



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:49 PM UTC

PDB ID : 8YFC / pdb_00008yfc
EMDB ID : EMD-39219
Title : Human PIEZO1-A1988V-MDFIC
Authors : Zhang, M.F.
Deposited on : 2024-02-24
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

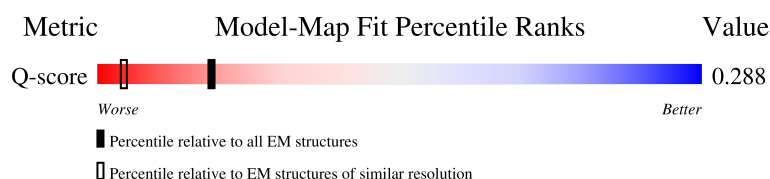
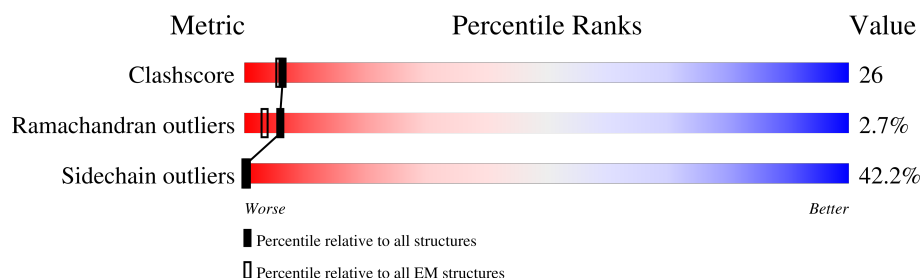
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2521	
1	B	2521	
1	D	2521	
2	C	246	

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Mol	Chain	Length	Quality of chain
2	E	246	 6% .. 91%
2	F	246	 6% .. 91%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	D12	E	301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32172 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

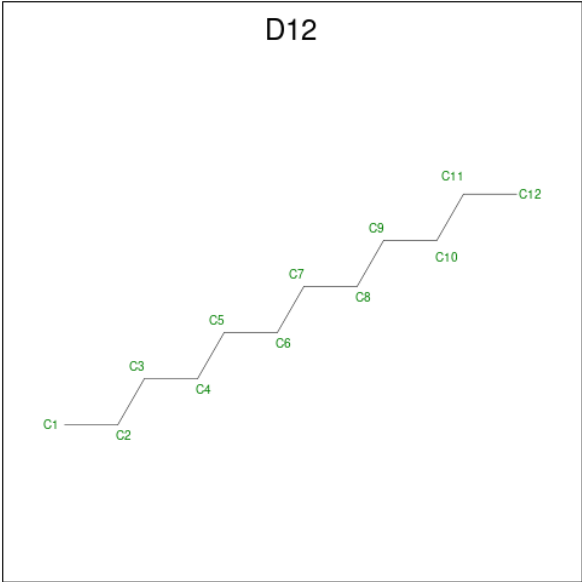
- Molecule 1 is a protein called Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1280	Total 10463	C 6920	N 1743	O 1739	S 61	0	0
1	B	1280	Total 10463	C 6920	N 1743	O 1739	S 61	0	0
1	D	1280	Total 10463	C 6920	N 1743	O 1739	S 61	0	0

- Molecule 2 is a protein called MyoD family inhibitor domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	21	Total 150	C 88	N 21	O 33	S 8	0	0
2	E	21	Total 150	C 88	N 21	O 33	S 8	0	0
2	F	21	Total 150	C 88	N 21	O 33	S 8	0	0

- Molecule 3 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆) (labeled as "Ligand of Interest" by depositor).



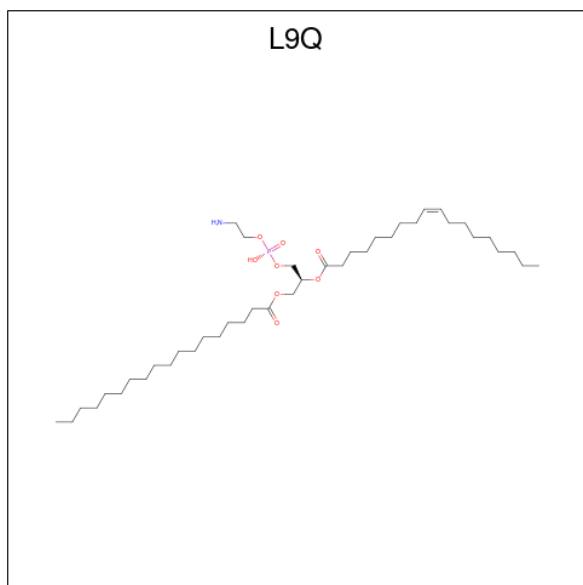
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	C	0
			12	12	
3	A	1	Total	C	0
			12	12	
3	B	1	Total	C	0
			12	12	
3	B	1	Total	C	0
			12	12	
3	D	1	Total	C	0
			12	12	
3	D	1	Total	C	0
			12	12	
3	C	1	Total	C	0
			12	12	
3	C	1	Total	C	0
			12	12	
3	C	1	Total	C	0
			12	12	
3	E	1	Total	C	0
			12	12	
3	E	1	Total	C	0
			12	12	
3	E	1	Total	C	0
			12	12	
3	F	1	Total	C	0
			12	12	
3	F	1	Total	C	0
			12	12	

