



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:08 PM UTC

PDB ID : 1KMH / pdb_00001kmh
Title : Crystal Structure of spinach chloroplast F1-ATPase complexed with tentoxin
Authors : Groth, G.
Deposited on : 2001-12-16
Resolution : 3.40 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

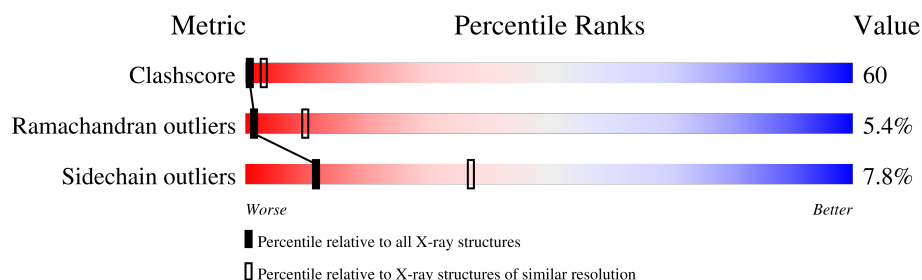
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	507	
2	B	498	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7217 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.

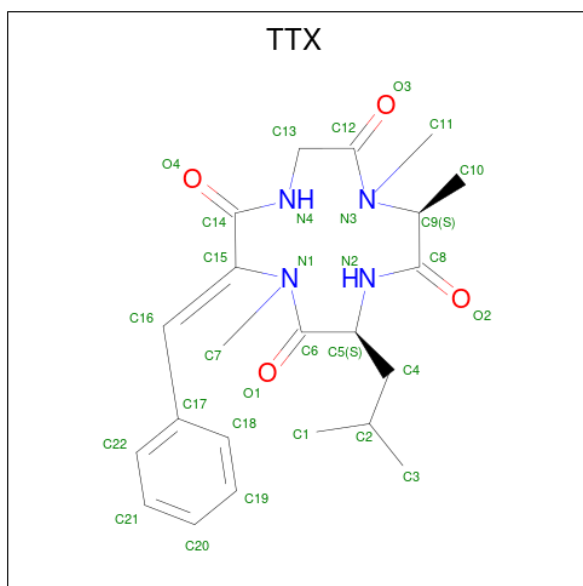
- Molecule 1 is a protein called ATPase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3647	2296	628	710	13			

- Molecule 2 is a protein called ATPase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	467	Total	C	N	O	S	0	0	0
			3540	2234	612	680	14			

- Molecule 3 is TENTOXIN (CCD ID: TTX) (formula: $C_{22}H_{30}N_4O_4$).



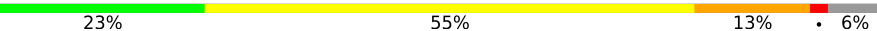
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			30	22	4	4		

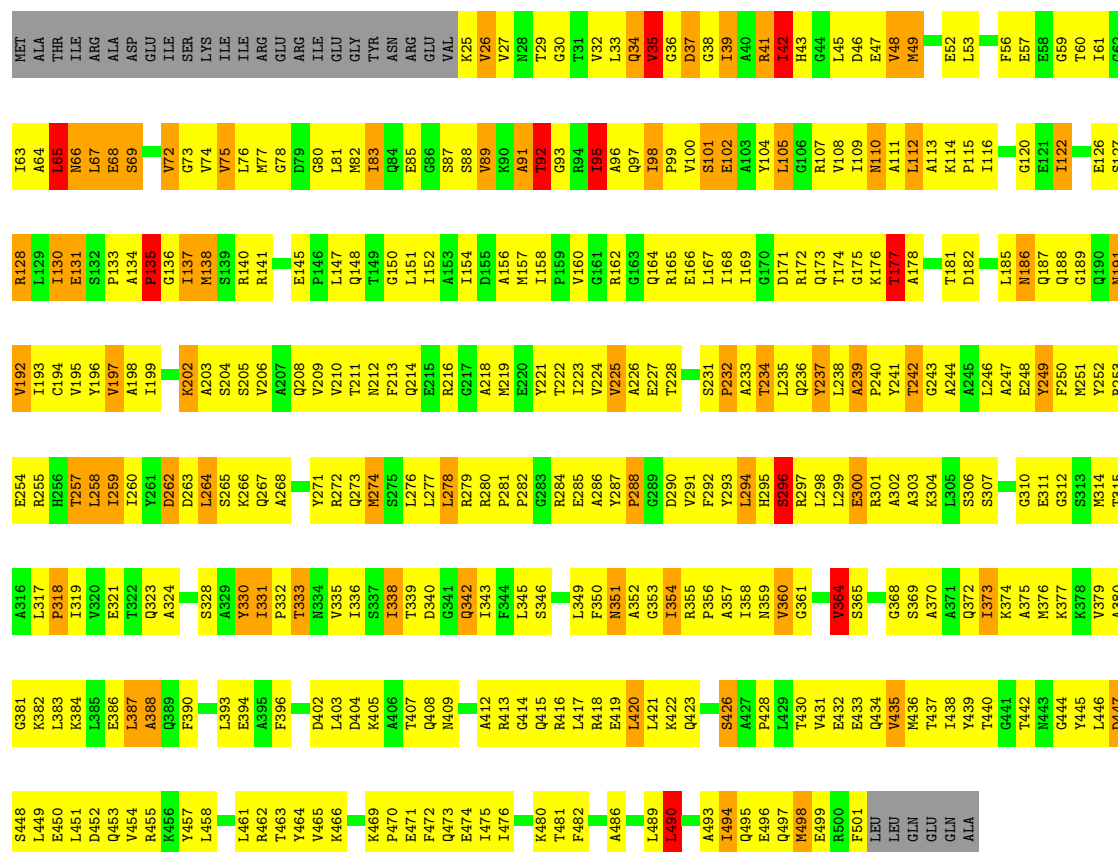
3 Residue-property plots

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

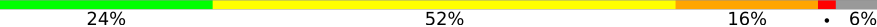
Note EDS was not executed.

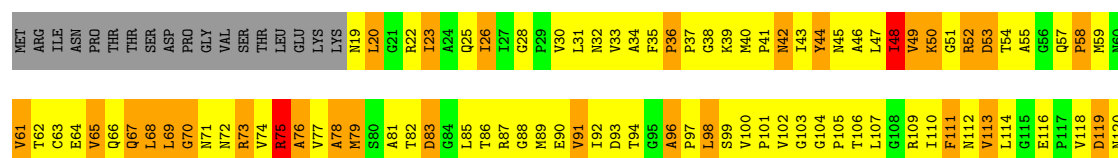
• Molecule 1: ATPase alpha subunit

Chain A: 



• Molecule 2: ATPase beta subunit

Chain B: 



L462	L463	G464	E465	L466	L469	P470	E471	Q472	A473	F474	Y475	L476	V477	I480	A483	T484	A485	LYS	MET	ALA	ASN	LEU	GLU	MET	GLU	SER	LYS	LEU	LYS	LYS	L482	L483	L484	L485	R122	P123	I126	R127	T128	T129	S130	P131	I132	H133	R134	S135	A136	P137	A138	F139	T140	Q141	L142	D143	T144	K145	L146	S147	I148	F149	G152	I153	K154	V155	V156	N157	L158	L159	A160	P161	Y162	R163	R164	G165	G166	K167	I168	G169	L170	F171	G175	V176	G177	K178	T179	V180	L181	I182	M183	E184
I387	A388	Q389	R390	V391	K392	E393	T394	L395	Q396	R397	Y398	K399	E400	Q401	Q402	D403	I404	A405	A406	T407	L408	G409	L410	D411	E412	L413	S414	D417	R418	L419	T420	V421	A422	R423	A424	R425	K426	I427	E428	R429	F430	L431	S432	Q433	P434	F435	A438	L451	T454	I455	F458	Q459	L460	I461																																				
S314	T315	G319	S320	I321	T322	S323	I324	Q325	A326	V327	Y328	V329	D333	L334	T335	A338	T341	T342	F343	A344	H345	L346	T350	V351	L352	S353	L356	A357	I361	Y362	P363	A364	P367	L368	D369	S370	T371	S372	T373	M374	L375	Q376	P377	R378	I379	V380	G381	Y385	E386																																									
G250	L251	T252	A253	L254	T255	M256	A257	E258	Y259	F260	R261	D262	V263	N264	E265	Q266	D267	V268	L269	F270	F271	I272	D273	N274	I275	F276	R277	F278	V279	Q280	A281	G282	S283	E284	V285	S286	A287	L288	L289	G290	R291	V296	G297	Y298	Q299	P300	T301	L302	M306	G307	S308	L309	G310	E311	R246	M247	R248																																	

4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	146.89Å 146.89Å 381.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.40	Depositor
% Data completeness (in resolution range)	92.5 (6.00-3.40)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0, CNS	Depositor
R, R_{free}	0.297 , 0.319	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7217	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.53	46/3695 (1.2%)	1.35	29/5002 (0.6%)
2	B	1.53	40/3598 (1.1%)	1.41	41/4883 (0.8%)
All	All	1.53	86/7293 (1.2%)	1.38	70/9885 (0.7%)

