA-CB	6.47	1.62	1.53
1	L	429	LEU	CG-CD2	6.47	1.74	1.52
1	J	316	ILE	CA-CB	6.46	1.63	1.54
1	B	414	ASN	CG-OD1	6.44	1.35	1.23
1	K	455	GLU	CD-OE1	6.44	1.37	1.25
1	B	167	GLU	CD-OE2	6.41	1.37	1.25
1	B	506	ARG	C-N	-6.38	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	421	GLN	CD-NE2	6.37	1.46	1.33
1	L	100	ASP	CG-OD2	6.36	1.37	1.25
1	L	154	THR	CA-CB	6.36	1.62	1.53
1	M	100	ASP	CG-OD2	6.32	1.37	1.25
1	M	315	VAL	CA-CB	6.32	1.63	1.54
1	O	316	ILE	CA-CB	6.32	1.63	1.54
1	D	108	THR	CA-CB	6.31	1.63	1.53
1	L	316	ILE	CA-CB	6.31	1.63	1.54
1	O	181	ILE	CA-CB	6.28	1.61	1.54
1	H	59	GLU	CD-OE1	6.28	1.37	1.25
1	O	94	THR	CA-CB	6.28	1.60	1.53
1	I	154	THR	CA-CB	6.27	1.62	1.53
1	E	502	VAL	CA-CB	-6.25	1.47	1.54
1	O	326	ARG	CZ-NH2	6.23	1.41	1.33
1	L	411	SER	CB-OG	6.22	1.54	1.42
1	H	423	ILE	CA-CB	6.21	1.61	1.54
1	C	268	GLN	CD-OE1	6.17	1.35	1.23
1	N	334	ASP	CG-OD2	6.17	1.37	1.25
1	E	315	VAL	CA-CB	6.14	1.62	1.54
1	L	429	LEU	CG-CD1	6.11	1.72	1.52
1	H	269	GLU	CD-OE2	6.11	1.36	1.25
1	D	315	VAL	CA-CB	6.08	1.62	1.54
1	F	421	GLN	CD-NE2	6.06	1.46	1.33
1	E	94	THR	CA-CB	6.04	1.60	1.53
1	C	423	ILE	CA-CB	6.03	1.61	1.54
1	D	423	ILE	CA-CB	6.01	1.61	1.54
1	L	423	ILE	CA-CB	6.01	1.61	1.54
1	C	164	GLU	CD-OE2	6.00	1.36	1.25
1	O	331	ILE	CA-CB	6.00	1.62	1.54
1	B	423	ILE	CA-CB	6.00	1.61	1.54
1	F	77	THR	CA-CB	5.98	1.62	1.53
1	B	487	THR	CA-CB	5.94	1.63	1.53
1	C	506	ARG	C-N	-5.92	1.25	1.33
1	G	425	GLN	CD-OE1	5.92	1.34	1.23
1	M	316	ILE	CA-CB	5.92	1.62	1.54
1	A	423	ILE	CA-CB	5.90	1.61	1.54
1	O	421	GLN	CD-OE1	5.89	1.34	1.23
1	F	506	ARG	C-N	-5.88	1.25	1.33
1	O	220	ASP	CG-OD1	5.86	1.36	1.25
1	M	387	THR	CA-CB	5.85	1.63	1.53
1	M	391	THR	CA-CB	5.85	1.62	1.53
1	N	197	ARG	CZ-NH1	5.82	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	102	SER	CB-OG	5.79	1.53	1.42
1	O	425	GLN	CD-OE1	5.79	1.34	1.23
1	A	159	VAL	CA-CB	5.79	1.62	1.54
1	A	331	ILE	CA-CB	5.78	1.60	1.54
1	A	506	ARG	C-N	-5.77	1.25	1.33
1	C	96	ILE	CA-CB	-5.77	1.47	1.53
1	N	506	ARG	C-N	-5.74	1.25	1.33
1	K	154	THR	CA-CB	5.73	1.61	1.53
1	J	315	VAL	CA-CB	5.73	1.62	1.54
1	H	444	ARG	CZ-NH2	5.73	1.40	1.33
1	L	289	VAL	CA-CB	5.72	1.60	1.54
1	G	423	ILE	CA-CB	5.72	1.61	1.54
1	J	391	THR	CA-CB	5.69	1.62	1.53
1	F	372	GLU	CD-OE1	5.69	1.36	1.25
1	K	360	THR	CA-CB	5.68	1.61	1.53
1	E	320	THR	CA-CB	5.67	1.63	1.53
1	J	444	ARG	CZ-NH1	5.67	1.40	1.32
1	E	209	LYS	CE-NZ	5.60	1.66	1.49
1	J	506	ARG	C-N	-5.60	1.25	1.33
1	K	316	ILE	CA-CB	5.58	1.62	1.54
1	O	325	LYS	CG-CD	5.58	1.69	1.52
1	M	506	ARG	C-N	-5.58	1.25	1.33
1	N	154	THR	CA-CB	5.57	1.61	1.53
1	M	416	GLN	CB-CG	5.57	1.69	1.52
1	B	316	ILE	CA-CB	5.56	1.62	1.54
1	I	230	VAL	CA-CB	5.56	1.61	1.54
1	N	203	GLU	CD-OE2	5.53	1.35	1.25
1	G	506	ARG	C-N	-5.52	1.25	1.33
1	E	269	GLU	CD-OE2	5.51	1.35	1.25
1	K	289	VAL	CA-CB	5.50	1.60	1.54
1	J	230	VAL	CA-CB	5.49	1.61	1.54
1	D	316	ILE	CA-CB	5.48	1.61	1.54
1	C	130	ASN	CB-CG	5.48	1.65	1.52
1	L	331	ILE	CA-CB	5.47	1.60	1.54
1	F	261	ILE	CA-CB	5.46	1.61	1.54
1	A	77	THR	CA-CB	5.45	1.61	1.53
1	O	425	GLN	CB-CG	5.44	1.68	1.52
1	G	425	GLN	CB-CG	5.43	1.68	1.52
1	A	108	THR	CA-CB	5.42	1.61	1.53
1	O	293	GLN	CD-NE2	5.42	1.44	1.33
1	G	425	GLN	CG-CD	5.41	1.65	1.52
1	N	289	VAL	CA-CB	5.41	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	233	ASN	CG-ND2	5.41	1.44	1.33
1	L	293	GLN	CD-OE1	5.41	1.33	1.23
1	O	154	THR	CA-CB	5.39	1.61	1.53
1	C	265	GLN	CD-OE1	5.39	1.33	1.23
1	N	159	VAL	CA-CB	5.38	1.61	1.54
1	A	154	THR	CA-CB	5.37	1.61	1.53
1	N	315	VAL	CA-CB	5.37	1.61	1.54
1	M	240	ILE	CB-CG2	-5.35	1.34	1.52
1	M	339	GLN	CD-NE2	5.35	1.44	1.33
1	D	506	ARG	C-N	-5.35	1.25	1.33
1	J	226	VAL	CA-CB	5.27	1.60	1.54
1	J	126	ILE	CA-CB	5.27	1.60	1.53
1	E	316	ILE	CA-CB	5.26	1.61	1.54
1	E	506	ARG	C-N	-5.25	1.25	1.33
1	E	423	ILE	CA-CB	5.24	1.60	1.54
1	L	195	VAL	CA-CB	5.24	1.61	1.54
1	D	386	VAL	CA-CB	-5.23	1.48	1.54
1	A	69	VAL	CA-CB	-5.22	1.48	1.54
1	G	372	GLU	CD-OE1	5.22	1.35	1.25
1	J	158	GLN	CD-OE1	5.22	1.33	1.23
1	J	142	LYS	CE-NZ	5.21	1.65	1.49
1	F	316	ILE	CA-CB	5.21	1.61	1.54
1	E	457	VAL	CA-CB	5.20	1.63	1.54
1	B	289	VAL	CA-CB	5.20	1.60	1.54
1	C	315	VAL	CA-CB	5.19	1.61	1.54
1	K	69	VAL	CA-CB	-5.17	1.48	1.54
1	M	331	ILE	CA-CB	5.17	1.60	1.54
1	K	263	LYS	CE-NZ	5.17	1.64	1.49
1	D	289	VAL	CA-CB	5.14	1.60	1.54
1	G	317	LYS	CE-NZ	5.13	1.64	1.49
1	I	320	THR	CA-CB	5.13	1.62	1.53
1	I	506	ARG	C-N	-5.13	1.26	1.33
1	F	315	VAL	CA-CB	5.13	1.61	1.54
1	A	491	VAL	CA-CB	5.12	1.58	1.53
1	H	154	THR	CA-CB	5.12	1.60	1.53
1	M	77	THR	CA-CB	5.12	1.61	1.53
1	M	110	THR	CA-CB	5.12	1.65	1.53
1	J	94	THR	CA-CB	5.12	1.59	1.53
1	E	273	ILE	CA-CB	5.12	1.60	1.54
1	B	240	ILE	CB-CG2	-5.11	1.35	1.52
1	L	317	LYS	CG-CD	5.11	1.67	1.52
1	A	480	ILE	CA-CB	5.10	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	454	SER	CB-OG	5.10	1.52	1.42
1	D	142	LYS	CE-NZ	5.09	1.64	1.49
1	M	95	VAL	CA-CB	-5.08	1.47	1.54
1	E	289	VAL	CA-CB	5.08	1.59	1.54
1	O	162	LYS	CG-CD	5.07	1.67	1.52
1	K	293	GLN	CD-NE2	5.04	1.43	1.33
1	F	372	GLU	CD-OE2	5.04	1.34	1.25
1	F	96	ILE	CA-CB	-5.03	1.46	1.53
1	O	216	ARG	CZ-NH2	5.03	1.40	1.33
1	G	317	LYS	CG-CD	5.03	1.67	1.52
1	O	239	ASP	N-CA	-5.02	1.39	1.46
1	F	274	THR	CA-CB	5.01	1.62	1.54
1	K	506	ARG	C-N	-5.00	1.26	1.33

All (316) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	424	ARG	NE-CZ-NH2	-13.33	107.20	119.20
1	C	157	LYS	CG-CD-CE	-12.19	83.26	111.30
1	F	227	MET	CA-C-N	-10.59	106.61	119.84
1	F	227	MET	C-N-CA	-10.59	106.61	119.84
1	I	227	MET	CA-C-N	-10.52	106.69	119.84
1	I	227	MET	C-N-CA	-10.52	106.69	119.84
1	M	416	GLN	OE1-CD-NE2	10.13	132.73	122.60
1	N	227	MET	CA-C-N	-10.05	107.28	119.84
1	N	227	MET	C-N-CA	-10.05	107.28	119.84
1	G	227	MET	CA-C-N	-10.00	107.34	119.84
1	G	227	MET	C-N-CA	-10.00	107.34	119.84
1	C	227	MET	CA-C-N	-9.97	107.38	119.84
1	C	227	MET	C-N-CA	-9.97	107.38	119.84
1	J	227	MET	CA-C-N	-9.87	107.51	119.84
1	J	227	MET	C-N-CA	-9.87	107.51	119.84
1	K	227	MET	CA-C-N	-9.81	107.58	119.84
1	K	227	MET	C-N-CA	-9.81	107.58	119.84
1	K	237	HIS	CA-C-N	-9.71	108.17	120.79
1	K	237	HIS	C-N-CA	-9.71	108.17	120.79
1	M	227	MET	CA-C-N	-9.64	107.78	119.84
1	M	227	MET	C-N-CA	-9.64	107.78	119.84
1	D	227	MET	CA-C-N	-9.61	107.83	119.84
1	D	227	MET	C-N-CA	-9.61	107.83	119.84
1	L	227	MET	CA-C-N	-9.61	107.83	119.84
1	L	227	MET	C-N-CA	-9.61	107.83	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	227	MET	CA-C-N	-9.59	107.86	119.84
1	H	227	MET	C-N-CA	-9.59	107.86	119.84
1	B	227	MET	CA-C-N	-9.57	107.88	119.84
1	B	227	MET	C-N-CA	-9.57	107.88	119.84
1	H	237	HIS	CA-C-N	-9.52	108.42	120.79
1	H	237	HIS	C-N-CA	-9.52	108.42	120.79
1	D	237	HIS	CA-C-N	-9.38	108.59	120.79
1	D	237	HIS	C-N-CA	-9.38	108.59	120.79
1	G	237	HIS	CA-C-N	-9.34	108.65	120.79
1	G	237	HIS	C-N-CA	-9.34	108.65	120.79
1	A	227	MET	CA-C-N	-9.25	108.28	119.84
1	A	227	MET	C-N-CA	-9.25	108.28	119.84
1	O	227	MET	CA-C-N	-9.24	108.29	119.84
1	O	227	MET	C-N-CA	-9.24	108.29	119.84
1	E	227	MET	CA-C-N	-9.20	108.34	119.84
1	E	227	MET	C-N-CA	-9.20	108.34	119.84
1	L	237	HIS	CA-C-N	-9.13	108.92	120.79
1	L	237	HIS	C-N-CA	-9.13	108.92	120.79
1	A	237	HIS	CA-C-N	-9.12	108.94	120.79
1	A	237	HIS	C-N-CA	-9.12	108.94	120.79
1	M	237	HIS	CA-C-N	-9.11	108.95	120.79
1	M	237	HIS	C-N-CA	-9.11	108.95	120.79
1	O	237	HIS	CA-C-N	-9.01	108.58	119.84
1	O	237	HIS	C-N-CA	-9.01	108.58	119.84
1	N	237	HIS	CA-C-N	-8.93	109.18	120.79
1	N	237	HIS	C-N-CA	-8.93	109.18	120.79
1	C	237	HIS	CA-C-N	-8.82	109.32	120.79
1	C	237	HIS	C-N-CA	-8.82	109.32	120.79
1	M	124	LYS	CG-CD-CE	-8.74	91.19	111.30
1	B	237	HIS	CA-C-N	-8.74	109.43	120.79
1	B	237	HIS	C-N-CA	-8.74	109.43	120.79
1	B	167	GLU	CB-CG-CD	-8.66	97.88	112.60
1	I	506	ARG	O-C-N	-8.53	109.35	123.00
1	F	241	ILE	N-CA-CB	-8.49	100.60	111.64
1	F	197	ARG	NE-CZ-NH2	-8.47	111.58	119.20
1	N	326	ARG	NE-CZ-NH2	-8.42	111.62	119.20
1	J	237	HIS	CA-C-N	-8.25	109.53	119.84
1	J	237	HIS	C-N-CA	-8.25	109.53	119.84
1	F	237	HIS	CA-C-N	-8.20	109.60	119.84
1	F	237	HIS	C-N-CA	-8.20	109.60	119.84
1	O	421	GLN	CG-CD-NE2	-7.99	104.41	116.40
1	I	237	HIS	CA-C-N	-7.82	110.07	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	237	HIS	C-N-CA	-7.82	110.07	119.84
1	E	237	HIS	CA-C-N	-7.79	110.10	119.84
1	E	237	HIS	C-N-CA	-7.79	110.10	119.84
1	L	502	VAL	CB-CA-C	-7.63	102.91	111.45
1	L	506	ARG	O-C-N	-7.59	110.86	123.00
1	K	313	LYS	CB-CG-CD	-7.58	93.88	111.30
1	N	421	GLN	OE1-CD-NE2	7.58	130.18	122.60
1	K	447	ALA	CA-C-N	-7.57	112.89	120.31
1	K	447	ALA	C-N-CA	-7.57	112.89	120.31
1	F	194	LYS	CG-CD-CE	-7.54	93.95	111.30
1	G	317	LYS	CG-CD-CE	-7.46	94.14	111.30
1	F	79	VAL	CB-CA-C	-7.41	102.33	112.04
1	H	447	ALA	CA-C-N	-7.41	113.05	120.31
1	H	447	ALA	C-N-CA	-7.41	113.05	120.31
1	F	194	LYS	CD-CE-NZ	-7.39	88.25	111.90
1	J	124	LYS	CG-CD-CE	-7.39	94.31	111.30
1	C	268	GLN	OE1-CD-NE2	7.36	129.96	122.60
1	G	506	ARG	O-C-N	-7.29	111.33	123.00
1	O	421	GLN	OE1-CD-NE2	7.28	129.88	122.60
1	C	135	ASN	N-CA-CB	-7.16	100.46	111.56
1	B	222	VAL	CB-CA-C	7.16	121.54	110.95
1	F	506	ARG	O-C-N	-7.14	111.57	123.00
1	E	447	ALA	CA-C-N	-7.11	113.34	120.31
1	E	447	ALA	C-N-CA	-7.11	113.34	120.31
1	C	447	ALA	CA-C-N	-7.04	113.41	120.31
1	C	447	ALA	C-N-CA	-7.04	113.41	120.31
1	N	181	ILE	CB-CA-C	-7.03	102.80	111.87
1	M	175	TYR	CA-CB-CG	7.00	126.49	113.90
1	M	79	VAL	CB-CA-C	-6.99	102.88	112.04
1	L	447	ALA	CA-C-N	-6.91	113.54	120.31
1	L	447	ALA	C-N-CA	-6.91	113.54	120.31
1	O	425	GLN	CB-CG-CD	-6.90	100.87	112.60
1	G	313	LYS	CB-CG-CD	-6.87	95.50	111.30
1	O	326	ARG	NE-CZ-NH2	-6.85	113.03	119.20
1	D	175	TYR	CA-CB-CG	6.82	126.18	113.90
1	N	506	ARG	O-C-N	-6.70	112.29	123.00
1	J	447	ALA	CA-C-N	-6.69	113.75	120.31
1	J	447	ALA	C-N-CA	-6.69	113.75	120.31
1	O	447	ALA	CA-C-N	-6.67	113.78	120.31
1	O	447	ALA	C-N-CA	-6.67	113.78	120.31
1	E	502	VAL	CB-CA-C	-6.58	104.08	111.45
1	G	175	TYR	CA-CB-CG	6.56	125.71	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	ALA	CA-C-N	-6.55	113.89	120.31
1	A	447	ALA	C-N-CA	-6.55	113.89	120.31
1	B	506	ARG	O-C-N	-6.54	112.53	123.00
1	N	502	VAL	CB-CA-C	-6.54	104.12	111.45
1	F	181	ILE	CB-CA-C	-6.49	103.50	111.87
1	C	157	LYS	CD-CE-NZ	-6.48	91.17	111.90
1	E	157	LYS	CG-CD-CE	-6.47	96.42	111.30
1	G	421	GLN	OE1-CD-NE2	6.43	129.03	122.60
1	L	386	VAL	CB-CA-C	-6.36	100.95	111.32
1	D	137	PHE	N-CA-CB	6.35	120.00	110.22
1	A	108	THR	CB-CA-C	-6.34	100.66	110.81
1	C	506	ARG	O-C-N	-6.33	112.88	123.00
1	N	386	VAL	CB-CA-C	-6.32	101.03	111.32
1	G	447	ALA	CA-C-N	-6.26	114.18	120.31
1	G	447	ALA	C-N-CA	-6.26	114.18	120.31
1	C	130	ASN	CB-CG-OD1	-6.25	108.29	120.80
1	H	457	VAL	CB-CA-C	6.21	115.42	109.33
1	B	206	ILE	CB-CA-C	6.20	119.87	111.87
1	I	447	ALA	CA-C-N	-6.19	114.24	120.31
1	I	447	ALA	C-N-CA	-6.19	114.24	120.31
1	K	380	ASP	CB-CA-C	6.19	121.02	110.56
1	B	447	ALA	CA-C-N	-6.14	114.29	120.31
1	B	447	ALA	C-N-CA	-6.14	114.29	120.31
1	N	397	PHE	CA-C-N	6.14	127.51	119.84
1	N	397	PHE	C-N-CA	6.14	127.51	119.84
1	I	421	GLN	CB-CA-C	-6.06	101.36	110.88
1	D	447	ALA	CA-C-N	-6.06	114.37	120.31
1	D	447	ALA	C-N-CA	-6.06	114.37	120.31
1	O	325	LYS	CG-CD-CE	-6.04	97.41	111.30
1	G	397	PHE	CA-C-N	6.00	127.34	119.84
1	G	397	PHE	C-N-CA	6.00	127.34	119.84
1	J	175	TYR	CA-CB-CG	6.00	124.70	113.90
1	J	181	ILE	CB-CA-C	-6.00	104.13	111.87
1	O	216	ARG	NE-CZ-NH2	-5.98	113.82	119.20
1	C	175	TYR	CA-CB-CG	5.96	124.63	113.90
1	B	397	PHE	CA-C-N	5.96	127.29	119.84
1	B	397	PHE	C-N-CA	5.96	127.29	119.84
1	F	339	GLN	OE1-CD-NE2	-5.95	116.66	122.60
1	I	356	ILE	N-CA-C	5.93	121.67	109.34
1	G	102	SER	CB-CA-C	-5.92	99.99	109.69
1	F	397	PHE	CA-C-N	5.92	127.23	119.84
1	F	397	PHE	C-N-CA	5.92	127.23	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	175	TYR	CA-CB-CG	5.88	124.49	113.90
1	M	416	GLN	CB-CG-CD	-5.88	102.61	112.60
1	K	384	ASP	CA-C-N	5.87	127.18	119.84
1	K	384	ASP	C-N-CA	5.87	127.18	119.84
1	G	356	ILE	N-CA-C	5.85	121.51	109.34
1	L	317	LYS	CG-CD-CE	-5.85	97.85	111.30
1	B	208	VAL	N-CA-CB	5.84	117.49	110.95
1	A	397	PHE	CA-C-N	5.84	127.14	119.84
1	A	397	PHE	C-N-CA	5.84	127.14	119.84
1	E	397	PHE	CA-C-N	5.82	127.11	119.84
1	E	397	PHE	C-N-CA	5.82	127.11	119.84
1	F	356	ILE	N-CA-C	5.81	121.43	109.34
1	N	295	SER	N-CA-C	5.79	119.34	107.69
1	H	356	ILE	N-CA-C	5.78	121.37	109.34
1	A	356	ILE	N-CA-C	5.76	121.33	109.34
1	L	356	ILE	N-CA-C	5.76	121.33	109.34
1	M	142	LYS	CG-CD-CE	-5.76	98.05	111.30
1	M	397	PHE	CA-C-N	5.76	127.04	119.84
1	M	397	PHE	C-N-CA	5.76	127.04	119.84
1	B	356	ILE	N-CA-C	5.74	121.28	109.34
1	L	397	PHE	CA-C-N	5.74	127.01	119.84
1	L	397	PHE	C-N-CA	5.74	127.01	119.84
1	O	424	ARG	NE-CZ-NH2	-5.74	114.04	119.20
1	K	356	ILE	N-CA-C	5.73	121.27	109.34
1	J	356	ILE	N-CA-C	5.72	121.24	109.34
1	O	506	ARG	O-C-N	-5.71	113.86	123.00
1	F	447	ALA	CA-C-N	-5.71	114.72	120.31
1	F	447	ALA	C-N-CA	-5.71	114.72	120.31
1	D	356	ILE	N-CA-C	5.71	121.21	109.34
1	G	317	LYS	CD-CE-NZ	-5.70	93.66	111.90
1	I	364	THR	N-CA-CB	5.67	118.39	110.11
1	C	356	ILE	N-CA-C	5.66	121.12	109.34
1	M	356	ILE	N-CA-C	5.66	121.11	109.34
1	O	94	THR	N-CA-CB	5.66	118.99	109.94
1	D	506	ARG	O-C-N	-5.66	113.95	123.00
1	M	254	ARG	CB-CA-C	5.65	119.53	110.09
1	E	66	THR	N-CA-C	5.65	122.83	110.80
1	C	66	THR	N-CA-C	5.64	122.82	110.80
1	B	108	THR	CB-CA-C	-5.62	101.82	110.81
1	O	397	PHE	CA-C-N	5.62	126.86	119.84
1	O	397	PHE	C-N-CA	5.62	126.86	119.84
1	A	487	THR	N-CA-CB	5.61	118.21	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	206	ILE	CB-CA-C	5.61	119.10	111.87
1	M	447	ALA	CA-C-N	-5.60	114.82	120.31
1	M	447	ALA	C-N-CA	-5.60	114.82	120.31
1	N	447	ALA	CA-C-N	-5.60	114.82	120.31
1	N	447	ALA	C-N-CA	-5.60	114.82	120.31
1	N	356	ILE	N-CA-C	5.58	120.95	109.34
1	C	397	PHE	CA-C-N	5.58	126.82	119.84
1	C	397	PHE	C-N-CA	5.58	126.82	119.84
1	O	356	ILE	N-CA-C	5.57	120.92	109.34
1	G	137	PHE	N-CA-CB	5.56	118.78	110.22
1	E	356	ILE	N-CA-C	5.55	120.89	109.34
1	D	108	THR	CB-CA-C	-5.55	101.93	110.81
1	J	506	ARG	O-C-N	-5.55	114.12	123.00
1	L	175	TYR	CA-CB-CG	5.51	123.82	113.90
1	O	63	LEU	CB-CA-C	-5.50	102.05	111.41
1	K	175	TYR	CA-CB-CG	5.47	123.75	113.90
1	E	111	ILE	CA-C-O	-5.47	115.05	120.85
1	O	414	ASN	N-CA-CB	5.47	119.35	110.32
1	N	237	HIS	CB-CA-C	5.46	120.92	110.17
1	D	66	THR	N-CA-C	5.45	122.41	110.80
1	O	386	VAL	CB-CA-C	-5.45	102.44	111.32
1	L	364	THR	N-CA-CB	5.40	118.00	110.11
1	A	506	ARG	O-C-N	-5.40	114.36	123.00
1	K	64	PHE	CB-CA-C	5.40	118.66	109.80
1	G	384	ASP	CA-C-N	5.40	126.59	119.84
1	G	384	ASP	C-N-CA	5.40	126.59	119.84
1	K	66	THR	N-CA-C	5.39	122.28	110.80
1	K	293	GLN	OE1-CD-NE2	5.38	127.98	122.60
1	B	333	ASN	CA-C-N	5.38	127.48	120.28
1	B	333	ASN	C-N-CA	5.38	127.48	120.28
1	M	465	THR	CB-CA-C	5.38	119.00	110.19
1	N	466	LEU	CB-CG-CD1	-5.36	94.62	110.70
1	B	414	ASN	OD1-CG-ND2	5.35	127.95	122.60
1	B	175	TYR	CA-CB-CG	5.35	123.53	113.90
1	N	66	THR	N-CA-C	5.35	122.19	110.80
1	J	237	HIS	CB-CA-C	5.34	120.70	110.17
1	J	52	ARG	CB-CA-C	5.34	119.33	110.78
1	N	384	ASP	CA-C-N	5.34	126.51	119.84
1	N	384	ASP	C-N-CA	5.34	126.51	119.84
1	A	66	THR	N-CA-C	5.33	122.16	110.80
1	F	111	ILE	CA-C-O	-5.32	115.21	120.85
1	M	142	LYS	CD-CE-NZ	-5.30	94.93	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	427	THR	CB-CA-C	-5.30	102.80	110.96
1	F	66	THR	N-CA-C	5.29	122.07	110.80
1	E	502	VAL	N-CA-C	5.29	116.19	110.21
1	D	397	PHE	CA-C-N	5.29	126.45	119.84
1	D	397	PHE	C-N-CA	5.29	126.45	119.84
1	J	111	ILE	CA-C-O	-5.28	115.25	120.85
1	G	380	ASP	CB-CA-C	5.28	119.47	110.56
1	L	66	THR	N-CA-C	5.27	122.03	110.80
1	N	147	VAL	CB-CA-C	-5.27	102.54	110.55
1	G	69	VAL	CB-CA-C	-5.27	102.80	110.81
1	E	480	ILE	CB-CA-C	-5.27	104.60	111.81
1	I	66	THR	N-CA-C	5.26	122.00	110.80
1	C	64	PHE	CB-CA-C	5.25	118.42	109.80
1	K	397	PHE	CA-C-N	5.25	126.41	119.84
1	K	397	PHE	C-N-CA	5.25	126.41	119.84
1	O	111	ILE	CA-C-O	-5.25	115.29	120.85
1	H	397	PHE	CA-C-N	5.24	126.39	119.84
1	H	397	PHE	C-N-CA	5.24	126.39	119.84
1	O	97	GLN	CB-CA-C	-5.24	104.72	111.22
1	J	206	ILE	CB-CA-C	5.24	118.63	111.87
1	O	431	HIS	CG-CD2-NE2	-5.23	101.97	107.20
1	G	506	ARG	CA-C-N	5.23	126.66	116.20
1	I	397	PHE	CA-C-N	5.23	126.37	119.84
1	I	397	PHE	C-N-CA	5.23	126.37	119.84
1	O	66	THR	N-CA-C	5.22	121.93	110.80
1	I	312	LEU	CB-CA-C	5.21	120.00	110.10
1	N	480	ILE	CB-CA-C	-5.21	104.67	111.81
1	E	237	HIS	CB-CA-C	5.21	120.42	110.17
1	G	96	ILE	N-CA-CB	-5.20	107.01	112.06
1	I	487	THR	N-CA-CB	5.20	117.61	109.97
1	A	502	VAL	N-CA-C	5.19	116.08	110.21
1	M	502	VAL	N-CA-C	5.18	116.07	110.21
1	D	97	GLN	CB-CA-C	-5.18	104.80	111.22
1	M	66	THR	N-CA-C	5.18	121.82	110.80
1	F	175	TYR	CA-CB-CG	5.17	123.21	113.90
1	A	384	ASP	CA-C-N	5.17	126.31	119.84
1	A	384	ASP	C-N-CA	5.17	126.31	119.84
1	J	52	ARG	N-CA-C	5.17	117.04	108.20
1	B	502	VAL	CB-CA-C	-5.17	105.66	111.45
1	C	111	ILE	CA-C-O	-5.17	115.37	120.85
1	J	66	THR	N-CA-C	5.17	121.80	110.80
1	H	66	THR	N-CA-C	5.16	121.78	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	111	ILE	CA-C-O	-5.16	115.38	120.85
1	A	64	PHE	CB-CA-C	5.16	118.25	109.80
1	L	363	CYS	CA-CB-SG	5.15	126.24	114.40
1	F	52	ARG	N-CA-C	5.14	116.99	108.20
1	H	126	ILE	CB-CA-C	5.13	117.53	111.32
1	J	94	THR	N-CA-CB	5.12	118.36	110.21
1	L	156	ASP	CB-CA-C	-5.12	105.00	111.86
1	J	480	ILE	CB-CA-C	-5.11	104.81	111.81
1	D	384	ASP	CA-C-N	5.11	126.22	119.84
1	D	384	ASP	C-N-CA	5.11	126.22	119.84
1	D	502	VAL	N-CA-C	5.10	115.98	110.21
1	D	364	THR	N-CA-CB	5.10	117.55	110.11
1	M	384	ASP	CA-C-N	5.10	126.21	119.84
1	M	384	ASP	C-N-CA	5.10	126.21	119.84
1	B	52	ARG	N-CA-C	5.09	116.91	108.20
1	N	175	TYR	CA-CB-CG	5.09	123.06	113.90
1	I	175	TYR	CA-CB-CG	5.08	123.04	113.90
1	L	384	ASP	CA-C-N	5.08	126.19	119.84
1	L	384	ASP	C-N-CA	5.08	126.19	119.84
1	A	137	PHE	N-CA-CB	5.04	117.98	110.22
1	H	506	ARG	O-C-N	-5.04	114.93	123.00
1	F	241	ILE	CB-CA-C	5.04	117.92	110.77
1	J	384	ASP	CA-C-N	5.04	126.14	119.84
1	J	384	ASP	C-N-CA	5.04	126.14	119.84
1	M	208	VAL	CB-CA-C	5.04	116.97	111.08
1	C	502	VAL	N-CA-C	5.04	115.90	110.21
1	G	502	VAL	N-CA-C	5.03	115.90	110.21
1	I	502	VAL	N-CA-C	5.02	115.88	110.21
1	K	480	ILE	N-CA-CB	5.02	117.62	111.60
1	F	222	VAL	CB-CA-C	-5.01	103.07	111.29
1	N	333	ASN	CA-C-N	5.01	127.00	120.28
1	N	333	ASN	C-N-CA	5.01	127.00	120.28
1	B	205	ASP	CB-CA-C	-5.01	102.89	111.46
1	I	384	ASP	CA-C-N	5.01	126.10	119.84
1	I	384	ASP	C-N-CA	5.01	126.10	119.84
1	B	130	ASN	CB-CA-C	5.00	118.99	111.18
1	G	66	THR	N-CA-C	5.00	121.46	110.80
1	L	432	VAL	N-CA-CB	5.00	118.09	110.58
1	B	66	THR	N-CA-C	5.00	121.45	110.80

There are no chirality outliers.