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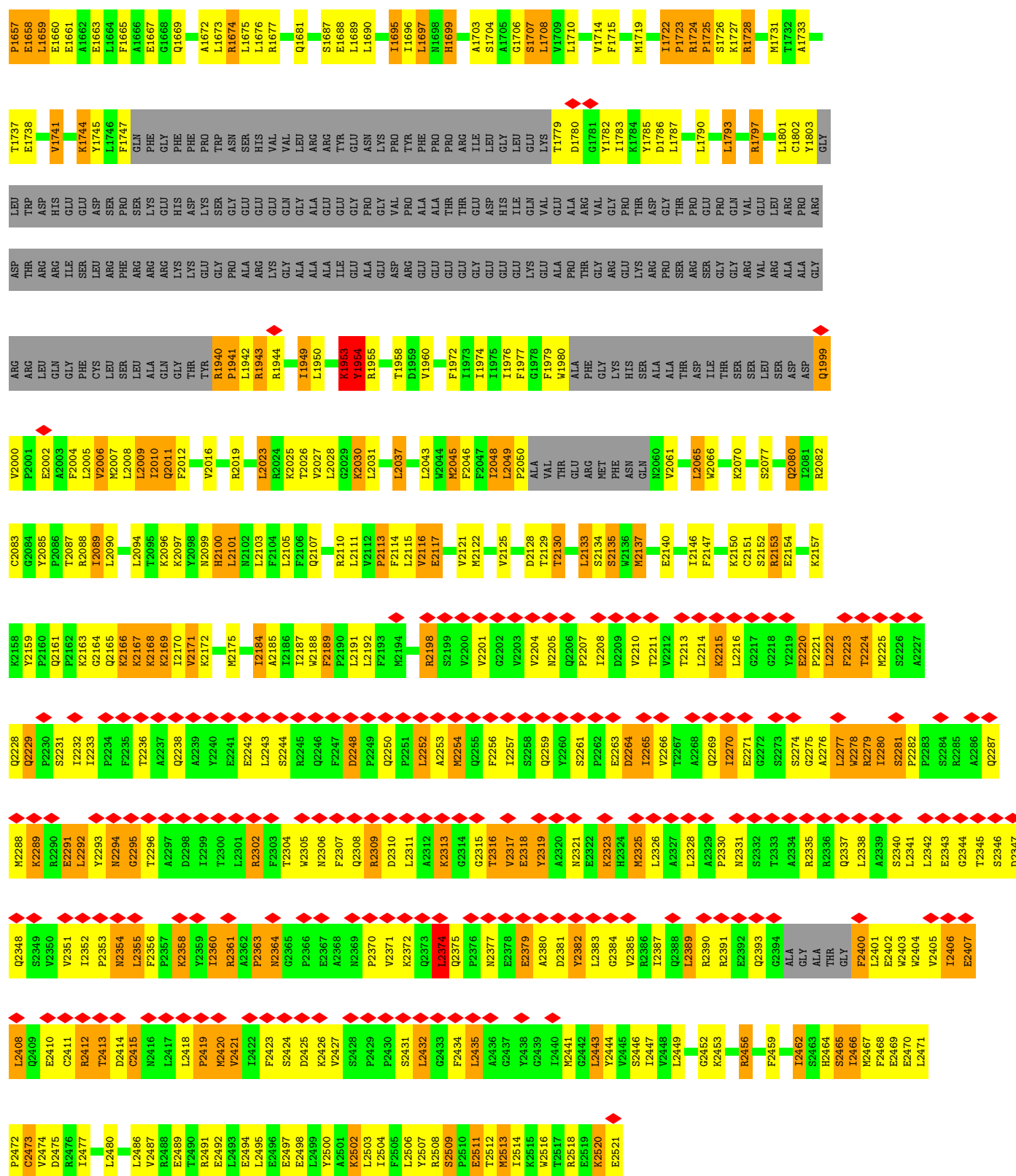
Mol	Chain	Residues	Atoms		AltConf
3	F	1	Total	C	0
			12	12	

- Molecule 4 is (1S)-2-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(octadecanoyloxymethyl)ethyl (9Z)-octadec-9-enoate (CCD ID: L9Q) (formula: C₄₁H₈₀NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	D	1	Total	C	N	O	P	0
			51	41	1	8	1	