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	77	VAL	CA-CB	-10.31	1.41	1.54
1	A	75	VAL	C-O	-9.97	1.12	1.23
1	A	72	VAL	CA-CB	-9.09	1.43	1.54
2	B	96	ALA	CA-C	-8.95	1.41	1.52
1	A	274	MET	SD-CE	8.78	2.01	1.79
2	B	73	ARG	CZ-NH1	8.76	1.45	1.32
1	A	91	ALA	CA-C	8.75	1.64	1.52
2	B	96	ALA	C-O	-8.37	1.13	1.24
1	A	35	VAL	CA-CB	8.17	1.62	1.53
1	A	209	VAL	C-O	-8.16	1.15	1.23
1	A	331	ILE	CA-CB	-8.11	1.43	1.54
2	B	34	ALA	CA-C	-8.07	1.43	1.52
2	B	237	GLY	C-O	-8.03	1.13	1.23
2	B	90	GLU	C-O	-8.00	1.14	1.23
1	A	137	ILE	CA-CB	-7.99	1.44	1.54
2	B	75	ARG	CA-C	-7.78	1.43	1.52
1	A	87	SER	CA-C	-7.56	1.43	1.52
1	A	65	LEU	CA-C	-7.55	1.43	1.52
1	A	192	VAL	C-O	-7.48	1.16	1.23
1	A	63	ILE	CA-CB	-7.36	1.42	1.55
2	B	91	VAL	CA-C	-7.34	1.43	1.53
2	B	34	ALA	CA-CB	-7.33	1.41	1.53
1	A	300	GLU	C-O	-7.31	1.15	1.24
2	B	28	GLY	C-O	-7.30	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	83	ASP	C-O	-7.30	1.15	1.24
1	A	206	VAL	CA-CB	7.13	1.63	1.54
1	A	138	MET	SD-CE	6.97	1.97	1.79
2	B	133	HIS	CA-C	6.91	1.60	1.53
1	A	92	THR	N-CA	-6.89	1.37	1.46
1	A	95	ILE	C-O	-6.89	1.15	1.24
2	B	244	GLY	C-O	6.85	1.33	1.23
2	B	240	ASN	CA-C	6.76	1.61	1.52
2	B	48	ILE	C-O	6.66	1.30	1.24
2	B	83	ASP	CA-C	-6.58	1.43	1.52
1	A	75	VAL	CA-CB	-6.57	1.46	1.53
1	A	135	PRO	CA-C	-6.50	1.44	1.52
1	A	69	SER	C-O	-6.46	1.16	1.24
1	A	177	THR	C-O	-6.41	1.16	1.24
2	B	113	VAL	CA-CB	-6.37	1.46	1.54
2	B	78	ALA	CA-CB	-6.35	1.42	1.53
1	A	95	ILE	CA-C	-6.30	1.44	1.52
1	A	197	VAL	CA-CB	-6.28	1.46	1.54
1	A	68	GLU	CA-C	-6.26	1.44	1.52
1	A	258	LEU	CA-C	-6.23	1.45	1.52
2	B	34	ALA	C-O	-6.21	1.17	1.24
2	B	65	VAL	C-O	-6.12	1.16	1.24
2	B	256	MET	SD-CE	-6.10	1.64	1.79
2	B	246	ARG	CA-C	6.01	1.60	1.52
1	A	242	THR	CA-C	-5.94	1.45	1.52
2	B	23	ILE	CA-C	-5.94	1.44	1.52
1	A	74	VAL	C-O	5.92	1.30	1.24
2	B	326	ALA	C-O	5.91	1.30	1.23
1	A	284	ARG	C-O	5.89	1.31	1.23
1	A	64	ALA	CA-CB	-5.86	1.44	1.53
2	B	119	ASP	C-O	-5.85	1.16	1.24
2	B	263	VAL	CA-CB	-5.82	1.46	1.54
2	B	44	TYR	C-O	-5.79	1.16	1.24
1	A	202	LYS	C-O	-5.76	1.16	1.23
1	A	259	ILE	CA-CB	5.70	1.61	1.54
2	B	333	ASP	CA-C	5.63	1.59	1.52
2	B	326	ALA	CA-C	5.60	1.59	1.52
1	A	296	SER	C-O	-5.59	1.17	1.24
2	B	100	VAL	N-CA	-5.55	1.39	1.46
1	A	130	ILE	CA-C	-5.53	1.46	1.52
1	A	42	ILE	C-O	-5.48	1.16	1.24
1	A	239	ALA	CA-CB	-5.46	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	ILE	C-O	5.42	1.30	1.23
1	A	130	ILE	C-O	-5.39	1.18	1.24
2	B	50	LYS	C-O	5.39	1.30	1.24
2	B	76	ALA	N-CA	5.38	1.52	1.46
2	B	96	ALA	CA-CB	-5.36	1.45	1.53
2	B	67	GLN	N-CA	-5.36	1.39	1.46
1	A	32	VAL	C-O	-5.33	1.18	1.24
2	B	163	ARG	C-O	-5.24	1.18	1.24
1	A	276	LEU	CA-C	5.22	1.59	1.52
2	B	50	LYS	N-CA	-5.22	1.39	1.46
1	A	67	LEU	CA-C	5.21	1.61	1.52
2	B	183	MET	SD-CE	5.20	1.92	1.79
1	A	197	VAL	CB-CG1	5.19	1.69	1.52
1	A	331	ILE	C-O	-5.18	1.17	1.24
1	A	231	SER	N-CA	5.17	1.51	1.45
2	B	288	LEU	CA-C	-5.15	1.46	1.52
2	B	213	TYR	C-O	-5.15	1.19	1.23
1	A	225	VAL	CA-C	-5.08	1.46	1.52
1	A	292	PHE	C-O	-5.04	1.17	1.24
1	A	338	ILE	CA-C	5.04	1.59	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	50	LYS	N-CA-C	12.50	126.32	111.82
2	B	50	LYS	CA-C-N	-11.15	113.03	121.61
2	B	50	LYS	C-N-CA	-11.15	113.03	121.61
2	B	70	GLY	N-CA-C	-9.96	100.28	112.33
2	B	312	ARG	N-CA-C	-9.76	101.94	114.04
1	A	102	GLU	N-CA-C	-8.99	102.46	113.97
2	B	250	GLY	N-CA-C	-8.31	104.11	114.16
1	A	130	ILE	N-CA-C	-8.21	103.27	110.74
1	A	294	LEU	N-CA-C	-7.53	104.59	114.31
1	A	264	LEU	N-CA-C	-7.13	104.31	113.16
1	A	265	SER	N-CA-C	-6.97	102.89	111.40
2	B	68	LEU	N-CA-C	-6.96	99.22	109.11
2	B	430	PHE	N-CA-C	-6.90	104.59	112.87
2	B	91	VAL	N-CA-C	-6.81	99.62	109.29
2	B	396	GLN	N-CA-C	-6.61	104.86	113.12
2	B	51	GLY	CA-C-O	-6.57	115.85	121.57
2	B	242	PRO	CA-C-O	-6.47	111.17	120.56
2	B	75	ARG	CA-C-O	-6.43	113.55	121.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	53	ASP	N-CA-C	6.31	118.86	110.53
1	A	242	THR	N-CA-C	-6.29	104.12	110.97
2	B	310	GLN	N-CA-C	-6.21	104.97	114.16
2	B	79	MET	N-CA-C	-6.17	105.91	113.50
2	B	189	ILE	N-CA-C	6.13	117.27	112.12
2	B	113	VAL	N-CA-C	-6.12	105.05	113.00
1	A	232	PRO	CA-C-O	-6.08	114.41	121.34
2	B	418	ARG	N-CA-C	-6.07	105.84	113.18
1	A	237	TYR	N-CA-C	-6.06	104.30	111.03
1	A	307	SER	N-CA-C	-6.06	105.87	113.20
2	B	99	SER	N-CA-C	6.06	118.56	108.20
2	B	20	LEU	N-CA-C	6.03	120.31	107.70
2	B	221	VAL	N-CA-C	-6.00	105.21	113.00
1	A	278	LEU	N-CA-C	-5.94	105.69	113.17
1	A	282	PRO	O-C-N	5.92	130.64	122.64
1	A	69	SER	N-CA-C	5.89	121.10	111.37
2	B	227	ILE	N-CA-C	-5.87	105.09	113.07
1	A	135	PRO	CA-C-O	-5.86	114.93	121.32
2	B	276	PHE	O-C-N	5.74	128.69	122.15
2	B	249	VAL	N-CA-C	-5.68	104.09	112.04
2	B	323	SER	N-CA-C	5.63	117.87	109.25
1	A	498	MET	N-CA-C	-5.63	105.24	111.71
2	B	75	ARG	N-CA-C	-5.63	101.87	110.14
2	B	333	ASP	N-CA-C	5.61	117.87	108.96
1	A	318	PRO	CA-C-O	-5.60	115.09	121.98
2	B	26	ILE	CA-C-O	-5.56	113.47	120.69
1	A	138	MET	N-CA-C	-5.55	104.86	111.69
1	A	420	LEU	N-CA-C	-5.51	104.92	111.69
2	B	73	ARG	NE-CZ-NH2	-5.49	114.26	119.20
2	B	255	THR	N-CA-C	-5.47	105.40	111.36
1	A	112	LEU	N-CA-C	-5.44	103.52	111.30
2	B	165	GLY	N-CA-C	-5.42	107.20	114.25
2	B	36	PRO	CA-C-O	-5.42	112.70	120.56
2	B	111	PHE	N-CA-C	5.41	118.89	110.17
1	A	63	ILE	CA-C-N	-5.40	115.55	123.00
1	A	63	ILE	C-N-CA	-5.40	115.55	123.00
1	A	208	GLN	N-CA-C	-5.35	104.90	111.75
2	B	132	ILE	N-CA-C	-5.29	106.13	113.00
1	A	133	PRO	CA-C-O	-5.23	115.29	121.67
1	A	364	VAL	N-CA-C	5.22	116.71	109.29
1	A	490	LEU	N-CA-C	-5.21	105.20	112.45
2	B	375	LEU	N-CA-C	-5.21	106.12	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	ILE	N-CA-C	5.20	115.41	110.42
1	A	81	LEU	N-CA-C	-5.16	105.63	112.34
2	B	371	THR	N-CA-C	5.16	117.37	109.95
2	B	49	VAL	N-CA-C	5.15	116.00	108.53
2	B	357	ALA	N-CA-C	-5.11	107.22	113.50
2	B	266	GLN	N-CA-C	5.10	117.10	110.53
1	A	388	ALA	N-CA-C	-5.09	108.09	114.56
1	A	206	VAL	N-CA-C	-5.07	105.60	110.72
1	A	278	LEU	CA-C-O	5.04	125.25	119.35
2	B	50	LYS	N-CA-CB	-5.02	102.50	110.28

There are no chirality outliers.

There are no planarity outliers.

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	3647	0	3715	457	1
2	B	3540	0	3589	433	0
3	B	30	0	29	20	0
All	All	7217	0	7333	878	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 60.