All (1667) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ASP	Sidechain
1	A	101	TYR	Sidechain
1	A	103	PRO	Mainchain
1	A	104	GLY	Mainchain
1	A	106	ALA	Mainchain
1	A	111	ILE	Mainchain
1	A	114	ASP	Sidechain
1	A	116	ARG	Sidechain
1	A	118	HIS	Sidechain
1	A	119	TRP	Mainchain
1	A	132	PRO	Mainchain
1	A	137	PHE	Mainchain,Sidechain
1	A	139	PHE	Sidechain
1	A	151	ARG	Mainchain
1	A	168	PHE	Sidechain
1	A	171	PRO	Mainchain
1	A	173	GLY	Mainchain
1	A	175	TYR	Sidechain
1	A	177	GLU	Mainchain
1	A	178	THR	Mainchain
1	A	181	ILE	Mainchain
1	A	192	TYR	Mainchain
1	A	197	ARG	Mainchain
1	A	203	GLU	Mainchain
1	A	205	ASP	Sidechain
1	A	206	ILE	Mainchain
1	A	210	PHE	Sidechain
1	A	213	ARG	Sidechain
1	A	215	PHE	Mainchain,Sidechain
1	A	219	PHE	Sidechain
1	A	220	ASP	Sidechain
1	A	231	TYR	Sidechain
1	A	236	PHE	Sidechain
1	A	238	PRO	Mainchain
1	A	239	ASP	Sidechain
1	A	249	ASP	Sidechain
1	A	250	PHE	Sidechain
1	A	254	ARG	Mainchain
1	A	258	LEU	Mainchain
1	A	260	GLY	Mainchain
1	A	262	ARG	Sidechain
1	A	264	ARG	Mainchain
1	A	270	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	A	271	PHE	Sidechain
1	A	272	ARG	Sidechain
1	A	275	TYR	Sidechain
1	A	288	ASP	Mainchain
1	A	289	VAL	Mainchain
1	A	294	ALA	Mainchain
1	A	315	VAL	Mainchain
1	A	322	ASP	Mainchain
1	A	323	SER	Mainchain
1	A	326	ARG	Sidechain
1	A	328	TYR	Sidechain
1	A	329	ASN	Mainchain
1	A	337	PHE	Sidechain
1	A	338	THR	Mainchain
1	A	347	TYR	Sidechain
1	A	349	TYR	Sidechain
1	A	355	GLY	Mainchain
1	A	368	THR	Mainchain
1	A	371	SER	Mainchain
1	A	372	GLU	Mainchain
1	A	375	TYR	Sidechain
1	A	378	LEU	Mainchain,Peptide
1	A	380	ASP	Sidechain
1	A	383	GLN	Mainchain
1	A	384	ASP	Sidechain
1	A	391	THR	Mainchain
1	A	394	ILE	Mainchain
1	A	410	LYS	Mainchain
1	A	413	TYR	Sidechain
1	A	415	ASP	Mainchain
1	A	419	TYR	Sidechain
1	A	424	ARG	Sidechain
1	A	427	THR	Mainchain
1	A	431	HIS	Sidechain
1	A	436	PHE	Sidechain
1	A	439	ASN	Mainchain
1	A	441	ILE	Mainchain
1	A	463	HIS	Sidechain
1	A	485	ARG	Mainchain
1	A	486	ARG	Sidechain
1	A	489	PRO	Mainchain
1	A	492	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	500	PRO	Mainchain
1	A	504	SER	Mainchain
1	A	506	ARG	Mainchain,Sidechain
1	A	52	ARG	Mainchain
1	A	56	ARG	Mainchain,Sidechain
1	A	57	TYR	Sidechain
1	A	58	SER	Mainchain
1	A	62	PRO	Mainchain
1	A	64	PHE	Mainchain,Sidechain
1	A	76	SER	Mainchain
1	A	78	ASP	Sidechain
1	A	79	VAL	Mainchain
1	A	84	TYR	Mainchain,Sidechain
1	A	88	HIS	Sidechain
1	A	91	PHE	Sidechain
1	A	98	ASN	Mainchain
1	A	99	ASN	Mainchain
1	B	100	ASP	Sidechain
1	B	103	PRO	Mainchain
1	B	104	GLY	Mainchain
1	B	106	ALA	Mainchain
1	B	111	ILE	Mainchain
1	B	116	ARG	Sidechain
1	B	118	HIS	Sidechain
1	B	119	TRP	Mainchain
1	B	128	HIS	Sidechain
1	B	132	PRO	Mainchain
1	B	137	PHE	Mainchain,Sidechain
1	B	151	ARG	Mainchain
1	B	168	PHE	Sidechain
1	B	171	PRO	Mainchain
1	B	173	GLY	Mainchain
1	B	174	ASN	Sidechain
1	B	175	TYR	Sidechain
1	B	177	GLU	Mainchain
1	B	178	THR	Mainchain
1	B	181	ILE	Mainchain
1	B	182	ASP	Sidechain
1	B	192	TYR	Mainchain
1	B	205	ASP	Sidechain
1	B	206	ILE	Mainchain
1	B	210	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	B	215	PHE	Mainchain,Sidechain
1	B	231	TYR	Sidechain
1	B	234	GLU	Mainchain
1	B	236	PHE	Sidechain
1	B	238	PRO	Mainchain
1	B	250	PHE	Mainchain
1	B	254	ARG	Mainchain
1	B	257	ASN	Sidechain
1	B	258	LEU	Mainchain
1	B	260	GLY	Mainchain
1	B	264	ARG	Mainchain
1	B	270	GLY	Mainchain
1	B	271	PHE	Sidechain
1	B	272	ARG	Sidechain
1	B	275	TYR	Sidechain
1	B	282	ASN	Sidechain
1	B	288	ASP	Mainchain
1	B	289	VAL	Mainchain
1	B	315	VAL	Mainchain
1	B	322	ASP	Mainchain
1	B	323	SER	Mainchain
1	B	326	ARG	Sidechain
1	B	328	TYR	Sidechain
1	B	329	ASN	Mainchain
1	B	334	ASP	Sidechain
1	B	338	THR	Mainchain
1	B	347	TYR	Sidechain
1	B	355	GLY	Mainchain
1	B	357	ARG	Sidechain
1	B	367	VAL	Mainchain
1	B	371	SER	Mainchain
1	B	372	GLU	Mainchain,Sidechain
1	B	375	TYR	Sidechain
1	B	378	LEU	Mainchain,Peptide
1	B	383	GLN	Mainchain
1	B	388	PHE	Sidechain
1	B	389	ARG	Sidechain
1	B	390	SER	Mainchain
1	B	391	THR	Mainchain
1	B	394	ILE	Mainchain
1	B	403	GLU	Sidechain
1	B	410	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	B	412	PHE	Mainchain
1	B	427	THR	Mainchain
1	B	435	ARG	Sidechain
1	B	439	ASN	Mainchain
1	B	441	ILE	Mainchain
1	B	443	ALA	Mainchain
1	B	476	GLN	Sidechain
1	B	477	ARG	Mainchain
1	B	480	ILE	Mainchain
1	B	485	ARG	Mainchain,Sidechain
1	B	489	PRO	Mainchain
1	B	492	TYR	Sidechain
1	B	500	PRO	Mainchain
1	B	501	ARG	Sidechain
1	B	504	SER	Mainchain
1	B	506	ARG	Mainchain
1	B	52	ARG	Mainchain
1	B	56	ARG	Mainchain
1	B	57	TYR	Sidechain
1	B	58	SER	Mainchain
1	B	62	PRO	Mainchain
1	B	64	PHE	Mainchain,Sidechain
1	B	70	TYR	Sidechain
1	B	76	SER	Mainchain
1	B	78	ASP	Mainchain
1	B	79	VAL	Mainchain
1	B	84	TYR	Mainchain,Sidechain
1	B	90	ASN	Sidechain
1	B	91	PHE	Sidechain
1	B	98	ASN	Mainchain
1	B	99	ASN	Mainchain
1	C	100	ASP	Sidechain
1	C	101	TYR	Sidechain
1	C	103	PRO	Mainchain
1	C	104	GLY	Mainchain
1	C	106	ALA	Mainchain
1	C	111	ILE	Mainchain
1	C	116	ARG	Sidechain
1	C	118	HIS	Sidechain
1	C	119	TRP	Mainchain
1	C	130	ASN	Sidechain
1	C	132	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	C	137	PHE	Mainchain,Sidechain
1	C	139	PHE	Sidechain
1	C	151	ARG	Mainchain,Sidechain
1	C	171	PRO	Mainchain
1	C	173	GLY	Mainchain
1	C	175	TYR	Sidechain
1	C	177	GLU	Mainchain,Sidechain
1	C	178	THR	Mainchain
1	C	181	ILE	Mainchain
1	C	203	GLU	Mainchain
1	C	205	ASP	Sidechain
1	C	206	ILE	Mainchain
1	C	213	ARG	Sidechain
1	C	215	PHE	Mainchain
1	C	219	PHE	Sidechain
1	C	231	TYR	Sidechain
1	C	236	PHE	Mainchain,Sidechain
1	C	238	PRO	Mainchain
1	C	248	VAL	Mainchain
1	C	249	ASP	Sidechain
1	C	250	PHE	Mainchain
1	C	254	ARG	Mainchain
1	C	260	GLY	Mainchain
1	C	264	ARG	Mainchain
1	C	267	PHE	Sidechain
1	C	270	GLY	Mainchain
1	C	271	PHE	Sidechain
1	C	275	TYR	Sidechain
1	C	277	ASP	Mainchain
1	C	288	ASP	Mainchain
1	C	289	VAL	Mainchain
1	C	315	VAL	Mainchain
1	C	322	ASP	Mainchain
1	C	323	SER	Mainchain
1	C	326	ARG	Sidechain
1	C	328	TYR	Sidechain
1	C	329	ASN	Mainchain
1	C	338	THR	Mainchain
1	C	340	TYR	Sidechain
1	C	344	TYR	Sidechain
1	C	347	TYR	Sidechain
1	C	349	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	355	GLY	Mainchain
1	C	366	ASP	Sidechain
1	C	368	THR	Mainchain
1	C	371	SER	Mainchain
1	C	375	TYR	Sidechain
1	C	378	LEU	Mainchain,Peptide
1	C	383	GLN	Mainchain
1	C	388	PHE	Sidechain
1	C	389	ARG	Sidechain
1	C	390	SER	Mainchain
1	C	391	THR	Mainchain
1	C	394	ILE	Mainchain
1	C	410	LYS	Mainchain
1	C	412	PHE	Mainchain
1	C	419	TYR	Sidechain
1	C	424	ARG	Sidechain
1	C	426	PHE	Sidechain
1	C	427	THR	Mainchain
1	C	438	GLU	Mainchain
1	C	439	ASN	Mainchain
1	C	441	ILE	Mainchain
1	C	443	ALA	Mainchain
1	C	463	HIS	Sidechain
1	C	469	ARG	Sidechain
1	C	477	ARG	Sidechain
1	C	480	ILE	Mainchain
1	C	485	ARG	Mainchain
1	C	489	PRO	Mainchain
1	C	491	VAL	Mainchain
1	C	492	TYR	Sidechain
1	C	500	PRO	Mainchain
1	C	504	SER	Mainchain
1	C	506	ARG	Mainchain,Sidechain
1	C	52	ARG	Mainchain,Sidechain
1	C	56	ARG	Mainchain
1	C	57	TYR	Sidechain
1	C	58	SER	Mainchain
1	C	62	PRO	Mainchain
1	C	64	PHE	Mainchain,Sidechain
1	C	68	ARG	Sidechain
1	C	70	TYR	Sidechain
1	C	73	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	C	76	SER	Mainchain
1	C	78	ASP	Mainchain
1	C	79	VAL	Mainchain
1	C	84	TYR	Mainchain,Sidechain
1	C	91	PHE	Sidechain
1	C	98	ASN	Mainchain
1	C	99	ASN	Mainchain
1	D	100	ASP	Sidechain
1	D	101	TYR	Sidechain
1	D	103	PRO	Mainchain
1	D	104	GLY	Mainchain
1	D	106	ALA	Mainchain
1	D	111	ILE	Mainchain
1	D	113	LEU	Mainchain
1	D	114	ASP	Sidechain
1	D	116	ARG	Sidechain
1	D	118	HIS	Sidechain
1	D	119	TRP	Mainchain
1	D	132	PRO	Mainchain
1	D	137	PHE	Mainchain
1	D	139	PHE	Sidechain
1	D	151	ARG	Mainchain
1	D	171	PRO	Mainchain
1	D	173	GLY	Mainchain
1	D	175	TYR	Sidechain
1	D	177	GLU	Mainchain
1	D	178	THR	Mainchain
1	D	181	ILE	Mainchain
1	D	192	TYR	Mainchain
1	D	197	ARG	Mainchain,Sidechain
1	D	206	ILE	Mainchain
1	D	215	PHE	Mainchain
1	D	231	TYR	Sidechain
1	D	238	PRO	Mainchain
1	D	239	ASP	Sidechain
1	D	241	ILE	Mainchain
1	D	250	PHE	Mainchain
1	D	252	HIS	Sidechain
1	D	254	ARG	Mainchain,Sidechain
1	D	258	LEU	Mainchain
1	D	260	GLY	Mainchain
1	D	262	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	264	ARG	Mainchain
1	D	270	GLY	Mainchain
1	D	271	PHE	Sidechain
1	D	272	ARG	Sidechain
1	D	275	TYR	Sidechain
1	D	288	ASP	Mainchain
1	D	289	VAL	Mainchain
1	D	294	ALA	Mainchain
1	D	315	VAL	Mainchain
1	D	322	ASP	Mainchain
1	D	323	SER	Mainchain
1	D	326	ARG	Sidechain
1	D	329	ASN	Mainchain
1	D	337	PHE	Sidechain
1	D	338	THR	Mainchain
1	D	341	ARG	Sidechain
1	D	344	TYR	Sidechain
1	D	347	TYR	Sidechain
1	D	349	TYR	Sidechain
1	D	355	GLY	Mainchain
1	D	371	SER	Mainchain
1	D	372	GLU	Mainchain
1	D	375	TYR	Sidechain
1	D	378	LEU	Mainchain,Peptide
1	D	383	GLN	Mainchain
1	D	388	PHE	Sidechain
1	D	391	THR	Mainchain
1	D	394	ILE	Mainchain
1	D	410	LYS	Mainchain
1	D	413	TYR	Sidechain
1	D	424	ARG	Sidechain
1	D	427	THR	Mainchain
1	D	433	PHE	Sidechain
1	D	439	ASN	Mainchain
1	D	441	ILE	Mainchain
1	D	443	ALA	Mainchain
1	D	456	ASN	Sidechain
1	D	463	HIS	Sidechain
1	D	469	ARG	Sidechain
1	D	470	ASN	Sidechain
1	D	477	ARG	Sidechain
1	D	480	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	D	484	ARG	Sidechain
1	D	485	ARG	Mainchain,Sidechain
1	D	486	ARG	Sidechain
1	D	489	PRO	Mainchain
1	D	490	TYR	Sidechain
1	D	491	VAL	Mainchain
1	D	492	TYR	Sidechain
1	D	500	PRO	Mainchain
1	D	501	ARG	Sidechain
1	D	504	SER	Mainchain
1	D	506	ARG	Mainchain
1	D	52	ARG	Mainchain
1	D	56	ARG	Mainchain
1	D	57	TYR	Sidechain
1	D	58	SER	Mainchain
1	D	62	PRO	Mainchain
1	D	64	PHE	Mainchain,Sidechain
1	D	76	SER	Mainchain
1	D	78	ASP	Mainchain
1	D	79	VAL	Mainchain
1	D	84	TYR	Mainchain,Sidechain
1	D	91	PHE	Sidechain
1	D	98	ASN	Mainchain
1	D	99	ASN	Mainchain
1	E	103	PRO	Mainchain
1	E	104	GLY	Mainchain
1	E	106	ALA	Mainchain
1	E	111	ILE	Mainchain
1	E	113	LEU	Mainchain
1	E	116	ARG	Sidechain
1	E	118	HIS	Sidechain
1	E	119	TRP	Mainchain
1	E	132	PRO	Mainchain
1	E	137	PHE	Mainchain,Sidechain
1	E	151	ARG	Mainchain,Sidechain
1	E	153	LEU	Mainchain
1	E	171	PRO	Mainchain
1	E	173	GLY	Mainchain
1	E	175	TYR	Sidechain
1	E	177	GLU	Mainchain
1	E	178	THR	Mainchain
1	E	181	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	E	192	TYR	Mainchain,Sidechain
1	E	206	ILE	Mainchain
1	E	213	ARG	Sidechain
1	E	215	PHE	Mainchain,Sidechain
1	E	231	TYR	Sidechain
1	E	236	PHE	Mainchain,Sidechain
1	E	238	PRO	Mainchain
1	E	239	ASP	Sidechain
1	E	249	ASP	Sidechain
1	E	254	ARG	Mainchain
1	E	258	LEU	Mainchain
1	E	260	GLY	Mainchain
1	E	262	ARG	Sidechain
1	E	264	ARG	Mainchain,Sidechain
1	E	270	GLY	Mainchain
1	E	275	TYR	Sidechain
1	E	283	ILE	Mainchain
1	E	288	ASP	Mainchain
1	E	289	VAL	Mainchain
1	E	315	VAL	Mainchain
1	E	322	ASP	Mainchain
1	E	323	SER	Mainchain
1	E	329	ASN	Mainchain,Sidechain
1	E	337	PHE	Sidechain
1	E	338	THR	Mainchain
1	E	340	TYR	Sidechain
1	E	344	TYR	Sidechain
1	E	347	TYR	Sidechain
1	E	355	GLY	Mainchain
1	E	366	ASP	Sidechain
1	E	367	VAL	Mainchain
1	E	371	SER	Mainchain
1	E	372	GLU	Mainchain
1	E	375	TYR	Sidechain
1	E	378	LEU	Mainchain,Peptide
1	E	383	GLN	Mainchain
1	E	388	PHE	Sidechain
1	E	390	SER	Mainchain
1	E	391	THR	Mainchain
1	E	394	ILE	Mainchain
1	E	408	HIS	Sidechain
1	E	410	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	E	419	TYR	Sidechain
1	E	424	ARG	Sidechain
1	E	426	PHE	Sidechain
1	E	435	ARG	Sidechain
1	E	439	ASN	Mainchain
1	E	441	ILE	Mainchain
1	E	469	ARG	Sidechain
1	E	470	ASN	Sidechain
1	E	477	ARG	Mainchain
1	E	482	ASP	Mainchain
1	E	484	ARG	Sidechain
1	E	485	ARG	Mainchain
1	E	486	ARG	Sidechain
1	E	489	PRO	Mainchain
1	E	490	TYR	Sidechain
1	E	491	VAL	Mainchain
1	E	492	TYR	Sidechain
1	E	500	PRO	Mainchain
1	E	501	ARG	Sidechain
1	E	504	SER	Mainchain
1	E	506	ARG	Mainchain
1	E	52	ARG	Mainchain
1	E	56	ARG	Mainchain
1	E	57	TYR	Sidechain
1	E	58	SER	Mainchain
1	E	62	PRO	Mainchain
1	E	64	PHE	Mainchain,Sidechain
1	E	70	TYR	Sidechain
1	E	73	ASP	Mainchain
1	E	76	SER	Mainchain
1	E	79	VAL	Mainchain
1	E	84	TYR	Mainchain
1	E	98	ASN	Mainchain
1	E	99	ASN	Mainchain
1	F	100	ASP	Sidechain
1	F	103	PRO	Mainchain
1	F	104	GLY	Mainchain
1	F	106	ALA	Mainchain
1	F	111	ILE	Mainchain
1	F	115	ASP	Sidechain
1	F	118	HIS	Sidechain
1	F	119	TRP	Mainchain

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Mol	Chain	Res	Type	Group
1	F	132	PRO	Mainchain
1	F	137	PHE	Mainchain,Sidechain
1	F	139	PHE	Sidechain
1	F	151	ARG	Mainchain
1	F	168	PHE	Sidechain
1	F	171	PRO	Mainchain
1	F	173	GLY	Mainchain
1	F	175	TYR	Sidechain
1	F	177	GLU	Mainchain
1	F	178	THR	Mainchain
1	F	181	ILE	Mainchain
1	F	191	HIS	Sidechain
1	F	197	ARG	Mainchain
1	F	206	ILE	Mainchain
1	F	213	ARG	Sidechain
1	F	215	PHE	Mainchain
1	F	219	PHE	Sidechain
1	F	231	TYR	Sidechain
1	F	236	PHE	Mainchain,Sidechain
1	F	238	PRO	Mainchain
1	F	249	ASP	Sidechain
1	F	254	ARG	Mainchain
1	F	258	LEU	Mainchain
1	F	260	GLY	Mainchain
1	F	262	ARG	Sidechain
1	F	264	ARG	Mainchain,Sidechain
1	F	270	GLY	Mainchain
1	F	271	PHE	Sidechain
1	F	275	TYR	Sidechain
1	F	288	ASP	Mainchain
1	F	289	VAL	Mainchain
1	F	292	TYR	Sidechain
1	F	315	VAL	Mainchain
1	F	322	ASP	Mainchain
1	F	323	SER	Mainchain
1	F	326	ARG	Sidechain
1	F	328	TYR	Sidechain
1	F	329	ASN	Mainchain
1	F	334	ASP	Sidechain
1	F	337	PHE	Sidechain
1	F	338	THR	Mainchain
1	F	340	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	F	344	TYR	Sidechain
1	F	347	TYR	Sidechain
1	F	351	ASP	Sidechain
1	F	355	GLY	Mainchain
1	F	371	SER	Mainchain
1	F	372	GLU	Sidechain
1	F	375	TYR	Sidechain
1	F	378	LEU	Mainchain,Peptide
1	F	383	GLN	Mainchain
1	F	390	SER	Mainchain
1	F	391	THR	Mainchain
1	F	394	ILE	Mainchain
1	F	397	PHE	Sidechain
1	F	410	LYS	Mainchain
1	F	413	TYR	Sidechain
1	F	419	TYR	Sidechain
1	F	431	HIS	Sidechain
1	F	434	ASN	Sidechain
1	F	436	PHE	Sidechain
1	F	439	ASN	Mainchain
1	F	441	ILE	Mainchain
1	F	462	ASP	Sidechain
1	F	463	HIS	Sidechain
1	F	477	ARG	Sidechain
1	F	480	ILE	Mainchain
1	F	485	ARG	Mainchain,Sidechain
1	F	486	ARG	Sidechain
1	F	489	PRO	Mainchain
1	F	490	TYR	Sidechain
1	F	491	VAL	Mainchain
1	F	492	TYR	Sidechain
1	F	500	PRO	Mainchain
1	F	501	ARG	Sidechain
1	F	504	SER	Mainchain
1	F	506	ARG	Mainchain,Sidechain
1	F	52	ARG	Mainchain
1	F	56	ARG	Mainchain
1	F	57	TYR	Sidechain
1	F	58	SER	Mainchain
1	F	59	GLU	Sidechain
1	F	62	PRO	Mainchain
1	F	64	PHE	Mainchain,Sidechain

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Mol	Chain	Res	Type	Group
1	F	68	ARG	Sidechain
1	F	76	SER	Mainchain
1	F	78	ASP	Mainchain
1	F	84	TYR	Mainchain,Sidechain
1	F	91	PHE	Sidechain
1	F	98	ASN	Mainchain
1	F	99	ASN	Mainchain,Sidechain
1	G	100	ASP	Sidechain
1	G	101	TYR	Sidechain
1	G	103	PRO	Mainchain
1	G	104	GLY	Mainchain
1	G	106	ALA	Mainchain
1	G	111	ILE	Mainchain
1	G	113	LEU	Mainchain
1	G	118	HIS	Sidechain
1	G	119	TRP	Mainchain
1	G	128	HIS	Sidechain
1	G	132	PRO	Mainchain
1	G	135	ASN	Sidechain
1	G	137	PHE	Mainchain,Sidechain
1	G	139	PHE	Sidechain
1	G	143	PHE	Sidechain
1	G	151	ARG	Mainchain
1	G	171	PRO	Mainchain
1	G	172	GLU	Sidechain
1	G	173	GLY	Mainchain
1	G	175	TYR	Sidechain
1	G	177	GLU	Mainchain
1	G	181	ILE	Mainchain
1	G	192	TYR	Mainchain
1	G	197	ARG	Mainchain
1	G	203	GLU	Mainchain
1	G	206	ILE	Mainchain
1	G	210	PHE	Sidechain
1	G	215	PHE	Mainchain
1	G	216	ARG	Sidechain
1	G	220	ASP	Sidechain
1	G	231	TYR	Sidechain
1	G	236	PHE	Sidechain
1	G	237	HIS	Sidechain
1	G	238	PRO	Mainchain
1	G	248	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	G	249	ASP	Sidechain
1	G	254	ARG	Mainchain
1	G	258	LEU	Mainchain
1	G	260	GLY	Mainchain
1	G	262	ARG	Sidechain
1	G	264	ARG	Mainchain
1	G	270	GLY	Mainchain
1	G	271	PHE	Sidechain
1	G	275	TYR	Sidechain
1	G	288	ASP	Mainchain
1	G	289	VAL	Mainchain
1	G	315	VAL	Mainchain
1	G	322	ASP	Mainchain
1	G	323	SER	Mainchain
1	G	326	ARG	Sidechain
1	G	328	TYR	Sidechain
1	G	329	ASN	Mainchain,Sidechain
1	G	337	PHE	Sidechain
1	G	338	THR	Mainchain
1	G	344	TYR	Sidechain
1	G	347	TYR	Sidechain
1	G	355	GLY	Mainchain
1	G	357	ARG	Sidechain
1	G	367	VAL	Mainchain
1	G	371	SER	Mainchain
1	G	372	GLU	Mainchain
1	G	375	TYR	Sidechain
1	G	378	LEU	Mainchain,Peptide
1	G	380	ASP	Sidechain
1	G	383	GLN	Mainchain
1	G	394	ILE	Mainchain
1	G	408	HIS	Sidechain
1	G	410	LYS	Mainchain
1	G	415	ASP	Mainchain
1	G	420	SER	Mainchain
1	G	424	ARG	Sidechain
1	G	426	PHE	Sidechain
1	G	427	THR	Mainchain
1	G	431	HIS	Sidechain
1	G	435	ARG	Sidechain
1	G	439	ASN	Mainchain
1	G	441	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	G	443	ALA	Mainchain
1	G	476	GLN	Sidechain
1	G	477	ARG	Sidechain
1	G	480	ILE	Mainchain
1	G	482	ASP	Sidechain
1	G	484	ARG	Sidechain
1	G	485	ARG	Mainchain
1	G	489	PRO	Mainchain
1	G	491	VAL	Mainchain
1	G	492	TYR	Sidechain
1	G	500	PRO	Mainchain
1	G	501	ARG	Sidechain
1	G	504	SER	Mainchain
1	G	506	ARG	Mainchain
1	G	52	ARG	Mainchain,Sidechain
1	G	56	ARG	Mainchain
1	G	57	TYR	Sidechain
1	G	58	SER	Mainchain
1	G	62	PRO	Mainchain
1	G	64	PHE	Mainchain,Sidechain
1	G	68	ARG	Sidechain
1	G	70	TYR	Sidechain
1	G	73	ASP	Mainchain,Sidechain
1	G	76	SER	Mainchain
1	G	78	ASP	Mainchain
1	G	79	VAL	Mainchain
1	G	84	TYR	Mainchain
1	G	91	PHE	Sidechain
1	G	98	ASN	Mainchain
1	G	99	ASN	Mainchain
1	H	100	ASP	Sidechain
1	H	101	TYR	Sidechain
1	H	103	PRO	Mainchain
1	H	104	GLY	Mainchain
1	H	106	ALA	Mainchain
1	H	111	ILE	Mainchain
1	H	116	ARG	Sidechain
1	H	118	HIS	Sidechain
1	H	119	TRP	Mainchain
1	H	122	ASP	Sidechain
1	H	132	PRO	Mainchain
1	H	137	PHE	Mainchain,Sidechain

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Mol	Chain	Res	Type	Group
1	H	151	ARG	Mainchain
1	H	160	GLU	Sidechain
1	H	163	TYR	Sidechain
1	H	168	PHE	Sidechain
1	H	171	PRO	Mainchain
1	H	173	GLY	Mainchain
1	H	175	TYR	Sidechain
1	H	177	GLU	Mainchain
1	H	178	THR	Mainchain
1	H	181	ILE	Mainchain
1	H	182	ASP	Sidechain
1	H	185	ASN	Sidechain
1	H	192	TYR	Mainchain
1	H	197	ARG	Mainchain
1	H	203	GLU	Mainchain
1	H	206	ILE	Mainchain
1	H	210	PHE	Sidechain
1	H	215	PHE	Mainchain,Sidechain
1	H	236	PHE	Sidechain
1	H	237	HIS	Sidechain
1	H	238	PRO	Mainchain
1	H	241	ILE	Mainchain
1	H	249	ASP	Sidechain
1	H	250	PHE	Mainchain
1	H	254	ARG	Mainchain
1	H	260	GLY	Mainchain
1	H	264	ARG	Mainchain,Sidechain
1	H	267	PHE	Sidechain
1	H	269	GLU	Sidechain
1	H	270	GLY	Mainchain
1	H	271	PHE	Sidechain
1	H	275	TYR	Sidechain
1	H	288	ASP	Mainchain
1	H	289	VAL	Mainchain
1	H	292	TYR	Sidechain
1	H	315	VAL	Mainchain
1	H	322	ASP	Mainchain
1	H	323	SER	Mainchain
1	H	328	TYR	Sidechain
1	H	329	ASN	Mainchain
1	H	337	PHE	Sidechain
1	H	338	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	H	347	TYR	Sidechain
1	H	349	TYR	Sidechain
1	H	355	GLY	Mainchain
1	H	366	ASP	Sidechain
1	H	371	SER	Mainchain
1	H	372	GLU	Mainchain
1	H	375	TYR	Sidechain
1	H	378	LEU	Mainchain,Peptide
1	H	383	GLN	Mainchain
1	H	384	ASP	Sidechain
1	H	390	SER	Mainchain
1	H	391	THR	Mainchain
1	H	394	ILE	Mainchain
1	H	397	PHE	Sidechain
1	H	408	HIS	Sidechain
1	H	410	LYS	Mainchain
1	H	413	TYR	Sidechain
1	H	415	ASP	Mainchain
1	H	424	ARG	Sidechain
1	H	426	PHE	Sidechain
1	H	427	THR	Mainchain
1	H	439	ASN	Mainchain
1	H	441	ILE	Mainchain
1	H	443	ALA	Mainchain
1	H	444	ARG	Sidechain
1	H	477	ARG	Mainchain
1	H	480	ILE	Mainchain
1	H	482	ASP	Mainchain
1	H	485	ARG	Mainchain,Sidechain
1	H	489	PRO	Mainchain
1	H	490	TYR	Sidechain
1	H	491	VAL	Mainchain
1	H	492	TYR	Sidechain
1	H	500	PRO	Mainchain
1	H	504	SER	Mainchain
1	H	506	ARG	Mainchain,Sidechain
1	H	52	ARG	Mainchain
1	H	53	ASN	Mainchain
1	H	56	ARG	Mainchain
1	H	57	TYR	Sidechain
1	H	58	SER	Mainchain
1	H	59	GLU	Sidechain