• Molecule 1: Piezo-type mechanosensitive ion channel component 1

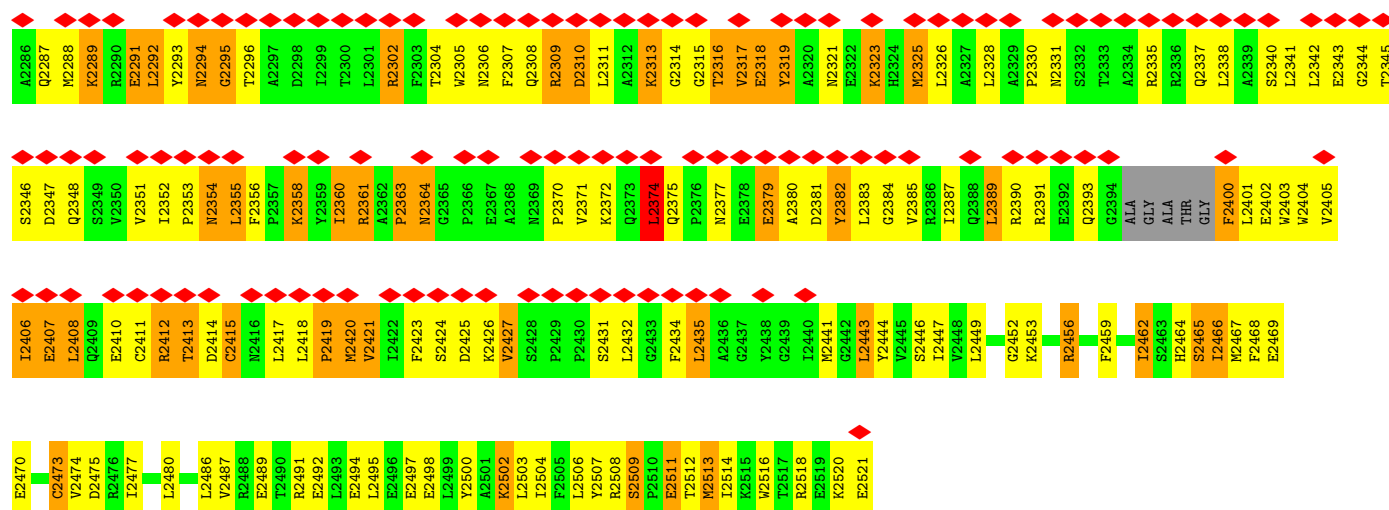






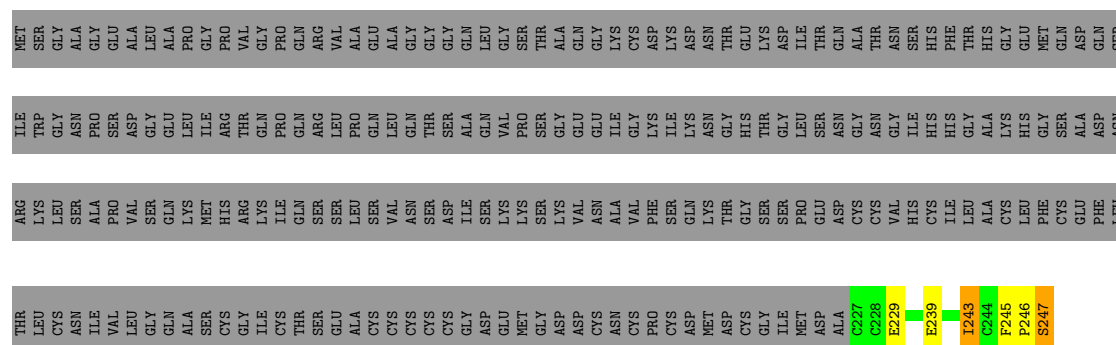






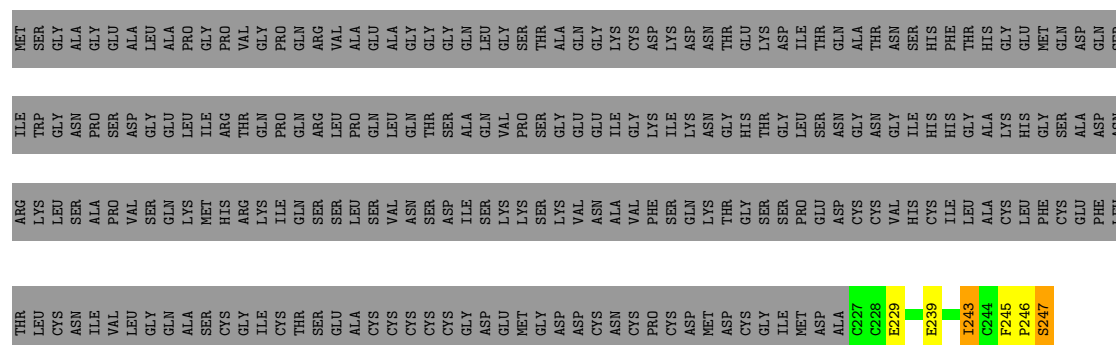
• Molecule 2: MyoD family inhibitor domain-containing protein

Chain C: 6% .. 91%



• Molecule 2: MyoD family inhibitor domain-containing protein

Chain E: 6% .. 91%



• Molecule 2: MyoD family inhibitor domain-containing protein

Chain F: 6% .. 91%



THR	ARG	ILE
LEU	LYS	TRP
CYS	LEU	GLY
ASN	SER	ASN
ILE	ALA	PRO
VAL	PRO	SER
LEU	VAL	ASP
GLY	SER	GLY
GLN	SER	GLN
ALA	LYS	LEU
ALA	SER	ILE
CYS	HIS	ARG
GLY	ARG	THR
ILE	LYS	GLN
CYS	ILE	PRO
THR	GLN	GLN
SER	SER	ARG
GLU	SER	LEU
ALA	LEU	PRO
CYS	SER	GLN
CYS	VAL	LEU
CYS	ASN	GLN
CYS	SER	THR
CYS	ASP	SER
GLY	ILE	ALA
ASP	SER	GLN
GLU	LYS	VAL
MET	LYS	GLY
ASN	ASN	GLU
CYS	ALA	ILE
PRO	VAL	GLY
CYS	PHE	LYS
ASP	SER	ILE
ASP	GLN	LYS
MET	LYS	ASN
ASP	THR	GLY
CYS	GLY	HIS
ILE	SER	THR
ILE	SER	GLY
MET	PRO	LEU
ASP	GLU	SER
ALA	ASP	ASN
C227	CYS	GLY
C228	CYS	ASN
E229	VAL	GLY
E239	HIS	ILE
E239	CYS	HIS
E239	ILE	HIS
E239	LEU	GLY
I243	ALA	ALA
C244	CYS	LYS
F245	LEU	HIS
P246	PHE	GLY
S247	CYS	SER
S247	GLU	ALA
S247	PHE	ASP
S247	LEU	ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40207	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI 10	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.385	Depositor
Minimum map value	-0.227	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	456.0, 456.0, 456.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.57, 0.57, 0.57	Depositor

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: D12, L9Q

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	0.55	2/10719 (0.0%)	0.91	51/14526 (0.4%)
1	B	0.55	2/10719 (0.0%)	0.96	53/14526 (0.4%)
1	D	0.55	2/10719 (0.0%)	0.91	51/14526 (0.4%)
2	C	0.71	0/151	1.16	0/200
2	E	0.71	0/151	1.16	0/200
2	F	0.70	0/151	1.16	0/200
All	All	0.55	6/32610 (0.0%)	0.93	155/44178 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1160	VAL	CA-CB	6.03	1.62	1.54
1	A	1160	VAL	CA-CB	6.02	1.62	1.54
1	B	1160	VAL	CA-CB	6.00	1.62	1.54
1	D	2289	LYS	C-N	-5.10	1.27	1.33
1	B	2289	LYS	C-N	-5.09	1.27	1.33
1	A	2289	LYS	C-N	-5.06	1.27	1.33