All (878) 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)
3:B:499:TTX:H181	3:B:499:TTX:C7	1.32	1.57
1:A:274:MET:SD	1:A:274:MET:CE	2.01	1.48
1:A:131:GLU:HG2	1:A:297:ARG:NH1	1.41	1.33
1:A:131:GLU:CG	1:A:297:ARG:NH1	1.92	1.32
3:B:499:TTX:C7	3:B:499:TTX:C18	2.14	1.25
3:B:499:TTX:C18	3:B:499:TTX:H73	1.74	1.17
1:A:131:GLU:CG	1:A:297:ARG:HH12	1.56	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:499:TTX:C18	3:B:499:TTX:H72	1.80	1.09
3:B:499:TTX:H181	3:B:499:TTX:H73	1.14	1.08
3:B:499:TTX:H181	3:B:499:TTX:H72	1.11	1.08
1:A:131:GLU:HG3	1:A:297:ARG:CZ	1.86	1.06
1:A:131:GLU:HG3	1:A:297:ARG:NH1	1.71	1.06
2:B:275:ILE:O	2:B:278:PHE:HB3	1.56	1.03
2:B:243:PRO:HA	2:B:246:ARG:HH21	1.19	1.03
1:A:240:PRO:HB2	1:A:298:LEU:HD21	1.44	1.00
1:A:152:ILE:H	1:A:423:GLN:HE22	1.04	0.99
2:B:19:ASN:HB3	2:B:39:LYS:HD3	1.43	0.99
1:A:39:ILE:HD11	1:A:277:LEU:HB3	1.43	0.99
1:A:210:VAL:HG13	1:A:219:MET:HE1	1.42	0.98
1:A:131:GLU:CG	1:A:297:ARG:CZ	2.40	0.97
1:A:39:ILE:CD1	1:A:277:LEU:HB3	1.97	0.94
2:B:41:PRO:HG2	2:B:74:VAL:HG11	1.51	0.92
2:B:69:LEU:HD21	2:B:75:ARG:HE	1.34	0.91
2:B:238:GLN:HE21	2:B:238:GLN:HA	1.33	0.90
2:B:183:MET:HE1	2:B:212:LEU:HB2	1.53	0.89
2:B:46:ALA:O	2:B:94:THR:HG22	1.71	0.88
2:B:222:ILE:HG22	2:B:223:ASN:H	1.38	0.88
1:A:437:THR:HG21	1:A:462:ARG:HH21	1.40	0.87
2:B:251:LEU:HD21	2:B:309:LEU:HD22	1.56	0.86
2:B:185:LEU:HD13	2:B:324:ILE:HG21	1.56	0.86
1:A:188:GLN:O	1:A:191:ASN:HB2	1.75	0.85
1:A:240:PRO:CB	1:A:298:LEU:HD21	2.06	0.85
1:A:152:ILE:H	1:A:423:GLN:NE2	1.73	0.85
2:B:96:ALA:HB1	2:B:97:PRO:HD2	1.59	0.85
1:A:131:GLU:HG2	1:A:297:ARG:HH12	0.72	0.85
2:B:155:VAL:HG22	2:B:431:LEU:HD22	1.59	0.85
2:B:132:ILE:HA	2:B:255:THR:OG1	1.77	0.84
2:B:134:ARG:H	2:B:312:ARG:NH1	1.75	0.84
2:B:246:ARG:HB2	2:B:246:ARG:CZ	2.08	0.84
1:A:152:ILE:N	1:A:423:GLN:HE22	1.77	0.83
1:A:174:THR:HA	1:A:350:PHE:HZ	1.45	0.81
1:A:393:LEU:HD13	1:A:407:THR:HG23	1.60	0.81
2:B:69:LEU:HD12	2:B:73:ARG:HG2	1.62	0.81
2:B:104:GLY:N	2:B:105:PRO:HD2	1.96	0.81
2:B:122:ARG:HB3	2:B:123:PRO:HD2	1.62	0.81
2:B:30:VAL:HG21	2:B:288:LEU:HD22	1.63	0.81
1:A:440:THR:HG22	1:A:446:LEU:HG	1.62	0.80
1:A:373:ILE:HG22	1:A:374:LYS:H	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:SER:O	2:B:374:MET:HE1	1.82	0.80
1:A:232:PRO:HG2	1:A:235:LEU:HD12	1.63	0.79
1:A:381:GLY:HA2	1:A:384:LYS:HD2	1.64	0.79
2:B:152:GLY:H	2:B:157:ASN:HD21	1.29	0.79
2:B:207:ARG:HH11	2:B:207:ARG:HB3	1.47	0.79
2:B:247:MET:SD	2:B:282:GLY:HA2	2.21	0.79
2:B:390:ARG:HA	2:B:393:GLU:OE1	1.83	0.79
2:B:158:LEU:HD22	2:B:454:THR:HG22	1.65	0.78
2:B:388:ALA:O	2:B:392:LYS:HG3	1.84	0.78
1:A:174:THR:HA	1:A:350:PHE:CZ	2.18	0.78
1:A:197:VAL:HG12	1:A:199:ILE:HD11	1.63	0.78
2:B:105:PRO:HG3	2:B:126:THR:HA	1.64	0.78
1:A:53:LEU:HD11	1:A:96:ALA:HA	1.64	0.78
1:A:264:LEU:HB3	1:A:295:HIS:CE1	2.19	0.78
2:B:41:PRO:HB2	2:B:65:VAL:HG21	1.65	0.78
2:B:302:LEU:O	2:B:302:LEU:HD23	1.83	0.78
1:A:66:ASN:HD22	1:A:68:GLU:CD	1.92	0.77
2:B:285:VAL:O	2:B:289:LEU:HD12	1.84	0.77
1:A:68:GLU:HA	2:B:25:GLN:HG2	1.67	0.77
2:B:109:ARG:NE	2:B:119:ASP:OD2	2.16	0.77
2:B:245:ALA:O	2:B:249:VAL:HG13	1.85	0.77
1:A:445:TYR:HB3	1:A:498:MET:SD	2.24	0.77
1:A:131:GLU:HB3	1:A:297:ARG:HH22	1.49	0.76
1:A:216:ARG:NH1	1:A:426:SER:HB2	2.00	0.76
2:B:389:GLN:O	2:B:393:GLU:HG3	1.84	0.76
2:B:243:PRO:HA	2:B:246:ARG:NH2	1.99	0.76
1:A:65:LEU:HD22	3:B:499:TTX:C18	2.15	0.76
2:B:387:ILE:O	2:B:391:VAL:HG23	1.85	0.76
1:A:138:MET:SD	2:B:119:ASP:C	2.68	0.75
2:B:429:ARG:HE	2:B:472:GLN:NE2	1.82	0.75
2:B:260:PHE:HB2	2:B:268:VAL:HG21	1.67	0.75
1:A:296:SER:HB2	2:B:239:MET:HB3	1.69	0.75
1:A:354:ILE:HG22	1:A:357:ALA:HA	1.69	0.75
1:A:211:THR:C	1:A:213:PHE:H	1.95	0.75
2:B:276:PHE:CD2	2:B:328:TYR:HB3	2.22	0.75
2:B:429:ARG:HE	2:B:472:GLN:HE22	1.35	0.74
1:A:293:TYR:OH	2:B:246:ARG:NH2	2.20	0.74
2:B:275:ILE:HG22	2:B:327:VAL:HG22	1.69	0.74
2:B:310:GLN:HA	2:B:313:ILE:HD12	1.69	0.74
1:A:287:TYR:HB3	1:A:291:VAL:HG21	1.68	0.74
2:B:425:ARG:HD3	2:B:471:GLU:OE2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:466:LEU:HB3	2:B:469:LEU:HD12	1.70	0.74
2:B:82:THR:O	2:B:85:LEU:HG	1.86	0.74
2:B:207:ARG:HB3	2:B:207:ARG:NH1	2.01	0.74
2:B:33:VAL:HG13	2:B:91:VAL:HG21	1.70	0.73
2:B:269:LEU:HD22	2:B:322:THR:HB	1.70	0.73
1:A:187:GLN:HE22	1:A:258:LEU:HD22	1.51	0.73
1:A:262:ASP:HA	1:A:319:ILE:HD12	1.69	0.73
2:B:343:PHE:HA	2:B:346:LEU:HD12	1.68	0.73
2:B:41:PRO:CG	2:B:74:VAL:HG11	2.18	0.73
1:A:413:ARG:HA	1:A:416:ARG:HD2	1.70	0.73
1:A:95:ILE:HG12	1:A:95:ILE:O	1.88	0.73
1:A:446:LEU:HA	1:A:449:LEU:HD12	1.69	0.73
1:A:338:ILE:HA	2:B:239:MET:HE1	1.70	0.72
1:A:364:VAL:HG12	1:A:365:SER:H	1.51	0.72
2:B:160:ALA:HA	2:B:372:SER:HB3	1.71	0.72
1:A:340:ASP:CG	2:B:207:ARG:HE	1.97	0.72
2:B:333:ASP:OD2	2:B:335:THR:OG1	2.08	0.72
1:A:281:PRO:HB2	2:B:287:ALA:HB1	1.70	0.72
1:A:293:TYR:CD1	1:A:293:TYR:N	2.53	0.72
2:B:131:PRO:HD2	2:B:134:ARG:HH21	1.55	0.72
1:A:187:GLN:OE1	1:A:192:VAL:HB	1.90	0.72
1:A:204:SER:OG	1:A:205:SER:N	2.20	0.72
1:A:49:MET:HG3	1:A:52:GLU:OE1	1.89	0.71
1:A:158:ILE:HG21	1:A:343:ILE:HG12	1.71	0.71
1:A:461:LEU:CD2	1:A:497:GLN:HB3	2.19	0.71
2:B:222:ILE:HG22	2:B:223:ASN:N	2.05	0.71
2:B:310:GLN:NE2	2:B:325:GLN:OE1	2.21	0.71
1:A:271:TYR:HD2	1:A:294:LEU:HD11	1.55	0.70
2:B:167:LYS:HZ1	2:B:310:GLN:HB3	1.56	0.70
2:B:310:GLN:HE22	2:B:325:GLN:CD	1.98	0.70
2:B:36:PRO:HD2	2:B:39:LYS:HB2	1.72	0.70
1:A:211:THR:O	1:A:213:PHE:N	2.25	0.70
1:A:247:ALA:HB1	1:A:257:THR:HG21	1.74	0.70
1:A:197:VAL:HG22	1:A:225:VAL:HB	1.71	0.70
2:B:286:SER:HA	2:B:291:ARG:NH1	2.07	0.70
2:B:395:LEU:HD21	2:B:428:GLU:HG2	1.73	0.70
2:B:167:LYS:HB3	2:B:325:GLN:NE2	2.05	0.70
1:A:264:LEU:HB3	1:A:295:HIS:HE1	1.54	0.69
2:B:35:PHE:HB3	2:B:36:PRO:HD2	1.73	0.69
2:B:302:LEU:HD23	2:B:302:LEU:C	2.16	0.69
2:B:149:PHE:CD1	2:B:164:ARG:HG2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:TYR:HA	2:B:401:LEU:HD12	1.74	0.69
1:A:131:GLU:CB	1:A:297:ARG:HH22	2.05	0.69
1:A:135:PRO:HB2	1:A:140:ARG:HH21	1.58	0.69
1:A:444:GLY:HA2	1:A:447:ASP:OD1	1.92	0.69
1:A:198:ALA:HB3	1:A:226:ALA:HB1	1.73	0.69
1:A:162:ARG:NH1	1:A:192:VAL:HG22	2.07	0.69
1:A:182:ASP:HA	1:A:185:LEU:HD12	1.75	0.69
2:B:82:THR:HB	2:B:85:LEU:HD12	1.75	0.68
2:B:396:GLN:HE21	2:B:400:GLU:CD	2.00	0.68
1:A:131:GLU:CG	1:A:297:ARG:NH2	2.57	0.68
2:B:19:ASN:O	2:B:92:ILE:HG13	1.93	0.68
1:A:350:PHE:HB3	1:A:355:ARG:NH2	2.09	0.68
2:B:37:PRO:HA	2:B:72:ASN:OD1	1.93	0.68
2:B:118:VAL:HG12	2:B:118:VAL:O	1.92	0.68
2:B:474:PHE:O	2:B:477:VAL:HG22	1.94	0.68
2:B:264:ASN:O	2:B:266:GLN:N	2.27	0.68
2:B:423:ARG:O	2:B:427:ILE:HG13	1.94	0.68
1:A:39:ILE:HD11	1:A:277:LEU:HD13	1.74	0.68
1:A:293:TYR:OH	2:B:246:ARG:CZ	2.42	0.68
1:A:434:GLN:O	1:A:438:ILE:HG12	1.94	0.68
1:A:486:ALA:HA	1:A:489:LEU:HB2	1.76	0.68
1:A:356:PRO:HD2	1:A:423:GLN:H	1.59	0.67
1:A:126:GLU:O	1:A:127:SER:OG	2.13	0.67
1:A:198:ALA:HB3	1:A:226:ALA:CB	2.25	0.67
1:A:450:GLU:HB2	1:A:453:GLN:OE1	1.94	0.67
1:A:250:PHE:O	1:A:255:ARG:HB2	1.94	0.67
2:B:353:SER:HB3	2:B:356:LEU:HB2	1.76	0.66
2:B:264:ASN:HB2	2:B:266:GLN:HG3	1.75	0.66
1:A:271:TYR:CD2	1:A:294:LEU:HD11	2.30	0.66
1:A:291:VAL:HA	1:A:294:LEU:HD11	1.78	0.66
2:B:25:GLN:HB2	2:B:32:ASN:HD22	1.60	0.66
2:B:148:ILE:HD13	2:B:451:LEU:HD11	1.78	0.66
1:A:293:TYR:CE1	2:B:284:GLU:OE2	2.48	0.66
2:B:104:GLY:N	2:B:105:PRO:CD	2.58	0.66
1:A:39:ILE:HD11	1:A:277:LEU:CB	2.22	0.66
1:A:131:GLU:CB	1:A:297:ARG:NH2	2.59	0.66
1:A:216:ARG:HH12	1:A:426:SER:HB2	1.58	0.66
2:B:79:MET:SD	2:B:244:GLY:O	2.54	0.66
1:A:197:VAL:HG12	1:A:199:ILE:CD1	2.25	0.66
1:A:187:GLN:NE2	1:A:194:CYS:SG	2.68	0.66
1:A:187:GLN:NE2	1:A:258:LEU:HD22	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:MET:HE1	2:B:342:THR:OG1	1.95	0.66
1:A:381:GLY:O	1:A:384:LYS:HB2	1.95	0.66
1:A:430:THR:HG22	1:A:431:VAL:H	1.60	0.66
2:B:107:LEU:HD21	2:B:196:VAL:HG13	1.76	0.66
2:B:104:GLY:O	2:B:107:LEU:HD12	1.96	0.65
2:B:435:PHE:HB2	2:B:438:ALA:HB3	1.78	0.65
1:A:295:HIS:CD2	1:A:335:VAL:HG22	2.31	0.65
1:A:33:LEU:HD21	1:A:43:HIS:HB2	1.78	0.65
1:A:42:ILE:HG21	1:A:45:LEU:HD12	1.78	0.65
1:A:293:TYR:HE1	2:B:284:GLU:OE2	1.80	0.65
1:A:356:PRO:HD2	1:A:423:GLN:N	2.10	0.65
2:B:83:ASP:OD1	3:B:499:TTX:O3	2.15	0.65
1:A:167:LEU:N	1:A:339:THR:HG21	2.12	0.65
2:B:471:GLU:C	2:B:473:ALA:H	2.03	0.65
2:B:171:PHE:HZ	2:B:342:THR:HB	1.63	0.64
2:B:178:LYS:O	2:B:181:LEU:HB3	1.98	0.64
2:B:149:PHE:HB2	2:B:162:TYR:O	1.96	0.64
2:B:83:ASP:OD1	3:B:499:TTX:C12	2.45	0.64
2:B:85:LEU:HD22	2:B:89:MET:HE1	1.78	0.64
1:A:232:PRO:HG2	1:A:235:LEU:CD1	2.28	0.64
2:B:216:MET:CE	2:B:232:VAL:HG21	2.28	0.64
1:A:61:ILE:HG22	1:A:77:MET:SD	2.38	0.64
1:A:160:VAL:HA	1:A:164:GLN:OE1	1.98	0.64
2:B:101:PRO:HB2	2:B:126:THR:HG21	1.80	0.64
1:A:386:GLU:C	1:A:388:ALA:H	2.06	0.64
1:A:65:LEU:HD11	1:A:75:VAL:CG2	2.28	0.63
1:A:126:GLU:OE2	1:A:253:ARG:NH2	2.31	0.63
2:B:286:SER:HA	2:B:291:ARG:HH12	1.63	0.63
1:A:135:PRO:HB2	1:A:140:ARG:HE	1.62	0.63
1:A:351:ASN:C	1:A:353:GLY:H	2.05	0.63
1:A:364:VAL:HG12	1:A:365:SER:N	2.12	0.63
1:A:376:MET:SD	1:A:435:VAL:HG22	2.38	0.63
2:B:69:LEU:HD22	2:B:75:ARG:HH21	1.63	0.63
2:B:163:ARG:HE	2:B:374:MET:CB	2.11	0.63
2:B:216:MET:HE1	2:B:232:VAL:HG21	1.78	0.63
1:A:104:TYR:O	1:A:105:LEU:C	2.41	0.63
1:A:258:LEU:C	1:A:259:ILE:HD12	2.24	0.63
1:A:422:LYS:HD3	1:A:455:ARG:HH21	1.62	0.63
2:B:170:LEU:HD22	2:B:181:LEU:HD21	1.79	0.63
1:A:53:LEU:CD1	1:A:96:ALA:HA	2.28	0.63
1:A:138:MET:SD	2:B:120:ASN:N	2.72	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:LYS:HB3	2:B:325:GLN:HE21	1.63	0.63
2:B:296:VAL:HG12	2:B:296:VAL:O	1.98	0.63
1:A:462:ARG:HB3	1:A:466:LYS:HE3	1.80	0.63