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Mol	Chain	Res	Type	Group
1	H	62	PRO	Mainchain
1	H	64	PHE	Mainchain
1	H	65	ASP	Sidechain
1	H	68	ARG	Sidechain
1	H	70	TYR	Sidechain
1	H	73	ASP	Mainchain
1	H	76	SER	Mainchain
1	H	79	VAL	Mainchain
1	H	84	TYR	Mainchain
1	H	91	PHE	Sidechain
1	H	98	ASN	Mainchain
1	H	99	ASN	Mainchain
1	I	101	TYR	Sidechain
1	I	103	PRO	Mainchain
1	I	104	GLY	Mainchain
1	I	106	ALA	Mainchain
1	I	111	ILE	Mainchain
1	I	113	LEU	Mainchain
1	I	118	HIS	Sidechain
1	I	119	TRP	Mainchain
1	I	122	ASP	Sidechain
1	I	128	HIS	Sidechain
1	I	132	PRO	Mainchain
1	I	135	ASN	Sidechain
1	I	137	PHE	Mainchain
1	I	151	ARG	Mainchain,Sidechain
1	I	163	TYR	Sidechain
1	I	167	GLU	Sidechain
1	I	168	PHE	Sidechain
1	I	171	PRO	Mainchain
1	I	173	GLY	Mainchain
1	I	175	TYR	Sidechain
1	I	177	GLU	Mainchain
1	I	178	THR	Mainchain
1	I	179	MET	Mainchain
1	I	181	ILE	Mainchain
1	I	182	ASP	Sidechain
1	I	191	HIS	Sidechain
1	I	192	TYR	Mainchain
1	I	203	GLU	Mainchain
1	I	206	ILE	Mainchain
1	I	215	PHE	Mainchain

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Mol	Chain	Res	Type	Group
1	I	219	PHE	Sidechain
1	I	220	ASP	Sidechain
1	I	231	TYR	Sidechain
1	I	236	PHE	Sidechain
1	I	238	PRO	Mainchain
1	I	249	ASP	Sidechain
1	I	250	PHE	Mainchain,Sidechain
1	I	254	ARG	Mainchain,Sidechain
1	I	260	GLY	Mainchain
1	I	262	ARG	Sidechain
1	I	264	ARG	Mainchain
1	I	267	PHE	Sidechain
1	I	270	GLY	Mainchain
1	I	271	PHE	Sidechain
1	I	272	ARG	Sidechain
1	I	275	TYR	Sidechain
1	I	288	ASP	Mainchain
1	I	289	VAL	Mainchain
1	I	292	TYR	Sidechain
1	I	312	LEU	Mainchain
1	I	315	VAL	Mainchain
1	I	322	ASP	Mainchain
1	I	323	SER	Mainchain
1	I	326	ARG	Sidechain
1	I	328	TYR	Sidechain
1	I	329	ASN	Mainchain
1	I	337	PHE	Sidechain
1	I	338	THR	Mainchain
1	I	341	ARG	Sidechain
1	I	344	TYR	Sidechain
1	I	347	TYR	Sidechain
1	I	349	TYR	Sidechain
1	I	355	GLY	Mainchain
1	I	357	ARG	Sidechain
1	I	371	SER	Mainchain
1	I	372	GLU	Mainchain
1	I	375	TYR	Sidechain
1	I	378	LEU	Mainchain,Peptide
1	I	383	GLN	Mainchain
1	I	390	SER	Mainchain
1	I	394	ILE	Mainchain
1	I	397	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	I	413	TYR	Sidechain
1	I	424	ARG	Sidechain
1	I	426	PHE	Sidechain
1	I	427	THR	Mainchain
1	I	432	VAL	Mainchain
1	I	436	PHE	Sidechain
1	I	438	GLU	Mainchain
1	I	439	ASN	Mainchain
1	I	441	ILE	Mainchain
1	I	443	ALA	Mainchain
1	I	444	ARG	Sidechain
1	I	469	ARG	Sidechain
1	I	477	ARG	Mainchain
1	I	485	ARG	Mainchain
1	I	486	ARG	Sidechain
1	I	489	PRO	Mainchain
1	I	490	TYR	Sidechain
1	I	492	TYR	Sidechain
1	I	500	PRO	Mainchain
1	I	501	ARG	Sidechain
1	I	504	SER	Mainchain
1	I	506	ARG	Mainchain,Sidechain
1	I	52	ARG	Mainchain,Sidechain
1	I	56	ARG	Mainchain
1	I	57	TYR	Sidechain
1	I	58	SER	Mainchain
1	I	62	PRO	Mainchain
1	I	64	PHE	Mainchain
1	I	70	TYR	Sidechain
1	I	76	SER	Mainchain
1	I	78	ASP	Mainchain
1	I	79	VAL	Mainchain
1	I	84	TYR	Mainchain
1	I	91	PHE	Sidechain
1	I	98	ASN	Mainchain,Sidechain
1	I	99	ASN	Mainchain
1	J	100	ASP	Sidechain
1	J	101	TYR	Sidechain
1	J	103	PRO	Mainchain
1	J	104	GLY	Mainchain
1	J	106	ALA	Mainchain
1	J	111	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	J	114	ASP	Sidechain
1	J	118	HIS	Sidechain
1	J	119	TRP	Mainchain
1	J	128	HIS	Sidechain
1	J	132	PRO	Mainchain
1	J	137	PHE	Mainchain,Sidechain
1	J	139	PHE	Sidechain
1	J	143	PHE	Sidechain
1	J	151	ARG	Mainchain,Sidechain
1	J	156	ASP	Sidechain
1	J	171	PRO	Mainchain
1	J	173	GLY	Mainchain
1	J	175	TYR	Sidechain
1	J	177	GLU	Mainchain
1	J	178	THR	Mainchain
1	J	181	ILE	Mainchain
1	J	191	HIS	Sidechain
1	J	192	TYR	Mainchain
1	J	197	ARG	Mainchain
1	J	206	ILE	Mainchain
1	J	213	ARG	Sidechain
1	J	215	PHE	Mainchain,Sidechain
1	J	220	ASP	Sidechain
1	J	233	ASN	Sidechain
1	J	234	GLU	Mainchain
1	J	236	PHE	Mainchain,Sidechain
1	J	238	PRO	Mainchain
1	J	241	ILE	Mainchain
1	J	248	VAL	Mainchain
1	J	250	PHE	Mainchain
1	J	252	HIS	Sidechain
1	J	254	ARG	Mainchain,Sidechain
1	J	260	GLY	Mainchain
1	J	264	ARG	Mainchain
1	J	270	GLY	Mainchain
1	J	271	PHE	Sidechain
1	J	275	TYR	Sidechain
1	J	288	ASP	Mainchain
1	J	289	VAL	Mainchain
1	J	295	SER	Mainchain
1	J	315	VAL	Mainchain
1	J	322	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	J	323	SER	Mainchain
1	J	326	ARG	Sidechain
1	J	329	ASN	Mainchain
1	J	334	ASP	Sidechain
1	J	338	THR	Mainchain
1	J	347	TYR	Sidechain
1	J	355	GLY	Mainchain
1	J	367	VAL	Mainchain
1	J	371	SER	Mainchain
1	J	375	TYR	Sidechain
1	J	378	LEU	Mainchain,Peptide
1	J	383	GLN	Mainchain
1	J	388	PHE	Sidechain
1	J	389	ARG	Sidechain
1	J	391	THR	Mainchain
1	J	394	ILE	Mainchain
1	J	397	PHE	Sidechain
1	J	410	LYS	Mainchain
1	J	413	TYR	Sidechain
1	J	415	ASP	Mainchain
1	J	419	TYR	Sidechain
1	J	424	ARG	Sidechain
1	J	426	PHE	Sidechain
1	J	427	THR	Mainchain
1	J	431	HIS	Sidechain
1	J	436	PHE	Sidechain
1	J	439	ASN	Mainchain
1	J	441	ILE	Mainchain
1	J	443	ALA	Mainchain
1	J	463	HIS	Sidechain
1	J	476	GLN	Sidechain
1	J	477	ARG	Sidechain
1	J	485	ARG	Mainchain,Sidechain
1	J	486	ARG	Sidechain
1	J	489	PRO	Mainchain
1	J	491	VAL	Mainchain
1	J	492	TYR	Sidechain
1	J	500	PRO	Mainchain
1	J	504	SER	Mainchain
1	J	506	ARG	Mainchain
1	J	52	ARG	Mainchain
1	J	56	ARG	Mainchain,Sidechain

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Mol	Chain	Res	Type	Group
1	J	57	TYR	Sidechain
1	J	58	SER	Mainchain
1	J	62	PRO	Mainchain
1	J	64	PHE	Mainchain,Sidechain
1	J	70	TYR	Sidechain
1	J	76	SER	Mainchain
1	J	78	ASP	Mainchain
1	J	79	VAL	Mainchain
1	J	84	TYR	Mainchain,Sidechain
1	J	91	PHE	Sidechain
1	J	98	ASN	Mainchain
1	J	99	ASN	Mainchain
1	K	100	ASP	Sidechain
1	K	101	TYR	Sidechain
1	K	103	PRO	Mainchain
1	K	104	GLY	Mainchain
1	K	106	ALA	Mainchain
1	K	111	ILE	Mainchain
1	K	114	ASP	Mainchain
1	K	115	ASP	Sidechain
1	K	118	HIS	Sidechain
1	K	119	TRP	Mainchain
1	K	128	HIS	Sidechain
1	K	132	PRO	Mainchain
1	K	137	PHE	Mainchain,Sidechain
1	K	142	LYS	Mainchain
1	K	151	ARG	Mainchain
1	K	163	TYR	Sidechain
1	K	168	PHE	Sidechain
1	K	171	PRO	Mainchain
1	K	173	GLY	Mainchain
1	K	175	TYR	Sidechain
1	K	177	GLU	Mainchain
1	K	181	ILE	Mainchain
1	K	192	TYR	Mainchain
1	K	203	GLU	Mainchain
1	K	205	ASP	Sidechain
1	K	206	ILE	Mainchain
1	K	210	PHE	Sidechain
1	K	215	PHE	Mainchain
1	K	236	PHE	Sidechain
1	K	238	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	K	239	ASP	Sidechain
1	K	248	VAL	Mainchain
1	K	249	ASP	Sidechain
1	K	250	PHE	Sidechain
1	K	254	ARG	Mainchain
1	K	258	LEU	Mainchain
1	K	260	GLY	Mainchain
1	K	262	ARG	Sidechain
1	K	264	ARG	Mainchain,Sidechain
1	K	267	PHE	Sidechain
1	K	270	GLY	Mainchain
1	K	271	PHE	Sidechain
1	K	272	ARG	Sidechain
1	K	275	TYR	Sidechain
1	K	288	ASP	Mainchain
1	K	289	VAL	Mainchain
1	K	315	VAL	Mainchain
1	K	322	ASP	Mainchain
1	K	323	SER	Mainchain
1	K	328	TYR	Sidechain
1	K	329	ASN	Mainchain
1	K	334	ASP	Sidechain
1	K	338	THR	Mainchain
1	K	344	TYR	Sidechain
1	K	347	TYR	Sidechain
1	K	349	TYR	Sidechain
1	K	355	GLY	Mainchain
1	K	371	SER	Mainchain
1	K	372	GLU	Mainchain
1	K	375	TYR	Sidechain
1	K	378	LEU	Mainchain,Peptide
1	K	383	GLN	Mainchain
1	K	384	ASP	Sidechain
1	K	388	PHE	Sidechain
1	K	391	THR	Mainchain
1	K	394	ILE	Mainchain
1	K	408	HIS	Sidechain
1	K	410	LYS	Mainchain
1	K	412	PHE	Sidechain
1	K	413	TYR	Sidechain
1	K	419	TYR	Sidechain
1	K	420	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	K	424	ARG	Sidechain
1	K	426	PHE	Sidechain
1	K	427	THR	Mainchain
1	K	436	PHE	Sidechain
1	K	439	ASN	Mainchain
1	K	441	ILE	Mainchain
1	K	443	ALA	Mainchain
1	K	444	ARG	Sidechain
1	K	455	GLU	Sidechain
1	K	463	HIS	Sidechain
1	K	469	ARG	Sidechain
1	K	477	ARG	Mainchain,Sidechain
1	K	480	ILE	Mainchain
1	K	485	ARG	Mainchain,Sidechain
1	K	486	ARG	Sidechain
1	K	489	PRO	Mainchain
1	K	490	TYR	Sidechain
1	K	492	TYR	Sidechain
1	K	500	PRO	Mainchain
1	K	501	ARG	Sidechain
1	K	504	SER	Mainchain
1	K	506	ARG	Sidechain
1	K	52	ARG	Mainchain
1	K	56	ARG	Mainchain
1	K	57	TYR	Sidechain
1	K	58	SER	Mainchain
1	K	62	PRO	Mainchain
1	K	64	PHE	Mainchain,Sidechain
1	K	65	ASP	Sidechain
1	K	68	ARG	Sidechain
1	K	70	TYR	Sidechain
1	K	73	ASP	Mainchain,Sidechain
1	K	76	SER	Mainchain
1	K	78	ASP	Mainchain,Sidechain
1	K	79	VAL	Mainchain
1	K	84	TYR	Mainchain,Sidechain
1	K	91	PHE	Sidechain
1	K	98	ASN	Mainchain
1	L	100	ASP	Sidechain
1	L	101	TYR	Sidechain
1	L	103	PRO	Mainchain
1	L	104	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	L	106	ALA	Mainchain
1	L	111	ILE	Mainchain
1	L	113	LEU	Mainchain
1	L	119	TRP	Mainchain
1	L	122	ASP	Sidechain
1	L	128	HIS	Sidechain
1	L	132	PRO	Mainchain
1	L	133	ASN	Sidechain
1	L	137	PHE	Mainchain,Sidechain
1	L	139	PHE	Sidechain
1	L	151	ARG	Mainchain
1	L	160	GLU	Sidechain
1	L	163	TYR	Sidechain
1	L	171	PRO	Mainchain
1	L	173	GLY	Mainchain
1	L	175	TYR	Sidechain
1	L	177	GLU	Mainchain
1	L	178	THR	Mainchain
1	L	179	MET	Mainchain
1	L	181	ILE	Mainchain
1	L	191	HIS	Sidechain
1	L	192	TYR	Mainchain
1	L	197	ARG	Mainchain,Sidechain
1	L	206	ILE	Mainchain
1	L	210	PHE	Sidechain
1	L	211	ASP	Sidechain
1	L	213	ARG	Sidechain
1	L	215	PHE	Mainchain,Sidechain
1	L	219	PHE	Sidechain
1	L	236	PHE	Sidechain
1	L	238	PRO	Mainchain
1	L	239	ASP	Sidechain
1	L	249	ASP	Sidechain
1	L	250	PHE	Mainchain,Sidechain
1	L	252	HIS	Sidechain
1	L	254	ARG	Mainchain,Sidechain
1	L	258	LEU	Mainchain
1	L	260	GLY	Mainchain
1	L	264	ARG	Mainchain
1	L	267	PHE	Sidechain
1	L	270	GLY	Mainchain
1	L	271	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	L	272	ARG	Sidechain
1	L	275	TYR	Sidechain
1	L	288	ASP	Mainchain
1	L	289	VAL	Mainchain
1	L	292	TYR	Sidechain
1	L	315	VAL	Mainchain
1	L	322	ASP	Mainchain
1	L	323	SER	Mainchain
1	L	326	ARG	Sidechain
1	L	328	TYR	Sidechain
1	L	329	ASN	Mainchain
1	L	338	THR	Mainchain
1	L	340	TYR	Sidechain
1	L	344	TYR	Sidechain
1	L	347	TYR	Sidechain
1	L	355	GLY	Mainchain
1	L	367	VAL	Mainchain
1	L	371	SER	Mainchain
1	L	372	GLU	Mainchain
1	L	375	TYR	Sidechain
1	L	378	LEU	Mainchain,Peptide
1	L	383	GLN	Mainchain
1	L	384	ASP	Sidechain
1	L	388	PHE	Sidechain
1	L	390	SER	Mainchain
1	L	391	THR	Mainchain
1	L	394	ILE	Mainchain
1	L	397	PHE	Sidechain
1	L	408	HIS	Sidechain
1	L	412	PHE	Mainchain,Sidechain
1	L	415	ASP	Mainchain
1	L	426	PHE	Sidechain
1	L	427	THR	Mainchain
1	L	436	PHE	Sidechain
1	L	439	ASN	Mainchain
1	L	441	ILE	Mainchain
1	L	443	ALA	Mainchain
1	L	463	HIS	Sidechain
1	L	477	ARG	Mainchain,Sidechain
1	L	480	ILE	Mainchain
1	L	485	ARG	Mainchain
1	L	486	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	L	489	PRO	Mainchain
1	L	492	TYR	Sidechain
1	L	500	PRO	Mainchain
1	L	504	SER	Mainchain
1	L	506	ARG	Mainchain
1	L	52	ARG	Mainchain
1	L	56	ARG	Mainchain
1	L	57	TYR	Sidechain
1	L	58	SER	Mainchain
1	L	62	PRO	Mainchain
1	L	64	PHE	Mainchain,Sidechain
1	L	70	TYR	Sidechain
1	L	76	SER	Mainchain
1	L	79	VAL	Mainchain
1	L	84	TYR	Mainchain
1	L	98	ASN	Mainchain
1	L	99	ASN	Mainchain,Sidechain
1	M	100	ASP	Sidechain
1	M	101	TYR	Sidechain
1	M	103	PRO	Mainchain
1	M	104	GLY	Mainchain
1	M	106	ALA	Mainchain
1	M	111	ILE	Mainchain
1	M	118	HIS	Sidechain
1	M	119	TRP	Mainchain
1	M	122	ASP	Sidechain
1	M	130	ASN	Sidechain
1	M	132	PRO	Mainchain
1	M	133	ASN	Sidechain
1	M	137	PHE	Mainchain,Sidechain
1	M	139	PHE	Sidechain
1	M	151	ARG	Mainchain
1	M	171	PRO	Mainchain
1	M	173	GLY	Mainchain
1	M	175	TYR	Sidechain
1	M	177	GLU	Mainchain
1	M	178	THR	Mainchain
1	M	181	ILE	Mainchain
1	M	182	ASP	Sidechain
1	M	191	HIS	Sidechain
1	M	192	TYR	Mainchain
1	M	197	ARG	Mainchain,Sidechain

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Mol	Chain	Res	Type	Group
1	M	203	GLU	Mainchain
1	M	205	ASP	Sidechain
1	M	206	ILE	Mainchain
1	M	210	PHE	Sidechain
1	M	215	PHE	Mainchain,Sidechain
1	M	231	TYR	Sidechain
1	M	234	GLU	Mainchain,Sidechain
1	M	236	PHE	Mainchain,Sidechain
1	M	238	PRO	Mainchain
1	M	241	ILE	Mainchain
1	M	249	ASP	Sidechain
1	M	250	PHE	Sidechain
1	M	252	HIS	Sidechain
1	M	254	ARG	Mainchain,Sidechain
1	M	260	GLY	Mainchain
1	M	264	ARG	Mainchain,Sidechain
1	M	270	GLY	Mainchain
1	M	271	PHE	Sidechain
1	M	275	TYR	Sidechain
1	M	288	ASP	Mainchain
1	M	289	VAL	Mainchain
1	M	292	TYR	Sidechain
1	M	315	VAL	Mainchain
1	M	322	ASP	Mainchain
1	M	323	SER	Mainchain
1	M	326	ARG	Sidechain
1	M	328	TYR	Sidechain
1	M	329	ASN	Mainchain
1	M	338	THR	Mainchain
1	M	344	TYR	Sidechain
1	M	347	TYR	Sidechain
1	M	355	GLY	Mainchain
1	M	371	SER	Mainchain
1	M	372	GLU	Mainchain
1	M	375	TYR	Sidechain
1	M	378	LEU	Mainchain,Peptide
1	M	383	GLN	Mainchain
1	M	388	PHE	Sidechain
1	M	390	SER	Mainchain
1	M	391	THR	Mainchain
1	M	394	ILE	Mainchain
1	M	397	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	M	410	LYS	Mainchain
1	M	419	TYR	Sidechain
1	M	427	THR	Mainchain
1	M	439	ASN	Mainchain
1	M	441	ILE	Mainchain
1	M	476	GLN	Sidechain
1	M	477	ARG	Mainchain,Sidechain
1	M	485	ARG	Mainchain
1	M	486	ARG	Sidechain
1	M	489	PRO	Mainchain
1	M	492	TYR	Sidechain
1	M	500	PRO	Mainchain
1	M	501	ARG	Sidechain
1	M	504	SER	Mainchain
1	M	506	ARG	Sidechain
1	M	52	ARG	Mainchain
1	M	56	ARG	Mainchain,Sidechain
1	M	57	TYR	Sidechain
1	M	58	SER	Mainchain
1	M	62	PRO	Mainchain
1	M	64	PHE	Mainchain,Sidechain
1	M	70	TYR	Sidechain
1	M	76	SER	Mainchain
1	M	84	TYR	Mainchain,Sidechain
1	M	98	ASN	Mainchain
1	M	99	ASN	Mainchain
1	N	101	TYR	Sidechain
1	N	103	PRO	Mainchain
1	N	104	GLY	Mainchain
1	N	106	ALA	Mainchain
1	N	111	ILE	Mainchain
1	N	119	TRP	Mainchain
1	N	128	HIS	Sidechain
1	N	132	PRO	Mainchain
1	N	133	ASN	Sidechain
1	N	137	PHE	Mainchain,Sidechain
1	N	139	PHE	Sidechain
1	N	143	PHE	Sidechain
1	N	151	ARG	Mainchain
1	N	153	LEU	Mainchain
1	N	168	PHE	Sidechain
1	N	171	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	N	173	GLY	Mainchain
1	N	174	ASN	Sidechain
1	N	175	TYR	Sidechain
1	N	177	GLU	Mainchain
1	N	178	THR	Mainchain
1	N	181	ILE	Mainchain
1	N	191	HIS	Sidechain
1	N	192	TYR	Mainchain,Sidechain
1	N	197	ARG	Sidechain
1	N	203	GLU	Mainchain
1	N	206	ILE	Mainchain
1	N	210	PHE	Sidechain
1	N	215	PHE	Mainchain,Sidechain
1	N	219	PHE	Sidechain
1	N	220	ASP	Sidechain
1	N	231	TYR	Sidechain
1	N	234	GLU	Mainchain
1	N	237	HIS	Sidechain
1	N	238	PRO	Mainchain
1	N	249	ASP	Sidechain
1	N	250	PHE	Sidechain
1	N	254	ARG	Mainchain
1	N	258	LEU	Mainchain
1	N	260	GLY	Mainchain
1	N	264	ARG	Mainchain,Sidechain
1	N	270	GLY	Mainchain
1	N	271	PHE	Sidechain
1	N	275	TYR	Sidechain
1	N	288	ASP	Mainchain
1	N	289	VAL	Mainchain
1	N	315	VAL	Mainchain
1	N	322	ASP	Mainchain
1	N	323	SER	Mainchain
1	N	326	ARG	Sidechain
1	N	328	TYR	Sidechain
1	N	329	ASN	Mainchain
1	N	334	ASP	Sidechain
1	N	337	PHE	Sidechain
1	N	338	THR	Mainchain
1	N	344	TYR	Sidechain
1	N	347	TYR	Sidechain
1	N	351	ASP	Sidechain

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Mol	Chain	Res	Type	Group
1	N	355	GLY	Mainchain
1	N	371	SER	Mainchain
1	N	372	GLU	Mainchain
1	N	375	TYR	Sidechain
1	N	378	LEU	Mainchain,Peptide
1	N	383	GLN	Mainchain
1	N	384	ASP	Sidechain
1	N	388	PHE	Sidechain
1	N	389	ARG	Sidechain
1	N	390	SER	Mainchain
1	N	394	ILE	Mainchain
1	N	397	PHE	Sidechain
1	N	408	HIS	Sidechain
1	N	413	TYR	Sidechain
1	N	415	ASP	Mainchain
1	N	424	ARG	Sidechain
1	N	426	PHE	Sidechain
1	N	427	THR	Mainchain
1	N	431	HIS	Sidechain
1	N	434	ASN	Sidechain
1	N	435	ARG	Sidechain
1	N	436	PHE	Sidechain
1	N	439	ASN	Mainchain
1	N	441	ILE	Mainchain
1	N	463	HIS	Sidechain
1	N	477	ARG	Sidechain
1	N	482	ASP	Sidechain
1	N	485	ARG	Mainchain,Sidechain
1	N	486	ARG	Sidechain
1	N	489	PRO	Mainchain
1	N	491	VAL	Mainchain
1	N	492	TYR	Sidechain
1	N	500	PRO	Mainchain
1	N	501	ARG	Sidechain
1	N	504	SER	Mainchain
1	N	506	ARG	Sidechain
1	N	52	ARG	Mainchain
1	N	56	ARG	Mainchain
1	N	57	TYR	Sidechain
1	N	58	SER	Mainchain
1	N	62	PRO	Mainchain
1	N	64	PHE	Mainchain,Sidechain

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Mol	Chain	Res	Type	Group
1	N	70	TYR	Sidechain
1	N	76	SER	Mainchain
1	N	78	ASP	Mainchain
1	N	79	VAL	Mainchain
1	N	84	TYR	Mainchain,Sidechain
1	N	91	PHE	Sidechain
1	N	98	ASN	Mainchain
1	N	99	ASN	Mainchain
1	O	100	ASP	Sidechain
1	O	101	TYR	Sidechain
1	O	103	PRO	Mainchain
1	O	104	GLY	Mainchain
1	O	106	ALA	Mainchain
1	O	111	ILE	Mainchain
1	O	119	TRP	Mainchain
1	O	128	HIS	Sidechain
1	O	132	PRO	Mainchain
1	O	137	PHE	Mainchain,Sidechain
1	O	139	PHE	Sidechain
1	O	143	PHE	Sidechain
1	O	151	ARG	Mainchain
1	O	168	PHE	Sidechain
1	O	171	PRO	Mainchain
1	O	173	GLY	Mainchain
1	O	175	TYR	Sidechain
1	O	177	GLU	Mainchain
1	O	181	ILE	Mainchain
1	O	191	HIS	Sidechain
1	O	192	TYR	Mainchain
1	O	197	ARG	Mainchain
1	O	206	ILE	Mainchain
1	O	210	PHE	Sidechain
1	O	213	ARG	Sidechain
1	O	215	PHE	Mainchain,Sidechain
1	O	216	ARG	Sidechain
1	O	219	PHE	Sidechain
1	O	231	TYR	Sidechain
1	O	238	PRO	Mainchain
1	O	241	ILE	Mainchain
1	O	250	PHE	Mainchain
1	O	254	ARG	Mainchain
1	O	258	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	O	260	GLY	Mainchain
1	O	262	ARG	Sidechain
1	O	264	ARG	Mainchain
1	O	267	PHE	Sidechain
1	O	270	GLY	Mainchain
1	O	271	PHE	Sidechain
1	O	272	ARG	Sidechain
1	O	275	TYR	Sidechain
1	O	283	ILE	Mainchain
1	O	288	ASP	Mainchain
1	O	289	VAL	Mainchain
1	O	292	TYR	Sidechain
1	O	315	VAL	Mainchain
1	O	322	ASP	Mainchain
1	O	323	SER	Mainchain
1	O	326	ARG	Sidechain
1	O	328	TYR	Sidechain
1	O	329	ASN	Mainchain,Sidechain
1	O	334	ASP	Sidechain
1	O	337	PHE	Sidechain
1	O	338	THR	Mainchain
1	O	347	TYR	Sidechain
1	O	355	GLY	Mainchain
1	O	357	ARG	Sidechain
1	O	367	VAL	Mainchain
1	O	368	THR	Mainchain
1	O	371	SER	Mainchain
1	O	372	GLU	Mainchain,Sidechain
1	O	375	TYR	Sidechain
1	O	378	LEU	Mainchain,Peptide
1	O	383	GLN	Mainchain
1	O	384	ASP	Sidechain
1	O	388	PHE	Sidechain
1	O	391	THR	Mainchain
1	O	394	ILE	Mainchain
1	O	397	PHE	Sidechain
1	O	408	HIS	Sidechain
1	O	410	LYS	Mainchain
1	O	412	PHE	Sidechain
1	O	413	TYR	Sidechain
1	O	419	TYR	Sidechain
1	O	426	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	O	427	THR	Mainchain
1	O	436	PHE	Sidechain
1	O	439	ASN	Mainchain
1	O	440	GLN	Sidechain
1	O	441	ILE	Mainchain
1	O	469	ARG	Sidechain
1	O	477	ARG	Mainchain,Sidechain
1	O	480	ILE	Mainchain
1	O	485	ARG	Mainchain
1	O	486	ARG	Sidechain
1	O	489	PRO	Mainchain
1	O	491	VAL	Mainchain
1	O	492	TYR	Sidechain
1	O	500	PRO	Mainchain
1	O	504	SER	Mainchain
1	O	52	ARG	Mainchain,Sidechain
1	O	56	ARG	Mainchain
1	O	57	TYR	Sidechain
1	O	58	SER	Mainchain
1	O	62	PRO	Mainchain
1	O	64	PHE	Mainchain,Sidechain
1	O	70	TYR	Sidechain
1	O	73	ASP	Mainchain,Sidechain
1	O	76	SER	Mainchain
1	O	78	ASP	Mainchain
1	O	79	VAL	Mainchain
1	O	84	TYR	Mainchain
1	O	91	PHE	Sidechain
1	O	98	ASN	Mainchain
1	O	99	ASN	Mainchain