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	584	CYS	CA-CB-SG	-35.48	29.68	104.20
1	B	930	GLN	N-CA-C	11.20	126.52	113.19
1	A	930	GLN	N-CA-C	11.19	126.51	113.19
1	D	930	GLN	N-CA-C	11.19	126.51	113.19
1	D	2374	LEU	N-CA-C	-10.05	100.31	111.07
1	B	2374	LEU	N-CA-C	-10.03	100.33	111.07
1	A	2374	LEU	N-CA-C	-10.03	100.33	111.07
1	A	2415	CYS	N-CA-C	-9.75	101.05	113.72
1	D	2415	CYS	N-CA-C	-9.74	101.06	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2415	CYS	N-CA-C	-9.72	101.08	113.72
1	A	688	GLY	N-CA-C	-9.51	100.99	112.49
1	B	688	GLY	N-CA-C	-9.51	100.99	112.49
1	D	688	GLY	N-CA-C	-9.49	101.00	112.49
1	A	1785	TYR	N-CA-C	-9.42	101.31	113.17
1	D	1785	TYR	N-CA-C	-9.41	101.31	113.17
1	B	1785	TYR	N-CA-C	-9.40	101.33	113.17
1	A	987	ILE	N-CA-C	-9.34	101.29	110.72
1	B	987	ILE	N-CA-C	-9.32	101.30	110.72
1	D	987	ILE	N-CA-C	-9.32	101.30	110.72
1	A	686	VAL	CA-C-N	-9.09	110.42	119.87
1	A	686	VAL	C-N-CA	-9.09	110.42	119.87
1	B	686	VAL	CA-C-N	-9.08	110.43	119.87
1	B	686	VAL	C-N-CA	-9.08	110.43	119.87
1	D	686	VAL	CA-C-N	-9.07	110.43	119.87
1	D	686	VAL	C-N-CA	-9.07	110.43	119.87
1	A	680	LEU	N-CA-C	-8.82	101.35	110.97
1	D	680	LEU	N-CA-C	-8.80	101.37	110.97
1	B	680	LEU	N-CA-C	-8.80	101.38	110.97
1	D	1197	LEU	N-CA-C	-8.38	102.65	113.12
1	A	1197	LEU	N-CA-C	-8.37	102.65	113.12
1	B	1197	LEU	N-CA-C	-8.37	102.66	113.12
1	A	1551	THR	N-CA-C	-8.02	105.47	114.62
1	B	1551	THR	N-CA-C	-8.02	105.48	114.62
1	D	1551	THR	N-CA-C	-8.01	105.49	114.62
1	A	1115	VAL	N-CA-C	-6.96	106.12	111.62
1	B	2282	PRO	N-CA-C	6.96	119.19	110.70
1	D	2282	PRO	N-CA-C	6.95	119.18	110.70
1	A	2282	PRO	N-CA-C	6.95	119.18	110.70
1	B	1115	VAL	N-CA-C	-6.95	106.13	111.62
1	D	1115	VAL	N-CA-C	-6.93	106.14	111.62
1	B	702	HIS	N-CA-C	-6.72	103.77	112.23
1	D	702	HIS	N-CA-C	-6.71	103.78	112.23
1	A	702	HIS	N-CA-C	-6.71	103.78	112.23
1	D	608	PHE	N-CA-C	-6.70	103.78	112.23
1	B	608	PHE	N-CA-C	-6.70	103.79	112.23
1	A	1204	LEU	N-CA-C	-6.69	104.14	112.90
1	B	1204	LEU	N-CA-C	-6.69	104.14	112.90
1	A	608	PHE	N-CA-C	-6.68	103.81	112.23
1	D	1204	LEU	N-CA-C	-6.68	104.15	112.90
1	A	612	LEU	N-CA-C	-6.46	104.15	111.07
1	B	612	LEU	N-CA-C	-6.46	104.16	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	612	LEU	N-CA-C	-6.44	104.18	111.07
1	B	817	VAL	N-CA-C	-6.28	106.59	113.43
1	D	817	VAL	N-CA-C	-6.27	106.60	113.43
1	B	1317	THR	N-CA-C	-6.26	104.53	111.36
1	A	817	VAL	N-CA-C	-6.26	106.61	113.43
1	A	1317	THR	N-CA-C	-6.24	104.56	111.36
1	D	1317	THR	N-CA-C	-6.24	104.56	111.36
1	B	2277	LEU	CA-C-N	-6.23	111.88	123.03
1	B	2277	LEU	C-N-CA	-6.23	111.88	123.03
1	A	2277	LEU	CA-C-N	-6.22	111.89	123.03
1	A	2277	LEU	C-N-CA	-6.22	111.89	123.03
1	D	2277	LEU	CA-C-N	-6.21	111.91	123.03
1	D	2277	LEU	C-N-CA	-6.21	111.91	123.03
1	B	687	PRO	N-CA-C	6.11	121.55	114.03
1	A	687	PRO	N-CA-C	6.10	121.53	114.03
1	D	687	PRO	N-CA-C	6.09	121.52	114.03
1	D	1706	GLY	N-CA-C	-6.06	102.54	111.03
1	A	1706	GLY	N-CA-C	-6.04	102.58	111.03
1	B	1706	GLY	N-CA-C	-6.03	102.58	111.03
1	D	1304	SER	N-CA-C	-6.02	105.86	112.72
1	B	1304	SER	N-CA-C	-6.01	105.87	112.72
1	A	1304	SER	N-CA-C	-5.98	105.90	112.72
1	D	1703	ALA	N-CA-C	5.98	116.18	108.34
1	A	1703	ALA	N-CA-C	5.98	116.17	108.34
1	B	1703	ALA	N-CA-C	5.96	116.15	108.34
1	A	2130	THR	N-CA-C	-5.76	106.41	113.50
1	D	2130	THR	N-CA-C	-5.75	106.42	113.50
1	B	2130	THR	N-CA-C	-5.74	106.44	113.50
1	A	632	LEU	N-CA-C	-5.73	104.94	111.07
1	A	703	ARG	N-CA-C	5.73	120.55	112.75
1	D	703	ARG	N-CA-C	5.73	120.54	112.75
1	B	632	LEU	N-CA-C	-5.72	104.94	111.07