2:B:410:LEU:O	2:B:418:ARG:CZ	2.47	0.63
1:A:461:LEU:O	1:A:465:VAL:HG23	1.99	0.62
2:B:163:ARG:HE	2:B:374:MET:CG	2.13	0.62
1:A:34:GLN:HG3	1:A:41:ARG:HB2	1.81	0.62
2:B:399:LYS:HA	2:B:402:GLN:HE21	1.65	0.62
1:A:156:ALA:O	1:A:380:ALA:HB1	2.00	0.62
1:A:233:ALA:C	1:A:235:LEU:H	2.08	0.62
1:A:461:LEU:HD22	1:A:497:GLN:HB3	1.81	0.62
2:B:64:GLU:CD	2:B:248:ARG:HE	2.08	0.62
2:B:219:SER:OG	2:B:221:VAL:HG23	2.00	0.62
1:A:194:CYS:O	1:A:222:THR:HA	1.99	0.62
2:B:61:VAL:HG21	2:B:85:LEU:HD21	1.81	0.62
1:A:137:ILE:HG21	2:B:110:ILE:HD13	1.82	0.62
1:A:300:GLU:C	1:A:302:ALA:H	2.08	0.62
1:A:150:GLY:N	1:A:186:ASN:ND2	2.47	0.61
1:A:111:ALA:C	1:A:112:LEU:HD23	2.25	0.61
1:A:45:LEU:HB3	1:A:48:VAL:HG13	1.82	0.61
2:B:101:PRO:HA	2:B:129:THR:HA	1.81	0.61
2:B:136:ALA:HB1	2:B:311:GLU:O	2.01	0.61
1:A:263:ASP:H	1:A:319:ILE:HB	1.64	0.61
2:B:149:PHE:HB3	2:B:162:TYR:HB2	1.83	0.61
1:A:67:LEU:O	2:B:87:ARG:HD3	1.99	0.61
2:B:179:THR:O	2:B:182:ILE:HG22	2.01	0.61
2:B:204:GLU:C	2:B:239:MET:HG3	2.26	0.61
2:B:105:PRO:CG	2:B:126:THR:HA	2.31	0.61
2:B:163:ARG:HH21	2:B:374:MET:HG3	1.66	0.61
1:A:110:ASN:HB2	1:A:114:LYS:O	2.00	0.60
2:B:245:ALA:O	2:B:249:VAL:CG1	2.49	0.60
1:A:346:SER:HB3	1:A:359:ASN:HD21	1.66	0.60
2:B:49:VAL:HG22	2:B:91:VAL:HG13	1.83	0.60
2:B:83:ASP:CG	3:B:499:TTX:O3	2.44	0.60
2:B:458:PHE:HA	2:B:461:ILE:HD12	1.83	0.60
1:A:359:ASN:O	1:A:361:GLY:N	2.34	0.60
2:B:68:LEU:O	2:B:69:LEU:C	2.44	0.60
2:B:378:ARG:O	2:B:379:ILE:HD13	2.01	0.60
3:B:499:TTX:C7	3:B:499:TTX:C17	2.62	0.60
2:B:167:LYS:HE2	2:B:325:GLN:HE22	1.67	0.60
1:A:100:VAL:HG23	1:A:246:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:ASN:HB2	2:B:45:ASN:OD1	2.01	0.60
2:B:81:ALA:HB1	3:B:499:TTX:H111	1.83	0.60
1:A:181:THR:HG23	1:A:213:PHE:CE1	2.36	0.60
2:B:203:GLY:HA3	2:B:277:ARG:HB3	1.84	0.60
1:A:130:ILE:HG23	1:A:241:TYR:HB3	1.84	0.60
2:B:422:ALA:HB1	2:B:426:LYS:NZ	2.17	0.59
1:A:225:VAL:HG21	1:A:243:GLY:HA2	1.83	0.59
2:B:319:GLY:O	2:B:320:SER:HB2	2.02	0.59
2:B:308:SER:O	2:B:309:LEU:HD23	2.02	0.59
2:B:46:ALA:O	2:B:94:THR:CG2	2.46	0.59
2:B:103:GLY:C	2:B:105:PRO:HD2	2.27	0.59
2:B:163:ARG:HE	2:B:374:MET:HB2	1.67	0.59
1:A:128:ARG:HH12	1:A:252:TYR:HE1	1.51	0.59
2:B:38:GLY:O	2:B:40:MET:HG3	2.02	0.59
2:B:121:LEU:O	2:B:122:ARG:HB2	2.03	0.59
3:B:499:TTX:H73	3:B:499:TTX:C17	2.28	0.59
1:A:65:LEU:HD22	3:B:499:TTX:C19	2.33	0.59
2:B:397:ARG:O	2:B:401:LEU:HG	2.02	0.59
1:A:181:THR:HG23	1:A:213:PHE:HE1	1.67	0.58
1:A:239:ALA:HB3	1:A:240:PRO:CD	2.33	0.58
1:A:296:SER:N	1:A:338:ILE:HD13	2.17	0.58
2:B:156:VAL:O	2:B:158:LEU:N	2.36	0.58
2:B:109:ARG:HE	2:B:119:ASP:CG	2.11	0.58
1:A:66:ASN:HD22	1:A:68:GLU:CG	2.15	0.58
1:A:111:ALA:HB2	1:A:227:GLU:CD	2.28	0.58
1:A:237:TYR:O	1:A:240:PRO:HD2	2.02	0.58
1:A:293:TYR:OH	2:B:246:ARG:NH1	2.37	0.58
1:A:138:MET:SD	2:B:119:ASP:CA	2.92	0.58
1:A:158:ILE:HD11	1:A:360:VAL:HG13	1.84	0.58
1:A:249:TYR:O	1:A:253:ARG:HG3	2.04	0.58
1:A:346:SER:OG	1:A:349:LEU:HB2	2.03	0.58
1:A:495:GLN:HA	1:A:498:MET:HE2	1.86	0.58
2:B:69:LEU:HD21	2:B:75:ARG:HB2	1.85	0.58
1:A:274:MET:CE	1:A:274:MET:CG	2.81	0.57
2:B:141:GLN:O	2:B:316:THR:HB	2.05	0.57
1:A:451:LEU:C	1:A:453:GLN:H	2.11	0.57
2:B:240:ASN:HD22	2:B:240:ASN:N	2.02	0.57
2:B:398:TYR:O	2:B:402:GLN:HG3	2.04	0.57
2:B:48:ILE:HG22	2:B:92:ILE:CG2	2.35	0.57
2:B:463:SER:OG	2:B:465:GLU:HG3	2.04	0.57
1:A:336:ILE:HG23	1:A:342:GLN:HE22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:ILE:N	2:B:326:ALA:O	2.30	0.57
2:B:396:GLN:NE2	2:B:400:GLU:CD	2.62	0.57
2:B:471:GLU:O	2:B:473:ALA:N	2.37	0.57
1:A:375:ALA:HB2	1:A:480:LYS:O	2.04	0.57
1:A:359:ASN:C	1:A:361:GLY:H	2.12	0.57
1:A:108:VAL:HA	1:A:224:VAL:HB	1.87	0.57
2:B:264:ASN:O	2:B:265:GLU:C	2.46	0.57
2:B:278:PHE:CZ	2:B:309:LEU:HD12	2.40	0.57
2:B:362:TYR:HA	2:B:363:PRO:C	2.29	0.57
1:A:422:LYS:C	1:A:423:GLN:HG3	2.30	0.57
2:B:196:VAL:HG11	2:B:260:PHE:CE2	2.40	0.57
2:B:285:VAL:O	2:B:289:LEU:CD1	2.52	0.57
2:B:53:ASP:OD1	2:B:58:PRO:HG3	2.04	0.56
1:A:56:PHE:CD1	1:A:89:VAL:CG1	2.88	0.56
1:A:167:LEU:H	1:A:339:THR:HG21	1.68	0.56
1:A:167:LEU:HG	1:A:169:ILE:HG13	1.87	0.56
1:A:233:ALA:O	1:A:235:LEU:N	2.37	0.56
1:A:433:GLU:OE2	1:A:466:LYS:HE2	2.05	0.56
2:B:222:ILE:CG2	2:B:223:ASN:H	2.12	0.56
1:A:266:LYS:NZ	1:A:321:GLU:OE1	2.38	0.56
1:A:254:GLU:HG2	1:A:310:GLY:CA	2.35	0.56
1:A:437:THR:HG23	1:A:458:LEU:HD22	1.88	0.56
2:B:310:GLN:HE22	2:B:325:GLN:NE2	2.03	0.56
1:A:446:LEU:HA	1:A:449:LEU:CD1	2.36	0.56
2:B:111:PHE:HB2	2:B:235:VAL:HG22	1.86	0.56
1:A:57:GLU:C	1:A:59:GLY:H	2.13	0.56
1:A:162:ARG:HA	1:A:315:THR:OG1	2.06	0.56
1:A:239:ALA:HB3	1:A:240:PRO:HD3	1.86	0.56
1:A:259:ILE:HD13	1:A:314:MET:HG3	1.87	0.56
1:A:451:LEU:O	1:A:453:GLN:N	2.39	0.56
1:A:148:GLN:HE21	1:A:431:VAL:HG21	1.70	0.56
1:A:472:PHE:O	1:A:476:ILE:HG12	2.06	0.56
1:A:236:GLN:O	1:A:267:GLN:HG3	2.05	0.56
1:A:431:VAL:O	1:A:434:GLN:HB2	2.06	0.56
2:B:186:ILE:HG23	2:B:190:ALA:HB3	1.88	0.56
1:A:359:ASN:C	1:A:361:GLY:N	2.64	0.56
2:B:35:PHE:HB3	2:B:36:PRO:CD	2.36	0.56
2:B:134:ARG:O	2:B:312:ARG:HD2	2.06	0.56
2:B:195:GLY:O	2:B:231:LYS:HE2	2.06	0.56
1:A:287:TYR:CZ	1:A:331:ILE:HD13	2.41	0.55
1:A:419:GLU:HA	1:A:422:LYS:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:OE2	1:A:239:ALA:HA	2.06	0.55
2:B:167:LYS:CE	2:B:310:GLN:NE2	2.69	0.55
2:B:237:GLY:HA3	2:B:249:VAL:HG11	1.88	0.55
2:B:280:GLN:O	2:B:284:GLU:HG3	2.06	0.55
1:A:37:ASP:O	1:A:277:LEU:HD13	2.07	0.55
2:B:96:ALA:HB1	2:B:97:PRO:CD	2.34	0.55
1:A:47:GLU:O	1:A:48:VAL:C	2.44	0.55
1:A:300:GLU:C	1:A:302:ALA:N	2.65	0.55
2:B:148:ILE:HG12	2:B:149:PHE:H	1.71	0.55
2:B:302:LEU:C	2:B:302:LEU:CD2	2.79	0.55
1:A:197:VAL:HA	1:A:225:VAL:O	2.07	0.55
2:B:240:ASN:N	2:B:240:ASN:ND2	2.55	0.55
2:B:274:ASN:HA	2:B:326:ALA:O	2.07	0.55
2:B:299:GLN:H	2:B:299:GLN:NE2	2.04	0.55
1:A:138:MET:SD	2:B:119:ASP:HA	2.47	0.55
1:A:196:TYR:CZ	1:A:262:ASP:OD2	2.60	0.55
1:A:340:ASP:OD1	2:B:207:ARG:NE	2.31	0.55
1:A:493:ALA:HB1	1:A:497:GLN:NE2	2.21	0.55
2:B:299:GLN:H	2:B:299:GLN:HE21	1.54	0.54
2:B:327:VAL:HG21	2:B:342:THR:HG21	1.89	0.54
1:A:241:TYR:HE1	1:A:267:GLN:HE22	1.55	0.54
1:A:387:LEU:HD13	1:A:421:LEU:HD11	1.90	0.54
2:B:146:LEU:HD13	2:B:163:ARG:NH2	2.21	0.54
2:B:158:LEU:HD22	2:B:454:THR:CG2	2.36	0.54
2:B:269:LEU:HD12	2:B:271:PHE:CZ	2.41	0.54
1:A:193:ILE:N	1:A:193:ILE:HD12	2.23	0.54
1:A:210:VAL:O	1:A:214:GLN:HG3	2.06	0.54
1:A:216:ARG:CZ	1:A:426:SER:HB2	2.37	0.54
2:B:270:LEU:HD22	2:B:313:ILE:HG23	1.89	0.54
1:A:387:LEU:HD21	1:A:417:LEU:HB2	1.89	0.54
1:A:496:GLU:O	1:A:499:GLU:HB2	2.08	0.54
1:A:111:ALA:HB2	1:A:227:GLU:CG	2.38	0.54
1:A:39:ILE:HD11	1:A:277:LEU:CD1	2.38	0.54
1:A:131:GLU:CD	3:B:499:TTX:H42	2.33	0.54
1:A:244:ALA:O	1:A:248:GLU:HG3	2.08	0.54
2:B:255:THR:HA	2:B:258:GLU:HG2	1.88	0.54
1:A:375:ALA:HB2	1:A:481:THR:HA	1.88	0.54
1:A:152:ILE:HG22	1:A:421:LEU:HD23	1.90	0.54
1:A:196:TYR:CE1	1:A:262:ASP:OD2	2.61	0.54
1:A:199:ILE:N	1:A:199:ILE:HD12	2.22	0.54
1:A:210:VAL:HG22	1:A:224:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:ILE:O	2:B:186:ILE:HG13	2.07	0.54
2:B:52:ARG:HD2	2:B:61:VAL:HG23	1.89	0.53
2:B:275:ILE:O	2:B:275:ILE:HG13	2.08	0.53
2:B:368:LEU:HD12	2:B:399:LYS:HD3	1.91	0.53
2:B:171:PHE:CZ	2:B:342:THR:HB	2.43	0.53
2:B:300:PRO:HG2	2:B:301:THR:HG23	1.90	0.53
2:B:470:PRO:HG2	2:B:473:ALA:HB2	1.90	0.53
2:B:45:ASN:O	2:B:65:VAL:HG23	2.08	0.53
2:B:351:VAL:HB	2:B:369:ASP:O	2.09	0.53
1:A:430:THR:HG22	1:A:431:VAL:N	2.24	0.53
1:A:115:PRO:HG3	1:A:120:GLY:O	2.09	0.53
1:A:131:GLU:HG2	1:A:297:ARG:CZ	2.21	0.53
1:A:182:ASP:O	1:A:185:LEU:HB2	2.08	0.53
2:B:278:PHE:HZ	2:B:309:LEU:HD12	1.74	0.53
1:A:65:LEU:HB2	1:A:280:ARG:HH22	1.74	0.53
1:A:295:HIS:C	1:A:297:ARG:N	2.67	0.53
1:A:390:PHE:O	1:A:394:GLU:HG3	2.08	0.53
1:A:412:ALA:HB1	1:A:416:ARG:NH2	2.24	0.53
1:A:457:TYR:O	1:A:461:LEU:HG	2.09	0.53
2:B:106:THR:O	2:B:111:PHE:HE1	1.92	0.53
2:B:201:GLY:O	2:B:249:VAL:HG21	2.08	0.53
2:B:429:ARG:HD2	2:B:471:GLU:HB3	1.90	0.53
2:B:171:PHE:HZ	2:B:342:THR:CB	2.22	0.52
2:B:361:ILE:N	2:B:361:ILE:HD12	2.24	0.52
1:A:122:ILE:HD13	1:A:122:ILE:H	1.73	0.52
1:A:295:HIS:C	1:A:297:ARG:H	2.17	0.52
2:B:260:PHE:HB2	2:B:268:VAL:CG2	2.38	0.52
2:B:411:ASP:C	2:B:418:ARG:HH22	2.17	0.52
1:A:350:PHE:HB3	1:A:355:ARG:CZ	2.39	0.52
2:B:276:PHE:C	2:B:278:PHE:H	2.18	0.52
1:A:386:GLU:O	1:A:388:ALA:N	2.42	0.52
1:A:387:LEU:CD1	1:A:421:LEU:HD11	2.39	0.52
2:B:209:GLY:HA2	2:B:236:TYR:OH	2.09	0.52
2:B:473:ALA:O	2:B:483:ALA:HA	2.09	0.52
1:A:66:ASN:HB2	1:A:73:GLY:HA3	1.92	0.52
1:A:195:VAL:HG12	1:A:197:VAL:HG23	1.91	0.52
2:B:107:LEU:HA	2:B:232:VAL:O	2.09	0.52
1:A:259:ILE:HD12	1:A:259:ILE:N	2.24	0.52
1:A:291:VAL:HA	1:A:294:LEU:CD1	2.40	0.52
1:A:419:GLU:OE1	1:A:451:LEU:HA	2.10	0.52
2:B:19:ASN:O	2:B:92:ILE:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:LEU:CD2	2:B:89:MET:HE1	2.39	0.52
2:B:207:ARG:O	2:B:208:GLU:C	2.52	0.52
2:B:270:LEU:CD2	2:B:313:ILE:HG23	2.40	0.52
1:A:164:GLN:O	1:A:315:THR:HG23	2.10	0.52
2:B:113:VAL:HG22	2:B:249:VAL:HG12	1.90	0.52
2:B:122:ARG:HB3	2:B:123:PRO:CD	2.37	0.52
2:B:246:ARG:HB2	2:B:246:ARG:NH1	2.25	0.52
2:B:274:ASN:H	2:B:326:ALA:HB3	1.73	0.52
1:A:466:LYS:HA	1:A:473:GLN:OE1	2.10	0.52
2:B:52:ARG:HD2	2:B:61:VAL:CG2	2.40	0.52
2:B:198:VAL:HG22	2:B:233:ALA:HB3	1.91	0.52
1:A:262:ASP:O	1:A:263:ASP:HB2	2.09	0.52
1:A:141:ARG:HG3	1:A:306:SER:HA	1.92	0.52
1:A:431:VAL:O	1:A:435:VAL:HG23	2.09	0.52
2:B:144:THR:O	2:B:146:LEU:HG	2.09	0.52
2:B:189:ILE:O	2:B:193:HIS:HB2	2.10	0.52
1:A:258:LEU:HA	1:A:315:THR:O	2.11	0.51
1:A:331:ILE:HG22	1:A:332:PRO:N	2.23	0.51
2:B:165:GLY:CA	2:B:315:SER:HB3	2.41	0.51