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	3534	0	3463	85	0
1	B	3534	0	3463	107	0
1	C	3534	0	3463	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3534	0	3463	82	0
1	E	3534	0	3463	106	0
1	F	3534	0	3463	95	0
1	G	3534	0	3463	91	0
1	H	3534	0	3463	86	0
1	I	3534	0	3463	99	0
1	J	3534	0	3463	109	0
1	K	3534	0	3463	109	0
1	L	3534	0	3463	106	0
1	M	3534	0	3463	93	0
1	N	3534	0	3463	100	0
1	O	3534	0	3463	92	0
All	All	53010	0	51945	1350	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1350) 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:J:124:LYS:CG	1:J:124:LYS:CD	1.78	1.62
1:K:422:LEU:CG	1:K:422:LEU:CD2	1.76	1.62
1:E:157:LYS:CE	1:E:157:LYS:CD	1.81	1.59
1:O:162:LYS:CE	1:O:162:LYS:CD	1.77	1.59
1:B:167:GLU:CD	1:B:167:GLU:CG	1.76	1.58
1:C:157:LYS:CD	1:C:157:LYS:CG	1.83	1.57
1:J:142:LYS:CE	1:J:142:LYS:CD	1.76	1.57
1:K:422:LEU:CG	1:K:422:LEU:CD1	1.78	1.56
1:L:317:LYS:CE	1:L:317:LYS:CD	1.83	1.56
1:J:124:LYS:CD	1:J:124:LYS:CE	1.80	1.55
1:G:313:LYS:CD	1:G:313:LYS:CG	1.84	1.53
1:H:155:LYS:CE	1:H:155:LYS:NZ	1.69	1.52
1:O:325:LYS:CE	1:O:325:LYS:CD	1.83	1.52
1:M:124:LYS:CD	1:M:124:LYS:CG	1.84	1.51
1:K:313:LYS:CD	1:K:313:LYS:CG	1.89	1.51
1:F:194:LYS:CE	1:F:194:LYS:CD	1.86	1.50
1:M:124:LYS:CD	1:M:124:LYS:CE	1.91	1.47
1:M:142:LYS:CE	1:M:142:LYS:CD	1.89	1.47
1:G:317:LYS:CE	1:G:317:LYS:CD	1.92	1.47
1:M:124:LYS:CE	1:M:124:LYS:NZ	1.79	1.45
1:A:144:LYS:CE	1:A:144:LYS:NZ	1.80	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:325:LYS:CE	1:K:325:LYS:NZ	1.82	1.42
1:E:144:LYS:NZ	1:E:144:LYS:CE	1.84	1.40
1:M:142:LYS:CE	1:M:142:LYS:NZ	1.83	1.39
1:C:157:LYS:CD	1:C:157:LYS:CE	2.01	1.38
1:D:324:LYS:CE	1:D:324:LYS:NZ	1.87	1.37
1:G:220:ASP:CG	1:G:220:ASP:OD2	1.68	1.36
1:F:194:LYS:CE	1:F:194:LYS:NZ	1.98	1.25
1:C:157:LYS:CE	1:C:157:LYS:NZ	2.07	1.17
1:A:133:ASN:HB2	1:A:175:TYR:HB3	1.34	1.10
1:E:133:ASN:HB2	1:E:175:TYR:HB3	1.27	1.07
1:M:133:ASN:HB2	1:M:175:TYR:HB3	1.36	1.06
1:G:133:ASN:HB2	1:G:175:TYR:HB3	1.35	1.06
1:O:133:ASN:HB2	1:O:175:TYR:HB3	1.36	1.06
1:C:133:ASN:HB2	1:C:175:TYR:HB3	1.41	1.00
1:D:133:ASN:HB2	1:D:175:TYR:HB3	1.44	0.99
1:N:133:ASN:HB2	1:N:175:TYR:HB3	1.46	0.98
1:H:133:ASN:HB2	1:H:175:TYR:HB3	1.47	0.97
1:J:176:SER:O	1:J:180:THR:OG1	1.83	0.96
1:B:133:ASN:HB2	1:B:175:TYR:HB3	1.48	0.95
1:F:133:ASN:HB2	1:F:175:TYR:HB3	1.50	0.94
1:K:111:ILE:HB	1:K:472:ILE:HB	1.51	0.90
1:N:381:MET:HE1	1:N:498:VAL:HG21	1.53	0.88
1:J:430:THR:HB	1:J:432:VAL:HG23	1.56	0.88
1:M:133:ASN:CB	1:M:175:TYR:HB3	2.02	0.87
1:C:69:VAL:HG23	1:C:498:VAL:HB	1.54	0.87
1:O:69:VAL:HG23	1:O:498:VAL:HB	1.56	0.87
1:G:430:THR:HB	1:G:432:VAL:HG23	1.57	0.86
1:N:133:ASN:HB2	1:N:175:TYR:CB	2.06	0.85
1:C:157:LYS:CG	1:C:157:LYS:CE	2.55	0.84
1:E:157:LYS:CE	1:E:157:LYS:CG	2.55	0.84
1:D:66:THR:HB	1:D:500:PRO:O	1.76	0.84
1:B:430:THR:HB	1:B:432:VAL:HG23	1.60	0.83
1:D:58:SER:OG	1:D:59:GLU:N	2.11	0.83
1:M:133:ASN:HB2	1:M:175:TYR:CB	2.08	0.83
1:I:111:ILE:HB	1:I:472:ILE:HB	1.61	0.83
1:E:430:THR:HB	1:E:432:VAL:HG23	1.60	0.82
1:I:430:THR:HB	1:I:432:VAL:HG23	1.59	0.82
1:F:133:ASN:HB2	1:F:175:TYR:CB	2.09	0.82
1:H:282:ASN:H	1:H:341:ARG:HG3	1.44	0.82
1:M:430:THR:HB	1:M:432:VAL:HG23	1.60	0.81
1:O:133:ASN:CB	1:O:175:TYR:HB3	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:LYS:CE	1:F:194:LYS:CG	2.57	0.81
1:B:240:ILE:HG23	1:B:344:TYR:H	1.46	0.81
1:C:100:ASP:HB2	1:D:389:ARG:HH21	1.46	0.81
1:G:313:LYS:CD	1:G:313:LYS:CB	2.59	0.81
1:I:133:ASN:HB2	1:I:175:TYR:HB3	1.63	0.80
1:J:133:ASN:HB2	1:J:175:TYR:HB3	1.63	0.80
1:C:238:PRO:HG2	1:C:362:LEU:HD11	1.64	0.79
1:B:167:GLU:CD	1:B:167:GLU:CB	2.56	0.79
1:F:430:THR:HB	1:F:432:VAL:HG23	1.64	0.79
1:A:240:ILE:HG23	1:A:344:TYR:H	1.46	0.78
1:N:203:GLU:HB2	1:N:326:ARG:HH12	1.47	0.78
1:L:430:THR:HB	1:L:432:VAL:HG23	1.64	0.78
1:E:326:ARG:HD2	1:E:439:ASN:HB2	1.64	0.78
1:A:356:ILE:O	1:A:360:THR:HG22	1.84	0.78
1:B:101:TYR:OH	1:L:390:SER:OG	2.02	0.77
1:O:356:ILE:O	1:O:360:THR:HG22	1.84	0.77
1:M:240:ILE:HG23	1:M:344:TYR:H	1.48	0.77
1:J:124:LYS:CG	1:J:124:LYS:CE	2.62	0.77
1:O:240:ILE:HG23	1:O:344:TYR:H	1.48	0.77
1:C:326:ARG:HD2	1:C:439:ASN:HB2	1.66	0.77
1:E:185:ASN:HD21	1:E:210:PHE:H	1.32	0.76
1:F:240:ILE:HG23	1:F:344:TYR:H	1.50	0.76
1:L:240:ILE:HG23	1:L:344:TYR:H	1.49	0.76
1:K:313:LYS:CD	1:K:313:LYS:CB	2.64	0.76
1:L:317:LYS:CE	1:L:317:LYS:CG	2.64	0.76
1:J:58:SER:OG	1:J:59:GLU:N	2.18	0.76
1:J:69:VAL:HG23	1:J:498:VAL:HB	1.67	0.76
1:C:133:ASN:HB2	1:C:175:TYR:CB	2.16	0.75
1:N:133:ASN:CB	1:N:175:TYR:HB3	2.15	0.75
1:F:326:ARG:HD2	1:F:439:ASN:HB2	1.67	0.75
1:O:325:LYS:CE	1:O:325:LYS:CG	2.64	0.75
1:B:133:ASN:HB2	1:B:175:TYR:CB	2.16	0.75
1:C:111:ILE:HB	1:C:472:ILE:HB	1.68	0.75
1:C:430:THR:HB	1:C:432:VAL:HG23	1.68	0.75
1:J:197:ARG:HG3	1:J:198:GLN:HE21	1.52	0.75
1:O:430:THR:HB	1:O:432:VAL:HG23	1.68	0.75
1:G:317:LYS:CE	1:G:317:LYS:CG	2.64	0.74
1:M:237:HIS:HB3	1:M:238:PRO:HD3	1.67	0.74
1:H:133:ASN:HB2	1:H:175:TYR:CB	2.18	0.74
1:K:100:ASP:HB2	1:L:389:ARG:HH21	1.52	0.74
1:L:133:ASN:HB2	1:L:175:TYR:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:142:LYS:CE	1:J:142:LYS:CG	2.66	0.74
1:O:111:ILE:HB	1:O:472:ILE:HB	1.69	0.74
1:L:69:VAL:HG23	1:L:498:VAL:HB	1.71	0.73
1:H:240:ILE:HG23	1:H:344:TYR:H	1.52	0.73
1:H:430:THR:HB	1:H:432:VAL:HG23	1.71	0.73
1:L:141:ASN:H	1:L:141:ASN:HD22	1.34	0.73
1:F:58:SER:OG	1:F:59:GLU:N	2.22	0.73
1:I:453:VAL:HG21	1:J:450:ILE:HG21	1.70	0.73
1:K:430:THR:HB	1:K:432:VAL:HG23	1.71	0.73
1:K:133:ASN:HB2	1:K:175:TYR:HB3	1.69	0.72
1:C:240:ILE:HG23	1:C:344:TYR:H	1.52	0.72
1:D:240:ILE:HG23	1:D:344:TYR:H	1.54	0.72
1:K:172:GLU:HB2	1:L:362:LEU:HD23	1.71	0.72
1:G:69:VAL:HG23	1:G:498:VAL:HB	1.71	0.72
1:N:282:ASN:H	1:N:341:ARG:HG3	1.54	0.71
1:C:133:ASN:CB	1:C:175:TYR:HB3	2.20	0.71
1:M:142:LYS:CE	1:M:142:LYS:CG	2.67	0.71
1:O:162:LYS:CE	1:O:162:LYS:CG	2.68	0.71
1:A:58:SER:OG	1:A:59:GLU:N	2.24	0.71
1:J:133:ASN:HB2	1:J:175:TYR:CB	2.20	0.71
1:L:133:ASN:HB2	1:L:175:TYR:CB	2.20	0.71
1:C:489:PRO:O	1:D:262:ARG:NH1	2.24	0.71
1:C:238:PRO:HG2	1:C:362:LEU:CD1	2.21	0.70
1:B:84:TYR:CZ	1:C:268:GLN:HG3	2.26	0.70
1:G:133:ASN:CB	1:G:175:TYR:HB3	2.17	0.70
1:C:73:ASP:OD1	1:C:73:ASP:N	2.18	0.70
1:H:155:LYS:NZ	1:H:155:LYS:CD	2.53	0.70
1:M:124:LYS:CG	1:M:124:LYS:CE	2.68	0.70
1:C:67:THR:OG1	1:C:68:ARG:N	2.23	0.70
1:M:416:GLN:OE1	1:N:415:ASP:HB3	1.92	0.70
1:O:136:GLU:HA	1:O:141:ASN:HD22	1.57	0.70
1:N:453:VAL:HG21	1:O:450:ILE:HG21	1.72	0.69
1:K:73:ASP:HB3	1:K:91:PHE:CE1	2.28	0.69
1:B:185:ASN:HA	1:B:188:ILE:HD12	1.74	0.69
1:D:430:THR:HB	1:D:432:VAL:HG23	1.73	0.69
1:O:470:ASN:OD1	1:O:470:ASN:N	2.24	0.69
1:I:240:ILE:HG23	1:I:344:TYR:H	1.58	0.69
1:K:422:LEU:CD1	1:K:422:LEU:CB	2.69	0.68
1:O:481:THR:OG1	1:O:485:ARG:HA	1.94	0.68
1:G:133:ASN:HB2	1:G:175:TYR:CB	2.17	0.68
1:N:356:ILE:O	1:N:360:THR:HG22	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:ASP:HA	1:F:319:LEU:HD12	1.76	0.68
1:D:288:ASP:HA	1:D:319:LEU:HD12	1.75	0.68
1:M:69:VAL:HG23	1:M:498:VAL:HB	1.76	0.68
1:L:453:VAL:HG21	1:M:450:ILE:HG21	1.76	0.68
1:N:430:THR:HB	1:N:432:VAL:HG23	1.75	0.68
1:G:57:TYR:OH	1:G:109:GLN:OE1	2.11	0.67
1:J:52:ARG:HB2	1:J:116:ARG:HD2	1.77	0.67
1:J:238:PRO:HG2	1:J:362:LEU:HD11	1.75	0.67
1:N:434:ASN:HD21	1:N:437:PRO:HB3	1.59	0.67
1:I:133:ASN:HB2	1:I:175:TYR:CB	2.24	0.67
1:N:382:MET:HG2	1:N:466:LEU:HD12	1.77	0.67
1:A:66:THR:OG1	1:A:500:PRO:O	2.10	0.66
1:C:113:LEU:HB3	1:C:119:TRP:CD1	2.30	0.66
1:I:58:SER:OG	1:I:59:GLU:N	2.22	0.66
1:D:185:ASN:HA	1:D:188:ILE:HD12	1.76	0.66
1:E:240:ILE:HG23	1:E:344:TYR:H	1.60	0.66
1:M:427:THR:HG22	1:M:428:SER:HB2	1.78	0.66
1:C:134:VAL:HA	1:C:140:THR:HB	1.78	0.66
1:C:356:ILE:O	1:C:360:THR:HG22	1.95	0.66
1:F:360:THR:OG1	1:F:361:LEU:N	2.28	0.66
1:J:356:ILE:O	1:J:360:THR:HG22	1.96	0.66
1:O:73:ASP:OD1	1:O:73:ASP:N	2.24	0.65
1:E:69:VAL:HG23	1:E:498:VAL:HB	1.78	0.65
1:K:422:LEU:CD2	1:K:422:LEU:HG	2.15	0.65
1:I:133:ASN:CB	1:I:175:TYR:HB3	2.26	0.65
1:J:124:LYS:CD	1:J:124:LYS:CB	2.72	0.65
1:O:381:MET:HE1	1:O:498:VAL:HG21	1.78	0.65
1:O:325:LYS:CD	1:O:325:LYS:NZ	2.60	0.65
1:E:133:ASN:CB	1:E:175:TYR:HB3	2.15	0.65
1:F:238:PRO:HG2	1:F:362:LEU:CD1	2.25	0.65
1:E:88:HIS:HB2	1:E:491:VAL:O	1.97	0.65
1:E:157:LYS:CD	1:E:157:LYS:NZ	2.60	0.65
1:G:240:ILE:HG23	1:G:344:TYR:H	1.61	0.65
1:H:141:ASN:HD22	1:H:141:ASN:H	1.44	0.65
1:K:470:ASN:OD1	1:K:470:ASN:N	2.29	0.65
1:G:55:ILE:HG12	1:G:113:LEU:HD23	1.78	0.64
1:K:240:ILE:HG23	1:K:344:TYR:H	1.62	0.64
1:C:88:HIS:HB2	1:C:491:VAL:O	1.98	0.64
1:L:72:VAL:H	1:L:93:THR:HG21	1.62	0.64
1:M:231:TYR:OH	1:M:284:PRO:O	2.12	0.64
1:J:136:GLU:HA	1:J:141:ASN:HD22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:133:ASN:HB2	1:K:175:TYR:CB	2.27	0.64
1:B:133:ASN:CB	1:B:175:TYR:HB3	2.25	0.64
1:E:67:THR:OG1	1:E:68:ARG:N	2.29	0.64
1:J:142:LYS:CD	1:J:142:LYS:NZ	2.60	0.64
1:J:240:ILE:HG23	1:J:344:TYR:H	1.63	0.64
1:K:249:ASP:OD1	1:K:251:THR:HB	1.98	0.64
1:E:113:LEU:HB3	1:E:119:TRP:CD1	2.32	0.64
1:L:58:SER:OG	1:L:59:GLU:N	2.27	0.64
1:F:213:ARG:O	1:F:240:ILE:HD11	1.98	0.64
1:J:282:ASN:H	1:J:341:ARG:HG3	1.63	0.64
1:M:145:ALA:HB3	1:M:168:PHE:HE1	1.63	0.63
1:O:197:ARG:HG3	1:O:198:GLN:HE21	1.64	0.63
1:A:130:ASN:HB3	1:B:363:CYS:HB3	1.81	0.63
1:B:69:VAL:HG23	1:B:498:VAL:HB	1.81	0.63
1:A:133:ASN:CB	1:A:175:TYR:HB3	2.21	0.63
1:A:343:TRP:HE1	1:A:360:THR:HG21	1.63	0.63
1:A:326:ARG:HH11	1:A:326:ARG:HB3	1.64	0.63
1:D:88:HIS:HB2	1:D:491:VAL:O	2.00	0.62
1:N:58:SER:OG	1:N:59:GLU:N	2.26	0.62
1:A:203:GLU:HB2	1:A:326:ARG:HH12	1.63	0.62
1:A:176:SER:O	1:A:180:THR:OG1	2.08	0.62
1:I:326:ARG:HD2	1:I:439:ASN:HB2	1.81	0.62
1:F:198:GLN:HA	1:F:198:GLN:HE21	1.65	0.62
1:G:317:LYS:CD	1:G:317:LYS:NZ	2.61	0.62
1:H:331:ILE:HD13	1:H:339:GLN:HG2	1.82	0.62
1:K:363:CYS:HB3	1:O:130:ASN:HB3	1.80	0.62
1:L:401:GLY:HA3	1:L:463:HIS:HD2	1.64	0.62
1:F:69:VAL:HG23	1:F:498:VAL:HB	1.81	0.62
1:I:145:ALA:HB3	1:I:168:PHE:HE1	1.62	0.62
1:M:124:LYS:CD	1:M:124:LYS:CB	2.78	0.61
1:K:197:ARG:HG3	1:K:198:GLN:HE21	1.64	0.61
1:A:282:ASN:H	1:A:341:ARG:HG3	1.64	0.61
1:H:465:THR:HG21	1:H:501:ARG:HH11	1.65	0.61
1:I:185:ASN:HD21	1:I:210:PHE:H	1.46	0.61
1:A:430:THR:HB	1:A:432:VAL:HG23	1.83	0.61
1:L:67:THR:OG1	1:L:68:ARG:N	2.32	0.61
1:E:427:THR:HG22	1:E:428:SER:HB2	1.82	0.61
1:C:157:LYS:CD	1:C:157:LYS:CB	2.77	0.61
1:D:254:ARG:HB3	1:D:369:CYS:HB3	1.82	0.61
1:H:326:ARG:HH11	1:H:326:ARG:HB3	1.64	0.61
1:A:238:PRO:HG2	1:A:362:LEU:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:238:PRO:HG2	1:N:362:LEU:HD11	1.82	0.61
1:O:150:SER:HB2	1:O:162:LYS:HB2	1.83	0.60
1:F:133:ASN:CB	1:F:175:TYR:HB3	2.28	0.60
1:N:212:THR:HA	1:N:239:ASP:HA	1.83	0.60
1:F:212:THR:HA	1:F:239:ASP:HA	1.83	0.60
1:G:102:SER:HB2	1:G:105:GLU:HB3	1.83	0.60
1:J:403:GLU:OE2	1:J:461:THR:OG1	2.18	0.60
1:M:342:SER:HB3	1:M:345:LEU:HG	1.84	0.60
1:K:231:TYR:OH	1:K:284:PRO:O	2.14	0.60
1:B:238:PRO:HG2	1:B:362:LEU:CD1	2.31	0.60
1:J:212:THR:HA	1:J:239:ASP:HA	1.84	0.60
1:J:88:HIS:HB2	1:J:491:VAL:O	2.02	0.60
1:E:472:ILE:HG22	1:E:476:GLN:HE21	1.66	0.60
1:C:389:ARG:HH11	1:L:389:ARG:NH1	2.00	0.59
1:A:238:PRO:HG2	1:A:362:LEU:HD11	1.83	0.59
1:I:212:THR:HA	1:I:239:ASP:HA	1.84	0.59
1:M:356:ILE:O	1:M:360:THR:HG22	2.03	0.59
1:O:212:THR:HA	1:O:239:ASP:HA	1.84	0.59
1:G:172:GLU:OE1	1:H:347:TYR:HE2	1.85	0.59
1:C:157:LYS:CE	1:C:157:LYS:HG3	2.32	0.59
1:M:212:THR:HA	1:M:239:ASP:HA	1.84	0.59
1:A:185:ASN:ND2	1:A:210:PHE:O	2.34	0.59
1:E:340:TYR:HD1	1:E:441:ILE:HD13	1.67	0.59
1:F:241:ILE:HD13	1:F:248:VAL:HG21	1.85	0.59
1:K:141:ASN:H	1:K:141:ASN:HD22	1.49	0.59
1:G:57:TYR:CD1	1:H:387:THR:HG22	2.38	0.59
1:K:174:ASN:HB2	1:K:179:MET:HE1	1.85	0.59
1:L:102:SER:HB3	1:L:105:GLU:HB3	1.84	0.59
1:E:212:THR:HA	1:E:239:ASP:HA	1.84	0.59
1:G:212:THR:HA	1:G:239:ASP:HA	1.85	0.59
1:M:403:GLU:OE2	1:M:461:THR:OG1	2.20	0.59
1:F:72:VAL:O	1:F:93:THR:OG1	2.20	0.59
1:H:133:ASN:CB	1:H:175:TYR:HB3	2.29	0.59
1:B:88:HIS:HB2	1:B:491:VAL:O	2.03	0.59
1:I:177:GLU:HG2	1:I:452:THR:H	1.67	0.59
1:L:212:THR:HA	1:L:239:ASP:HA	1.85	0.59
1:L:360:THR:OG1	1:L:361:LEU:N	2.35	0.59
1:B:238:PRO:HG2	1:B:362:LEU:HD11	1.84	0.58
1:G:203:GLU:O	1:G:206:ILE:HG12	2.02	0.58
1:N:240:ILE:HG23	1:N:344:TYR:H	1.67	0.58
1:A:144:LYS:NZ	1:A:144:LYS:CD	2.64	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:THR:HA	1:D:239:ASP:HA	1.84	0.58
1:D:324:LYS:NZ	1:D:324:LYS:CD	2.64	0.58
1:G:89:SER:HA	1:G:480:ILE:HG12	1.84	0.58
1:M:95:VAL:HG21	1:M:476:GLN:HG2	1.84	0.58
1:N:176:SER:O	1:N:180:THR:HB	2.03	0.58
1:I:88:HIS:HB2	1:I:491:VAL:O	2.04	0.58
1:E:322:ASP:HB2	1:E:328:TYR:HE2	1.69	0.58
1:K:422:LEU:CD2	1:K:422:LEU:CB	2.76	0.58
1:C:212:THR:HA	1:C:239:ASP:HA	1.85	0.58
1:J:73:ASP:OD1	1:J:73:ASP:N	2.33	0.58
1:G:427:THR:HG22	1:G:428:SER:HB2	1.86	0.58
1:M:88:HIS:HB2	1:M:491:VAL:O	2.04	0.58
1:M:282:ASN:H	1:M:341:ARG:HG3	1.66	0.58
1:N:104:GLY:O	1:N:107:SER:OG	2.18	0.58
1:J:57:TYR:OH	1:J:109:GLN:OE1	2.19	0.58
1:K:325:LYS:NZ	1:K:325:LYS:CD	2.66	0.58
1:F:419:TYR:HB3	1:F:422:LEU:HB2	1.86	0.58
1:M:72:VAL:O	1:M:93:THR:OG1	2.21	0.58
1:B:212:THR:HA	1:B:239:ASP:HA	1.85	0.57
1:D:241:ILE:HD12	1:D:273:ILE:HD11	1.85	0.57
1:E:83:ASN:HA	1:E:86:ASN:HD22	1.69	0.57
1:I:427:THR:HG22	1:I:428:SER:HB2	1.86	0.57
1:O:288:ASP:HA	1:O:319:LEU:HD12	1.85	0.57
1:A:212:THR:HA	1:A:239:ASP:HA	1.86	0.57
1:M:240:ILE:HG21	1:M:342:SER:OG	2.04	0.57
1:B:403:GLU:OE2	1:B:461:THR:OG1	2.21	0.57
1:K:212:THR:HA	1:K:239:ASP:HA	1.85	0.57
1:K:359:TRP:HD1	1:K:360:THR:HG22	1.68	0.57
1:O:326:ARG:CD	1:O:439:ASN:HB2	2.34	0.57
1:I:213:ARG:O	1:I:240:ILE:HD11	2.05	0.57
1:L:240:ILE:HG21	1:L:342:SER:OG	2.03	0.57
1:K:134:VAL:HA	1:K:140:THR:HB	1.86	0.57
1:M:343:TRP:HH2	1:M:362:LEU:HD13	1.68	0.57
1:H:89:SER:HA	1:H:480:ILE:HG12	1.86	0.57
1:A:207:GLY:HA2	1:A:244:PRO:HD2	1.86	0.57
1:D:89:SER:HA	1:D:480:ILE:HG12	1.86	0.57
1:G:138:MET:HB3	1:G:254:ARG:HH12	1.69	0.57
1:J:135:ASN:HA	1:J:172:GLU:HG2	1.87	0.57
1:K:326:ARG:HD2	1:K:439:ASN:HB2	1.87	0.57
1:E:240:ILE:HD13	1:E:342:SER:OG	2.05	0.56
1:E:382:MET:HE3	1:E:466:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:LYS:CD	1:F:194:LYS:NZ	2.68	0.56
1:H:185:ASN:HA	1:H:188:ILE:HD12	1.87	0.56
1:I:185:ASN:HA	1:I:188:ILE:HD12	1.86	0.56
1:F:207:GLY:HA2	1:F:244:PRO:HD2	1.87	0.56
1:K:69:VAL:HG23	1:K:498:VAL:HB	1.88	0.56
1:G:177:GLU:HG2	1:G:452:THR:H	1.69	0.56
1:G:381:MET:HB2	1:G:476:GLN:OE1	2.05	0.56
1:H:172:GLU:CB	1:I:362:LEU:HD23	2.36	0.56
1:H:212:THR:HA	1:H:239:ASP:HA	1.86	0.56
1:L:288:ASP:HA	1:L:319:LEU:HD12	1.88	0.56
1:L:254:ARG:HB3	1:L:369:CYS:HB3	1.85	0.56
1:B:100:ASP:HB2	1:C:389:ARG:HH21	1.69	0.56
1:F:402:ALA:HB3	1:J:497:ILE:HD11	1.87	0.56
1:H:134:VAL:HG13	1:H:140:THR:O	2.06	0.56
1:I:356:ILE:O	1:I:360:THR:HG22	2.05	0.56
1:E:220:ASP:HB2	1:E:227:MET:HG2	1.86	0.56
1:M:57:TYR:CD2	1:N:387:THR:HA	2.41	0.56
1:N:381:MET:CE	1:N:498:VAL:HG21	2.31	0.56
1:O:326:ARG:HD3	1:O:439:ASN:HB2	1.87	0.56
1:B:326:ARG:HH11	1:B:326:ARG:HB3	1.71	0.56
1:H:172:GLU:HB2	1:I:362:LEU:HD23	1.88	0.56
1:C:113:LEU:HB3	1:C:119:TRP:NE1	2.21	0.56
1:D:69:VAL:HG23	1:D:498:VAL:HB	1.88	0.56
1:F:434:ASN:HD21	1:F:437:PRO:HB3	1.71	0.56
1:G:381:MET:HG3	1:G:472:ILE:HD13	1.88	0.56
1:H:185:ASN:HD21	1:H:210:PHE:H	1.53	0.56
1:I:96:ILE:HA	1:J:387:THR:HG21	1.88	0.56
1:D:134:VAL:HA	1:D:140:THR:HB	1.88	0.55
1:F:102:SER:HB3	1:F:105:GLU:HB3	1.88	0.55
1:B:241:ILE:HD13	1:B:248:VAL:HG21	1.88	0.55
1:G:88:HIS:HB2	1:G:491:VAL:O	2.06	0.55
1:O:213:ARG:O	1:O:240:ILE:HD11	2.05	0.55
1:F:133:ASN:HD21	1:F:367:VAL:HG22	1.71	0.55
1:I:241:ILE:HD12	1:I:248:VAL:HG21	1.88	0.55
1:M:177:GLU:HG2	1:M:452:THR:H	1.70	0.55
1:C:58:SER:OG	1:C:59:GLU:N	2.39	0.55
1:K:57:TYR:OH	1:K:109:GLN:OE1	2.23	0.55
1:F:237:HIS:HB2	1:F:238:PRO:HD3	1.87	0.55
1:C:67:THR:HG1	1:C:68:ARG:H	1.55	0.55
1:O:251:THR:OG1	1:O:270:GLY:HA2	2.07	0.55
1:H:240:ILE:HG21	1:H:342:SER:OG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:SER:HB3	1:C:345:LEU:HG	1.88	0.55
1:E:73:ASP:OD1	1:E:73:ASP:N	2.40	0.55
1:F:88:HIS:HB2	1:F:491:VAL:O	2.07	0.55
1:G:69:VAL:HG21	1:G:381:MET:HE1	1.88	0.55
1:L:55:ILE:HG12	1:L:113:LEU:HD23	1.89	0.55
1:L:380:ASP:OD2	1:L:380:ASP:N	2.40	0.55
1:A:94:THR:HA	1:A:474:GLY:O	2.07	0.55
1:C:215:PHE:HB2	1:C:345:LEU:HD21	1.88	0.55
1:H:470:ASN:OD1	1:H:470:ASN:N	2.38	0.55
1:N:326:ARG:HH11	1:N:326:ARG:HB3	1.72	0.55
1:K:133:ASN:CB	1:K:175:TYR:HB3	2.37	0.54
1:M:94:THR:HA	1:M:474:GLY:O	2.07	0.54
1:N:401:GLY:HA3	1:N:463:HIS:HD2	1.72	0.54
1:O:67:THR:OG1	1:O:68:ARG:N	2.40	0.54
1:H:130:ASN:HB3	1:I:363:CYS:HB3	1.89	0.54
1:C:71:LEU:HD11	1:C:381:MET:HE1	1.88	0.54
1:C:214:ASN:HB3	1:C:217:LEU:HD22	1.89	0.54
1:I:197:ARG:HE	1:I:198:GLN:HE22	1.54	0.54
1:J:176:SER:HB2	1:J:179:MET:HB3	1.88	0.54
1:B:57:TYR:OH	1:B:109:GLN:OE1	2.15	0.54
1:E:176:SER:HB3	1:E:179:MET:HB3	1.89	0.54
1:G:326:ARG:HD2	1:G:439:ASN:HB2	1.88	0.54
1:N:240:ILE:HG22	1:N:241:ILE:N	2.22	0.54
1:E:111:ILE:HB	1:E:472:ILE:HB	1.88	0.54
1:L:88:HIS:HB2	1:L:491:VAL:O	2.06	0.54
1:L:282:ASN:H	1:L:341:ARG:HG3	1.71	0.54
1:D:240:ILE:HG22	1:D:241:ILE:N	2.23	0.54
1:K:115:ASP:HA	1:K:470:ASN:HD22	1.73	0.54
1:B:96:ILE:HD12	1:B:474:GLY:HA3	1.90	0.54
1:D:282:ASN:H	1:D:341:ARG:HG3	1.72	0.54
1:I:275:TYR:CE1	1:I:341:ARG:HD3	2.42	0.54
1:L:133:ASN:CB	1:L:175:TYR:HB3	2.38	0.54
1:L:172:GLU:HB2	1:M:362:LEU:HD23	1.89	0.54
1:N:133:ASN:HD21	1:N:367:VAL:HG22	1.73	0.54
1:A:216:ARG:HG3	1:A:345:LEU:HD13	1.90	0.54
1:G:183:LEU:HD21	1:H:236:PHE:HE2	1.72	0.54
1:H:207:GLY:HA2	1:H:244:PRO:HD2	1.90	0.54
1:A:326:ARG:HD2	1:A:439:ASN:HB2	1.90	0.54
1:D:356:ILE:O	1:D:360:THR:HG22	2.08	0.54
1:J:138:MET:O	1:J:254:ARG:NH1	2.41	0.54
1:K:282:ASN:H	1:K:341:ARG:HG3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:57:TYR:CD1	1:M:387:THR:HG22	2.43	0.54
1:F:282:ASN:H	1:F:341:ARG:HG3	1.73	0.54
1:L:94:THR:HA	1:L:474:GLY:O	2.08	0.54
1:A:89:SER:HA	1:A:480:ILE:HG12	1.89	0.53
1:C:94:THR:HA	1:C:474:GLY:O	2.08	0.53
1:G:313:LYS:CG	1:G:313:LYS:CE	2.81	0.53
1:J:124:LYS:CD	1:J:124:LYS:NZ	2.68	0.53
1:N:150:SER:HB2	1:N:162:LYS:HB2	1.90	0.53
1:B:220:ASP:HB2	1:B:227:MET:HG2	1.90	0.53
1:L:326:ARG:HD2	1:L:439:ASN:HB2	1.89	0.53
1:M:225:LEU:HD12	1:M:287:LEU:HD12	1.89	0.53
1:M:343:TRP:CH2	1:M:362:LEU:HD13	2.43	0.53
1:A:434:ASN:HD21	1:A:437:PRO:HB3	1.74	0.53
1:B:111:ILE:HB	1:B:472:ILE:HB	1.90	0.53
1:N:254:ARG:O	1:N:257:ASN:HB2	2.08	0.53
1:O:380:ASP:HB2	1:O:476:GLN:HE22	1.73	0.53
1:K:150:SER:HB2	1:K:162:LYS:HB2	1.91	0.53
1:N:207:GLY:HA2	1:N:244:PRO:HD2	1.91	0.53
1:D:172:GLU:HB2	1:E:362:LEU:HD23	1.91	0.53
1:L:497:ILE:HD11	1:M:402:ALA:HB3	1.89	0.53
1:D:131:MET:HA	1:D:490:TYR:CD2	2.44	0.53
1:I:94:THR:HA	1:I:474:GLY:O	2.09	0.53
1:L:207:GLY:HA2	1:L:244:PRO:HD2	1.91	0.53
1:M:67:THR:HG23	1:M:68:ARG:N	2.24	0.53
1:O:88:HIS:HB2	1:O:491:VAL:O	2.08	0.53
1:O:185:ASN:HA	1:O:188:ILE:HD12	1.91	0.53
1:D:275:TYR:CE1	1:D:341:ARG:HD3	2.44	0.53
1:H:58:SER:OG	1:H:59:GLU:N	2.41	0.53
1:I:136:GLU:HB2	1:I:172:GLU:OE2	2.08	0.53
1:L:481:THR:HB	1:L:485:ARG:HA	1.91	0.53
1:A:69:VAL:HG23	1:A:498:VAL:HB	1.90	0.53
1:D:382:MET:SD	1:D:382:MET:N	2.82	0.53
1:H:198:GLN:HE21	1:H:198:GLN:HA	1.74	0.53
1:D:427:THR:HG22	1:D:428:SER:HB2	1.91	0.52
1:F:238:PRO:HG2	1:F:362:LEU:HD11	1.90	0.52
1:F:389:ARG:NH2	1:J:98:ASN:HD21	2.06	0.52
1:G:69:VAL:CG2	1:G:498:VAL:HB	2.38	0.52
1:L:419:TYR:HB3	1:L:422:LEU:HB2	1.90	0.52
1:H:69:VAL:HG23	1:H:498:VAL:HB	1.91	0.52
1:O:427:THR:HG22	1:O:428:SER:HB2	1.91	0.52
1:A:362:LEU:HD23	1:E:172:GLU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:ILE:HG21	1:G:356:ILE:HD11	1.90	0.52
1:H:94:THR:HA	1:H:474:GLY:O	2.09	0.52
1:N:326:ARG:HD3	1:N:439:ASN:HD22	1.75	0.52
1:E:126:ILE:HD12	1:E:495:LEU:HD23	1.92	0.52
1:F:340:TYR:CD1	1:F:441:ILE:HG21	2.45	0.52
1:I:381:MET:HE1	1:I:498:VAL:HG21	1.92	0.52
1:C:213:ARG:O	1:C:240:ILE:HD11	2.10	0.52
1:J:135:ASN:OD1	1:J:136:GLU:N	2.43	0.52
1:J:238:PRO:HG2	1:J:362:LEU:CD1	2.40	0.52
1:L:113:LEU:HB3	1:L:119:TRP:CD1	2.45	0.52
1:N:95:VAL:HG21	1:N:476:GLN:HG2	1.92	0.52
1:B:377:SER:O	1:B:378:LEU:HD23	2.10	0.52
1:E:244:PRO:HA	1:E:275:TYR:CE1	2.45	0.52
1:K:88:HIS:HB2	1:K:491:VAL:O	2.09	0.52
1:O:102:SER:HB2	1:O:105:GLU:HB3	1.90	0.52
1:A:114:ASP:N	1:A:119:TRP:HE1	2.08	0.52
1:F:498:VAL:HG12	1:F:500:PRO:HD3	1.92	0.52
1:G:465:THR:HG21	1:G:501:ARG:HH11	1.74	0.52
1:H:203:GLU:HB2	1:H:326:ARG:HH12	1.75	0.52
1:M:172:GLU:HB2	1:N:362:LEU:HD23	1.91	0.52
1:C:154:THR:HG22	1:C:157:LYS:HA	1.90	0.52
1:C:207:GLY:HA2	1:C:244:PRO:HD2	1.91	0.52
1:B:209:LYS:NZ	1:B:443:ALA:O	2.41	0.52
1:A:55:ILE:HG12	1:A:113:LEU:HD23	1.91	0.51
1:C:185:ASN:HA	1:C:188:ILE:HD12	1.91	0.51
1:F:427:THR:HG22	1:F:428:SER:HB2	1.92	0.51
1:K:331:ILE:HD13	1:K:339:GLN:HG2	1.92	0.51
1:K:386:VAL:O	1:K:387:THR:OG1	2.27	0.51
1:A:213:ARG:O	1:A:240:ILE:HD11	2.10	0.51
1:B:94:THR:HA	1:B:474:GLY:O	2.10	0.51
1:H:88:HIS:HB2	1:H:491:VAL:O	2.10	0.51
1:I:209:LYS:HB3	1:I:242:LEU:HD12	1.93	0.51
1:I:211:ASP:HB2	1:I:242:LEU:HD11	1.92	0.51
1:M:238:PRO:HG2	1:M:362:LEU:CD1	2.40	0.51
1:N:239:ASP:OD1	1:N:259:LEU:HA	2.10	0.51
1:B:197:ARG:HG3	1:B:198:GLN:HE21	1.75	0.51
1:D:326:ARG:HD3	1:D:439:ASN:HB2	1.92	0.51
1:J:411:SER:HB3	1:J:452:THR:HG22	1.92	0.51
1:J:209:LYS:HD2	1:J:442:LEU:HA	1.92	0.51
1:N:238:PRO:HG2	1:N:362:LEU:CD1	2.40	0.51
1:D:326:ARG:HB3	1:D:326:ARG:HH11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:TYR:HD2	1:G:60:LEU:HB2	1.76	0.51
1:J:240:ILE:HG22	1:J:241:ILE:N	2.26	0.51
1:M:97:GLN:HB2	1:N:388:PHE:CE2	2.46	0.51
1:M:264:ARG:NH1	1:M:357:ARG:O	2.44	0.51
1:N:88:HIS:HB2	1:N:491:VAL:O	2.10	0.51
1:N:145:ALA:HB3	1:N:168:PHE:HE1	1.75	0.51
1:I:69:VAL:CG2	1:I:498:VAL:HB	2.41	0.51
1:I:138:MET:HB3	1:I:254:ARG:HH12	1.74	0.51
1:B:96:ILE:HA	1:C:387:THR:HG21	1.93	0.51
1:C:83:ASN:HA	1:C:86:ASN:HB2	1.93	0.51
1:K:313:LYS:CG	1:K:313:LYS:CE	2.82	0.51
1:B:343:TRP:HH2	1:B:362:LEU:HD13	1.76	0.51
1:F:113:LEU:HB3	1:F:119:TRP:CD1	2.46	0.51
1:K:207:GLY:HA2	1:K:244:PRO:HD2	1.92	0.51
1:K:419:TYR:HB3	1:K:422:LEU:HB2	1.93	0.51
1:E:213:ARG:O	1:E:240:ILE:HD11	2.10	0.51
1:E:340:TYR:CD1	1:E:441:ILE:HD13	2.45	0.51
1:F:94:THR:HA	1:F:474:GLY:O	2.11	0.51
1:K:102:SER:HB2	1:K:105:GLU:HB3	1.93	0.51
1:L:331:ILE:HD13	1:L:339:GLN:HG2	1.92	0.51
1:M:142:LYS:CD	1:M:142:LYS:NZ	2.74	0.51
1:N:94:THR:HA	1:N:474:GLY:O	2.11	0.51
1:D:94:THR:HA	1:D:474:GLY:O	2.10	0.50
1:H:72:VAL:H	1:H:93:THR:HG21	1.76	0.50
1:F:83:ASN:HA	1:F:86:ASN:HB2	1.93	0.50
1:G:94:THR:HA	1:G:474:GLY:O	2.11	0.50
1:M:96:ILE:HA	1:N:387:THR:HG21	1.93	0.50
1:O:52:ARG:HB3	1:O:114:ASP:OD2	2.11	0.50
1:J:57:TYR:CG	1:J:58:SER:N	2.78	0.50
1:K:225:LEU:HD12	1:K:287:LEU:HD12	1.93	0.50
1:O:207:GLY:HA2	1:O:244:PRO:HD2	1.94	0.50
1:A:388:PHE:CD2	1:A:398:PRO:HA	2.47	0.50
1:F:236:PHE:HE2	1:J:183:LEU:HD21	1.76	0.50
1:I:240:ILE:HG12	1:I:344:TYR:HB2	1.93	0.50
1:J:470:ASN:HD21	1:J:506:ARG:HH22	1.59	0.50
1:K:481:THR:HB	1:K:485:ARG:HA	1.93	0.50
1:M:207:GLY:HA2	1:M:244:PRO:HD2	1.93	0.50
1:N:213:ARG:O	1:N:240:ILE:HD11	2.12	0.50
1:O:136:GLU:HA	1:O:141:ASN:ND2	2.25	0.50
1:C:203:GLU:O	1:C:206:ILE:HG12	2.11	0.50
1:D:73:ASP:OD1	1:D:73:ASP:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:HIS:CD2	1:J:174:ASN:HA	2.46	0.50
1:I:470:ASN:N	1:I:470:ASN:OD1	2.44	0.50
1:J:207:GLY:HA2	1:J:244:PRO:HD2	1.94	0.50
1:N:237:HIS:O	1:N:239:ASP:OD2	2.29	0.50
1:O:237:HIS:HB2	1:O:238:PRO:HD3	1.94	0.50
1:A:113:LEU:HB3	1:A:119:TRP:CD1	2.46	0.50
1:F:244:PRO:HG3	1:F:340:TYR:HE2	1.76	0.50
1:J:94:THR:HA	1:J:474:GLY:O	2.12	0.50
1:B:254:ARG:HB3	1:B:369:CYS:HB3	1.94	0.50
1:D:57:TYR:CD1	1:E:387:THR:HG22	2.46	0.50
1:E:94:THR:HA	1:E:474:GLY:O	2.12	0.50
1:J:102:SER:HB3	1:J:105:GLU:HB3	1.93	0.50
1:L:403:GLU:OE2	1:L:461:THR:OG1	2.29	0.50
1:N:211:ASP:HB2	1:N:242:LEU:HD11	1.94	0.50
1:B:135:ASN:HB3	1:B:138:MET:HB2	1.94	0.50
1:B:258:LEU:HD22	1:B:367:VAL:HA	1.93	0.50
1:F:111:ILE:HB	1:F:472:ILE:HB	1.93	0.50
1:F:465:THR:O	1:J:68:ARG:NH2	2.45	0.50
1:G:141:ASN:H	1:G:141:ASN:HD22	1.60	0.50
1:K:482:ASP:CG	1:K:483:ALA:N	2.69	0.50
1:L:57:TYR:CD2	1:M:387:THR:HA	2.47	0.50
1:N:113:LEU:HD22	1:N:119:TRP:CD2	2.47	0.50
1:B:326:ARG:HD3	1:B:439:ASN:HB2	1.94	0.49
1:D:172:GLU:CB	1:E:362:LEU:HD23	2.41	0.49
1:D:343:TRP:HE1	1:D:360:THR:HG21	1.77	0.49
1:E:133:ASN:HD21	1:E:367:VAL:HG22	1.77	0.49
1:L:177:GLU:HG2	1:L:452:THR:H	1.77	0.49
1:L:209:LYS:NZ	1:L:443:ALA:O	2.44	0.49
1:M:382:MET:N	1:M:382:MET:SD	2.85	0.49
1:C:176:SER:O	1:C:180:THR:OG1	2.21	0.49
1:G:492:TYR:CZ	1:H:262:ARG:HG3	2.46	0.49
1:N:133:ASN:HB2	1:N:175:TYR:HB2	1.91	0.49
1:D:154:THR:HG22	1:D:157:LYS:HA	1.93	0.49
1:E:58:SER:OG	1:E:59:GLU:N	2.44	0.49
1:J:133:ASN:CB	1:J:175:TYR:HB3	2.38	0.49
1:B:172:GLU:HB2	1:C:362:LEU:HD23	1.95	0.49
1:E:240:ILE:HD13	1:E:342:SER:HG	1.78	0.49
1:G:57:TYR:CG	1:G:58:SER:N	2.80	0.49
1:G:244:PRO:HA	1:G:275:TYR:CD1	2.47	0.49
1:K:185:ASN:ND2	1:K:210:PHE:O	2.45	0.49
1:O:240:ILE:HD13	1:O:342:SER:OG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:137:PHE:HD1	1:L:138:MET:HE2	1.77	0.49
1:E:114:ASP:N	1:E:119:TRP:HE1	2.10	0.49
1:H:213:ARG:O	1:H:240:ILE:HD11	2.13	0.49
1:I:436:PHE:CD1	1:I:442:LEU:HB3	2.47	0.49
1:J:177:GLU:HG2	1:J:452:THR:H	1.77	0.49
1:K:237:HIS:HD2	1:O:174:ASN:HA	1.78	0.49
1:N:381:MET:HG2	1:N:468:LEU:HD11	1.94	0.49
1:B:102:SER:HB3	1:B:105:GLU:HB3	1.95	0.49
1:G:320:THR:HG23	1:G:321:GLU:HG3	1.94	0.49
1:L:141:ASN:H	1:L:141:ASN:ND2	2.07	0.49
1:B:360:THR:OG1	1:B:361:LEU:N	2.40	0.49
1:D:258:LEU:HD23	1:D:369:CYS:SG	2.52	0.49
1:G:391:THR:HG21	1:G:396:ASN:HB3	1.94	0.49
1:I:57:TYR:CD2	1:J:387:THR:HA	2.47	0.49
1:K:240:ILE:HG22	1:K:241:ILE:N	2.28	0.49
1:A:111:ILE:HB	1:A:472:ILE:HB	1.94	0.49
1:B:154:THR:HG22	1:B:157:LYS:HA	1.95	0.49
1:B:240:ILE:CG2	1:B:344:TYR:H	2.22	0.49
1:M:71:LEU:HA	1:M:93:THR:HG21	1.95	0.49
1:B:242:LEU:HA	1:B:341:ARG:O	2.13	0.49
1:B:465:THR:HG21	1:B:501:ARG:HH11	1.77	0.49
1:E:203:GLU:O	1:E:206:ILE:HG12	2.13	0.49
1:I:197:ARG:HE	1:I:198:GLN:NE2	2.10	0.49
1:L:68:ARG:NH1	1:L:499:SER:OG	2.45	0.49
1:O:154:THR:HG22	1:O:157:LYS:HA	1.95	0.49
1:A:67:THR:HG21	1:B:386:VAL:HG13	1.95	0.48
1:A:419:TYR:HB3	1:A:422:LEU:HB2	1.95	0.48
1:B:58:SER:OG	1:B:59:GLU:N	2.42	0.48
1:F:57:TYR:OH	1:F:109:GLN:OE1	2.29	0.48
1:G:240:ILE:HG22	1:G:241:ILE:N	2.27	0.48
1:B:71:LEU:HA	1:B:93:THR:HG21	1.95	0.48
1:D:188:ILE:HD13	1:D:208:VAL:O	2.12	0.48
1:K:52:ARG:HG3	1:K:116:ARG:CZ	2.43	0.48
1:N:130:ASN:HB3	1:O:363:CYS:HB3	1.95	0.48
1:A:197:ARG:HG3	1:A:198:GLN:HE21	1.78	0.48
1:F:278:LEU:HB3	1:F:341:ARG:HG2	1.93	0.48
1:G:185:ASN:ND2	1:G:210:PHE:O	2.46	0.48
1:G:207:GLY:HA2	1:G:244:PRO:HD2	1.94	0.48
1:N:439:ASN:ND2	1:N:442:LEU:HD23	2.27	0.48
1:F:171:PRO:HA	1:G:348:ASN:CG	2.39	0.48
1:H:145:ALA:HB1	1:H:208:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:LYS:HG2	1:J:167:GLU:HG3	1.95	0.48
1:K:497:ILE:HD11	1:L:402:ALA:HB3	1.94	0.48
1:N:375:TYR:HB3	1:N:399:VAL:HG13	1.93	0.48
1:D:130:ASN:HB3	1:E:363:CYS:HB3	1.94	0.48
1:F:481:THR:HB	1:F:485:ARG:HA	1.94	0.48
1:H:504:SER:HB2	1:H:505:SER:H	1.47	0.48
1:K:113:LEU:HB3	1:K:119:TRP:CD1	2.49	0.48
1:A:387:THR:HG22	1:E:57:TYR:CD1	2.48	0.48
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.68	0.48
1:B:481:THR:HB	1:B:485:ARG:HA	1.95	0.48
1:C:242:LEU:HA	1:C:341:ARG:O	2.14	0.48
1:I:237:HIS:O	1:I:239:ASP:N	2.47	0.48
1:K:427:THR:HG22	1:K:428:SER:HB2	1.95	0.48
1:B:343:TRP:CH2	1:B:362:LEU:HD13	2.49	0.48
1:F:71:LEU:HA	1:F:93:THR:HG21	1.94	0.48
1:F:468:LEU:HD12	1:F:468:LEU:HA	1.61	0.48
1:K:359:TRP:CD1	1:K:360:THR:HG22	2.48	0.48
1:L:137:PHE:CD1	1:L:138:MET:HE2	2.48	0.48
1:G:188:ILE:HG12	1:G:208:VAL:HG23	1.95	0.48
1:K:72:VAL:H	1:K:93:THR:HG21	1.79	0.48
1:L:213:ARG:O	1:L:240:ILE:HD11	2.14	0.48
1:L:391:THR:HG21	1:L:396:ASN:HB3	1.96	0.48
1:O:133:ASN:HB2	1:O:175:TYR:CB	2.26	0.48
1:B:174:ASN:ND2	1:B:183:LEU:HD23	2.29	0.48
1:I:397:PHE:HA	1:I:398:PRO:HD2	1.69	0.48
1:J:206:ILE:HD13	1:J:206:ILE:HA	1.69	0.48
1:K:94:THR:HA	1:K:474:GLY:O	2.13	0.48
1:M:320:THR:HA	1:M:330:LEU:HD11	1.96	0.48
1:D:343:TRP:CH2	1:D:362:LEU:HD13	2.49	0.48
1:D:391:THR:HG21	1:D:396:ASN:HB3	1.96	0.48
1:G:361:LEU:HD23	1:G:363:CYS:SG	2.54	0.48
1:H:239:ASP:HB2	1:H:259:LEU:HD23	1.96	0.48
1:O:242:LEU:HA	1:O:341:ARG:O	2.13	0.48
1:E:138:MET:O	1:E:254:ARG:HD3	2.14	0.47
1:E:240:ILE:HG22	1:E:241:ILE:N	2.29	0.47
1:H:102:SER:HB2	1:H:105:GLU:HG2	1.96	0.47
1:I:102:SER:HB3	1:I:105:GLU:HB3	1.95	0.47
1:K:91:PHE:CE2	1:K:478:VAL:HB	2.49	0.47
1:L:85:GLN:HE21	1:L:85:GLN:HB3	1.51	0.47
1:L:317:LYS:CD	1:L:317:LYS:NZ	2.74	0.47
1:M:342:SER:CB	1:M:345:LEU:HG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:237:HIS:O	1:O:239:ASP:N	2.47	0.47
1:E:388:PHE:CD2	1:E:398:PRO:HA	2.49	0.47
1:F:237:HIS:O	1:F:239:ASP:N	2.48	0.47
1:G:133:ASN:HB3	1:G:134:VAL:H	1.37	0.47
1:H:237:HIS:O	1:H:239:ASP:N	2.47	0.47
1:I:185:ASN:HD21	1:I:210:PHE:N	2.11	0.47
1:K:453:VAL:HG21	1:L:450:ILE:HG21	1.96	0.47
1:N:154:THR:HG22	1:N:157:LYS:HA	1.96	0.47
1:N:241:ILE:HD12	1:N:273:ILE:HD11	1.96	0.47
1:D:111:ILE:HB	1:D:472:ILE:HB	1.95	0.47
1:H:237:HIS:CE1	1:H:448:PRO:HB3	2.48	0.47
1:B:203:GLU:HB2	1:B:326:ARG:HH12	1.79	0.47
1:K:177:GLU:HG2	1:K:452:THR:H	1.78	0.47
1:L:185:ASN:ND2	1:L:210:PHE:O	2.47	0.47
1:L:211:ASP:HB3	1:L:240:ILE:HD12	1.95	0.47
1:G:71:LEU:HA	1:G:93:THR:HG21	1.97	0.47
1:G:93:THR:HG22	1:G:95:VAL:HG22	1.96	0.47
1:J:67:THR:O	1:J:500:PRO:HD2	2.15	0.47
1:J:154:THR:HG22	1:J:157:LYS:HA	1.96	0.47
1:L:453:VAL:HG11	1:M:450:ILE:HD13	1.96	0.47
1:M:237:HIS:O	1:M:239:ASP:N	2.47	0.47
1:N:111:ILE:HB	1:N:472:ILE:HB	1.95	0.47
1:B:136:GLU:OE1	1:C:357:ARG:NH1	2.47	0.47
1:B:400:VAL:HB	1:B:466:LEU:HD13	1.97	0.47
1:C:282:ASN:H	1:C:341:ARG:HG3	1.80	0.47
1:D:242:LEU:HA	1:D:341:ARG:O	2.15	0.47
1:D:383:GLN:HE21	1:D:467:PRO:HB2	1.79	0.47
1:E:69:VAL:HG21	1:E:381:MET:HE1	1.96	0.47
1:E:144:LYS:NZ	1:E:144:LYS:CD	2.72	0.47
1:F:450:ILE:HG21	1:J:453:VAL:HG21	1.97	0.47
1:G:67:THR:HG21	1:H:386:VAL:HG13	1.97	0.47
1:N:492:TYR:CZ	1:O:262:ARG:HG3	2.49	0.47
1:A:237:HIS:O	1:A:239:ASP:N	2.47	0.47
1:A:254:ARG:HB3	1:A:369:CYS:HB3	1.95	0.47
1:B:243:LEU:HD13	1:B:247:GLY:HA2	1.96	0.47
1:B:381:MET:HG3	1:B:472:ILE:HD13	1.97	0.47
1:B:391:THR:HG21	1:B:396:ASN:HB3	1.96	0.47
1:C:57:TYR:CD2	1:D:387:THR:HA	2.49	0.47
1:C:238:PRO:CG	1:C:362:LEU:HD11	2.38	0.47
1:D:241:ILE:HD13	1:D:248:VAL:HG21	1.97	0.47
1:F:133:ASN:HB2	1:F:175:TYR:HB2	1.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:ASP:HB2	1:F:227:MET:HG2	1.97	0.47