1	B	703	ARG	N-CA-C	5.72	120.53	112.75
1	D	632	LEU	N-CA-C	-5.71	104.96	111.07
1	D	591	VAL	N-CA-C	-5.70	103.80	111.44
1	D	1656	ILE	CA-C-N	-5.69	115.90	121.65
1	D	1656	ILE	C-N-CA	-5.69	115.90	121.65
1	A	2413	THR	N-CA-C	-5.69	104.55	113.02
1	B	2413	THR	N-CA-C	-5.68	104.56	113.02
1	A	1013	PHE	N-CA-C	-5.68	106.51	113.50
1	B	591	VAL	N-CA-C	-5.68	103.83	111.44
1	A	591	VAL	N-CA-C	-5.68	103.83	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2413	THR	N-CA-C	-5.67	104.57	113.02
1	D	1013	PHE	N-CA-C	-5.67	106.53	113.50
1	B	1656	ILE	CA-C-N	-5.66	115.93	121.65
1	B	1656	ILE	C-N-CA	-5.66	115.93	121.65
1	B	1013	PHE	N-CA-C	-5.66	106.54	113.50
1	A	1656	ILE	CA-C-N	-5.66	115.94	121.65
1	A	1656	ILE	C-N-CA	-5.66	115.94	121.65
1	D	923	PHE	CA-C-N	-5.59	114.50	120.03
1	D	923	PHE	C-N-CA	-5.59	114.50	120.03
1	A	923	PHE	CA-C-N	-5.59	114.50	120.03
1	A	923	PHE	C-N-CA	-5.59	114.50	120.03
1	D	1541	ASP	N-CA-C	-5.58	106.82	113.97
1	D	1657	PRO	CA-C-O	-5.58	117.08	121.38
1	A	1541	ASP	N-CA-C	-5.58	106.83	113.97
1	B	1541	ASP	N-CA-C	-5.57	106.84	113.97
1	B	923	PHE	CA-C-N	-5.57	114.52	120.03
1	B	923	PHE	C-N-CA	-5.57	114.52	120.03
1	A	1657	PRO	CA-C-O	-5.57	117.09	121.38
1	B	1657	PRO	CA-C-O	-5.55	117.10	121.38
1	D	841	CYS	N-CA-C	-5.53	105.15	111.07
1	B	841	CYS	N-CA-C	-5.51	105.17	111.07
1	A	841	CYS	N-CA-C	-5.51	105.17	111.07
1	D	2379	GLU	N-CA-C	-5.50	99.09	110.80
1	B	2379	GLU	N-CA-C	-5.49	99.12	110.80
1	A	2379	GLU	N-CA-C	-5.48	99.12	110.80
1	D	577	ALA	N-CA-C	-5.47	106.11	112.89
1	B	577	ALA	N-CA-C	-5.46	106.12	112.89
1	A	577	ALA	N-CA-C	-5.45	106.13	112.89
1	B	1016	THR	N-CA-C	-5.41	105.54	111.82
1	A	1016	THR	N-CA-C	-5.40	105.55	111.82
1	D	1016	THR	N-CA-C	-5.38	105.58	111.82
1	D	1037	LEU	N-CA-C	-5.36	106.79	113.38
1	A	1037	LEU	N-CA-C	-5.36	106.79	113.38
1	B	1037	LEU	N-CA-C	-5.35	106.80	113.38
1	B	2264	ASP	N-CA-C	-5.32	103.41	111.34
1	D	1554	LEU	CB-CA-C	-5.32	110.42	116.54
1	A	2264	ASP	N-CA-C	-5.32	103.42	111.34
1	B	1554	LEU	CB-CA-C	-5.31	110.43	116.54
1	A	1554	LEU	CB-CA-C	-5.31	110.43	116.54
1	D	2264	ASP	N-CA-C	-5.31	103.43	111.34
1	D	2412	ARG	N-CA-C	-5.23	104.59	111.96
1	B	1055	LEU	N-CA-C	-5.22	107.04	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2412	ARG	N-CA-C	-5.21	104.62	111.96
1	B	2412	ARG	N-CA-C	-5.21	104.62	111.96
1	D	1055	LEU	N-CA-C	-5.21	107.06	113.41
1	B	607	LEU	N-CA-C	-5.20	106.78	113.23
1	A	607	LEU	N-CA-C	-5.19	106.79	113.23
1	A	1055	LEU	N-CA-C	-5.19	107.08	113.41
1	B	2233	ILE	N-CA-C	5.18	113.14	107.60
1	A	2233	ILE	N-CA-C	5.18	113.14	107.60
1	D	607	LEU	N-CA-C	-5.18	106.81	113.23
1	D	2233	ILE	N-CA-C	5.17	113.13	107.60
1	B	1953	LYS	N-CA-C	5.08	121.63	110.80
1	A	1953	LYS	N-CA-C	5.08	121.62	110.80
1	D	1953	LYS	N-CA-C	5.08	121.62	110.80
1	A	2337	GLN	N-CA-C	-5.03	105.88	111.36
1	D	1363	LYS	N-CA-C	-5.03	105.90	112.23
1	B	2337	GLN	N-CA-C	-5.02	105.89	111.36
1	B	1545	ALA	N-CA-C	-5.02	105.89	111.36
1	A	1363	LYS	N-CA-C	-5.01	105.92	112.23
1	D	2337	GLN	N-CA-C	-5.01	105.90	111.36
1	B	1363	LYS	N-CA-C	-5.01	105.92	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10463	0	10689	610	0
1	B	10463	0	10689	603	0
1	D	10463	0	10689	603	0
2	C	150	0	132	11	0
2	E	150	0	132	12	0
2	F	150	0	132	11	0
3	A	24	0	52	3	0
3	B	24	0	52	4	0
3	C	36	0	78	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	24	0	52	4	0
3	E	36	0	78	10	0
3	F	36	0	78	8	0
4	A	51	0	79	8	0
4	B	51	0	79	9	0
4	D	51	0	79	8	0
All	All	32172	0	33090	1679	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 26.