1:A:52:GLU:OE2	1:A:91:ALA:HB1	2.10	0.51
1:A:288:PRO:HG2	1:A:291:VAL:HG22	1.90	0.51
2:B:19:ASN:O	2:B:20:LEU:HD23	2.09	0.51
2:B:184:GLU:OE2	2:B:435:PHE:HA	2.11	0.51
2:B:202:VAL:HB	2:B:274:ASN:O	2.10	0.51
1:A:158:ILE:N	1:A:158:ILE:HD12	2.25	0.51
1:A:237:TYR:O	1:A:267:GLN:NE2	2.43	0.51
1:A:238:LEU:O	1:A:239:ALA:C	2.51	0.51
1:A:498:MET:HA	1:A:501:PHE:HD1	1.74	0.51
2:B:63:CYS:SG	2:B:78:ALA:HA	2.50	0.51
2:B:299:GLN:HB2	2:B:300:PRO:HD2	1.91	0.51
2:B:255:THR:HA	2:B:258:GLU:OE2	2.10	0.51
1:A:187:GLN:OE1	1:A:194:CYS:SG	2.69	0.51
2:B:167:LYS:HE2	2:B:325:GLN:NE2	2.26	0.51
2:B:167:LYS:HG2	2:B:323:SER:OG	2.10	0.51
1:A:273:GLN:O	1:A:277:LEU:HG	2.10	0.51
2:B:429:ARG:C	2:B:431:LEU:N	2.63	0.51
1:A:210:VAL:CG1	1:A:219:MET:HE1	2.28	0.51
1:A:351:ASN:C	1:A:353:GLY:N	2.69	0.51
1:A:440:THR:CG2	1:A:446:LEU:HG	2.37	0.51
2:B:207:ARG:O	2:B:209:GLY:N	2.44	0.51
1:A:36:GLY:O	1:A:37:ASP:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ILE:HD11	1:A:255:ARG:HH11	1.76	0.51
1:A:219:MET:O	1:A:219:MET:HG2	2.11	0.51
1:A:272:ARG:HG3	1:A:286:ALA:O	2.11	0.51
1:A:76:LEU:HD11	1:A:83:ILE:HG13	1.92	0.51
1:A:109:ILE:HG23	1:A:225:VAL:HA	1.92	0.51
1:A:248:GLU:OE2	1:A:301:ARG:HB3	2.11	0.51
1:A:419:GLU:HG2	1:A:422:LYS:HE3	1.93	0.51
2:B:163:ARG:NE	2:B:374:MET:HB2	2.25	0.51
2:B:176:VAL:HG23	2:B:352:LEU:HD23	1.92	0.51
1:A:254:GLU:HG2	1:A:310:GLY:HA3	1.94	0.50
2:B:112:ASN:HB3	2:B:114:LEU:H	1.76	0.50
2:B:429:ARG:C	2:B:431:LEU:H	2.17	0.50
1:A:166:GLU:O	1:A:317:LEU:HA	2.12	0.50
1:A:471:GLU:O	1:A:475:ILE:HG12	2.11	0.50
2:B:106:THR:HA	2:B:111:PHE:HZ	1.76	0.50
2:B:276:PHE:CG	2:B:328:TYR:HB3	2.46	0.50
2:B:377:PRO:HD3	2:B:385:TYR:CE2	2.45	0.50
1:A:25:LYS:C	1:A:27:VAL:H	2.20	0.50
1:A:152:ILE:HG23	1:A:438:ILE:HD11	1.92	0.50
2:B:264:ASN:C	2:B:266:GLN:N	2.68	0.50
1:A:197:VAL:CG1	1:A:199:ILE:HD11	2.36	0.50
2:B:134:ARG:H	2:B:312:ARG:HH12	1.53	0.50
1:A:259:ILE:HD13	1:A:314:MET:CG	2.41	0.50
1:A:278:LEU:O	1:A:279:ARG:HB2	2.11	0.50
1:A:493:ALA:HB1	1:A:497:GLN:HE22	1.76	0.50
2:B:203:GLY:O	2:B:277:ARG:HG3	2.12	0.50
2:B:243:PRO:HB3	2:B:284:GLU:OE1	2.12	0.50
1:A:80:GLY:C	1:A:82:MET:N	2.68	0.50
1:A:165:ARG:HG2	1:A:299:LEU:O	2.12	0.50
1:A:166:GLU:HA	1:A:166:GLU:OE1	2.11	0.50
2:B:251:LEU:HD21	2:B:309:LEU:HD13	1.93	0.50
2:B:410:LEU:O	2:B:418:ARG:NH2	2.45	0.50
2:B:423:ARG:HA	2:B:426:LYS:HD2	1.93	0.50
1:A:65:LEU:CD1	1:A:278:LEU:CD1	2.90	0.50
1:A:101:SER:OG	1:A:102:GLU:N	2.39	0.50
1:A:166:GLU:O	1:A:318:PRO:HD2	2.12	0.50
2:B:247:MET:C	2:B:248:ARG:HG2	2.36	0.50
1:A:157:MET:SD	1:A:360:VAL:HG11	2.51	0.50
1:A:436:MET:O	1:A:439:TYR:HB3	2.11	0.50
1:A:100:VAL:O	1:A:101:SER:HB3	2.10	0.50
1:A:351:ASN:O	1:A:353:GLY:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:ILE:HA	2:B:374:MET:CE	2.42	0.50
2:B:238:GLN:HE21	2:B:238:GLN:CA	2.08	0.50
2:B:255:THR:O	2:B:258:GLU:HG2	2.12	0.50
1:A:39:ILE:HD13	1:A:277:LEU:HB3	1.89	0.49
2:B:110:ILE:HB	2:B:119:ASP:HB3	1.94	0.49
1:A:145:GLU:OE1	1:A:304:LYS:NZ	2.31	0.49
1:A:345:LEU:CD2	1:A:358:ILE:HD13	2.42	0.49
2:B:83:ASP:CG	3:B:499:TTX:C12	2.85	0.49
1:A:210:VAL:O	1:A:210:VAL:CG1	2.60	0.49
2:B:275:ILE:CG2	2:B:327:VAL:HG22	2.41	0.49
1:A:339:THR:HG22	1:A:340:ASP:N	2.26	0.49
2:B:235:VAL:HG11	2:B:252:THR:CG2	2.43	0.49
1:A:33:LEU:CD2	1:A:43:HIS:HB2	2.43	0.49
1:A:47:GLU:O	1:A:48:VAL:O	2.30	0.49
1:A:57:GLU:OE2	1:A:88:SER:N	2.33	0.49
2:B:48:ILE:O	2:B:92:ILE:HG22	2.13	0.49
1:A:202:LYS:O	1:A:203:ALA:C	2.54	0.49
1:A:260:ILE:HA	1:A:317:LEU:O	2.13	0.49
2:B:107:LEU:HD23	2:B:232:VAL:C	2.37	0.49
2:B:279:VAL:O	2:B:282:GLY:N	2.42	0.49
1:A:394:GLU:CD	1:A:418:ARG:HH21	2.21	0.49
1:A:56:PHE:CE1	1:A:89:VAL:HG11	2.48	0.49
1:A:263:ASP:HA	1:A:319:ILE:O	2.13	0.49
2:B:197:SER:O	2:B:232:VAL:HA	2.12	0.49
1:A:240:PRO:HB2	1:A:298:LEU:CD2	2.29	0.48
2:B:94:THR:HG23	2:B:96:ALA:H	1.78	0.48
2:B:148:ILE:HA	2:B:374:MET:HE1	1.94	0.48
1:A:35:VAL:HG11	1:A:83:ILE:HB	1.94	0.48
2:B:251:LEU:CD2	2:B:309:LEU:HD22	2.37	0.48
1:A:386:GLU:OE2	1:A:442:THR:HG23	2.14	0.48
2:B:341:THR:O	2:B:342:THR:C	2.55	0.48
2:B:475:TYR:CE1	2:B:476:LEU:HG	2.48	0.48
1:A:440:THR:HG23	1:A:494:ILE:HG21	1.96	0.48
2:B:75:ARG:CG	2:B:76:ALA:N	2.76	0.48
2:B:196:VAL:HG11	2:B:260:PHE:CD2	2.49	0.48
2:B:276:PHE:C	2:B:278:PHE:N	2.72	0.48
1:A:310:GLY:C	1:A:312:GLY:H	2.20	0.48
2:B:156:VAL:C	2:B:158:LEU:H	2.20	0.48
1:A:95:ILE:O	1:A:95:ILE:HG23	2.12	0.48
1:A:498:MET:HA	1:A:501:PHE:CD1	2.48	0.48
2:B:69:LEU:CD2	2:B:75:ARG:HH21	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:PHE:O	2:B:142:LEU:HD12	2.14	0.48
2:B:391:VAL:HG13	2:B:427:ILE:CG2	2.44	0.48
2:B:186:ILE:HA	2:B:190:ALA:HB3	1.96	0.48
2:B:422:ALA:HB1	2:B:426:LYS:HZ1	1.79	0.48
1:A:69:SER:HB3	2:B:25:GLN:HE21	1.79	0.48
2:B:286:SER:HB2	2:B:299:GLN:HB3	1.95	0.48
1:A:405:LYS:HA	1:A:408:GLN:HG3	1.96	0.48
2:B:207:ARG:NH1	2:B:207:ARG:CB	2.75	0.48
2:B:31:LEU:O	2:B:76:ALA:N	2.47	0.47
2:B:42:ASN:ND2	2:B:45:ASN:ND2	2.62	0.47
2:B:247:MET:O	2:B:248:ARG:HG2	2.14	0.47
2:B:251:LEU:HD21	2:B:309:LEU:CD2	2.34	0.47
2:B:374:MET:C	2:B:376:GLN:H	2.22	0.47
1:A:36:GLY:O	1:A:37:ASP:HB2	2.14	0.47
1:A:396:PHE:CD1	1:A:396:PHE:N	2.82	0.47
2:B:149:PHE:HB3	2:B:162:TYR:CB	2.44	0.47
1:A:218:ALA:HA	1:A:221:TYR:CE2	2.49	0.47
2:B:413:LEU:HD22	2:B:417:ASP:HB3	1.96	0.47
2:B:381:GLY:O	2:B:385:TYR:HB2	2.15	0.47
1:A:211:THR:C	1:A:213:PHE:N	2.60	0.47
1:A:383:LEU:HD12	1:A:417:LEU:HD13	1.96	0.47
1:A:463:THR:HA	1:A:466:LYS:HD2	1.96	0.47
2:B:47:LEU:HD23	2:B:93:ASP:HA	1.97	0.47
2:B:168:ILE:O	2:B:325:GLN:HG3	2.14	0.47
2:B:333:ASP:OD1	2:B:335:THR:OG1	2.33	0.47
3:B:499:TTX:H71	3:B:499:TTX:H21	1.96	0.47
1:A:33:LEU:HB2	1:A:41:ARG:O	2.14	0.47
1:A:223:ILE:HD12	1:A:223:ILE:N	2.30	0.47
1:A:439:TYR:CD1	1:A:490:LEU:HD13	2.49	0.47
2:B:26:ILE:HD12	2:B:26:ILE:N	2.30	0.47
1:A:176:LYS:O	1:A:177:THR:C	2.58	0.47
1:A:432:GLU:OE2	1:A:473:GLN:O	2.32	0.47
2:B:19:ASN:CB	2:B:39:LYS:HD3	2.31	0.47
2:B:62:THR:O	2:B:79:MET:HG2	2.15	0.47
2:B:163:ARG:HG2	2:B:374:MET:SD	2.54	0.47
2:B:386:GLU:OE1	2:B:390:ARG:NH2	2.48	0.47
2:B:333:ASP:CG	2:B:335:THR:OG1	2.58	0.47
2:B:391:VAL:HG13	2:B:427:ILE:HG21	1.96	0.47
1:A:65:LEU:CD1	1:A:278:LEU:HD11	2.45	0.47
1:A:135:PRO:HB2	1:A:140:ARG:NH2	2.28	0.47
1:A:302:ALA:HA	1:A:314:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:GLU:HB2	2:B:435:PHE:CD2	2.50	0.47
1:A:242:THR:O	1:A:244:ALA:N	2.48	0.46
1:A:386:GLU:C	1:A:388:ALA:N	2.73	0.46
1:A:430:THR:O	1:A:434:GLN:HG3	2.14	0.46
2:B:156:VAL:C	2:B:158:LEU:N	2.73	0.46
1:A:349:LEU:O	1:A:354:ILE:HB	2.15	0.46
1:A:469:LYS:N	1:A:470:PRO:CD	2.78	0.46
2:B:131:PRO:C	2:B:133:HIS:H	2.22	0.46
2:B:361:ILE:HD12	2:B:361:ILE:H	1.80	0.46
3:B:499:TTX:H72	3:B:499:TTX:C17	2.35	0.46
1:A:27:VAL:HG13	1:A:47:GLU:HG3	1.96	0.46
1:A:33:LEU:CG	1:A:43:HIS:HB2	2.45	0.46
1:A:145:GLU:CD	1:A:304:LYS:HZ3	2.18	0.46
1:A:176:LYS:HG2	1:A:345:LEU:HD12	1.97	0.46
1:A:197:VAL:HG21	1:A:243:GLY:HA3	1.98	0.46
2:B:50:LYS:HG2	2:B:59:MET:HE2	1.96	0.46
2:B:86:THR:HG22	2:B:87:ARG:N	2.30	0.46
2:B:466:LEU:HD13	2:B:480:ILE:HD11	1.97	0.46
3:B:499:TTX:C6	3:B:499:TTX:HN41	2.28	0.46
1:A:165:ARG:NH2	2:B:205:ARG:HD3	2.30	0.46
1:A:323:GLN:O	1:A:324:ALA:HB3	2.16	0.46
1:A:454:VAL:O	1:A:457:TYR:HB2	2.15	0.46
1:A:151:LEU:HA	1:A:423:GLN:HE22	1.81	0.46
1:A:199:ILE:HG13	1:A:239:ALA:CB	2.46	0.46
1:A:272:ARG:HD2	1:A:286:ALA:HB3	1.97	0.46
1:A:356:PRO:CD	1:A:423:GLN:H	2.25	0.46
1:A:417:LEU:O	1:A:421:LEU:HG	2.16	0.46
1:A:457:TYR:HA	1:A:501:PHE:CZ	2.51	0.46
2:B:148:ILE:HG12	2:B:149:PHE:N	2.30	0.46
1:A:91:ALA:O	1:A:93:GLY:N	2.49	0.46
1:A:264:LEU:HD11	1:A:318:PRO:HB2	1.96	0.46
2:B:298:TYR:CE1	2:B:338:ALA:HB2	2.51	0.46
1:A:65:LEU:HD11	1:A:278:LEU:HD11	1.98	0.46
1:A:128:ARG:HH11	1:A:248:GLU:HB2	1.81	0.46
1:A:158:ILE:HG21	1:A:343:ILE:CG1	2.44	0.46
2:B:40:MET:O	2:B:41:PRO:C	2.53	0.46
2:B:227:ILE:O	2:B:227:ILE:HG22	2.16	0.46
1:A:91:ALA:O	1:A:92:THR:C	2.57	0.45
1:A:167:LEU:HD12	1:A:168:ILE:H	1.81	0.45
1:A:310:GLY:C	1:A:312:GLY:N	2.74	0.45
2:B:163:ARG:HG2	2:B:374:MET:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:ILE:CG2	2:B:190:ALA:HB3	2.46	0.45
1:A:187:GLN:CD	1:A:194:CYS:SG	2.99	0.45
1:A:281:PRO:CB	2:B:287:ALA:HB1	2.41	0.45
2:B:19:ASN:ND2	2:B:93:ASP:OD2	2.49	0.45
2:B:131:PRO:C	2:B:133:HIS:N	2.73	0.45
1:A:451:LEU:C	1:A:453:GLN:N	2.74	0.45
1:A:486:ALA:O	1:A:490:LEU:HB2	2.16	0.45
2:B:66:GLN:O	2:B:67:GLN:HG2	2.15	0.45
2:B:161:PRO:HD2	2:B:375:LEU:HG	1.97	0.45
2:B:238:GLN:HA	2:B:238:GLN:NE2	2.16	0.45
1:A:214:GLN:C	1:A:216:ARG:N	2.74	0.45
1:A:259:ILE:HD13	1:A:314:MET:SD	2.56	0.45
2:B:402:GLN:O	2:B:404:ILE:N	2.49	0.45
1:A:211:THR:O	1:A:214:GLN:N	2.45	0.45
1:A:240:PRO:CG	1:A:298:LEU:HD21	2.47	0.45
2:B:143:ASP:OD2	2:B:316:THR:C	2.59	0.45
2:B:222:ILE:CG2	2:B:223:ASN:N	2.74	0.45
1:A:154:ILE:O	1:A:158:ILE:O	2.35	0.45
2:B:107:LEU:HD23	2:B:232:VAL:N	2.32	0.45
2:B:413:LEU:O	2:B:418:ARG:NE	2.42	0.45
1:A:128:ARG:HH11	1:A:248:GLU:CB	2.29	0.45
2:B:160:ALA:CA	2:B:372:SER:HB3	2.43	0.45
2:B:223:ASN:OD1	2:B:228:ALA:HA	2.16	0.45
2:B:310:GLN:HE22	2:B:325:GLN:HE22	1.65	0.45
2:B:329:VAL:HG11	2:B:334:LEU:HD23	1.99	0.45
2:B:434:PRO:HD3	2:B:476:LEU:HD22	1.99	0.45
1:A:111:ALA:O	1:A:112:LEU:HD23	2.17	0.45
1:A:414:GLY:C	1:A:416:ARG:H	2.25	0.45
1:A:418:ARG:O	1:A:422:LYS:HG3	2.17	0.45
2:B:33:VAL:CG1	2:B:91:VAL:HG21	2.43	0.45
2:B:261:ARG:HD3	2:B:321:ILE:HG12	1.99	0.45
2:B:315:SER:HA	2:B:320:SER:HA	1.97	0.45
2:B:430:PHE:HD1	2:B:474:PHE:HB3	1.82	0.45
1:A:29:THR:HA	1:A:89:VAL:O	2.16	0.45
1:A:165:ARG:NH2	1:A:338:ILE:O	2.49	0.45
1:A:167:LEU:HD21	1:A:169:ILE:HD11	1.97	0.45