1:F:244:PRO:HG3	1:F:340:TYR:CE2	2.50	0.47
1:H:241:ILE:HD12	1:H:273:ILE:HD11	1.95	0.47
1:I:216:ARG:HG3	1:I:345:LEU:HD13	1.96	0.47
1:J:185:ASN:ND2	1:J:210:PHE:O	2.48	0.47
1:K:348:ASN:OD1	1:O:171:PRO:HA	2.14	0.47
1:K:379:PRO:HB3	1:K:398:PRO:HG2	1.97	0.47
1:L:133:ASN:HB2	1:L:175:TYR:HB2	1.93	0.47
1:M:154:THR:HG22	1:M:157:LYS:HA	1.97	0.47
1:M:242:LEU:HA	1:M:341:ARG:O	2.15	0.47
1:N:386:VAL:O	1:N:387:THR:OG1	2.28	0.47
1:C:436:PHE:CD1	1:C:442:LEU:HB3	2.50	0.47
1:D:237:HIS:O	1:D:239:ASP:N	2.48	0.47
1:G:120:GLY:O	1:G:500:PRO:HA	2.15	0.47
1:J:343:TRP:CH2	1:J:362:LEU:HD13	2.50	0.47
1:L:254:ARG:NH2	1:L:368:THR:O	2.48	0.47
1:N:237:HIS:O	1:N:239:ASP:N	2.47	0.47
1:O:424:ARG:HH21	1:O:444:ARG:HB2	1.80	0.47
1:F:242:LEU:HA	1:F:341:ARG:O	2.15	0.47
1:I:251:THR:OG1	1:I:270:GLY:HA2	2.14	0.47
1:J:286:LEU:HA	1:J:286:LEU:HD23	1.67	0.47
1:M:185:ASN:ND2	1:M:210:PHE:O	2.47	0.47
1:B:427:THR:HG22	1:B:428:SER:HB2	1.96	0.47
1:E:237:HIS:O	1:E:239:ASP:N	2.48	0.47
1:H:388:PHE:CD2	1:H:398:PRO:HA	2.50	0.47
1:L:186:ASN:ND2	1:L:190:GLU:HG3	2.30	0.47
1:O:52:ARG:HG3	1:O:116:ARG:HE	1.79	0.47
1:O:439:ASN:O	1:O:443:ALA:HB2	2.15	0.47
1:A:262:ARG:NH1	1:E:489:PRO:O	2.48	0.46
1:J:211:ASP:HB2	1:J:242:LEU:HD11	1.97	0.46
1:K:237:HIS:O	1:K:239:ASP:N	2.49	0.46
1:L:89:SER:HB2	1:L:480:ILE:HB	1.96	0.46
1:M:133:ASN:HB3	1:M:175:TYR:HB3	1.95	0.46
1:C:254:ARG:O	1:C:257:ASN:HB2	2.15	0.46
1:F:391:THR:HG21	1:F:396:ASN:HB3	1.97	0.46
1:H:67:THR:O	1:H:500:PRO:HD2	2.15	0.46
1:J:384:ASP:HA	1:J:385:PRO:HD2	1.79	0.46
1:M:73:ASP:OD1	1:M:73:ASP:N	2.46	0.46
1:N:244:PRO:HA	1:N:275:TYR:CE1	2.50	0.46
1:A:391:THR:HG21	1:A:396:ASN:HB3	1.96	0.46
1:B:120:GLY:O	1:B:500:PRO:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.70	0.46
1:E:57:TYR:OH	1:E:109:GLN:OE1	2.19	0.46
1:F:397:PHE:HA	1:F:398:PRO:HD2	1.55	0.46
1:G:343:TRP:CH2	1:G:362:LEU:HD13	2.50	0.46
1:J:237:HIS:O	1:J:239:ASP:N	2.48	0.46
1:K:242:LEU:HA	1:K:341:ARG:O	2.16	0.46
1:N:343:TRP:CH2	1:N:362:LEU:HD13	2.51	0.46
1:O:176:SER:HB2	1:O:179:MET:HB3	1.96	0.46
1:A:150:SER:HB2	1:A:162:LYS:HB2	1.97	0.46
1:B:397:PHE:HA	1:B:398:PRO:HD2	1.62	0.46
1:C:75:LYS:O	1:C:79:VAL:HG23	2.16	0.46
1:E:242:LEU:HA	1:E:341:ARG:O	2.15	0.46
1:H:188:ILE:HD11	1:H:210:PHE:CE1	2.51	0.46
1:I:282:ASN:H	1:I:341:ARG:HG3	1.80	0.46
1:L:237:HIS:O	1:L:239:ASP:N	2.49	0.46
1:O:94:THR:HA	1:O:474:GLY:O	2.14	0.46
1:O:254:ARG:O	1:O:257:ASN:HB2	2.16	0.46
1:A:394:ILE:HA	1:A:397:PHE:CE2	2.50	0.46
1:B:470:ASN:OD1	1:B:470:ASN:N	2.47	0.46
1:E:206:ILE:HD13	1:E:206:ILE:HA	1.80	0.46
1:E:241:ILE:HD11	1:E:261:ILE:HD12	1.98	0.46
1:E:283:ILE:HD11	1:E:441:ILE:HG12	1.96	0.46
1:F:111:ILE:HD13	1:F:111:ILE:HA	1.82	0.46
1:H:288:ASP:HA	1:H:319:LEU:HD12	1.97	0.46
1:H:393:GLN:C	1:H:395:SER:H	2.24	0.46
1:K:397:PHE:HA	1:K:398:PRO:HD2	1.67	0.46
1:K:492:TYR:CZ	1:L:262:ARG:HG3	2.50	0.46
1:N:242:LEU:HA	1:N:341:ARG:O	2.14	0.46
1:O:393:GLN:C	1:O:395:SER:H	2.24	0.46
1:A:242:LEU:HA	1:A:341:ARG:O	2.15	0.46
1:B:237:HIS:O	1:B:239:ASP:N	2.48	0.46
1:C:237:HIS:O	1:C:239:ASP:N	2.48	0.46
1:E:378:LEU:HD12	1:E:382:MET:HE1	1.97	0.46
1:G:237:HIS:HB2	1:G:238:PRO:HD3	1.96	0.46
1:J:83:ASN:HA	1:J:86:ASN:HD22	1.80	0.46
1:A:88:HIS:HB2	1:A:491:VAL:O	2.16	0.46
1:G:220:ASP:HB2	1:G:227:MET:HG2	1.97	0.46
1:I:67:THR:OG1	1:I:68:ARG:N	2.47	0.46
1:I:215:PHE:HB2	1:I:345:LEU:HD21	1.97	0.46
1:I:242:LEU:HA	1:I:341:ARG:O	2.15	0.46
1:K:120:GLY:O	1:K:500:PRO:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:179:MET:HE2	1:K:179:MET:HB3	1.88	0.46
1:N:251:THR:OG1	1:N:270:GLY:HA2	2.15	0.46
1:A:83:ASN:HA	1:A:86:ASN:HB2	1.98	0.46
1:C:120:GLY:O	1:C:500:PRO:HA	2.16	0.46
1:G:242:LEU:HA	1:G:341:ARG:O	2.14	0.46
1:I:455:GLU:OE1	1:J:411:SER:OG	2.34	0.46
1:J:120:GLY:O	1:J:500:PRO:HA	2.16	0.46
1:J:242:LEU:HA	1:J:341:ARG:O	2.16	0.46
1:N:343:TRP:CD1	1:N:356:ILE:HD13	2.50	0.46
1:O:240:ILE:HG21	1:O:342:SER:OG	2.15	0.46
1:A:120:GLY:O	1:A:500:PRO:HA	2.16	0.46
1:C:492:TYR:OH	1:D:262:ARG:HB2	2.16	0.46
1:C:504:SER:HB2	1:C:505:SER:H	1.47	0.46
1:D:207:GLY:HA2	1:D:244:PRO:HD2	1.97	0.46
1:E:67:THR:HG1	1:E:68:ARG:N	2.13	0.46
1:I:100:ASP:HB2	1:J:389:ARG:HH21	1.81	0.46
1:I:380:ASP:N	1:I:380:ASP:OD1	2.48	0.46
1:L:242:LEU:HA	1:L:341:ARG:O	2.16	0.46
1:A:326:ARG:CD	1:A:439:ASN:HB2	2.45	0.46
1:G:185:ASN:HD21	1:G:210:PHE:H	1.64	0.46
1:A:397:PHE:HA	1:A:398:PRO:HD2	1.59	0.45
1:B:240:ILE:HD13	1:B:342:SER:OG	2.15	0.45
1:D:66:THR:CB	1:D:500:PRO:O	2.57	0.45
1:E:238:PRO:HG2	1:E:362:LEU:HD11	1.97	0.45
1:F:120:GLY:O	1:F:500:PRO:HA	2.16	0.45
1:F:216:ARG:HB2	1:F:345:LEU:HD22	1.98	0.45
1:F:286:LEU:HA	1:F:286:LEU:HD23	1.69	0.45
1:H:215:PHE:HE1	1:H:242:LEU:HD21	1.81	0.45
1:I:96:ILE:HD12	1:I:474:GLY:HA3	1.97	0.45
1:I:174:ASN:HA	1:J:237:HIS:HD2	1.81	0.45
1:K:393:GLN:C	1:K:395:SER:H	2.24	0.45
1:M:497:ILE:HD11	1:N:402:ALA:HB3	1.98	0.45
1:N:120:GLY:O	1:N:500:PRO:HA	2.16	0.45
1:N:343:TRP:HH2	1:N:362:LEU:HD13	1.80	0.45
1:C:382:MET:HE3	1:C:466:LEU:HD13	1.97	0.45
1:F:154:THR:HG22	1:F:157:LYS:HA	1.98	0.45
1:F:192:TYR:CZ	1:F:197:ARG:HB3	2.51	0.45
1:G:135:ASN:HA	1:G:172:GLU:HG2	1.97	0.45
1:O:57:TYR:CG	1:O:58:SER:N	2.81	0.45
1:C:83:ASN:HA	1:C:86:ASN:HD22	1.81	0.45
1:C:288:ASP:HB3	1:C:291:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ILE:HD13	1:D:111:ILE:HA	1.84	0.45
1:G:83:ASN:HA	1:G:86:ASN:HD22	1.81	0.45
1:G:215:PHE:O	1:G:217:LEU:N	2.49	0.45
1:H:67:THR:OG1	1:H:68:ARG:N	2.48	0.45
1:I:240:ILE:HG22	1:I:241:ILE:N	2.31	0.45
1:K:492:TYR:CE2	1:L:262:ARG:HG3	2.51	0.45
1:L:226:VAL:HG12	1:L:228:PRO:HD2	1.98	0.45
1:N:113:LEU:HB3	1:N:119:TRP:CD1	2.51	0.45
1:O:239:ASP:N	1:O:239:ASP:OD1	2.43	0.45
1:A:399:VAL:HG12	1:E:70:TYR:OH	2.17	0.45
1:C:135:ASN:HB3	1:C:138:MET:HB2	1.99	0.45
1:C:176:SER:HB2	1:C:179:MET:HB3	1.97	0.45
1:D:119:TRP:HD1	1:D:470:ASN:HD22	1.64	0.45
1:G:188:ILE:HD11	1:G:210:PHE:HE1	1.80	0.45
1:M:208:VAL:HG12	1:M:243:LEU:HD22	1.98	0.45
1:N:393:GLN:C	1:N:395:SER:H	2.25	0.45
1:B:453:VAL:HG21	1:C:450:ILE:HG21	1.98	0.45
1:C:397:PHE:HA	1:C:398:PRO:HD2	1.61	0.45
1:F:177:GLU:HG2	1:F:452:THR:H	1.81	0.45
1:F:254:ARG:O	1:F:257:ASN:HB2	2.16	0.45
1:H:120:GLY:O	1:H:500:PRO:HA	2.17	0.45
1:H:128:HIS:HE1	1:I:366:ASP:OD2	1.98	0.45
1:K:67:THR:O	1:K:500:PRO:HD2	2.17	0.45
1:M:213:ARG:O	1:M:240:ILE:HD11	2.16	0.45
1:M:238:PRO:HG2	1:M:362:LEU:HD11	1.98	0.45
1:N:504:SER:HB2	1:N:505:SER:H	1.49	0.45
1:A:58:SER:HG	1:A:59:GLU:H	1.60	0.45
1:A:229:GLY:C	1:A:286:LEU:HD22	2.41	0.45
1:A:439:ASN:O	1:A:443:ALA:HB2	2.16	0.45
1:B:331:ILE:HD13	1:B:339:GLN:HG2	1.98	0.45
1:F:52:ARG:HG3	1:F:116:ARG:NH2	2.32	0.45
1:F:420:SER:HA	1:F:423:ILE:HD12	1.98	0.45
1:I:192:TYR:CZ	1:I:197:ARG:HB3	2.52	0.45
1:J:133:ASN:HB3	1:J:134:VAL:H	1.43	0.45
1:J:215:PHE:H	1:J:345:LEU:HD21	1.82	0.45
1:J:220:ASP:HB2	1:J:227:MET:HG2	1.99	0.45
1:N:52:ARG:HG3	1:N:116:ARG:NH1	2.32	0.45
1:N:96:ILE:HA	1:O:387:THR:HG21	1.98	0.45
1:D:133:ASN:HB3	1:D:134:VAL:H	1.40	0.45
1:D:393:GLN:C	1:D:395:SER:H	2.23	0.45
1:G:343:TRP:HH2	1:G:362:LEU:HD13	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220:ASP:HB2	1:H:227:MET:HG2	1.99	0.45
1:J:251:THR:OG1	1:J:270:GLY:HA2	2.17	0.45
1:K:171:PRO:HA	1:L:348:ASN:OD1	2.17	0.45
1:O:323:SER:HB3	1:O:438:GLU:HB2	1.97	0.45
1:O:450:ILE:H	1:O:450:ILE:HG13	1.57	0.45
1:A:215:PHE:O	1:A:217:LEU:N	2.50	0.45
1:B:207:GLY:HA2	1:B:244:PRO:HD2	1.99	0.45
1:C:389:ARG:HD2	1:L:389:ARG:CZ	2.47	0.45
1:D:326:ARG:CD	1:D:439:ASN:HB2	2.47	0.45
1:G:215:PHE:C	1:G:217:LEU:H	2.25	0.45
1:J:391:THR:HG21	1:J:396:ASN:HB3	1.99	0.45
1:K:504:SER:HB2	1:K:505:SER:H	1.47	0.45
1:M:393:GLN:C	1:M:395:SER:H	2.25	0.45
1:A:393:GLN:C	1:A:395:SER:H	2.24	0.45
1:B:331:ILE:H	1:B:331:ILE:HG12	1.66	0.45
1:D:57:TYR:CG	1:D:58:SER:N	2.85	0.45
1:E:152:SER:OG	1:E:159:VAL:HA	2.16	0.45
1:F:504:SER:HB2	1:F:505:SER:H	1.56	0.45
1:G:183:LEU:HD21	1:H:236:PHE:CE2	2.51	0.45
1:H:388:PHE:HD2	1:H:398:PRO:HA	1.82	0.45
1:I:120:GLY:O	1:I:500:PRO:HA	2.17	0.45
1:J:240:ILE:HD13	1:J:342:SER:OG	2.16	0.45
1:N:135:ASN:OD1	1:N:136:GLU:N	2.50	0.45
1:N:288:ASP:HA	1:N:319:LEU:HD12	1.98	0.45
1:N:419:TYR:HB3	1:N:422:LEU:HB2	1.98	0.45
1:C:414:ASN:HD21	1:D:415:ASP:HB2	1.82	0.45
1:E:286:LEU:HD23	1:E:286:LEU:HA	1.77	0.45
1:F:264:ARG:HD2	1:F:360:THR:O	2.16	0.45
1:G:237:HIS:O	1:G:239:ASP:N	2.50	0.45
1:G:450:ILE:H	1:G:450:ILE:HG13	1.64	0.45
1:I:55:ILE:HG12	1:I:113:LEU:HD23	1.99	0.45
1:I:207:GLY:HA2	1:I:244:PRO:HD2	1.97	0.45
1:L:71:LEU:HA	1:L:71:LEU:HD23	1.81	0.45
1:D:120:GLY:O	1:D:500:PRO:HA	2.18	0.44
1:D:150:SER:HB2	1:D:162:LYS:HB2	1.98	0.44
1:E:326:ARG:CD	1:E:439:ASN:HB2	2.42	0.44
1:F:74:ASN:HB2	1:G:373:GLN:HE22	1.83	0.44
1:G:206:ILE:HD13	1:G:206:ILE:HA	1.93	0.44
1:G:213:ARG:O	1:G:240:ILE:HD11	2.16	0.44
1:K:213:ARG:O	1:K:240:ILE:HD11	2.17	0.44
1:N:481:THR:HB	1:N:485:ARG:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:343:TRP:HE1	1:O:360:THR:HG21	1.82	0.44
1:A:72:VAL:H	1:A:93:THR:HG21	1.82	0.44
1:D:342:SER:HB3	1:D:345:LEU:HG	1.99	0.44
1:E:72:VAL:HG12	1:E:495:LEU:HD11	1.99	0.44
1:E:381:MET:HE3	1:E:472:ILE:HG21	1.99	0.44
1:J:192:TYR:CZ	1:J:197:ARG:HB3	2.52	0.44
1:L:215:PHE:O	1:L:217:LEU:N	2.50	0.44
1:L:379:PRO:HD2	1:L:380:ASP:OD2	2.17	0.44
1:M:120:GLY:O	1:M:500:PRO:HA	2.18	0.44
1:O:215:PHE:C	1:O:217:LEU:H	2.26	0.44
1:O:322:ASP:OD2	1:O:328:TYR:OH	2.34	0.44
1:A:177:GLU:HG2	1:A:452:THR:H	1.82	0.44
1:C:237:HIS:HB2	1:C:238:PRO:HD3	1.99	0.44
1:H:57:TYR:CD1	1:I:387:THR:HG22	2.52	0.44
1:I:111:ILE:HD13	1:I:111:ILE:HA	1.89	0.44
1:K:70:TYR:HE1	1:L:399:VAL:HB	1.81	0.44
1:M:400:VAL:HB	1:M:466:LEU:HD13	1.98	0.44
1:A:226:VAL:HG21	1:A:231:TYR:CE2	2.53	0.44
1:C:133:ASN:HD21	1:C:367:VAL:HG22	1.82	0.44
1:H:57:TYR:CD2	1:I:387:THR:HA	2.51	0.44
1:I:69:VAL:HG23	1:I:498:VAL:HB	1.99	0.44
1:L:323:SER:HB3	1:L:438:GLU:HB2	1.99	0.44
1:M:356:ILE:HG12	1:M:359:TRP:HB3	1.98	0.44
1:O:120:GLY:O	1:O:500:PRO:HA	2.17	0.44
1:E:215:PHE:HB2	1:E:345:LEU:HD21	1.99	0.44
1:E:251:THR:OG1	1:E:270:GLY:HA2	2.17	0.44
1:E:393:GLN:C	1:E:395:SER:H	2.25	0.44
1:G:288:ASP:HA	1:G:319:LEU:HD12	1.99	0.44
1:I:154:THR:HG22	1:I:157:LYS:HA	1.99	0.44
1:I:244:PRO:HA	1:I:275:TYR:CE1	2.52	0.44
1:M:113:LEU:HB3	1:M:119:TRP:CD1	2.52	0.44
1:B:135:ASN:HD22	1:B:138:MET:HG2	1.83	0.44
1:B:208:VAL:HG12	1:B:243:LEU:HD22	1.99	0.44
1:E:495:LEU:HD12	1:E:495:LEU:HA	1.77	0.44
1:G:323:SER:HB3	1:G:438:GLU:HB2	1.99	0.44
1:H:100:ASP:HB2	1:I:389:ARG:HH21	1.83	0.44
1:H:215:PHE:O	1:H:217:LEU:N	2.51	0.44
1:J:215:PHE:C	1:J:217:LEU:H	2.25	0.44
1:L:120:GLY:O	1:L:500:PRO:HA	2.16	0.44
1:L:215:PHE:C	1:L:217:LEU:H	2.26	0.44
1:B:380:ASP:OD2	1:B:380:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ILE:H	1:D:331:ILE:HG12	1.64	0.44
1:E:419:TYR:HB3	1:E:422:LEU:HB2	1.98	0.44
1:F:89:SER:HA	1:F:480:ILE:HG12	2.00	0.44
1:G:393:GLN:C	1:G:395:SER:H	2.24	0.44
1:G:441:ILE:HG22	1:G:442:LEU:HD13	2.00	0.44
1:H:206:ILE:HD13	1:H:206:ILE:HA	1.79	0.44
1:I:83:ASN:HA	1:I:86:ASN:HD22	1.82	0.44
1:J:85:GLN:HE21	1:J:85:GLN:HB3	1.69	0.44
1:M:251:THR:OG1	1:M:270:GLY:HA2	2.17	0.44
1:B:174:ASN:HA	1:C:237:HIS:HD2	1.83	0.44
1:C:70:TYR:OH	1:D:399:VAL:HG12	2.18	0.44
1:C:388:PHE:CD2	1:C:398:PRO:HA	2.53	0.44
1:E:120:GLY:O	1:E:500:PRO:HA	2.18	0.44
1:F:262:ARG:HB2	1:J:492:TYR:OH	2.17	0.44
1:H:148:MET:HE2	1:H:163:TYR:HE2	1.83	0.44
1:H:150:SER:HB2	1:H:162:LYS:HB2	1.99	0.44
1:H:397:PHE:HA	1:H:398:PRO:HD2	1.66	0.44
1:I:393:GLN:C	1:I:395:SER:H	2.26	0.44
1:N:174:ASN:HA	1:O:237:HIS:CD2	2.53	0.44
1:O:57:TYR:OH	1:O:109:GLN:OE1	2.27	0.44
1:A:203:GLU:O	1:A:206:ILE:HG12	2.18	0.44
1:B:215:PHE:O	1:B:217:LEU:N	2.51	0.44
1:B:283:ILE:HD13	1:B:441:ILE:HD11	2.00	0.44
1:E:377:SER:O	1:E:378:LEU:HD23	2.17	0.44
1:F:439:ASN:O	1:F:443:ALA:HB2	2.18	0.44
1:J:397:PHE:HA	1:J:398:PRO:HD2	1.70	0.44
1:K:498:VAL:HG12	1:K:500:PRO:HD3	2.00	0.44
1:L:55:ILE:HD13	1:L:67:THR:HG22	1.99	0.44
1:L:240:ILE:CG2	1:L:344:TYR:H	2.27	0.44
1:M:286:LEU:HA	1:M:286:LEU:HD23	1.62	0.44
1:M:439:ASN:O	1:M:443:ALA:HB2	2.18	0.44
1:A:215:PHE:C	1:A:217:LEU:H	2.25	0.43
1:B:215:PHE:C	1:B:217:LEU:H	2.26	0.43
1:C:393:GLN:C	1:C:395:SER:H	2.26	0.43
1:E:177:GLU:HG2	1:E:452:THR:H	1.82	0.43
1:E:207:GLY:HA2	1:E:244:PRO:HD2	1.99	0.43
1:F:179:MET:HE2	1:F:179:MET:HB3	1.85	0.43
1:G:155:LYS:HD3	1:G:155:LYS:HA	1.85	0.43
1:G:470:ASN:N	1:G:470:ASN:OD1	2.50	0.43
1:H:242:LEU:HA	1:H:341:ARG:O	2.18	0.43
1:H:455:GLU:OE1	1:I:411:SER:OG	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:215:PHE:O	1:I:217:LEU:N	2.51	0.43
1:K:215:PHE:O	1:K:217:LEU:N	2.51	0.43
1:K:243:LEU:HD22	1:K:247:GLY:HA2	1.99	0.43
1:M:215:PHE:O	1:M:217:LEU:N	2.51	0.43
1:O:223:THR:HG22	1:O:225:LEU:HD12	1.99	0.43
1:A:96:ILE:HA	1:B:387:THR:HG21	1.98	0.43
1:A:129:THR:OG1	1:A:406:PRO:HG2	2.18	0.43
1:A:206:ILE:HD13	1:A:206:ILE:HA	1.82	0.43
1:B:240:ILE:HG22	1:B:241:ILE:N	2.33	0.43
1:C:379:PRO:HB3	1:C:398:PRO:HG2	1.99	0.43
1:D:215:PHE:C	1:D:217:LEU:H	2.26	0.43
1:E:113:LEU:HB2	1:E:470:ASN:HA	2.00	0.43
1:E:439:ASN:O	1:E:443:ALA:HB2	2.18	0.43
1:F:381:MET:HG2	1:F:468:LEU:HD11	1.98	0.43
1:G:188:ILE:HD11	1:G:210:PHE:CE1	2.53	0.43
1:H:286:LEU:HD23	1:H:286:LEU:HA	1.65	0.43
1:J:393:GLN:C	1:J:395:SER:H	2.25	0.43
1:L:238:PRO:HG2	1:L:362:LEU:CD1	2.48	0.43
1:L:393:GLN:C	1:L:395:SER:H	2.25	0.43
1:B:83:ASN:HA	1:B:86:ASN:HB2	2.00	0.43
1:B:381:MET:HB2	1:B:476:GLN:OE1	2.18	0.43
1:E:146:ARG:HD2	1:E:246:CYS:HA	2.00	0.43
1:E:243:LEU:HD13	1:E:247:GLY:HA2	2.01	0.43
1:H:343:TRP:HH2	1:H:362:LEU:HD13	1.82	0.43
1:I:215:PHE:C	1:I:217:LEU:H	2.25	0.43
1:I:489:PRO:O	1:J:262:ARG:NH1	2.50	0.43
1:K:138:MET:HB3	1:K:254:ARG:HH12	1.83	0.43
1:L:383:GLN:HB2	1:L:467:PRO:HG2	2.00	0.43
1:F:133:ASN:HB3	1:F:134:VAL:H	1.42	0.43
1:F:251:THR:OG1	1:F:270:GLY:HA2	2.18	0.43
1:F:326:ARG:CD	1:F:439:ASN:HB2	2.45	0.43
1:I:68:ARG:NH2	1:J:465:THR:O	2.51	0.43
1:I:113:LEU:HB3	1:I:119:TRP:CD1	2.52	0.43
1:I:367:VAL:HG12	1:I:409:SER:HB2	2.01	0.43
1:L:381:MET:HB3	1:L:382:MET:HE2	2.01	0.43
1:O:215:PHE:O	1:O:217:LEU:N	2.51	0.43
1:D:116:ARG:HE	1:D:116:ARG:HB2	1.65	0.43
1:D:215:PHE:O	1:D:217:LEU:N	2.51	0.43
1:D:244:PRO:HA	1:D:275:TYR:CE1	2.53	0.43
1:F:363:CYS:HB3	1:J:130:ASN:HB3	1.99	0.43
1:G:243:LEU:HD22	1:G:247:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:240:ILE:HG22	1:H:241:ILE:N	2.34	0.43
1:I:52:ARG:HB2	1:I:116:ARG:HD2	2.00	0.43
1:N:229:GLY:C	1:N:286:LEU:HD22	2.44	0.43
1:N:439:ASN:O	1:N:443:ALA:HB2	2.17	0.43
1:B:52:ARG:HB2	1:B:116:ARG:HD2	2.01	0.43
1:C:229:GLY:C	1:C:286:LEU:HD22	2.44	0.43
1:E:83:ASN:HA	1:E:86:ASN:HB2	2.00	0.43
1:F:57:TYR:CG	1:F:58:SER:N	2.86	0.43
1:F:215:PHE:C	1:F:217:LEU:H	2.27	0.43
1:F:241:ILE:HG23	1:F:243:LEU:HD21	2.01	0.43
1:J:241:ILE:HD12	1:J:273:ILE:HD11	2.00	0.43
1:K:211:ASP:HB2	1:K:242:LEU:HD11	2.01	0.43
1:K:322:ASP:OD2	1:K:328:TYR:OH	2.26	0.43
1:N:240:ILE:HG21	1:N:342:SER:OG	2.17	0.43
1:O:130:ASN:HD22	1:O:130:ASN:HA	1.57	0.43
1:B:238:PRO:HG2	1:B:362:LEU:HD12	2.00	0.43
1:C:296:LEU:HD11	1:C:313:LYS:HG2	2.00	0.43
1:E:113:LEU:HA	1:E:113:LEU:HD23	1.74	0.43
1:H:172:GLU:HB3	1:I:362:LEU:HD23	2.01	0.43
1:J:135:ASN:HB3	1:J:138:MET:HB2	2.01	0.43
1:M:453:VAL:HG21	1:N:450:ILE:HG21	1.99	0.43
1:N:282:ASN:N	1:N:341:ARG:HG3	2.28	0.43
1:B:240:ILE:HG12	1:B:344:TYR:HB2	2.00	0.43
1:C:114:ASP:N	1:C:119:TRP:HE1	2.17	0.43
1:C:326:ARG:HB2	1:C:439:ASN:HD22	1.84	0.43
1:E:282:ASN:H	1:E:341:ARG:HG3	1.84	0.43
1:F:215:PHE:O	1:F:217:LEU:N	2.52	0.43
1:K:215:PHE:C	1:K:217:LEU:H	2.27	0.43
1:D:56:ARG:HG2	1:D:62:PRO:HG3	2.00	0.43
1:F:236:PHE:CE2	1:J:183:LEU:HD21	2.53	0.43
1:F:393:GLN:C	1:F:395:SER:H	2.25	0.43
1:G:130:ASN:HB3	1:H:363:CYS:HB3	2.00	0.43
1:H:378:LEU:HD12	1:H:382:MET:HE2	2.01	0.43
1:J:450:ILE:H	1:J:450:ILE:HG13	1.68	0.43
1:K:387:THR:HG22	1:O:57:TYR:CD1	2.54	0.43
1:M:237:HIS:HB3	1:M:238:PRO:CD	2.42	0.43
1:N:217:LEU:HD12	1:N:217:LEU:HA	1.71	0.43
1:N:343:TRP:HD1	1:N:356:ILE:HD13	1.83	0.43
1:B:89:SER:HB2	1:B:480:ILE:HB	2.00	0.43
1:C:106:ALA:HA	1:C:109:GLN:HE21	1.83	0.43
1:D:134:VAL:HG13	1:D:141:ASN:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ALA:HB3	1:D:168:PHE:CE1	2.54	0.43
1:J:238:PRO:CG	1:J:362:LEU:HD11	2.47	0.43
1:J:493:LYS:HD2	1:J:495:LEU:HD13	2.00	0.43
1:K:154:THR:HG22	1:K:157:LYS:HA	2.00	0.43
1:K:331:ILE:H	1:K:331:ILE:HG12	1.63	0.43
1:M:213:ARG:HG3	1:M:215:PHE:CE1	2.54	0.43
1:N:215:PHE:O	1:N:217:LEU:N	2.51	0.43
1:O:436:PHE:CD1	1:O:442:LEU:HB3	2.54	0.43
1:A:413:TYR:HD1	1:A:450:ILE:HG23	1.84	0.42
1:B:393:GLN:C	1:B:395:SER:H	2.25	0.42
1:B:439:ASN:O	1:B:443:ALA:HB2	2.19	0.42
1:D:497:ILE:HD11	1:E:402:ALA:HB3	2.01	0.42
1:E:185:ASN:HD21	1:E:210:PHE:N	2.07	0.42
1:G:292:TYR:HE1	1:G:313:LYS:HE2	1.84	0.42
1:H:343:TRP:CH2	1:H:362:LEU:HD13	2.54	0.42
1:I:217:LEU:HA	1:I:217:LEU:HD12	1.64	0.42
1:I:248:VAL:HG23	1:I:273:ILE:HG13	2.00	0.42
1:K:215:PHE:H	1:K:345:LEU:HD21	1.84	0.42
1:K:402:ALA:HB3	1:O:497:ILE:HD11	2.00	0.42
1:L:75:LYS:HB2	1:L:78:ASP:OD1	2.19	0.42
1:L:206:ILE:HD13	1:L:206:ILE:HA	1.65	0.42
1:M:124:LYS:CG	1:M:124:LYS:HE3	2.49	0.42
1:N:286:LEU:HD23	1:N:286:LEU:HA	1.87	0.42
1:N:368:THR:C	1:N:369:CYS:SG	3.02	0.42
1:E:391:THR:HG21	1:E:396:ASN:HB3	2.01	0.42
1:E:481:THR:HB	1:E:485:ARG:HA	2.00	0.42
1:H:133:ASN:HB3	1:H:134:VAL:H	1.33	0.42
1:H:215:PHE:C	1:H:217:LEU:H	2.27	0.42
1:J:215:PHE:O	1:J:217:LEU:N	2.51	0.42
1:J:258:LEU:HD22	1:J:367:VAL:HA	2.01	0.42
1:K:360:THR:OG1	1:K:361:LEU:N	2.52	0.42
1:K:381:MET:HB2	1:K:476:GLN:OE1	2.19	0.42
1:L:75:LYS:NZ	1:M:485:ARG:HH22	2.18	0.42
1:N:113:LEU:HB2	1:N:470:ASN:HA	2.01	0.42
1:A:113:LEU:HB3	1:A:119:TRP:NE1	2.34	0.42
1:B:113:LEU:HB2	1:B:470:ASN:HA	2.01	0.42
1:B:133:ASN:HB3	1:B:134:VAL:H	1.38	0.42
1:F:198:GLN:HE21	1:F:198:GLN:CA	2.29	0.42
1:G:397:PHE:HA	1:G:398:PRO:HD2	1.56	0.42
1:J:124:LYS:CG	1:J:124:LYS:HE3	2.48	0.42
1:L:504:SER:HB2	1:L:505:SER:H	1.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASP:HB2	1:A:227:MET:HG2	2.02	0.42
1:A:378:LEU:HD12	1:A:400:VAL:HG21	2.01	0.42
1:C:215:PHE:O	1:C:217:LEU:N	2.52	0.42
1:E:52:ARG:HB2	1:E:116:ARG:HD2	2.01	0.42
1:E:244:PRO:HG3	1:E:340:TYR:CE2	2.53	0.42
1:F:317:LYS:HA	1:F:318:PRO:HD3	1.90	0.42
1:L:492:TYR:CE2	1:M:262:ARG:HG3	2.54	0.42
1:M:215:PHE:C	1:M:217:LEU:H	2.27	0.42
1:O:383:GLN:HB2	1:O:467:PRO:HB2	2.02	0.42
1:A:95:VAL:HG23	1:A:474:GLY:HA2	2.01	0.42
1:C:114:ASP:OD1	1:C:116:ARG:HB2	2.19	0.42
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.89	0.42
1:E:215:PHE:C	1:E:217:LEU:H	2.27	0.42
1:G:254:ARG:HB3	1:G:369:CYS:HB3	2.00	0.42
1:K:403:GLU:OE2	1:K:461:THR:OG1	2.37	0.42
1:L:134:VAL:HG13	1:L:141:ASN:HA	2.01	0.42
1:E:96:ILE:HD12	1:E:474:GLY:HA3	2.01	0.42
1:K:118:HIS:HB2	1:K:504:SER:OG	2.20	0.42
1:N:239:ASP:OD2	1:N:239:ASP:N	2.39	0.42
1:A:243:LEU:HD22	1:A:247:GLY:HA2	2.02	0.42
1:B:57:TYR:CG	1:B:58:SER:N	2.87	0.42
1:B:254:ARG:O	1:B:257:ASN:HB2	2.19	0.42
1:E:238:PRO:HG2	1:E:362:LEU:CD1	2.49	0.42
1:E:397:PHE:HA	1:E:398:PRO:HD2	1.63	0.42
1:G:154:THR:HG22	1:G:158:GLN:H	1.84	0.42
1:H:209:LYS:HB3	1:H:242:LEU:HD12	2.01	0.42
1:H:224:GLY:O	1:H:336:THR:HB	2.19	0.42
1:K:96:ILE:HD12	1:K:474:GLY:HA3	2.02	0.42
1:L:145:ALA:HB3	1:L:168:PHE:HE1	1.85	0.42
1:L:243:LEU:HD22	1:L:247:GLY:HA2	2.00	0.42
1:M:288:ASP:HA	1:M:319:LEU:HD12	2.01	0.42
1:M:397:PHE:HA	1:M:398:PRO:HD2	1.56	0.42
1:A:135:ASN:HB3	1:A:138:MET:HB2	2.01	0.42
1:A:384:ASP:OD1	1:A:384:ASP:N	2.39	0.42
1:B:113:LEU:HB3	1:B:119:TRP:CD1	2.55	0.42
1:C:215:PHE:C	1:C:217:LEU:H	2.26	0.42
1:D:315:VAL:HG23	1:D:316:ILE:HG23	2.01	0.42
1:J:96:ILE:HD12	1:J:474:GLY:HA3	2.02	0.42
1:K:439:ASN:O	1:K:443:ALA:HB2	2.20	0.42
1:N:206:ILE:HD13	1:N:206:ILE:HA	1.78	0.42
1:N:273:ILE:HD12	1:N:278:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:TYR:OH	1:A:203:GLU:HG2	2.20	0.42
1:A:381:MET:HB2	1:A:476:GLN:OE1	2.19	0.42
1:D:215:PHE:HB2	1:D:345:LEU:HD21	2.02	0.42
1:E:229:GLY:C	1:E:286:LEU:HD22	2.45	0.42
1:G:504:SER:HB2	1:G:505:SER:H	1.54	0.42
1:I:85:GLN:H	1:I:85:GLN:HG2	1.77	0.42
1:I:213:ARG:HH11	1:I:446:PRO:HD3	1.84	0.42
1:J:136:GLU:HA	1:J:141:ASN:ND2	2.30	0.42
1:K:384:ASP:HA	1:K:385:PRO:HD3	1.85	0.42
1:K:389:ARG:HH21	1:O:100:ASP:HB2	1.84	0.42
1:N:133:ASN:CB	1:N:175:TYR:CB	2.85	0.42
1:O:146:ARG:HD2	1:O:246:CYS:HA	2.01	0.42
1:B:323:SER:HB3	1:B:438:GLU:HB2	2.01	0.42
1:C:179:MET:HG2	1:C:183:LEU:HD22	2.02	0.42
1:C:367:VAL:HG12	1:C:409:SER:HB3	2.01	0.42
1:E:69:VAL:CG2	1:E:498:VAL:HB	2.47	0.42
1:I:411:SER:HB3	1:I:452:THR:HG22	2.01	0.42
1:I:482:ASP:CG	1:I:483:ALA:N	2.76	0.42
1:J:343:TRP:HE1	1:J:360:THR:HG21	1.84	0.42
1:K:96:ILE:HA	1:L:387:THR:HG21	2.02	0.42
1:L:133:ASN:HB3	1:L:134:VAL:H	1.46	0.42
1:M:75:LYS:O	1:M:79:VAL:HG23	2.20	0.42
1:A:114:ASP:OD1	1:A:116:ARG:HB2	2.20	0.41
1:A:236:PHE:HE2	1:E:183:LEU:HD21	1.84	0.41
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.85	0.41
1:A:414:ASN:HD21	1:B:415:ASP:HB2	1.84	0.41
1:C:273:ILE:HG21	1:C:356:ILE:HD11	2.01	0.41
1:F:315:VAL:HG23	1:F:316:ILE:HG23	2.01	0.41
1:H:439:ASN:O	1:H:443:ALA:HB2	2.20	0.41
1:K:113:LEU:HB2	1:K:470:ASN:HA	2.02	0.41
1:K:206:ILE:HD13	1:K:206:ILE:HA	1.82	0.41
1:A:131:MET:HA	1:A:490:TYR:CD2	2.56	0.41
1:C:113:LEU:HB2	1:C:470:ASN:HA	2.01	0.41
1:E:482:ASP:CG	1:E:484:ARG:H	2.28	0.41
1:H:83:ASN:HA	1:H:86:ASN:HB2	2.01	0.41
1:J:241:ILE:HD13	1:J:248:VAL:HG21	2.01	0.41
1:J:273:ILE:HG21	1:J:356:ILE:HD11	2.01	0.41
1:K:130:ASN:HD22	1:K:130:ASN:HA	1.65	0.41
1:K:237:HIS:HB2	1:K:238:PRO:HD3	2.01	0.41
1:L:366:ASP:OD1	1:L:369:CYS:N	2.44	0.41
1:L:401:GLY:HA3	1:L:463:HIS:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:367:VAL:HG12	1:M:409:SER:HB2	2.02	0.41
1:N:282:ASN:CG	1:N:341:ARG:HD2	2.46	0.41
1:O:479:THR:HG22	1:O:481:THR:HG22	2.02	0.41
1:A:275:TYR:HE1	1:A:341:ARG:HB2	1.85	0.41
1:C:146:ARG:HD2	1:C:246:CYS:HA	2.02	0.41
1:C:468:LEU:HA	1:C:468:LEU:HD12	1.40	0.41
1:D:326:ARG:HB2	1:D:439:ASN:HD22	1.83	0.41
1:G:111:ILE:HB	1:G:472:ILE:HB	2.01	0.41
1:I:481:THR:HB	1:I:485:ARG:HA	2.01	0.41
1:J:217:LEU:HA	1:J:217:LEU:HD12	1.79	0.41
1:L:295:SER:OG	1:L:296:LEU:N	2.53	0.41
1:M:126:ILE:HG21	1:N:404:LEU:HD13	2.03	0.41
1:O:68:ARG:HD3	1:O:68:ARG:HA	1.79	0.41
1:O:473:GLY:C	1:O:475:VAL:H	2.28	0.41
1:B:85:GLN:HE21	1:B:85:GLN:HB3	1.60	0.41
1:B:224:GLY:O	1:B:336:THR:HB	2.21	0.41
1:B:381:MET:HG2	1:B:468:LEU:HD11	2.01	0.41
1:C:495:LEU:HA	1:C:495:LEU:HD12	1.78	0.41
1:D:178:THR:O	1:D:181:ILE:HG12	2.18	0.41
1:D:229:GLY:C	1:D:286:LEU:HD22	2.44	0.41
1:D:286:LEU:HD23	1:D:286:LEU:HA	1.83	0.41
1:D:342:SER:CB	1:D:345:LEU:HG	2.51	0.41
1:F:133:ASN:HD22	1:F:175:TYR:HB2	1.84	0.41
1:G:244:PRO:HA	1:G:275:TYR:CE1	2.56	0.41
1:I:96:ILE:CD1	1:I:474:GLY:HA3	2.50	0.41
1:I:381:MET:HE1	1:I:498:VAL:HG11	2.03	0.41
1:I:439:ASN:O	1:I:443:ALA:HB2	2.20	0.41
1:J:72:VAL:HG12	1:J:495:LEU:HD11	2.02	0.41
1:J:343:TRP:CD1	1:J:356:ILE:HD13	2.56	0.41
1:L:217:LEU:HD12	1:L:217:LEU:HA	1.96	0.41
1:L:427:THR:HG22	1:L:428:SER:HB2	2.01	0.41
1:M:263:LYS:NZ	1:M:270:GLY:O	2.49	0.41
1:N:178:THR:OG1	1:N:448:PRO:HD2	2.20	0.41
1:O:367:VAL:HG12	1:O:409:SER:HB2	2.03	0.41
1:O:394:ILE:H	1:O:394:ILE:HG13	1.67	0.41
1:O:397:PHE:HA	1:O:398:PRO:HD2	1.64	0.41
1:O:480:ILE:H	1:O:480:ILE:HG12	1.63	0.41
1:A:113:LEU:HB2	1:A:470:ASN:HA	2.02	0.41
1:A:504:SER:HB2	1:A:505:SER:H	1.57	0.41
1:B:495:LEU:HD12	1:B:495:LEU:HA	1.79	0.41
1:D:426:PHE:HD2	1:D:426:PHE:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:PHE:O	1:E:217:LEU:N	2.53	0.41
1:I:71:LEU:HB2	1:I:496:GLY:HA3	2.02	0.41
1:J:243:LEU:HD22	1:J:247:GLY:HA2	2.02	0.41
1:K:323:SER:HB3	1:K:438:GLU:HB2	2.03	0.41
1:L:197:ARG:HG3	1:L:198:GLN:HE21	1.86	0.41
1:L:203:GLU:HB2	1:L:326:ARG:HH12	1.84	0.41
1:M:129:THR:C	1:M:130:ASN:HD22	2.28	0.41
1:N:439:ASN:HD21	1:N:442:LEU:HD23	1.84	0.41
1:O:286:LEU:HD23	1:O:286:LEU:HA	1.86	0.41
1:D:87:ASP:O	1:E:267:PHE:HE1	2.03	0.41
1:E:135:ASN:OD1	1:E:136:GLU:N	2.54	0.41
1:I:404:LEU:HD12	1:I:404:LEU:HA	1.85	0.41
1:K:262:ARG:HG3	1:O:492:TYR:CZ	2.56	0.41
1:B:176:SER:HB2	1:B:179:MET:HB3	2.02	0.41
1:B:326:ARG:HD2	1:B:438:GLU:HG2	2.02	0.41
1:D:249:ASP:OD2	1:D:272:ARG:HB3	2.20	0.41
1:I:185:ASN:ND2	1:I:210:PHE:O	2.53	0.41
1:K:262:ARG:NH1	1:O:489:PRO:O	2.53	0.41
1:L:473:GLY:C	1:L:475:VAL:H	2.29	0.41
1:O:488:CYS:HA	1:O:489:PRO:HD3	1.90	0.41
1:B:244:PRO:HA	1:B:275:TYR:CE1	2.55	0.41
1:B:282:ASN:H	1:B:341:ARG:HG3	1.85	0.41
1:C:439:ASN:O	1:C:443:ALA:HB2	2.20	0.41
1:F:217:LEU:HD12	1:F:217:LEU:HA	1.80	0.41
1:F:473:GLY:C	1:F:475:VAL:H	2.28	0.41
1:M:138:MET:O	1:M:254:ARG:NH1	2.54	0.41
1:N:215:PHE:H	1:N:345:LEU:HD21	1.85	0.41
1:B:240:ILE:HG23	1:B:344:TYR:N	2.26	0.41
1:B:288:ASP:HB3	1:B:291:ALA:HB3	2.02	0.41
1:B:434:ASN:ND2	1:B:437:PRO:HG3	2.36	0.41
1:C:98:ASN:HD21	1:D:389:ARG:CZ	2.33	0.41
1:C:133:ASN:ND2	1:C:367:VAL:HG22	2.35	0.41
1:C:188:ILE:HD13	1:C:208:VAL:O	2.21	0.41
1:C:220:ASP:HA	1:C:221:PRO:HD2	1.88	0.41
1:C:243:LEU:HD22	1:C:247:GLY:HA2	2.03	0.41
1:C:248:VAL:HG23	1:C:273:ILE:HG13	2.03	0.41
1:D:261:ILE:HG12	1:D:343:TRP:CH2	2.56	0.41
1:E:254:ARG:HB3	1:E:369:CYS:HB3	2.02	0.41
1:G:367:VAL:HB	1:G:452:THR:OG1	2.21	0.41
1:G:468:LEU:HD12	1:G:468:LEU:HA	1.45	0.41
1:I:323:SER:HB3	1:I:438:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:288:ASP:HB3	1:J:291:ALA:HB3	2.03	0.41
1:J:343:TRP:HH2	1:J:362:LEU:HD13	1.86	0.41
1:J:439:ASN:O	1:J:443:ALA:HB2	2.20	0.41
1:K:264:ARG:NH1	1:K:357:ARG:O	2.54	0.41
1:K:351:ASP:HB3	1:K:354:THR:HB	2.02	0.41
1:L:154:THR:HG22	1:L:157:LYS:HA	2.03	0.41
1:M:240:ILE:HG22	1:M:241:ILE:N	2.36	0.41
1:N:215:PHE:C	1:N:217:LEU:H	2.27	0.41
1:N:243:LEU:HD13	1:N:247:GLY:HA2	2.03	0.41
1:N:397:PHE:HA	1:N:398:PRO:HD2	1.53	0.41
1:N:495:LEU:HD12	1:N:495:LEU:HA	1.68	0.41
1:O:89:SER:OG	1:O:480:ILE:O	2.39	0.41
1:A:226:VAL:HG21	1:A:231:TYR:HE2	1.86	0.41
1:C:470:ASN:OD1	1:C:470:ASN:N	2.54	0.41
1:E:504:SER:HB2	1:E:505:SER:H	1.57	0.41
1:F:136:GLU:HA	1:F:141:ASN:HD22	1.86	0.41
1:H:326:ARG:CD	1:H:439:ASN:HB2	2.51	0.41
1:H:379:PRO:HB3	1:H:398:PRO:HG2	2.03	0.41
1:I:243:LEU:HD22	1:I:247:GLY:HA2	2.02	0.41
1:I:381:MET:HE2	1:I:382:MET:SD	2.61	0.41
1:L:185:ASN:HD21	1:L:210:PHE:H	1.69	0.41
1:M:343:TRP:HE1	1:M:360:THR:HG21	1.86	0.41
1:N:71:LEU:HD23	1:N:71:LEU:HA	1.92	0.41
1:B:87:ASP:HB2	1:B:88:HIS:H	1.77	0.40
1:E:114:ASP:OD1	1:E:116:ARG:HB2	2.20	0.40
1:E:244:PRO:HG3	1:E:340:TYR:HE2	1.86	0.40
1:E:340:TYR:CD1	1:E:441:ILE:HG21	2.56	0.40
1:I:113:LEU:HB2	1:I:470:ASN:HA	2.03	0.40
1:L:397:PHE:HA	1:L:398:PRO:HD2	1.62	0.40
1:O:412:PHE:O	1:O:450:ILE:HA	2.21	0.40
1:A:133:ASN:H	1:A:175:TYR:HD2	1.69	0.40
1:B:113:LEU:HA	1:B:113:LEU:HD23	1.80	0.40
1:E:102:SER:HB3	1:E:105:GLU:HB3	2.03	0.40
1:E:178:THR:OG1	1:E:448:PRO:HD2	2.20	0.40
1:E:250:PHE:HB2	1:E:271:PHE:HD2	1.85	0.40
1:F:387:THR:HG21	1:J:96:ILE:HA	2.02	0.40
1:G:473:GLY:C	1:G:475:VAL:H	2.28	0.40
1:H:243:LEU:HD22	1:H:247:GLY:HA2	2.02	0.40
1:H:473:GLY:C	1:H:475:VAL:H	2.29	0.40
1:I:72:VAL:H	1:I:93:THR:HG21	1.85	0.40
1:I:492:TYR:CZ	1:J:262:ARG:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:52:ARG:HB3	1:K:114:ASP:OD2	2.21	0.40
1:K:89:SER:HA	1:K:480:ILE:HG12	2.02	0.40
1:K:387:THR:HG21	1:O:96:ILE:HA	2.04	0.40
1:L:83:ASN:HA	1:L:86:ASN:HB2	2.03	0.40
1:L:326:ARG:HB2	1:L:439:ASN:HD22	1.86	0.40
1:M:113:LEU:HB2	1:M:470:ASN:HA	2.03	0.40
1:N:184:MET:HE3	1:N:255:LEU:HD22	2.03	0.40
1:N:238:PRO:CG	1:N:362:LEU:HD11	2.49	0.40
1:N:412:PHE:O	1:N:450:ILE:HA	2.20	0.40
1:O:177:GLU:HG2	1:O:452:THR:H	1.87	0.40
1:O:391:THR:HG21	1:O:396:ASN:HB3	2.04	0.40
1:B:72:VAL:HG12	1:B:495:LEU:HD11	2.03	0.40
1:B:423:ILE:HD13	1:B:423:ILE:HG21	1.92	0.40
1:C:286:LEU:HA	1:C:286:LEU:HD23	1.78	0.40
1:C:326:ARG:NE	1:C:438:GLU:OE1	2.51	0.40
1:C:450:ILE:H	1:C:450:ILE:HG13	1.74	0.40
1:E:150:SER:HB2	1:E:162:LYS:HB2	2.03	0.40
1:G:254:ARG:O	1:G:257:ASN:HB2	2.21	0.40
1:H:316:ILE:H	1:H:316:ILE:HG13	1.70	0.40
1:H:326:ARG:HD2	1:H:439:ASN:HB2	2.03	0.40
1:H:391:THR:HG21	1:H:396:ASN:HB3	2.03	0.40
1:I:111:ILE:HD12	1:I:111:ILE:HG23	1.76	0.40
1:J:133:ASN:HB2	1:J:175:TYR:HB2	2.00	0.40
1:K:130:ASN:HB3	1:L:363:CYS:HB3	2.03	0.40
1:K:286:LEU:HD23	1:K:286:LEU:HA	1.96	0.40
1:L:278:LEU:HB3	1:L:341:ARG:HG2	2.04	0.40
1:M:220:ASP:HA	1:M:221:PRO:HD2	1.93	0.40
1:N:378:LEU:HD23	1:N:378:LEU:HA	1.83	0.40
1:B:206:ILE:HA	1:B:206:ILE:HD13	1.60	0.40
1:C:113:LEU:HD22	1:C:119:TRP:CD2	2.56	0.40
1:D:504:SER:HB2	1:D:505:SER:H	1.55	0.40
1:F:378:LEU:HA	1:F:378:LEU:HD23	1.73	0.40
1:F:385:PRO:HG2	1:F:388:PHE:CD1	2.57	0.40
1:G:453:VAL:HG11	1:H:450:ILE:HD13	2.03	0.40
1:I:57:TYR:CD1	1:J:387:THR:HG22	2.56	0.40
1:I:473:GLY:C	1:I:475:VAL:H	2.30	0.40
1:J:347:TYR:CE2	1:J:362:LEU:HB2	2.56	0.40
1:K:73:ASP:OD2	1:K:73:ASP:N	2.45	0.40
1:K:411:SER:HB3	1:K:452:THR:HG22	2.04	0.40
1:L:480:ILE:H	1:L:480:ILE:HG12	1.76	0.40
1:M:83:ASN:HA	1:M:86:ASN:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:111:ILE:HD13	1:M:111:ILE:HA	1.99	0.40
1:M:391:THR:OG1	1:M:392:SER:N	2.51	0.40
1:O:342:SER:HG	1:O:345:LEU:HG	1.86	0.40
1:A:111:ILE:HD13	1:A:111:ILE:HA	1.93	0.40
1:A:241:ILE:HD12	1:A:273:ILE:HD11	2.03	0.40
1:B:192:TYR:CZ	1:B:197:ARG:HB3	2.56	0.40
1:B:213:ARG:O	1:B:240:ILE:HD11	2.21	0.40
1:C:473:GLY:C	1:C:475:VAL:H	2.30	0.40
1:E:364:THR:HA	1:E:365:PRO:HD2	1.87	0.40
1:F:113:LEU:HB2	1:F:470:ASN:HA	2.04	0.40
1:G:111:ILE:HD13	1:G:111:ILE:HA	1.91	0.40
1:I:391:THR:HG21	1:I:396:ASN:HB3	2.03	0.40
1:J:256:SER:HB2	1:J:271:PHE:HE2	1.86	0.40
1:J:427:THR:HG22	1:J:428:SER:HB2	2.03	0.40
1:L:378:LEU:HD23	1:L:378:LEU:HA	1.77	0.40
1:N:473:GLY:C	1:N:475:VAL:H	2.30	0.40
1:O:326:ARG:HB2	1:O:439:ASN:HD22	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/523 (84%)	357 (81%)	65 (15%)	18 (4%)	2	19
1	B	440/523 (84%)	360 (82%)	62 (14%)	18 (4%)	2	19
1	C	440/523 (84%)	357 (81%)	65 (15%)	18 (4%)	2	19
1	D	440/523 (84%)	360 (82%)	62 (14%)	18 (4%)	2	19
1	E	440/523 (84%)	358 (81%)	63 (14%)	19 (4%)	2	18
1	F	440/523 (84%)	359 (82%)	62 (14%)	19 (4%)	2	18
1	G	440/523 (84%)	359 (82%)	63 (14%)	18 (4%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	440/523 (84%)	359 (82%)	63 (14%)	18 (4%)	2	19
1	I	440/523 (84%)	360 (82%)	62 (14%)	18 (4%)	2	19
1	J	440/523 (84%)	358 (81%)	64 (14%)	18 (4%)	2	19
1	K	440/523 (84%)	356 (81%)	65 (15%)	19 (4%)	2	18
1	L	440/523 (84%)	359 (82%)	63 (14%)	18 (4%)	2	19
1	M	440/523 (84%)	358 (81%)	64 (14%)	18 (4%)	2	19
1	N	440/523 (84%)	361 (82%)	61 (14%)	18 (4%)	2	19
1	O	440/523 (84%)	361 (82%)	61 (14%)	18 (4%)	2	19
All	All	6600/7845 (84%)	5382 (82%)	945 (14%)	273 (4%)	2	19