All (1679) 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:A:2459:PHE:CD1	1:D:2137:MET:HE2	1.54	1.42
1:B:2137:MET:HE2	1:D:2459:PHE:CD1	1.54	1.39
1:D:1650:LEU:CD2	1:D:1654:LEU:HD12	1.53	1.39
1:A:2137:MET:HE2	1:B:2459:PHE:CD1	1.54	1.38
1:B:1650:LEU:CD2	1:B:1654:LEU:HD12	1.53	1.38
1:A:1650:LEU:CD2	1:A:1654:LEU:HD12	1.53	1.36
1:A:1695:ILE:HD11	1:A:1714:VAL:CG2	1.55	1.36
1:D:1695:ILE:HD11	1:D:1714:VAL:CG2	1.55	1.35
1:B:2507:TYR:CB	1:D:2466:ILE:HD11	1.58	1.34
1:B:1695:ILE:HD11	1:B:1714:VAL:CG2	1.55	1.33
1:A:2466:ILE:HD11	1:D:2507:TYR:CB	1.58	1.33
1:A:2507:TYR:CB	1:B:2466:ILE:HD11	1.58	1.32
1:A:1695:ILE:CD1	1:A:1714:VAL:HG21	1.59	1.32
1:B:1695:ILE:CD1	1:B:1714:VAL:HG21	1.59	1.31
1:D:1695:ILE:CD1	1:D:1714:VAL:HG21	1.59	1.30
1:D:2443:LEU:HD21	1:D:2447:ILE:CD1	1.63	1.28
1:A:2443:LEU:HD21	1:A:2447:ILE:CD1	1.63	1.28
1:A:2459:PHE:CG	1:D:2137:MET:HE2	1.70	1.27
1:B:2443:LEU:HD21	1:B:2447:ILE:CD1	1.63	1.27
1:B:2137:MET:HE2	1:D:2459:PHE:CG	1.70	1.25
1:A:2137:MET:HE2	1:B:2459:PHE:CG	1.70	1.25
1:B:2443:LEU:CD2	1:B:2443:LEU:C	2.10	1.23
1:A:2443:LEU:C	1:A:2443:LEU:CD2	2.10	1.22
1:B:2323:LYS:NZ	1:B:2323:LYS:CB	2.01	1.22
1:D:2443:LEU:C	1:D:2443:LEU:CD2	2.10	1.22
1:D:2323:LYS:HB3	1:D:2323:LYS:NZ	1.11	1.21
1:B:2133:LEU:CD1	2:C:243:ILE:HD11	1.71	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2323:LYS:HZ3	1:D:2323:LYS:CB	1.50	1.21
1:A:2133:LEU:CD1	2:F:243:ILE:HD11	1.71	1.20
1:D:2133:LEU:CD1	2:E:243:ILE:HD11	1.71	1.20
1:B:2323:LYS:NZ	1:B:2323:LYS:HB3	1.11	1.19
1:D:2323:LYS:NZ	1:D:2323:LYS:CB	2.01	1.18
1:A:2012:PHE:CE2	1:B:2184:ILE:HD11	1.79	1.17
1:B:2012:PHE:CE2	1:D:2184:ILE:HD11	1.79	1.17
1:D:2048:ILE:N	1:D:2048:ILE:HD13	1.56	1.16
1:A:2184:ILE:HD11	1:D:2012:PHE:CE2	1.79	1.16
1:B:1515:TRP:CE3	1:B:1516:MET:HE2	1.80	1.16
1:D:1515:TRP:CE3	1:D:1516:MET:HE2	1.80	1.16
1:A:1515:TRP:CE3	1:A:1516:MET:HE2	1.80	1.16
1:B:2443:LEU:C	1:B:2443:LEU:HD22	1.69	1.15
1:A:2323:LYS:NZ	1:A:2323:LYS:HB3	1.11	1.15
1:A:2089:ILE:HD13	1:A:2089:ILE:H	1.01	1.15
1:D:1057:LEU:HG	1:D:1058:GLY:H	1.09	1.15
1:B:2048:ILE:H	1:B:2048:ILE:CD1	1.55	1.15
1:B:1052:GLN:HB3	1:B:1099:LEU:HD11	1.19	1.14
1:D:1052:GLN:HB3	1:D:1099:LEU:HD11	1.19	1.14
1:A:1057:LEU:HG	1:A:1058:GLY:H	1.09	1.14
1:A:2323:LYS:NZ	1:A:2323:LYS:CB	2.01	1.14
1:B:2048:ILE:HD13	1:B:2048:ILE:N	1.56	1.13
1:A:2443:LEU:C	1:A:2443:LEU:HD22	1.69	1.13
1:B:1699:HIS:NE2	1:B:1708:LEU:HD12	1.64	1.12
1:D:2048:ILE:H	1:D:2048:ILE:CD1	1.56	1.12
1:A:2443:LEU:HD21	1:A:2447:ILE:HD12	1.16	1.11
1:A:2358:LYS:HG3	1:A:2383:LEU:HD22	1.31	1.11
1:D:2045:MET:O	1:D:2048:ILE:HD12	1.50	1.11
1:A:1699:HIS:NE2	1:A:1708:LEU:HD12	1.64	1.11
1:A:2166:LYS:HE3	1:D:2128:ASP:HB3	1.32	1.10
1:D:2080:GLN:HA	1:D:2080:GLN:HE21	1.09	1.10
1:A:2045:MET:O	1:A:2048:ILE:HD12	1.50	1.10
1:A:1052:GLN:HB3	1:A:1099:LEU:HD11	1.19	1.10
1:A:2048:ILE:H	1:A:2048:ILE:CD1	1.55	1.10
1:A:2128:ASP:HB3	1:B:2166:LYS:HE3	1.32	1.09
1:D:1699:HIS:NE2	1:D:1708:LEU:HD12	1.64	1.09
1:B:2128:ASP:HB3	1:D:2166:LYS:HE3	1.32	1.09
1:B:2323:LYS:CB	1:B:2323:LYS:HZ3	1.61	1.09
1:A:2048:ILE:HD13	1:A:2048:ILE:N	1.56	1.09
1:B:1568:LEU:O	1:B:1653:ARG:HB3	1.53	1.09
1:D:635:ALA:O	1:D:639:LEU:HD12	1.53	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1568:LEU:O	1:D:1653:ARG:HB3	1.53	1.09
1:D:2443:LEU:C	1:D:2443:LEU:HD22	1.69	1.09
1:B:2089:ILE:HD13	1:B:2089:ILE:H	1.01	1.09
1:B:2443:LEU:HD21	1:B:2447:ILE:HD12	1.16	1.09
1:D:2089:ILE:HD13	1:D:2089:ILE:H	1.01	1.08
1:A:635:ALA:O	1:A:639:LEU:HD12	1.53	1.08
1:A:1057:LEU:HG	1:A:1058:GLY:N	1.59	1.08
1:B:635:ALA:O	1:B:639:LEU:HD12	1.53	1.08
1:B:2045:MET:O	1:B:2048:ILE:HD12	1.50	1.08
1:D:2443:LEU:HD21	1:D:2447:ILE:HD12	1.16	1.08
1:A:1515:TRP:CE3	1:A:1516:MET:CE	2.36	1.08
1:A:1568:LEU:O	1:A:1653:ARG:HB3	1.53	1.08
1:D:1515:TRP:CE3	1:D:1516:MET:CE	2.36	1.08
1:B:2358:LYS:HG3	1:B:2383:LEU:HD22	1.31	1.08
1:B:1057:LEU:HG	1:B:1058:GLY:H	1.09	1.07
1:B:2252:LEU:O	1:B:2256:PHE:HD1	1.37	1.07
1:B:1515:TRP:CE3	1:B:1516:MET:CE	2.36	1.07