1:A:415:GLN:O	1:A:451:LEU:HD22	2.17	0.45
2:B:204:GLU:O	2:B:238:GLN:NE2	2.50	0.45
2:B:480:ILE:O	2:B:483:ALA:HB3	2.17	0.45
1:A:418:ARG:O	1:A:421:LEU:HB2	2.17	0.45
2:B:350:THR:O	2:B:352:LEU:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HA	1:A:390:PHE:CD1	2.52	0.44
1:A:65:LEU:CD2	3:B:499:TTX:C19	2.95	0.44
1:A:130:ILE:HD13	1:A:238:LEU:HD13	1.98	0.44
2:B:98:LEU:O	2:B:132:ILE:HG12	2.18	0.44
1:A:26:VAL:HG12	1:A:26:VAL:O	2.17	0.44
1:A:151:LEU:HB3	1:A:154:ILE:HD13	1.99	0.44
1:A:490:LEU:O	1:A:493:ALA:HB3	2.17	0.44
2:B:183:MET:CE	2:B:212:LEU:HB2	2.38	0.44
2:B:207:ARG:C	2:B:209:GLY:N	2.73	0.44
2:B:377:PRO:HD3	2:B:385:TYR:CD2	2.53	0.44
1:A:56:PHE:CG	1:A:83:ILE:HD12	2.52	0.44
1:A:78:GLY:HA2	1:A:232:PRO:HG3	1.98	0.44
1:A:251:MET:C	1:A:253:ARG:H	2.25	0.44
1:A:302:ALA:HB2	1:A:314:MET:HE3	1.99	0.44
2:B:66:GLN:O	2:B:67:GLN:CG	2.65	0.44
1:A:56:PHE:HD2	1:A:60:THR:O	2.01	0.44
1:A:210:VAL:O	1:A:210:VAL:HG12	2.17	0.44
2:B:199:PHE:CZ	2:B:273:ASP:HB2	2.53	0.44
2:B:204:GLU:O	2:B:239:MET:HG3	2.17	0.44
2:B:271:PHE:HE1	2:B:324:ILE:HD12	1.82	0.44
2:B:402:GLN:C	2:B:404:ILE:N	2.75	0.44
1:A:38:GLY:O	1:A:76:LEU:HB2	2.17	0.44
1:A:264:LEU:HD11	1:A:318:PRO:CB	2.48	0.44
2:B:203:GLY:HA3	2:B:277:ARG:CB	2.46	0.44
2:B:241:GLU:HB2	2:B:246:ARG:HD3	2.00	0.44
1:A:27:VAL:CG1	1:A:47:GLU:HG3	2.48	0.44
1:A:494:ILE:O	1:A:498:MET:HG3	2.17	0.44
2:B:112:ASN:ND2	2:B:116:GLU:OE1	2.50	0.44
2:B:401:LEU:O	2:B:404:ILE:HB	2.18	0.44
1:A:56:PHE:CD1	1:A:89:VAL:HG13	2.53	0.44
1:A:174:THR:HG23	1:A:350:PHE:CZ	2.53	0.44
1:A:241:TYR:HE1	1:A:267:GLN:NE2	2.14	0.44
1:A:99:PRO:HD2	1:A:113:ALA:HB3	2.00	0.43
1:A:486:ALA:O	1:A:490:LEU:N	2.51	0.43
2:B:23:ILE:HG21	2:B:26:ILE:HD11	1.99	0.43
2:B:132:ILE:HG22	2:B:251:LEU:O	2.17	0.43
2:B:153:ILE:HA	2:B:433:GLN:OE1	2.18	0.43
2:B:168:ILE:HB	2:B:324:ILE:HA	2.00	0.43
2:B:235:VAL:HG11	2:B:252:THR:HG21	2.00	0.43
1:A:30:GLY:O	1:A:88:SER:HA	2.17	0.43
1:A:39:ILE:HG21	1:A:278:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:C	1:A:59:GLY:N	2.75	0.43
1:A:76:LEU:O	1:A:234:THR:CB	2.66	0.43
1:A:176:LYS:CG	1:A:345:LEU:HD12	2.48	0.43
2:B:43:ILE:HG22	2:B:44:TYR:CD1	2.53	0.43
2:B:299:GLN:HG3	2:B:301:THR:OG1	2.18	0.43
2:B:460:LEU:HD12	2:B:480:ILE:HG12	1.99	0.43
1:A:310:GLY:O	1:A:311:GLU:HB2	2.18	0.43
2:B:73:ARG:HE	2:B:73:ARG:HB2	1.43	0.43
2:B:106:THR:HA	2:B:111:PHE:CZ	2.53	0.43
2:B:167:LYS:CE	2:B:325:GLN:HE22	2.31	0.43
2:B:209:GLY:O	2:B:210:ASN:C	2.61	0.43
1:A:112:LEU:HD23	1:A:112:LEU:N	2.32	0.43
1:A:126:GLU:C	1:A:127:SER:OG	2.61	0.43
1:A:185:LEU:C	1:A:187:GLN:H	2.26	0.43
1:A:233:ALA:C	1:A:235:LEU:N	2.69	0.43
2:B:135:SER:O	2:B:136:ALA:O	2.36	0.43
2:B:203:GLY:CA	2:B:246:ARG:HG2	2.49	0.43
2:B:410:LEU:HA	2:B:413:LEU:HD12	2.00	0.43
1:A:134:ALA:HB1	1:A:301:ARG:HA	2.00	0.43
1:A:136:GLY:O	1:A:140:ARG:HG3	2.18	0.43
1:A:235:LEU:C	1:A:237:TYR:N	2.73	0.43
1:A:264:LEU:CD1	1:A:318:PRO:HB2	2.49	0.43
1:A:97:GLN:O	1:A:98:ILE:HD12	2.19	0.43
1:A:98:ILE:HA	1:A:99:PRO:HD3	1.86	0.43
1:A:107:ARG:NH2	1:A:115:PRO:HB3	2.34	0.43
2:B:22:ARG:O	2:B:23:ILE:C	2.61	0.43
2:B:167:LYS:HD2	2:B:313:ILE:O	2.19	0.43
2:B:414:SER:O	2:B:418:ARG:HG3	2.19	0.43
1:A:76:LEU:O	1:A:234:THR:HB	2.19	0.43
1:A:404:ASP:O	1:A:408:GLN:HG3	2.19	0.43
2:B:128:THR:HG22	2:B:129:THR:N	2.33	0.43
2:B:186:ILE:HA	2:B:190:ALA:CB	2.48	0.43
2:B:206:THR:O	2:B:209:GLY:N	2.47	0.43
1:A:438:ILE:HG22	1:A:442:THR:OG1	2.19	0.43
2:B:42:ASN:ND2	2:B:45:ASN:HD21	2.17	0.43
2:B:43:ILE:O	2:B:44:TYR:HB2	2.18	0.43
2:B:367:PRO:HB3	2:B:431:LEU:HD13	2.00	0.43
2:B:430:PHE:CD2	2:B:461:ILE:HD11	2.53	0.43
2:B:30:VAL:CG2	2:B:288:LEU:HD22	2.39	0.43
2:B:121:LEU:O	2:B:122:ARG:CB	2.65	0.43
2:B:238:GLN:O	2:B:239:MET:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:PHE:CE1	2:B:324:ILE:HD12	2.53	0.43
1:A:80:GLY:C	1:A:82:MET:H	2.26	0.43
1:A:174:THR:HG22	1:A:174:THR:O	2.18	0.43
1:A:175:GLY:O	1:A:178:ALA:HB3	2.19	0.43
1:A:368:GLY:C	1:A:370:ALA:N	2.77	0.43
2:B:35:PHE:CE1	2:B:41:PRO:HG3	2.54	0.43
2:B:269:LEU:HD22	2:B:322:THR:CB	2.46	0.43
2:B:387:ILE:HG23	2:B:462:LEU:HD11	2.01	0.43
1:A:109:ILE:CG2	1:A:225:VAL:HA	2.49	0.42
1:A:128:ARG:NH1	1:A:248:GLU:HB3	2.34	0.42
1:A:162:ARG:CZ	1:A:192:VAL:HG22	2.49	0.42
1:A:189:GLY:C	1:A:191:ASN:H	2.26	0.42
1:A:300:GLU:O	1:A:302:ALA:N	2.51	0.42
1:A:369:SER:HB2	1:A:372:GLN:OE1	2.19	0.42
1:A:382:LYS:O	1:A:386:GLU:HG3	2.19	0.42
2:B:86:THR:CG2	2:B:87:ARG:N	2.82	0.42
2:B:186:ILE:HG23	2:B:190:ALA:CB	2.49	0.42
1:A:440:THR:HA	1:A:494:ILE:HD13	2.00	0.42
2:B:23:ILE:HD11	2:B:49:VAL:HG11	2.02	0.42
1:A:268:ALA:O	1:A:271:TYR:HB3	2.19	0.42
1:A:403:LEU:HD13	1:A:407:THR:HG21	2.01	0.42
1:A:419:GLU:HA	1:A:422:LYS:CD	2.48	0.42
2:B:22:ARG:HB3	2:B:88:GLY:HA2	2.01	0.42
2:B:156:VAL:HG12	2:B:157:ASN:N	2.33	0.42
2:B:423:ARG:NH2	2:B:464:GLY:HA3	2.34	0.42
1:A:137:ILE:HD11	2:B:209:GLY:C	2.44	0.42
1:A:394:GLU:CD	1:A:418:ARG:NH2	2.78	0.42
2:B:138:ALA:N	2:B:141:GLN:OE1	2.40	0.42
1:A:138:MET:HE2	2:B:118:VAL:O	2.19	0.42
1:A:240:PRO:O	1:A:241:TYR:C	2.62	0.42
1:A:272:ARG:HA	1:A:288:PRO:HD3	2.00	0.42
1:A:339:THR:CG2	1:A:340:ASP:N	2.82	0.42
2:B:225:GLN:C	2:B:227:ILE:H	2.27	0.42
2:B:308:SER:C	2:B:309:LEU:HD23	2.45	0.42
1:A:104:TYR:CE2	1:A:109:ILE:HD12	2.54	0.42
1:A:130:ILE:CG2	1:A:241:TYR:HB3	2.49	0.42
2:B:430:PHE:CD1	2:B:474:PHE:HB3	2.54	0.42
1:A:122:ILE:HD13	1:A:122:ILE:N	2.35	0.42
1:A:157:MET:SD	1:A:387:LEU:HD12	2.60	0.42
1:A:173:GLN:OE1	1:A:173:GLN:HA	2.19	0.42
2:B:69:LEU:HD21	2:B:75:ARG:NE	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:VAL:HG11	2:B:438:ALA:HB2	2.01	0.42
1:A:227:GLU:OE1	1:A:235:LEU:O	2.38	0.42
1:A:419:GLU:HA	1:A:422:LYS:CG	2.49	0.42
1:A:481:THR:HG22	1:A:482:PHE:N	2.34	0.42
2:B:109:ARG:CD	2:B:119:ASP:OD2	2.67	0.42
2:B:458:PHE:HA	2:B:461:ILE:CD1	2.47	0.42
1:A:100:VAL:HA	1:A:104:TYR:HE1	1.85	0.42
1:A:172:ARG:H	1:A:172:ARG:HG2	1.72	0.42
1:A:186:ASN:CG	1:A:428:PRO:HB2	2.45	0.42
1:A:214:GLN:C	1:A:216:ARG:H	2.27	0.42
1:A:260:ILE:CD1	1:A:317:LEU:HB2	2.49	0.42
1:A:330:TYR:O	1:A:333:THR:HB	2.20	0.42
1:A:373:ILE:HG22	1:A:374:LYS:N	2.23	0.42
2:B:70:GLY:O	2:B:71:ASN:CB	2.67	0.42
1:A:53:LEU:HB2	1:A:92:THR:OG1	2.19	0.41
1:A:65:LEU:CD1	1:A:278:LEU:HD13	2.50	0.41
1:A:293:TYR:N	1:A:293:TYR:HD1	2.08	0.41
2:B:36:PRO:CD	2:B:39:LYS:HD2	2.50	0.41
2:B:254:LEU:HD22	2:B:313:ILE:HG12	2.01	0.41
1:A:373:ILE:O	1:A:377:LYS:HG3	2.20	0.41
1:A:447:ASP:C	1:A:449:LEU:H	2.26	0.41
2:B:102:VAL:HG12	2:B:256:MET:HG3	2.01	0.41
2:B:211:ASP:C	2:B:213:TYR:N	2.77	0.41
2:B:367:PRO:HB2	2:B:395:LEU:HD13	2.02	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.84	0.41
1:A:157:MET:C	1:A:158:ILE:HD12	2.45	0.41
1:A:167:LEU:HD12	1:A:318:PRO:O	2.20	0.41
2:B:48:ILE:HG22	2:B:92:ILE:HG22	2.00	0.41
2:B:431:LEU:HD23	2:B:431:LEU:HA	1.91	0.41
1:A:242:THR:C	1:A:244:ALA:N	2.78	0.41
2:B:169:GLY:HA3	2:B:346:LEU:HD13	2.02	0.41
2:B:170:LEU:HD13	2:B:181:LEU:CD2	2.50	0.41
2:B:261:ARG:HG2	2:B:262:ASP:OD1	2.20	0.41
1:A:295:HIS:HB2	1:A:338:ILE:CD1	2.50	0.41
1:A:457:TYR:HA	1:A:501:PHE:CE2	2.55	0.41
1:A:490:LEU:HD22	1:A:494:ILE:HD11	2.02	0.41
2:B:65:VAL:HG13	2:B:74:VAL:HB	2.03	0.41
1:A:154:ILE:HD12	1:A:154:ILE:N	2.36	0.41
2:B:72:ASN:O	2:B:73:ARG:HB2	2.20	0.41
2:B:212:LEU:O	2:B:212:LEU:HG	2.21	0.41
1:A:46:ASP:OD1	1:A:46:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ARG:O	1:A:173:GLN:C	2.63	0.41
1:A:470:PRO:O	1:A:474:GLU:HG3	2.20	0.41
2:B:42:ASN:O	2:B:45:ASN:HB2	2.21	0.41
2:B:105:PRO:HG2	2:B:126:THR:HG22	2.03	0.41
2:B:165:GLY:HA2	2:B:315:SER:HB3	2.02	0.41
1:A:216:ARG:NH2	1:A:426:SER:HB2	2.36	0.41
1:A:249:TYR:CD1	1:A:249:TYR:C	2.98	0.41
1:A:271:TYR:OH	1:A:290:ASP:HB2	2.21	0.41
1:A:454:VAL:HA	1:A:457:TYR:CD1	2.56	0.41
2:B:163:ARG:NE	2:B:374:MET:CB	2.81	0.41
2:B:251:LEU:CG	2:B:309:LEU:HD13	2.50	0.41
2:B:387:ILE:CD1	2:B:459:GLN:HB2	2.51	0.41
1:A:67:LEU:HB3	2:B:87:ARG:HE	1.86	0.41
1:A:134:ALA:CB	1:A:301:ARG:HA	2.51	0.41
1:A:148:GLN:HE21	1:A:431:VAL:CG2	2.34	0.41
1:A:235:LEU:C	1:A:237:TYR:H	2.29	0.41
1:A:285:GLU:C	1:A:287:TYR:H	2.28	0.41
1:A:380:ALA:O	1:A:381:GLY:C	2.63	0.41
2:B:52:ARG:HG2	2:B:53:ASP:N	2.35	0.41
2:B:259:TYR:HE2	2:B:264:ASN:HD21	1.69	0.41
2:B:423:ARG:O	2:B:426:LYS:HB2	2.21	0.41
1:A:138:MET:C	1:A:140:ARG:H	2.28	0.41
1:A:409:ASN:O	1:A:413:ARG:HG3	2.21	0.41
1:A:417:LEU:HA	1:A:420:LEU:HG	2.03	0.41
2:B:68:LEU:O	2:B:70:GLY:N	2.53	0.41
2:B:405:ILE:HG13	2:B:406:ALA:N	2.35	0.41
2:B:419:LEU:HD11	2:B:423:ARG:HE	1.85	0.41
2:B:276:PHE:CZ	2:B:280:GLN:HB2	2.56	0.40
2:B:298:TYR:CZ	2:B:338:ALA:HB2	2.55	0.40
1:A:135:PRO:O	1:A:140:ARG:NH2	2.54	0.40
2:B:240:ASN:O	2:B:241:GLU:C	2.63	0.40
2:B:353:SER:HB3	2:B:356:LEU:HD12	2.02	0.40
2:B:387:ILE:HA	2:B:390:ARG:HD2	2.02	0.40
2:B:50:LYS:HG2	2:B:59:MET:CE	2.51	0.40
1:A:56:PHE:CE2	1:A:76:LEU:HD22	2.56	0.40
1:A:108:VAL:HG12	1:A:116:ILE:HD11	2.03	0.40
1:A:189:GLY:C	1:A:191:ASN:N	2.79	0.40
1:A:302:ALA:O	1:A:303:ALA:HB2	2.22	0.40
2:B:64:GLU:O	2:B:65:VAL:C	2.63	0.40
2:B:161:PRO:HD2	2:B:372:SER:HB3	2.04	0.40
2:B:167:LYS:HE3	2:B:310:GLN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:399:LYS:HA	2:B:402:GLN:NE2	2.35	0.40
1:A:181:THR:O	1:A:185:LEU:HD12	2.21	0.40
1:A:271:TYR:O	1:A:272:ARG:C	2.64	0.40
1:A:422:LYS:O	1:A:423:GLN:HG3	2.21	0.40
1:A:461:LEU:O	1:A:464:TYR:HB2	2.22	0.40
2:B:269:LEU:HD12	2:B:271:PHE:HZ	1.85	0.40
2:B:299:GLN:HG2	2:B:301:THR:C	2.46	0.40
2:B:357:ALA:HB2	2:B:364:ALA:CB	2.52	0.40
2:B:404:ILE:O	2:B:408:LEU:HB2	2.22	0.40
2:B:417:ASP:HA	2:B:420:THR:HG23	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:GLU:OE1	1:A:499:GLU:OE1[4_555]	1.69	0.51