All (273) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	172	GLU
1	A	237	HIS
1	A	286	LEU
1	A	323	SER
1	B	66	THR
1	B	172	GLU
1	B	237	HIS
1	B	286	LEU
1	B	323	SER
1	C	66	THR
1	C	172	GLU
1	C	237	HIS
1	C	286	LEU
1	C	323	SER
1	D	66	THR
1	D	172	GLU
1	D	237	HIS
1	D	286	LEU
1	D	323	SER
1	E	66	THR
1	E	172	GLU
1	E	237	HIS
1	E	286	LEU
1	E	323	SER
1	F	66	THR

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Mol	Chain	Res	Type
1	F	172	GLU
1	F	237	HIS
1	F	286	LEU
1	F	323	SER
1	G	66	THR
1	G	172	GLU
1	G	237	HIS
1	G	286	LEU
1	G	323	SER
1	H	66	THR
1	H	172	GLU
1	H	237	HIS
1	H	286	LEU
1	H	323	SER
1	I	66	THR
1	I	172	GLU
1	I	237	HIS
1	I	286	LEU
1	I	323	SER
1	J	66	THR
1	J	172	GLU
1	J	237	HIS
1	J	286	LEU
1	J	323	SER
1	K	66	THR
1	K	172	GLU
1	K	237	HIS
1	K	286	LEU
1	K	323	SER
1	L	66	THR
1	L	172	GLU
1	L	237	HIS
1	L	286	LEU
1	L	323	SER
1	M	66	THR
1	M	172	GLU
1	M	237	HIS
1	M	286	LEU
1	M	323	SER
1	N	66	THR
1	N	172	GLU
1	N	237	HIS