1:D:1057:LEU:HG	1:D:1058:GLY:N	1.59	1.07
1:A:2466:ILE:CD1	1:D:2507:TYR:HB3	1.84	1.07
1:A:2507:TYR:HB3	1:B:2466:ILE:CD1	1.84	1.07
1:B:2080:GLN:HE21	1:B:2080:GLN:HA	1.09	1.07
1:D:1160:VAL:HA	1:D:1550:LEU:HD21	1.35	1.07
1:D:2358:LYS:HG3	1:D:2383:LEU:HD22	1.31	1.07
1:D:2443:LEU:O	1:D:2443:LEU:HD23	1.53	1.07
1:A:2443:LEU:O	1:A:2443:LEU:HD23	1.53	1.06
1:D:2252:LEU:O	1:D:2256:PHE:HD1	1.37	1.06
1:B:2443:LEU:HD23	1:B:2443:LEU:O	1.53	1.06
1:D:1733:ALA:O	1:D:1737:THR:HG23	1.56	1.06
1:A:2252:LEU:O	1:A:2256:PHE:HD1	1.37	1.05
1:B:2507:TYR:HB3	1:D:2466:ILE:CD1	1.84	1.05
1:A:2080:GLN:HE21	1:A:2080:GLN:HA	1.09	1.05
1:B:1057:LEU:HG	1:B:1058:GLY:N	1.59	1.05
1:B:1733:ALA:O	1:B:1737:THR:HG23	1.56	1.05
1:A:1650:LEU:HD22	1:A:1654:LEU:HD12	1.39	1.04
1:B:1737:THR:O	1:B:1741:VAL:HG23	1.57	1.04
1:A:1160:VAL:HA	1:A:1550:LEU:HD21	1.35	1.04
1:B:2443:LEU:CD2	1:B:2447:ILE:HD12	1.86	1.04
1:D:2443:LEU:CD2	1:D:2447:ILE:HD12	1.86	1.03
1:A:2443:LEU:CD2	1:A:2447:ILE:HD12	1.86	1.03
1:D:1737:THR:O	1:D:1741:VAL:HG23	1.57	1.03
1:D:2261:SER:O	1:D:2264:ASP:HB2	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1733:ALA:O	1:A:1737:THR:HG23	1.56	1.03
1:A:2468:PHE:CD2	1:B:2464:HIS:ND1	2.27	1.03
1:A:2358:LYS:HZ3	1:A:2383:LEU:HD21	1.17	1.03
1:B:1160:VAL:HA	1:B:1550:LEU:HD21	1.35	1.03
1:B:2468:PHE:CD2	1:D:2464:HIS:ND1	2.27	1.03
1:D:1516:MET:HA	1:D:1519:GLN:OE1	1.59	1.02
1:A:1516:MET:HA	1:A:1519:GLN:OE1	1.59	1.02
1:B:2261:SER:O	1:B:2264:ASP:HB2	1.58	1.02
1:D:1650:LEU:HD22	1:D:1654:LEU:HD12	1.39	1.02
1:A:1515:TRP:CZ3	1:A:1516:MET:HE1	1.95	1.02
1:A:2464:HIS:ND1	1:D:2468:PHE:CD2	2.27	1.02
1:B:1516:MET:HA	1:B:1519:GLN:OE1	1.59	1.02
1:A:1737:THR:O	1:A:1741:VAL:HG23	1.57	1.02
1:B:1650:LEU:CD2	1:B:1654:LEU:CD1	2.39	1.01
1:D:1515:TRP:CZ3	1:D:1516:MET:HE1	1.95	1.01
1:A:2137:MET:CE	1:B:2459:PHE:CD1	2.43	1.01
1:B:2137:MET:CE	1:D:2459:PHE:CD1	2.43	1.01
1:B:2507:TYR:CB	1:D:2466:ILE:CD1	2.38	1.01
1:A:2261:SER:O	1:A:2264:ASP:HB2	1.58	1.01
1:B:1515:TRP:CZ3	1:B:1516:MET:HE1	1.95	1.01
1:D:1650:LEU:CD2	1:D:1654:LEU:CD1	2.39	1.01
1:A:2128:ASP:CB	1:B:2166:LYS:HE3	1.91	1.00
1:A:2459:PHE:CD1	1:D:2137:MET:CE	2.43	1.00
1:A:2466:ILE:CD1	1:D:2507:TYR:CB	2.38	1.00
1:B:2128:ASP:CB	1:D:2166:LYS:HE3	1.91	1.00
1:A:2466:ILE:HD11	1:D:2507:TYR:HB3	1.02	1.00
1:A:2507:TYR:HB3	1:B:2466:ILE:HD11	1.02	1.00
1:A:2166:LYS:HE3	1:D:2128:ASP:CB	1.91	1.00
1:D:587:MET:HE2	1:D:587:MET:N	1.77	1.00
1:A:2507:TYR:CB	1:B:2466:ILE:CD1	2.38	0.99
1:B:1650:LEU:HD22	1:B:1654:LEU:HD12	1.40	0.99
1:B:2443:LEU:HD22	1:B:2444:TYR:N	1.78	0.99
1:A:1650:LEU:CD2	1:A:1654:LEU:CD1	2.39	0.99
1:A:2323:LYS:CB	1:A:2323:LYS:HZ3	1.66	0.99
1:B:2507:TYR:HB3	1:D:2466:ILE:HD11	1.02	0.99
1:D:1695:ILE:CD1	1:D:1714:VAL:CG2	2.29	0.99
1:A:1161:ALA:HA	1:A:1165:TYR:CE2	1.98	0.99
1:A:2443:LEU:HD22	1:A:2444:TYR:N	1.78	0.98
1:B:2265:ILE:HD11	1:B:2423:PHE:CD2	1.98	0.98
1:A:587:MET:N	1:A:587:MET:HE2	1.77	0.98
1:B:2089:ILE:H	1:B:2089:ILE:CD1	1.77	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:MET:HE2	1:B:587:MET:N	1.77	0.98
1:B:1161:ALA:HA	1:B:1165:TYR:CE2	1.98	0.98
1:B:2265:ILE:CD1	1:B:2423:PHE:CD2	2.47	0.98
1:B:2358:LYS:HZ3	1:B:2383:LEU:HD21	1.24	0.98
1:D:2443:LEU:HD22	1:D:2444:TYR:N	1.78	0.97
1:D:2265:ILE:CD1	1:D:2423:PHE:CD2	2.47	0.97
1:A:2265:ILE:HD11	1:A:2423:PHE:CD2	1.98	0.97
1:A:2265:ILE:CD1	1:A:2423:PHE:CD2	2.47	0.97
1:D:2089:ILE:H	1:D:2089:ILE:CD1	1.77	0.97
1:D:1161:ALA:HA	1:D:1165:TYR:CE2	1.98	0.97
1:D:2265:ILE:HD11	1:D:2423:PHE:CD2	1.98	0.97
1:A:2133:LEU:HD12	2:F:243:ILE:HD11	1.45	0.97
1:A:586:GLY:C	1:A:587:MET:HE2	1.90	0.97
1:A:2265:ILE:HD13	1:A:2423:PHE:CG	2.00	0.97
1:D:1699:HIS:CE1	1:D:1708:LEU:HD12	2.00	0.97
1:B:2265:ILE:HD13	1:B:2423:PHE:CG	2.00	0.96
1:B:1695:ILE:CD1	1:B:1714:VAL:CG2	2.28	0.96
1:D:2358:LYS:HZ3	1:D:2383:LEU:HD21	1.27	0.96
1:A:1699:HIS:CE1	1:A:1708:LEU:HD12	2.00	0.96
1:B:2133:LEU:HD12	2:C:243:ILE:HD11	1.45	0.96
1:B:1699:HIS:CE1	1:B:1708:LEU:HD12	2.00	0.95
1:B:586:GLY:C	1:B:587:MET:HE2	1.90	0.95
1:A:2089:ILE:H	1:A:2089:ILE:CD1	1.77	0.95