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	475/507 (94%)	362 (76%)	86 (18%)	27 (6%)	1	9
2	B	465/498 (93%)	365 (78%)	76 (16%)	24 (5%)	1	10
All	All	940/1005 (94%)	727 (77%)	162 (17%)	51 (5%)	1	10

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	SER
1	A	212	ASN
1	A	447	ASP

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Mol	Chain	Res	Type
2	B	265	GLU
2	B	343	PHE
1	A	48	VAL
1	A	85	GLU
1	A	92	THR
1	A	110	ASN
1	A	171	ASP
1	A	330	TYR
1	A	352	ALA
1	A	354	ILE
1	A	360	VAL
1	A	387	LEU
1	A	448	SER
2	B	55	ALA
2	B	157	ASN
2	B	208	GLU
2	B	286	SER
2	B	472	GLN
1	A	37	ASP
1	A	105	LEU
1	A	186	ASN
1	A	234	THR
1	A	262	ASP
1	A	296	SER
1	A	351	ASN
1	A	452	ASP
2	B	54	THR
2	B	69	LEU
2	B	239	MET
2	B	402	GLN
2	B	403	ASP
2	B	451	LEU
1	A	26	VAL
1	A	288	PRO
2	B	122	ARG
2	B	154	LYS
2	B	156	VAL
2	B	240	ASN
1	A	328	SER
1	A	402	ASP
2	B	52	ARG
2	B	345	HIS