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Mol	Chain	Res	Type
1	N	286	LEU
1	N	323	SER
1	O	66	THR
1	O	172	GLU
1	O	237	HIS
1	O	286	LEU
1	O	323	SER
1	A	152	SER
1	A	232	THR
1	A	244	PRO
1	A	316	ILE
1	A	434	ASN
1	B	232	THR
1	B	244	PRO
1	B	316	ILE
1	B	356	ILE
1	B	434	ASN
1	C	232	THR
1	C	244	PRO
1	C	316	ILE
1	C	434	ASN
1	D	232	THR
1	D	244	PRO
1	D	316	ILE
1	D	434	ASN
1	E	152	SER
1	E	232	THR
1	E	244	PRO
1	E	295	SER
1	E	316	ILE
1	E	434	ASN
1	F	232	THR
1	F	244	PRO
1	F	316	ILE
1	F	434	ASN
1	G	152	SER
1	G	232	THR
1	G	244	PRO
1	G	316	ILE
1	G	434	ASN
1	H	152	SER
1	H	232	THR

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Mol	Chain	Res	Type
1	H	244	PRO
1	H	316	ILE
1	H	434	ASN
1	I	232	THR
1	I	244	PRO
1	I	316	ILE
1	I	434	ASN
1	J	152	SER
1	J	232	THR
1	J	244	PRO
1	J	316	ILE
1	J	434	ASN
1	K	232	THR
1	K	244	PRO
1	K	316	ILE
1	K	434	ASN
1	L	152	SER
1	L	232	THR
1	L	244	PRO
1	L	316	ILE
1	L	434	ASN
1	M	152	SER
1	M	232	THR
1	M	244	PRO
1	M	316	ILE
1	M	434	ASN
1	N	152	SER
1	N	232	THR
1	N	244	PRO
1	N	316	ILE
1	N	434	ASN
1	O	152	SER
1	O	232	THR
1	O	244	PRO
1	O	316	ILE
1	O	356	ILE
1	O	434	ASN
1	A	133	ASN
1	B	133	ASN
1	B	152	SER
1	C	152	SER
1	C	157	LYS

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Mol	Chain	Res	Type
1	D	152	SER
1	E	133	ASN
1	E	356	ILE
1	F	152	SER
1	F	295	SER
1	F	356	ILE
1	G	133	ASN
1	H	133	ASN
1	I	133	ASN
1	I	152	SER
1	J	133	ASN
1	K	133	ASN
1	K	152	SER
1	L	133	ASN
1	M	133	ASN
1	O	133	ASN
1	A	157	LYS
1	A	356	ILE
1	B	157	LYS
1	C	133	ASN
1	D	133	ASN
1	D	157	LYS
1	D	356	ILE
1	E	157	LYS
1	F	133	ASN
1	F	157	LYS
1	G	157	LYS
1	H	157	LYS
1	H	356	ILE
1	I	157	LYS
1	I	356	ILE
1	J	157	LYS
1	K	157	LYS
1	K	295	SER
1	K	356	ILE
1	L	157	LYS
1	L	356	ILE
1	M	157	LYS
1	N	133	ASN
1	N	157	LYS
1	N	356	ILE
1	O	157	LYS

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Mol	Chain	Res	Type
1	A	65	ASP
1	A	370	GLY
1	B	58	SER
1	B	65	ASP
1	B	370	GLY
1	C	58	SER
1	C	65	ASP
1	C	356	ILE
1	C	370	GLY
1	D	58	SER
1	D	65	ASP
1	D	370	GLY
1	E	58	SER
1	E	65	ASP
1	E	370	GLY
1	F	58	SER
1	F	65	ASP
1	F	370	GLY
1	G	58	SER
1	G	65	ASP
1	G	356	ILE
1	G	370	GLY
1	H	65	ASP
1	H	370	GLY
1	I	58	SER
1	I	65	ASP
1	I	370	GLY
1	J	65	ASP
1	J	356	ILE
1	J	370	GLY
1	K	58	SER
1	K	65	ASP
1	K	370	GLY
1	L	65	ASP
1	L	370	GLY
1	M	58	SER
1	M	65	ASP
1	M	356	ILE
1	M	370	GLY
1	N	58	SER
1	N	65	ASP
1	N	370	GLY

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Mol	Chain	Res	Type
1	O	65	ASP
1	O	370	GLY
1	A	58	SER
1	H	58	SER
1	J	58	SER
1	L	58	SER
1	O	58	SER
1	B	51	GLY
1	C	51	GLY
1	D	51	GLY
1	E	51	GLY
1	F	51	GLY
1	G	51	GLY
1	H	51	GLY
1	I	51	GLY
1	J	51	GLY
1	K	51	GLY
1	L	51	GLY
1	M	51	GLY
1	N	51	GLY
1	O	51	GLY
1	A	51	GLY
1	B	475	VAL
1	J	475	VAL
1	K	475	VAL
1	A	475	VAL
1	C	475	VAL
1	D	475	VAL
1	F	475	VAL
1	G	475	VAL
1	H	475	VAL
1	I	475	VAL
1	L	475	VAL
1	M	475	VAL
1	N	475	VAL
1	O	475	VAL
1	E	475	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	400/451 (89%)	304 (76%)	96 (24%)	1	5
1	B	400/451 (89%)	318 (80%)	82 (20%)	1	8
1	C	400/451 (89%)	312 (78%)	88 (22%)	1	6
1	D	400/451 (89%)	307 (77%)	93 (23%)	1	5
1	E	400/451 (89%)	310 (78%)	90 (22%)	1	6
1	F	400/451 (89%)	311 (78%)	89 (22%)	1	6
1	G	400/451 (89%)	307 (77%)	93 (23%)	1	5
1	H	400/451 (89%)	301 (75%)	99 (25%)	1	4
1	I	400/451 (89%)	312 (78%)	88 (22%)	1	6
1	J	400/451 (89%)	307 (77%)	93 (23%)	1	5
1	K	400/451 (89%)	287 (72%)	113 (28%)	0	3
1	L	400/451 (89%)	298 (74%)	102 (26%)	0	4
1	M	400/451 (89%)	303 (76%)	97 (24%)	1	5
1	N	400/451 (89%)	297 (74%)	103 (26%)	0	4
1	O	400/451 (89%)	312 (78%)	88 (22%)	1	6
All	All	6000/6765 (89%)	4586 (76%)	1414 (24%)	1	5

All (1414) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	67	THR
1	A	68	ARG
1	A	69	VAL
1	A	72	VAL
1	A	74	ASN
1	A	77	THR
1	A	82	LEU
1	A	92	LEU
1	A	95	VAL
1	A	97	GLN
1	A	105	GLU
1	A	110	THR
1	A	111	ILE

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Mol	Chain	Res	Type
1	A	115	ASP
1	A	116	ARG
1	A	117	SER
1	A	129	THR
1	A	130	ASN
1	A	136	GLU
1	A	138	MET
1	A	141	ASN
1	A	147	VAL
1	A	150	SER
1	A	152	SER
1	A	154	THR
1	A	156	ASP
1	A	159	VAL
1	A	161	LEU
1	A	166	VAL
1	A	175	TYR
1	A	179	MET
1	A	183	LEU
1	A	188	ILE
1	A	194	LYS
1	A	195	VAL
1	A	203	GLU
1	A	204	SER
1	A	206	ILE
1	A	208	VAL
1	A	212	THR
1	A	232	THR
1	A	239	ASP
1	A	240	ILE
1	A	241	ILE
1	A	243	LEU
1	A	251	THR
1	A	257	ASN
1	A	258	LEU
1	A	283	ILE
1	A	295	SER
1	A	296	LEU
1	A	315	VAL
1	A	319	LEU
1	A	320	THR
1	A	323	SER

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Mol	Chain	Res	Type
1	A	325	LYS
1	A	326	ARG
1	A	329	ASN
1	A	331	ILE
1	A	338	THR
1	A	341	ARG
1	A	356	ILE
1	A	362	LEU
1	A	364	THR
1	A	368	THR
1	A	377	SER
1	A	382	MET
1	A	384	ASP
1	A	386	VAL
1	A	395	SER
1	A	400	VAL
1	A	407	VAL
1	A	410	LYS
1	A	419	TYR
1	A	426	PHE
1	A	441	ILE
1	A	442	LEU
1	A	444	ARG
1	A	450	ILE
1	A	453	VAL
1	A	457	VAL
1	A	460	LEU
1	A	465	THR
1	A	468	LEU
1	A	470	ASN
1	A	475	VAL
1	A	477	ARG
1	A	480	ILE
1	A	492	TYR
1	A	493	LYS
1	A	495	LEU
1	A	498	VAL
1	A	499	SER
1	A	502	VAL
1	A	503	LEU
1	B	54	SER
1	B	60	LEU

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Mol	Chain	Res	Type
1	B	64	PHE
1	B	67	THR
1	B	69	VAL
1	B	72	VAL
1	B	73	ASP
1	B	75	LYS
1	B	77	THR
1	B	82	LEU
1	B	85	GLN
1	B	95	VAL
1	B	99	ASN
1	B	108	THR
1	B	111	ILE
1	B	115	ASP
1	B	117	SER
1	B	124	LYS
1	B	154	THR
1	B	156	ASP
1	B	159	VAL
1	B	161	LEU
1	B	166	VAL
1	B	175	TYR
1	B	183	LEU
1	B	194	LYS
1	B	195	VAL
1	B	203	GLU
1	B	206	ILE
1	B	209	LYS
1	B	212	THR
1	B	222	VAL
1	B	223	THR
1	B	239	ASP
1	B	243	LEU
1	B	256	SER
1	B	258	LEU
1	B	262	ARG
1	B	268	GLN
1	B	312	LEU
1	B	315	VAL
1	B	316	ILE
1	B	319	LEU
1	B	326	ARG

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Mol	Chain	Res	Type
1	B	327	SER
1	B	331	ILE
1	B	332	SER
1	B	334	ASP
1	B	335	SER
1	B	337	PHE
1	B	341	ARG
1	B	356	ILE
1	B	360	THR
1	B	364	THR
1	B	375	TYR
1	B	377	SER
1	B	380	ASP
1	B	384	ASP
1	B	386	VAL
1	B	394	ILE
1	B	405	LEU
1	B	407	VAL
1	B	410	LYS
1	B	411	SER
1	B	419	TYR
1	B	426	PHE
1	B	430	THR
1	B	441	ILE
1	B	442	LEU
1	B	449	THR
1	B	450	ILE
1	B	454	SER
1	B	460	LEU
1	B	461	THR
1	B	470	ASN
1	B	475	VAL
1	B	481	THR
1	B	492	TYR
1	B	493	LYS
1	B	498	VAL
1	B	499	SER
1	B	503	LEU
1	C	60	LEU
1	C	63	LEU
1	C	64	PHE
1	C	67	THR

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Mol	Chain	Res	Type
1	C	69	VAL
1	C	72	VAL
1	C	73	ASP
1	C	74	ASN
1	C	82	LEU
1	C	85	GLN
1	C	97	GLN
1	C	105	GLU
1	C	108	THR
1	C	110	THR
1	C	111	ILE
1	C	115	ASP
1	C	116	ARG
1	C	122	ASP
1	C	124	LYS
1	C	126	ILE
1	C	136	GLU
1	C	140	THR
1	C	141	ASN
1	C	150	SER
1	C	151	ARG
1	C	154	THR
1	C	159	VAL
1	C	161	LEU
1	C	166	VAL
1	C	175	TYR
1	C	177	GLU
1	C	182	ASP
1	C	183	LEU
1	C	186	ASN
1	C	195	VAL
1	C	198	GLN
1	C	206	ILE
1	C	216	ARG
1	C	232	THR
1	C	239	ASP
1	C	240	ILE
1	C	243	LEU
1	C	248	VAL
1	C	251	THR
1	C	272	ARG
1	C	283	ILE

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Mol	Chain	Res	Type
1	C	289	VAL
1	C	296	LEU
1	C	326	ARG
1	C	329	ASN
1	C	335	SER
1	C	341	ARG
1	C	345	LEU
1	C	356	ILE
1	C	362	LEU
1	C	364	THR
1	C	368	THR
1	C	371	SER
1	C	374	VAL
1	C	375	TYR
1	C	377	SER
1	C	384	ASP
1	C	386	VAL
1	C	394	ILE
1	C	407	VAL
1	C	409	SER
1	C	410	LYS
1	C	415	ASP
1	C	419	TYR
1	C	430	THR
1	C	438	GLU
1	C	441	ILE
1	C	442	LEU
1	C	444	ARG
1	C	449	THR
1	C	450	ILE
1	C	457	VAL
1	C	460	LEU
1	C	461	THR
1	C	465	THR
1	C	470	ASN
1	C	475	VAL
1	C	481	THR
1	C	487	THR
1	C	493	LYS
1	C	499	SER
1	C	502	VAL
1	C	503	LEU

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Mol	Chain	Res	Type
1	D	49	THR
1	D	54	SER
1	D	58	SER
1	D	63	LEU
1	D	64	PHE
1	D	66	THR
1	D	69	VAL
1	D	72	VAL
1	D	82	LEU
1	D	85	GLN
1	D	90	ASN
1	D	92	LEU
1	D	110	THR
1	D	111	ILE
1	D	115	ASP
1	D	116	ARG
1	D	117	SER
1	D	136	GLU
1	D	138	MET
1	D	140	THR
1	D	159	VAL
1	D	160	GLU
1	D	175	TYR
1	D	183	LEU
1	D	184	MET
1	D	193	LEU
1	D	195	VAL
1	D	206	ILE
1	D	208	VAL
1	D	209	LYS
1	D	216	ARG
1	D	227	MET
1	D	232	THR
1	D	234	GLU
1	D	239	ASP
1	D	243	LEU
1	D	256	SER
1	D	258	LEU
1	D	259	LEU
1	D	283	ILE
1	D	289	VAL
1	D	312	LEU

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Mol	Chain	Res	Type
1	D	319	LEU
1	D	323	SER
1	D	326	ARG
1	D	329	ASN
1	D	331	ILE
1	D	341	ARG
1	D	353	GLN
1	D	356	ILE
1	D	360	THR
1	D	364	THR
1	D	368	THR
1	D	374	VAL
1	D	377	SER
1	D	380	ASP
1	D	382	MET
1	D	386	VAL
1	D	396	ASN
1	D	403	GLU
1	D	407	VAL
1	D	410	LYS
1	D	411	SER
1	D	415	ASP
1	D	419	TYR
1	D	426	PHE
1	D	430	THR
1	D	438	GLU
1	D	440	GLN
1	D	441	ILE
1	D	442	LEU
1	D	449	THR
1	D	450	ILE
1	D	453	VAL
1	D	455	GLU
1	D	460	LEU
1	D	461	THR
1	D	468	LEU
1	D	470	ASN
1	D	475	VAL
1	D	479	THR
1	D	480	ILE
1	D	481	THR
1	D	484	ARG