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Mol	Chain	Res	Type
1	A	373	ILE
2	B	136	ALA
2	B	296	VAL
2	B	175	GLY
2	B	61	VAL
2	B	455	ILE

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	388/414 (94%)	358 (92%)	30 (8%)	12	37
2	B	381/410 (93%)	351 (92%)	30 (8%)	11	36
All	All	769/824 (93%)	709 (92%)	60 (8%)	11	37

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	35	VAL
1	A	39	ILE
1	A	41	ARG
1	A	42	ILE
1	A	49	MET
1	A	65	LEU
1	A	66	ASN
1	A	72	VAL
1	A	83	ILE
1	A	89	VAL
1	A	95	ILE
1	A	98	ILE
1	A	122	ILE
1	A	128	ARG
1	A	131	GLU
1	A	135	PRO

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Mol	Chain	Res	Type
1	A	147	LEU
1	A	177	THR
1	A	191	ASN
1	A	228	THR
1	A	249	TYR
1	A	257	THR
1	A	333	THR
1	A	342	GLN
1	A	364	VAL
1	A	379	VAL
1	A	426	SER
1	A	435	VAL
1	A	490	LEU
2	B	42	ASN
2	B	48	ILE
2	B	57	GLN
2	B	58	PRO
2	B	75	ARG
2	B	98	LEU
2	B	129	THR
2	B	132	ILE
2	B	140	THR
2	B	149	PHE
2	B	167	LYS
2	B	215	GLU
2	B	238	GLN
2	B	240	ASN
2	B	246	ARG
2	B	249	VAL
2	B	268	VAL
2	B	269	LEU
2	B	288	LEU
2	B	299	GLN
2	B	306	MET
2	B	308	SER
2	B	310	GLN
2	B	316	THR
2	B	325	GLN
2	B	352	LEU
2	B	395	LEU
2	B	413	LEU
2	B	417	ASP

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Mol	Chain	Res	Type
2	B	425	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	70	ASN
1	A	148	GLN
1	A	186	ASN
1	A	273	GLN
1	A	295	HIS
1	A	409	ASN
1	A	423	GLN
1	A	425	GLN
1	A	434	GLN
1	A	497	GLN
2	B	19	ASN
2	B	25	GLN
2	B	42	ASN
2	B	45	ASN
2	B	60	ASN
2	B	187	ASN
2	B	238	GLN
2	B	240	ASN
2	B	264	ASN
2	B	299	GLN
2	B	310	GLN
2	B	325	GLN
2	B	396	GLN
2	B	402	GLN
2	B	459	GLN
2	B	472	GLN
2	B	479	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	TTX	B	499	-	31,31,31	3.42	9 (29%)	38,43,43	4.58	12 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TTX	B	499	-	-	17/45/45/45	0/1/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	499	TTX	O1-C6	11.78	1.43	1.22
3	B	499	TTX	C15-C14	-7.80	1.33	1.49
3	B	499	TTX	C6-N1	6.65	1.45	1.35
3	B	499	TTX	C5-C6	5.74	1.64	1.53
3	B	499	TTX	C7-N1	-4.58	1.38	1.47
3	B	499	TTX	C12-N3	-3.94	1.29	1.35
3	B	499	TTX	C15-N1	-3.32	1.34	1.42
3	B	499	TTX	C9-N3	-3.09	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	499	TTX	C5-N2	2.07	1.50	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	499	TTX	C5-C6-N1	-18.03	91.91	118.61
3	B	499	TTX	C7-N1-C6	-17.42	95.53	118.87
3	B	499	TTX	C4-C5-C6	6.41	121.72	109.28
3	B	499	TTX	C13-N4-C14	5.72	130.12	121.29
3	B	499	TTX	C11-N3-C12	-3.37	114.64	122.16
3	B	499	TTX	C9-C8-N2	3.32	122.07	115.64
3	B	499	TTX	C6-C5-N2	-2.81	101.68	108.97
3	B	499	TTX	C18-C17-C16	2.78	130.78	121.22
3	B	499	TTX	C15-C14-N4	2.41	121.72	117.20
3	B	499	TTX	C21-C22-C17	2.22	123.24	120.64
3	B	499	TTX	C2-C4-C5	2.10	121.05	115.40
3	B	499	TTX	C18-C17-C22	-2.06	114.60	117.65

There are no chirality outliers.

All (17) torsion outliers are listed below:

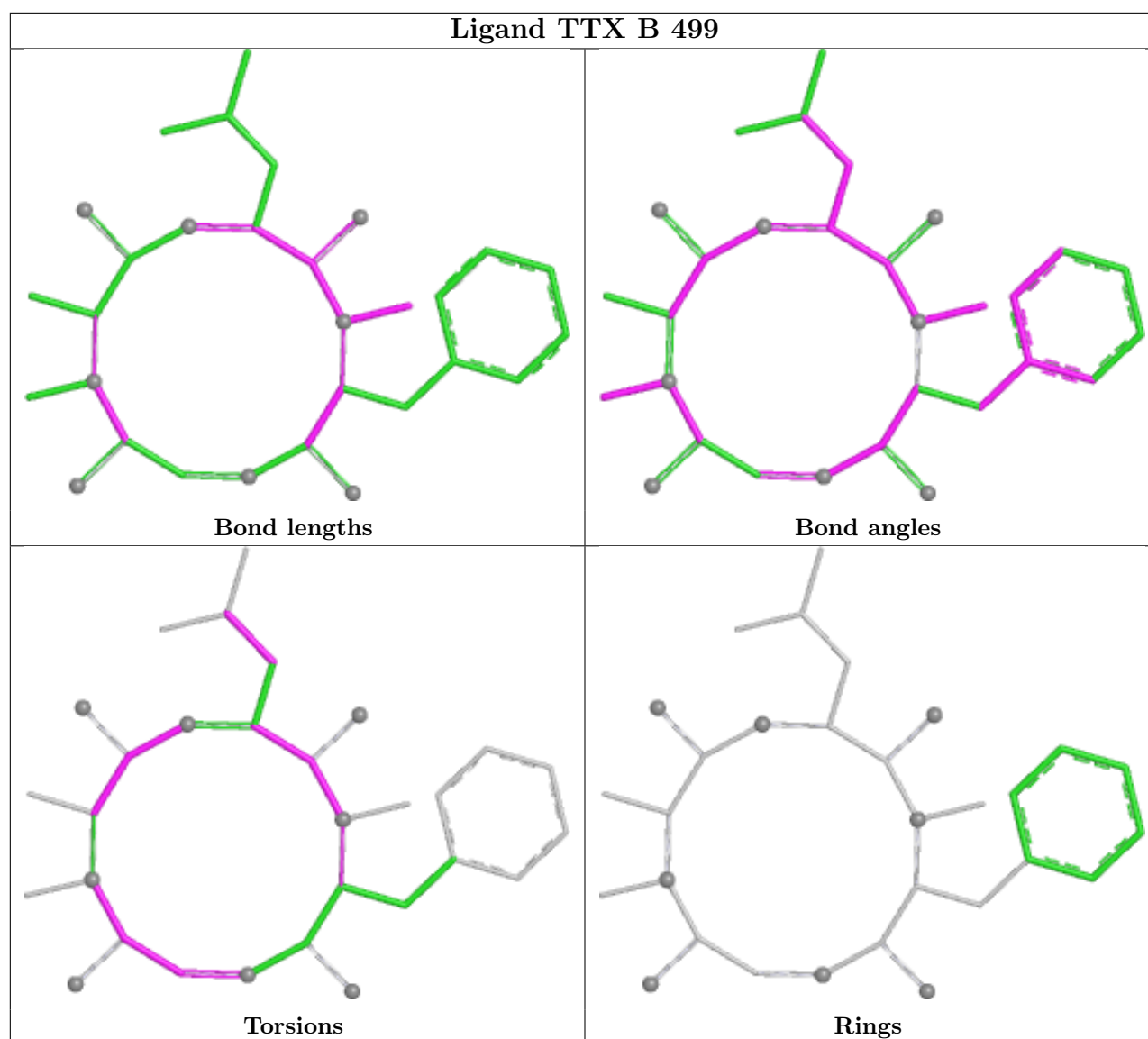
Mol	Chain	Res	Type	Atoms
3	B	499	TTX	C14-C15-N1-C6
3	B	499	TTX	O1-C6-N1-C7
3	B	499	TTX	C5-C6-N1-C7
3	B	499	TTX	C5-C6-N1-C15
3	B	499	TTX	O2-C8-N2-C5
3	B	499	TTX	C9-C8-N2-C5
3	B	499	TTX	O3-C12-C13-N4
3	B	499	TTX	C4-C5-C6-O1
3	B	499	TTX	N3-C12-C13-N4
3	B	499	TTX	N2-C5-C6-O1
3	B	499	TTX	C13-C12-N3-C9
3	B	499	TTX	C13-C12-N3-C11
3	B	499	TTX	C1-C2-C4-C5
3	B	499	TTX	N2-C8-C9-N3
3	B	499	TTX	C12-C13-N4-C14
3	B	499	TTX	C16-C15-N1-C6
3	B	499	TTX	O2-C8-C9-N3

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	499	TTX	20	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.