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Mol	Chain	Res	Type
1	D	493	LYS
1	D	495	LEU
1	D	498	VAL
1	D	499	SER
1	D	501	ARG
1	D	502	VAL
1	D	503	LEU
1	D	504	SER
1	D	506	ARG
1	E	54	SER
1	E	60	LEU
1	E	63	LEU
1	E	67	THR
1	E	72	VAL
1	E	75	LYS
1	E	76	SER
1	E	77	THR
1	E	81	SER
1	E	82	LEU
1	E	89	SER
1	E	97	GLN
1	E	105	GLU
1	E	107	SER
1	E	108	THR
1	E	111	ILE
1	E	115	ASP
1	E	117	SER
1	E	126	ILE
1	E	136	GLU
1	E	138	MET
1	E	150	SER
1	E	154	THR
1	E	156	ASP
1	E	158	GLN
1	E	159	VAL
1	E	160	GLU
1	E	164	GLU
1	E	166	VAL
1	E	169	THR
1	E	175	TYR
1	E	183	LEU
1	E	186	ASN

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Mol	Chain	Res	Type
1	E	188	ILE
1	E	195	VAL
1	E	206	ILE
1	E	208	VAL
1	E	211	ASP
1	E	216	ARG
1	E	223	THR
1	E	239	ASP
1	E	241	ILE
1	E	243	LEU
1	E	251	THR
1	E	256	SER
1	E	261	ILE
1	E	268	GLN
1	E	283	ILE
1	E	287	LEU
1	E	290	ASP
1	E	293	GLN
1	E	296	LEU
1	E	312	LEU
1	E	315	VAL
1	E	322	ASP
1	E	323	SER
1	E	325	LYS
1	E	326	ARG
1	E	329	ASN
1	E	335	SER
1	E	341	ARG
1	E	353	GLN
1	E	356	ILE
1	E	360	THR
1	E	367	VAL
1	E	368	THR
1	E	374	VAL
1	E	377	SER
1	E	384	ASP
1	E	385	PRO
1	E	386	VAL
1	E	394	ILE
1	E	395	SER
1	E	407	VAL
1	E	428	SER

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Mol	Chain	Res	Type
1	E	430	THR
1	E	442	LEU
1	E	449	THR
1	E	450	ILE
1	E	453	VAL
1	E	460	LEU
1	E	461	THR
1	E	466	LEU
1	E	472	ILE
1	E	475	VAL
1	E	487	THR
1	E	493	LYS
1	E	499	SER
1	E	502	VAL
1	E	503	LEU
1	F	56	ARG
1	F	64	PHE
1	F	69	VAL
1	F	72	VAL
1	F	75	LYS
1	F	82	LEU
1	F	93	THR
1	F	95	VAL
1	F	97	GLN
1	F	105	GLU
1	F	110	THR
1	F	111	ILE
1	F	116	ARG
1	F	138	MET
1	F	141	ASN
1	F	147	VAL
1	F	150	SER
1	F	154	THR
1	F	156	ASP
1	F	157	LYS
1	F	158	GLN
1	F	160	GLU
1	F	164	GLU
1	F	166	VAL
1	F	169	THR
1	F	183	LEU
1	F	186	ASN

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Mol	Chain	Res	Type
1	F	194	LYS
1	F	195	VAL
1	F	198	GLN
1	F	202	LEU
1	F	206	ILE
1	F	216	ARG
1	F	222	VAL
1	F	239	ASP
1	F	241	ILE
1	F	243	LEU
1	F	251	THR
1	F	258	LEU
1	F	262	ARG
1	F	265	GLN
1	F	278	LEU
1	F	293	GLN
1	F	312	LEU
1	F	319	LEU
1	F	320	THR
1	F	321	GLU
1	F	325	LYS
1	F	326	ARG
1	F	330	LEU
1	F	331	ILE
1	F	336	THR
1	F	338	THR
1	F	341	ARG
1	F	356	ILE
1	F	360	THR
1	F	362	LEU
1	F	364	THR
1	F	368	THR
1	F	374	VAL
1	F	377	SER
1	F	386	VAL
1	F	394	ILE
1	F	395	SER
1	F	407	VAL
1	F	410	LYS
1	F	424	ARG
1	F	428	SER
1	F	430	THR

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Mol	Chain	Res	Type
1	F	431	HIS
1	F	438	GLU
1	F	441	ILE
1	F	444	ARG
1	F	449	THR
1	F	450	ILE
1	F	451	THR
1	F	453	VAL
1	F	454	SER
1	F	460	LEU
1	F	465	THR
1	F	466	LEU
1	F	468	LEU
1	F	470	ASN
1	F	475	VAL
1	F	480	ILE
1	F	487	THR
1	F	499	SER
1	F	502	VAL
1	F	503	LEU
1	G	63	LEU
1	G	64	PHE
1	G	69	VAL
1	G	72	VAL
1	G	74	ASN
1	G	75	LYS
1	G	81	SER
1	G	82	LEU
1	G	85	GLN
1	G	92	LEU
1	G	93	THR
1	G	95	VAL
1	G	97	GLN
1	G	105	GLU
1	G	110	THR
1	G	111	ILE
1	G	130	ASN
1	G	135	ASN
1	G	136	GLU
1	G	141	ASN
1	G	150	SER
1	G	154	THR

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Mol	Chain	Res	Type
1	G	159	VAL
1	G	161	LEU
1	G	166	VAL
1	G	169	THR
1	G	175	TYR
1	G	177	GLU
1	G	179	MET
1	G	183	LEU
1	G	188	ILE
1	G	198	GLN
1	G	206	ILE
1	G	208	VAL
1	G	222	VAL
1	G	234	GLU
1	G	239	ASP
1	G	240	ILE
1	G	241	ILE
1	G	243	LEU
1	G	251	THR
1	G	255	LEU
1	G	258	LEU
1	G	262	ARG
1	G	264	ARG
1	G	268	GLN
1	G	275	TYR
1	G	279	GLU
1	G	287	LEU
1	G	293	GLN
1	G	296	LEU
1	G	315	VAL
1	G	319	LEU
1	G	326	ARG
1	G	329	ASN
1	G	330	LEU
1	G	338	THR
1	G	341	ARG
1	G	348	ASN
1	G	356	ILE
1	G	360	THR
1	G	362	LEU
1	G	364	THR
1	G	374	VAL

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Mol	Chain	Res	Type
1	G	377	SER
1	G	378	LEU
1	G	380	ASP
1	G	395	SER
1	G	403	GLU
1	G	405	LEU
1	G	407	VAL
1	G	409	SER
1	G	426	PHE
1	G	430	THR
1	G	431	HIS
1	G	435	ARG
1	G	441	ILE
1	G	442	LEU
1	G	450	ILE
1	G	452	THR
1	G	460	LEU
1	G	461	THR
1	G	470	ASN
1	G	472	ILE
1	G	475	VAL
1	G	480	ILE
1	G	481	THR
1	G	487	THR
1	G	492	TYR
1	G	493	LYS
1	G	498	VAL
1	G	502	VAL
1	G	503	LEU
1	H	63	LEU
1	H	64	PHE
1	H	67	THR
1	H	69	VAL
1	H	72	VAL
1	H	74	ASN
1	H	75	LYS
1	H	77	THR
1	H	82	LEU
1	H	89	SER
1	H	95	VAL
1	H	97	GLN
1	H	105	GLU

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Mol	Chain	Res	Type
1	H	107	SER
1	H	108	THR
1	H	111	ILE
1	H	115	ASP
1	H	117	SER
1	H	126	ILE
1	H	130	ASN
1	H	140	THR
1	H	141	ASN
1	H	154	THR
1	H	155	LYS
1	H	159	VAL
1	H	160	GLU
1	H	164	GLU
1	H	166	VAL
1	H	169	THR
1	H	175	TYR
1	H	179	MET
1	H	183	LEU
1	H	186	ASN
1	H	195	VAL
1	H	198	GLN
1	H	202	LEU
1	H	206	ILE
1	H	208	VAL
1	H	212	THR
1	H	222	VAL
1	H	233	ASN
1	H	239	ASP
1	H	240	ILE
1	H	241	ILE
1	H	243	LEU
1	H	258	LEU
1	H	262	ARG
1	H	268	GLN
1	H	272	ARG
1	H	276	ASP
1	H	279	GLU
1	H	315	VAL
1	H	316	ILE
1	H	319	LEU
1	H	323	SER

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Mol	Chain	Res	Type
1	H	326	ARG
1	H	330	LEU
1	H	331	ILE
1	H	333	ASN
1	H	338	THR
1	H	341	ARG
1	H	351	ASP
1	H	356	ILE
1	H	360	THR
1	H	362	LEU
1	H	364	THR
1	H	368	THR
1	H	374	VAL
1	H	375	TYR
1	H	377	SER
1	H	382	MET
1	H	384	ASP
1	H	394	ILE
1	H	405	LEU
1	H	407	VAL
1	H	409	SER
1	H	410	LYS
1	H	415	ASP
1	H	430	THR
1	H	441	ILE
1	H	442	LEU
1	H	449	THR
1	H	450	ILE
1	H	453	VAL
1	H	460	LEU
1	H	465	THR
1	H	468	LEU
1	H	470	ASN
1	H	475	VAL
1	H	480	ILE
1	H	481	THR
1	H	492	TYR
1	H	497	ILE
1	H	498	VAL
1	H	499	SER
1	H	502	VAL
1	H	504	SER

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Mol	Chain	Res	Type
1	H	505	SER
1	H	506	ARG
1	I	58	SER
1	I	60	LEU
1	I	64	PHE
1	I	68	ARG
1	I	75	LYS
1	I	77	THR
1	I	79	VAL
1	I	82	LEU
1	I	85	GLN
1	I	95	VAL
1	I	97	GLN
1	I	105	GLU
1	I	111	ILE
1	I	115	ASP
1	I	116	ARG
1	I	117	SER
1	I	150	SER
1	I	154	THR
1	I	156	ASP
1	I	158	GLN
1	I	164	GLU
1	I	166	VAL
1	I	175	TYR
1	I	183	LEU
1	I	189	VAL
1	I	195	VAL
1	I	206	ILE
1	I	212	THR
1	I	239	ASP
1	I	241	ILE
1	I	243	LEU
1	I	251	THR
1	I	262	ARG
1	I	265	GLN
1	I	273	ILE
1	I	278	LEU
1	I	279	GLU
1	I	283	ILE
1	I	296	LEU
1	I	315	VAL

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Mol	Chain	Res	Type
1	I	316	ILE
1	I	329	ASN
1	I	330	LEU
1	I	331	ILE
1	I	334	ASP
1	I	336	THR
1	I	338	THR
1	I	339	GLN
1	I	341	ARG
1	I	345	LEU
1	I	356	ILE
1	I	364	THR
1	I	368	THR
1	I	374	VAL
1	I	377	SER
1	I	380	ASP
1	I	382	MET
1	I	384	ASP
1	I	386	VAL
1	I	395	SER
1	I	405	LEU
1	I	407	VAL
1	I	409	SER
1	I	410	LYS
1	I	411	SER
1	I	429	LEU
1	I	430	THR
1	I	438	GLU
1	I	441	ILE
1	I	442	LEU
1	I	444	ARG
1	I	449	THR
1	I	451	THR
1	I	457	VAL
1	I	460	LEU
1	I	461	THR
1	I	470	ASN
1	I	471	SER
1	I	475	VAL
1	I	480	ILE
1	I	482	ASP
1	I	484	ARG

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Mol	Chain	Res	Type
1	I	487	THR
1	I	493	LYS
1	I	498	VAL
1	I	499	SER
1	I	502	VAL
1	I	503	LEU
1	J	54	SER
1	J	62	PRO
1	J	63	LEU
1	J	67	THR
1	J	69	VAL
1	J	72	VAL
1	J	75	LYS
1	J	77	THR
1	J	79	VAL
1	J	82	LEU
1	J	85	GLN
1	J	90	ASN
1	J	92	LEU
1	J	95	VAL
1	J	105	GLU
1	J	111	ILE
1	J	115	ASP
1	J	117	SER
1	J	136	GLU
1	J	138	MET
1	J	150	SER
1	J	152	SER
1	J	153	LEU
1	J	156	ASP
1	J	159	VAL
1	J	160	GLU
1	J	166	VAL
1	J	169	THR
1	J	175	TYR
1	J	177	GLU
1	J	180	THR
1	J	183	LEU
1	J	186	ASN
1	J	188	ILE
1	J	194	LYS
1	J	201	VAL

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Mol	Chain	Res	Type
1	J	204	SER
1	J	206	ILE
1	J	208	VAL
1	J	209	LYS
1	J	239	ASP
1	J	241	ILE
1	J	243	LEU
1	J	251	THR
1	J	258	LEU
1	J	268	GLN
1	J	274	THR
1	J	289	VAL
1	J	315	VAL
1	J	323	SER
1	J	326	ARG
1	J	327	SER
1	J	329	ASN
1	J	330	LEU
1	J	331	ILE
1	J	335	SER
1	J	336	THR
1	J	338	THR
1	J	341	ARG
1	J	345	LEU
1	J	351	ASP
1	J	356	ILE
1	J	368	THR
1	J	374	VAL
1	J	377	SER
1	J	379	PRO
1	J	382	MET
1	J	392	SER
1	J	394	ILE
1	J	395	SER
1	J	407	VAL
1	J	410	LYS
1	J	430	THR
1	J	431	HIS
1	J	441	ILE
1	J	442	LEU
1	J	450	ILE
1	J	457	VAL

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Mol	Chain	Res	Type
1	J	460	LEU
1	J	461	THR
1	J	469	ARG
1	J	470	ASN
1	J	472	ILE
1	J	475	VAL
1	J	480	ILE
1	J	493	LYS
1	J	495	LEU
1	J	498	VAL
1	J	499	SER
1	J	501	ARG
1	J	502	VAL
1	J	503	LEU
1	J	506	ARG
1	K	63	LEU
1	K	64	PHE
1	K	67	THR
1	K	69	VAL
1	K	72	VAL
1	K	74	ASN
1	K	75	LYS
1	K	77	THR
1	K	79	VAL
1	K	82	LEU
1	K	85	GLN
1	K	91	PHE
1	K	92	LEU
1	K	99	ASN
1	K	105	GLU
1	K	108	THR
1	K	110	THR
1	K	111	ILE
1	K	117	SER
1	K	125	THR
1	K	130	ASN
1	K	136	GLU
1	K	140	THR
1	K	141	ASN
1	K	154	THR
1	K	159	VAL
1	K	160	GLU

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Mol	Chain	Res	Type
1	K	161	LEU
1	K	162	LYS
1	K	166	VAL
1	K	169	THR
1	K	175	TYR
1	K	177	GLU
1	K	179	MET
1	K	183	LEU
1	K	188	ILE
1	K	204	SER
1	K	206	ILE
1	K	208	VAL
1	K	212	THR
1	K	222	VAL
1	K	230	VAL
1	K	233	ASN
1	K	239	ASP
1	K	241	ILE
1	K	243	LEU
1	K	248	VAL
1	K	251	THR
1	K	257	ASN
1	K	258	LEU
1	K	262	ARG
1	K	265	GLN
1	K	287	LEU
1	K	289	VAL
1	K	293	GLN
1	K	312	LEU
1	K	321	GLU
1	K	326	ARG
1	K	329	ASN
1	K	331	ILE
1	K	333	ASN
1	K	338	THR
1	K	341	ARG
1	K	345	LEU
1	K	354	THR
1	K	356	ILE
1	K	358	SER
1	K	360	THR
1	K	362	LEU

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Mol	Chain	Res	Type
1	K	364	THR
1	K	368	THR
1	K	374	VAL
1	K	375	TYR
1	K	377	SER
1	K	378	LEU
1	K	380	ASP
1	K	381	MET
1	K	384	ASP
1	K	394	ILE
1	K	395	SER
1	K	400	VAL
1	K	403	GLU
1	K	405	LEU
1	K	407	VAL
1	K	410	LYS
1	K	415	ASP
1	K	425	GLN
1	K	427	THR
1	K	428	SER
1	K	430	THR
1	K	435	ARG
1	K	438	GLU
1	K	449	THR
1	K	450	ILE
1	K	453	VAL
1	K	457	VAL
1	K	460	LEU
1	K	461	THR
1	K	465	THR
1	K	468	LEU
1	K	470	ASN
1	K	471	SER
1	K	472	ILE
1	K	475	VAL
1	K	478	VAL
1	K	480	ILE
1	K	482	ASP
1	K	492	TYR
1	K	499	SER
1	K	502	VAL
1	K	503	LEU

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Mol	Chain	Res	Type
1	K	504	SER
1	K	506	ARG
1	L	58	SER
1	L	60	LEU
1	L	63	LEU
1	L	64	PHE
1	L	66	THR
1	L	67	THR
1	L	68	ARG
1	L	69	VAL
1	L	74	ASN
1	L	82	LEU
1	L	85	GLN
1	L	92	LEU
1	L	95	VAL
1	L	97	GLN
1	L	99	ASN
1	L	105	GLU
1	L	110	THR
1	L	116	ARG
1	L	117	SER
1	L	125	THR
1	L	126	ILE
1	L	141	ASN
1	L	154	THR
1	L	158	GLN
1	L	159	VAL
1	L	166	VAL
1	L	175	TYR
1	L	177	GLU
1	L	179	MET
1	L	183	LEU
1	L	186	ASN
1	L	188	ILE
1	L	194	LYS
1	L	197	ARG
1	L	206	ILE
1	L	208	VAL
1	L	211	ASP
1	L	213	ARG
1	L	222	VAL
1	L	230	VAL

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Mol	Chain	Res	Type
1	L	239	ASP
1	L	240	ILE
1	L	241	ILE
1	L	243	LEU
1	L	251	THR
1	L	256	SER
1	L	257	ASN
1	L	258	LEU
1	L	261	ILE
1	L	265	GLN
1	L	268	GLN
1	L	272	ARG
1	L	289	VAL
1	L	296	LEU
1	L	315	VAL
1	L	319	LEU
1	L	326	ARG
1	L	329	ASN
1	L	331	ILE
1	L	332	SER
1	L	338	THR
1	L	341	ARG
1	L	356	ILE
1	L	358	SER
1	L	360	THR
1	L	364	THR
1	L	373	GLN
1	L	374	VAL
1	L	377	SER
1	L	380	ASP
1	L	384	ASP
1	L	386	VAL
1	L	389	ARG
1	L	390	SER
1	L	394	ILE
1	L	396	ASN
1	L	407	VAL
1	L	410	LYS
1	L	415	ASP
1	L	441	ILE
1	L	449	THR
1	L	450	ILE

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Mol	Chain	Res	Type
1	L	453	VAL
1	L	457	VAL
1	L	458	PRO
1	L	460	LEU
1	L	465	THR
1	L	469	ARG
1	L	470	ASN
1	L	471	SER
1	L	472	ILE
1	L	475	VAL
1	L	480	ILE
1	L	482	ASP
1	L	487	THR
1	L	493	LYS
1	L	495	LEU
1	L	498	VAL
1	L	501	ARG
1	L	502	VAL
1	L	503	LEU
1	L	504	SER
1	M	60	LEU
1	M	67	THR
1	M	69	VAL
1	M	73	ASP
1	M	74	ASN
1	M	75	LYS
1	M	77	THR
1	M	82	LEU
1	M	85	GLN
1	M	93	THR
1	M	95	VAL
1	M	97	GLN
1	M	108	THR
1	M	110	THR
1	M	115	ASP
1	M	116	ARG
1	M	117	SER
1	M	138	MET
1	M	141	ASN
1	M	150	SER
1	M	155	LYS
1	M	156	ASP

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Mol	Chain	Res	Type
1	M	159	VAL
1	M	166	VAL
1	M	175	TYR
1	M	177	GLU
1	M	183	LEU
1	M	186	ASN
1	M	189	VAL
1	M	190	GLU
1	M	194	LYS
1	M	195	VAL
1	M	197	ARG
1	M	206	ILE
1	M	222	VAL
1	M	223	THR
1	M	239	ASP
1	M	240	ILE
1	M	241	ILE
1	M	243	LEU
1	M	251	THR
1	M	258	LEU
1	M	265	GLN
1	M	268	GLN
1	M	276	ASP
1	M	283	ILE
1	M	289	VAL
1	M	295	SER
1	M	315	VAL
1	M	316	ILE
1	M	319	LEU
1	M	327	SER
1	M	331	ILE
1	M	332	SER
1	M	334	ASP
1	M	338	THR
1	M	341	ARG
1	M	356	ILE
1	M	362	LEU
1	M	363	CYS
1	M	368	THR
1	M	375	TYR
1	M	377	SER
1	M	380	ASP

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Mol	Chain	Res	Type
1	M	382	MET
1	M	386	VAL
1	M	393	GLN
1	M	394	ILE
1	M	395	SER
1	M	403	GLU
1	M	407	VAL
1	M	409	SER
1	M	410	LYS
1	M	426	PHE
1	M	428	SER
1	M	431	HIS
1	M	438	GLU
1	M	441	ILE
1	M	442	LEU
1	M	450	ILE
1	M	451	THR
1	M	454	SER
1	M	457	VAL
1	M	458	PRO
1	M	460	LEU
1	M	461	THR
1	M	466	LEU
1	M	470	ASN
1	M	472	ILE
1	M	475	VAL
1	M	480	ILE
1	M	481	THR
1	M	493	LYS
1	M	495	LEU
1	M	498	VAL
1	M	499	SER
1	M	503	LEU
1	N	49	THR
1	N	53	ASN
1	N	60	LEU
1	N	62	PRO
1	N	64	PHE
1	N	69	VAL
1	N	74	ASN
1	N	81	SER
1	N	82	LEU

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Mol	Chain	Res	Type
1	N	93	THR
1	N	95	VAL
1	N	97	GLN
1	N	105	GLU
1	N	108	THR
1	N	110	THR
1	N	111	ILE
1	N	115	ASP
1	N	116	ARG
1	N	124	LYS
1	N	126	ILE
1	N	136	GLU
1	N	138	MET
1	N	147	VAL
1	N	156	ASP
1	N	158	GLN
1	N	160	GLU
1	N	161	LEU
1	N	166	VAL
1	N	169	THR
1	N	174	ASN
1	N	175	TYR
1	N	177	GLU
1	N	179	MET
1	N	180	THR
1	N	183	LEU
1	N	194	LYS
1	N	203	GLU
1	N	206	ILE
1	N	208	VAL
1	N	216	ARG
1	N	222	VAL
1	N	230	VAL
1	N	239	ASP
1	N	241	ILE
1	N	243	LEU
1	N	251	THR
1	N	255	LEU
1	N	256	SER
1	N	258	LEU
1	N	265	GLN
1	N	283	ILE

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Mol	Chain	Res	Type
1	N	289	VAL
1	N	293	GLN
1	N	313	LYS
1	N	316	ILE
1	N	319	LEU
1	N	323	SER
1	N	325	LYS
1	N	326	ARG
1	N	329	ASN
1	N	331	ILE
1	N	338	THR
1	N	341	ARG
1	N	351	ASP
1	N	354	THR
1	N	356	ILE
1	N	362	LEU
1	N	363	CYS
1	N	367	VAL
1	N	368	THR
1	N	374	VAL
1	N	377	SER
1	N	385	PRO
1	N	386	VAL
1	N	392	SER
1	N	393	GLN
1	N	394	ILE
1	N	405	LEU
1	N	407	VAL
1	N	409	SER
1	N	410	LYS
1	N	424	ARG
1	N	429	LEU
1	N	430	THR
1	N	431	HIS
1	N	441	ILE
1	N	444	ARG
1	N	449	THR
1	N	450	ILE
1	N	460	LEU
1	N	466	LEU
1	N	468	LEU
1	N	469	ARG

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Mol	Chain	Res	Type
1	N	470	ASN
1	N	471	SER
1	N	475	VAL
1	N	480	ILE
1	N	493	LYS
1	N	498	VAL
1	N	499	SER
1	N	502	VAL
1	N	503	LEU
1	N	504	SER
1	O	54	SER
1	O	64	PHE
1	O	69	VAL
1	O	72	VAL
1	O	73	ASP
1	O	74	ASN
1	O	75	LYS
1	O	82	LEU
1	O	93	THR
1	O	94	THR
1	O	95	VAL
1	O	97	GLN
1	O	105	GLU
1	O	108	THR
1	O	110	THR
1	O	111	ILE
1	O	117	SER
1	O	125	THR
1	O	130	ASN
1	O	140	THR
1	O	154	THR
1	O	160	GLU
1	O	161	LEU
1	O	166	VAL
1	O	175	TYR
1	O	177	GLU
1	O	180	THR
1	O	183	LEU
1	O	195	VAL
1	O	206	ILE
1	O	208	VAL
1	O	212	THR

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Mol	Chain	Res	Type
1	O	216	ARG
1	O	222	VAL
1	O	234	GLU
1	O	239	ASP
1	O	240	ILE
1	O	243	LEU
1	O	248	VAL
1	O	251	THR
1	O	258	LEU
1	O	262	ARG
1	O	265	GLN
1	O	268	GLN
1	O	293	GLN
1	O	296	LEU
1	O	319	LEU
1	O	326	ARG
1	O	327	SER
1	O	329	ASN
1	O	331	ILE
1	O	332	SER
1	O	334	ASP
1	O	338	THR
1	O	341	ARG
1	O	356	ILE
1	O	367	VAL
1	O	368	THR
1	O	377	SER
1	O	380	ASP
1	O	386	VAL
1	O	394	ILE
1	O	395	SER
1	O	400	VAL
1	O	407	VAL
1	O	409	SER
1	O	419	TYR
1	O	430	THR
1	O	435	ARG
1	O	444	ARG
1	O	449	THR
1	O	450	ILE
1	O	460	LEU
1	O	465	THR

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Mol	Chain	Res	Type
1	O	468	LEU
1	O	470	ASN
1	O	471	SER
1	O	475	VAL
1	O	478	VAL
1	O	480	ILE
1	O	481	THR
1	O	482	ASP
1	O	484	ARG
1	O	487	THR
1	O	493	LYS
1	O	499	SER
1	O	502	VAL
1	O	503	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (174) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	130	ASN
1	A	133	ASN
1	A	198	GLN
1	A	233	ASN
1	A	268	GLN
1	A	396	ASN
1	A	414	ASN
1	A	425	GLN
1	A	434	ASN
1	B	74	ASN
1	B	85	GLN
1	B	90	ASN
1	B	99	ASN
1	B	130	ASN
1	B	141	ASN
1	B	198	GLN
1	B	252	HIS
1	B	348	ASN
1	B	396	ASN
1	B	431	HIS
1	C	74	ASN
1	C	85	GLN
1	C	86	ASN

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Mol	Chain	Res	Type
1	C	90	ASN
1	C	112	ASN
1	C	130	ASN
1	C	133	ASN
1	C	237	HIS
1	C	265	GLN
1	C	373	GLN
1	C	396	ASN
1	C	414	ASN
1	D	85	GLN
1	D	86	ASN
1	D	133	ASN
1	D	252	HIS
1	D	265	GLN
1	D	268	GLN
1	D	353	GLN
1	D	383	GLN
1	D	414	ASN
1	D	470	ASN
1	E	86	ASN
1	E	130	ASN
1	E	133	ASN
1	E	185	ASN
1	E	237	HIS
1	E	268	GLN
1	E	339	GLN
1	E	393	GLN
1	E	396	ASN
1	E	408	HIS
1	E	414	ASN
1	F	130	ASN
1	F	133	ASN
1	F	141	ASN
1	F	198	GLN
1	F	237	HIS
1	F	268	GLN
1	F	434	ASN
1	F	463	HIS
1	G	74	ASN
1	G	85	GLN
1	G	86	ASN
1	G	97	GLN

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Mol	Chain	Res	Type
1	G	130	ASN
1	G	133	ASN
1	G	135	ASN
1	G	141	ASN
1	G	198	GLN
1	G	237	HIS
1	G	373	GLN
1	G	393	GLN
1	G	440	GLN
1	G	463	HIS
1	H	86	ASN
1	H	90	ASN
1	H	97	GLN
1	H	128	HIS
1	H	133	ASN
1	H	141	ASN
1	H	185	ASN
1	H	191	HIS
1	H	198	GLN
1	H	214	ASN
1	H	237	HIS
1	H	257	ASN
1	H	265	GLN
1	H	431	HIS
1	H	463	HIS
1	I	85	GLN
1	I	86	ASN
1	I	141	ASN
1	I	198	GLN
1	I	237	HIS
1	I	257	ASN
1	I	268	GLN
1	I	339	GLN
1	I	396	ASN
1	I	425	GLN
1	J	85	GLN
1	J	86	ASN
1	J	130	ASN
1	J	133	ASN
1	J	141	ASN
1	J	198	GLN
1	J	233	ASN

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Mol	Chain	Res	Type
1	J	237	HIS
1	J	257	ASN
1	J	268	GLN
1	J	396	ASN
1	J	421	GLN
1	J	440	GLN
1	K	85	GLN
1	K	97	GLN
1	K	99	ASN
1	K	130	ASN
1	K	141	ASN
1	K	191	HIS
1	K	198	GLN
1	K	237	HIS
1	K	265	GLN
1	K	329	ASN
1	K	383	GLN
1	K	396	ASN
1	L	85	GLN
1	L	86	ASN
1	L	99	ASN
1	L	112	ASN
1	L	133	ASN
1	L	141	ASN
1	L	186	ASN
1	L	198	GLN
1	L	268	GLN
1	L	393	GLN
1	L	396	ASN
1	L	416	GLN
1	L	463	HIS
1	M	74	ASN
1	M	85	GLN
1	M	90	ASN
1	M	97	GLN
1	M	112	ASN
1	M	118	HIS
1	M	268	GLN
1	M	396	ASN
1	M	414	ASN
1	M	439	ASN
1	M	456	ASN

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Mol	Chain	Res	Type
1	N	74	ASN
1	N	86	ASN
1	N	97	GLN
1	N	128	HIS
1	N	133	ASN
1	N	198	GLN
1	N	233	ASN
1	N	396	ASN
1	N	425	GLN
1	N	434	ASN
1	N	439	ASN
1	O	74	ASN
1	O	86	ASN
1	O	97	GLN
1	O	130	ASN
1	O	141	ASN
1	O	198	GLN
1	O	237	HIS
1	O	268	GLN
1	O	282	ASN
1	O	329	ASN
1	O	396	ASN
1	O	408	HIS
1	O	416	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/523 (84%)	-0.26	2 (0%) 87 66	96, 131, 195, 200	0
1	B	444/523 (84%)	-0.25	2 (0%) 87 66	96, 131, 195, 200	0
1	C	444/523 (84%)	-0.25	0 100 100	95, 131, 196, 200	0
1	D	444/523 (84%)	-0.24	0 100 100	96, 131, 195, 200	0
1	E	444/523 (84%)	-0.23	0 100 100	96, 131, 195, 200	0
1	F	444/523 (84%)	-0.21	3 (0%) 84 61	94, 131, 196, 200	0
1	G	444/523 (84%)	-0.22	0 100 100	94, 132, 195, 200	0
1	H	444/523 (84%)	-0.18	0 100 100	95, 131, 195, 200	0
1	I	444/523 (84%)	-0.24	1 (0%) 91 80	96, 131, 195, 200	0
1	J	444/523 (84%)	-0.17	0 100 100	95, 131, 196, 200	0
1	K	444/523 (84%)	-0.16	2 (0%) 87 66	96, 131, 196, 200	0
1	L	444/523 (84%)	-0.22	0 100 100	95, 131, 196, 200	0
1	M	444/523 (84%)	-0.23	0 100 100	95, 132, 196, 200	0
1	N	444/523 (84%)	-0.17	4 (0%) 81 56	95, 131, 196, 200	0
1	O	444/523 (84%)	-0.12	2 (0%) 87 66	94, 131, 195, 200	0
All	All	6660/7845 (84%)	-0.21	16 (0%) 91 80	94, 131, 196, 200	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	239	ASP	4.1
1	N	444	ARG	3.1
1	F	239	ASP	2.9
1	O	239	ASP	2.8
1	K	237	HIS	2.6
1	A	485	ARG	2.6
1	O	366	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	454	SER	2.3
1	A	444	ARG	2.2
1	B	278	LEU	2.2
1	F	429	LEU	2.2
1	F	485	ARG	2.1
1	N	417	ALA	2.1
1	B	422	LEU	2.1
1	N	238	PRO	2.0
1	N	445	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.