1:D:2265:ILE:HD13	1:D:2423:PHE:CG	2.00	0.95
1:D:586:GLY:C	1:D:587:MET:HE2	1.90	0.95
1:A:2133:LEU:HD13	2:F:243:ILE:HD11	1.48	0.95
1:A:2358:LYS:O	1:A:2421:VAL:HG23	1.67	0.95
1:D:2443:LEU:C	1:D:2443:LEU:HD23	1.90	0.94
1:A:1695:ILE:CD1	1:A:1714:VAL:CG2	2.29	0.94
1:B:2323:LYS:HB3	1:B:2323:LYS:HZ2	1.21	0.94
1:A:2323:LYS:HB3	1:A:2323:LYS:HZ2	1.17	0.94
1:D:2133:LEU:HD12	2:E:243:ILE:HD11	1.45	0.94
1:B:1160:VAL:HA	1:B:1550:LEU:CD2	1.98	0.94
1:D:1160:VAL:HA	1:D:1550:LEU:CD2	1.98	0.94
1:D:2358:LYS:O	1:D:2421:VAL:HG23	1.67	0.94
1:A:1699:HIS:ND1	1:A:1707:SER:HB2	1.83	0.94
1:D:1699:HIS:ND1	1:D:1707:SER:HB2	1.83	0.94
1:A:1052:GLN:HB3	1:A:1099:LEU:CD1	1.97	0.93
1:B:2358:LYS:O	1:B:2421:VAL:HG23	1.67	0.93
1:B:1052:GLN:HB3	1:B:1099:LEU:CD1	1.97	0.93
1:D:1052:GLN:HB3	1:D:1099:LEU:CD1	1.97	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2133:LEU:CD1	2:F:243:ILE:CD1	2.47	0.93
1:A:2184:ILE:HD11	1:D:2012:PHE:HE2	1.30	0.93
1:A:1160:VAL:HA	1:A:1550:LEU:CD2	1.98	0.93
1:D:2048:ILE:HD13	1:D:2048:ILE:H	0.76	0.92
1:B:2133:LEU:CD1	2:C:243:ILE:CD1	2.47	0.92
1:B:1699:HIS:ND1	1:B:1707:SER:HB2	1.83	0.92
1:B:2358:LYS:NZ	1:B:2383:LEU:CD2	2.33	0.92
1:A:2358:LYS:HZ3	1:A:2383:LEU:CD2	1.82	0.92
1:B:2048:ILE:H	1:B:2048:ILE:HD13	0.76	0.92
1:D:2133:LEU:CD1	2:E:243:ILE:CD1	2.47	0.92
1:B:2133:LEU:HD13	2:C:243:ILE:HD11	1.48	0.92
1:A:2168:LYS:HB3	1:A:2171:VAL:HG23	1.52	0.91
1:B:2089:ILE:HD13	1:B:2089:ILE:N	1.84	0.91
1:D:2089:ILE:HD13	1:D:2089:ILE:N	1.84	0.91
1:A:2443:LEU:HD21	1:A:2447:ILE:HD11	1.52	0.91
1:A:2443:LEU:CD2	1:A:2447:ILE:CD1	2.47	0.91
1:B:2168:LYS:HB3	1:B:2171:VAL:HG23	1.52	0.91
1:D:2168:LYS:HB3	1:D:2171:VAL:HG23	1.52	0.91
1:D:2358:LYS:NZ	1:D:2383:LEU:CD2	2.33	0.91
1:D:2443:LEU:HD21	1:D:2447:ILE:HD11	1.52	0.91
1:B:2443:LEU:CD2	1:B:2447:ILE:CD1	2.47	0.91
1:D:2133:LEU:HD13	2:E:243:ILE:HD11	1.48	0.91
1:B:2443:LEU:HD21	1:B:2447:ILE:HD11	1.52	0.91
1:D:600:TYR:OH	1:D:644:VAL:HG11	1.71	0.90
1:A:2358:LYS:NZ	1:A:2383:LEU:CD2	2.33	0.90
1:B:1999:GLN:HB2	1:B:2050:PRO:C	1.97	0.90
1:B:2252:LEU:O	1:B:2256:PHE:CD1	2.25	0.90
1:A:2252:LEU:O	1:A:2256:PHE:CD1	2.25	0.90
1:B:600:TYR:OH	1:B:644:VAL:HG11	1.71	0.90
1:B:2133:LEU:HD13	2:C:243:ILE:CD1	2.02	0.90
1:A:2089:ILE:HD13	1:A:2089:ILE:N	1.84	0.90
1:A:1052:GLN:CB	1:A:1099:LEU:HD11	2.01	0.89
1:D:2323:LYS:HB3	1:D:2323:LYS:HZ2	1.31	0.89
1:A:1999:GLN:HB2	1:A:2050:PRO:C	1.97	0.89
1:A:2012:PHE:HE2	1:B:2184:ILE:HD11	1.31	0.89
1:B:924:PRO:HG2	1:B:928:TYR:HB2	1.55	0.89
1:B:1052:GLN:CB	1:B:1099:LEU:HD11	2.01	0.89
1:A:2048:ILE:H	1:A:2048:ILE:HD13	0.75	0.89
1:D:1999:GLN:HB2	1:D:2050:PRO:C	1.97	0.89
1:D:2252:LEU:O	1:D:2256:PHE:CD1	2.25	0.89
1:A:2150:LYS:HE3	1:A:2475:ASP:OD1	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1052:GLN:CB	1:D:1099:LEU:HD11	2.02	0.89
1:A:2133:LEU:HD13	2:F:243:ILE:CD1	2.02	0.89
1:D:2150:LYS:HE3	1:D:2475:ASP:OD1	1.73	0.88
1:A:600:TYR:OH	1:A:644:VAL:HG11	1.71	0.88
1:B:2150:LYS:HE3	1:B:2475:ASP:OD1	1.73	0.88
1:B:2443:LEU:CD2	1:B:2443:LEU:O	2.16	0.88
1:B:2443:LEU:C	1:B:2443:LEU:HD23	1.90	0.88
1:A:2137:MET:HE2	1:B:2459:PHE:CE1	2.08	0.88
1:A:2358:LYS:CG	1:A:2383:LEU:HD22	2.04	0.88
1:A:924:PRO:HG2	1:A:928:TYR:HB2	1.55	0.87
1:A:1650:LEU:HD23	1:A:1654:LEU:HD12	1.56	0.87
1:A:2167:LYS:HE3	1:A:2167:LYS:HA	1.56	0.87
1:A:2459:PHE:CE1	1:D:2137:MET:HE2	2.08	0.87
1:B:2137:MET:HE2	1:D:2459:PHE:CE1	2.08	0.87
1:D:2133:LEU:HD13	2:E:243:ILE:CD1	2.02	0.87
1:B:2265:ILE:CD1	1:B:2423:PHE:CG	2.58	0.87
1:D:1650:LEU:HD23	1:D:1654:LEU:HD12	1.56	0.87
1:A:2265:ILE:CD1	1:A:2423:PHE:CG	2.58	0.87
1:D:2302:ARG:HB3	1:D:2323:LYS:HZ2	1.38	0.87
1:A:2443:LEU:CD2	1:A:2443:LEU:O	2.16	0.86
1:D:2265:ILE:CD1	1:D:2423:PHE:CG	2.58	0.86
1:B:2012:PHE:HE2	1:D:2184:ILE:HD11	1.31	0.86
1:B:2358:LYS:CG	1:B:2383:LEU:HD22	2.04	0.86
1:D:2358:LYS:CG	1:D:2383:LEU:HD22	2.04	0.86
1:D:2167:LYS:HE3	1:D:2167:LYS:HA	1.56	0.86
1:D:924:PRO:HG2	1:D:928:TYR:HB2	1.55	0.86
1:A:2302:ARG:HB2	1:A:2323:LYS:HZ1	1.40	0.86
1:B:2128:ASP:CG	1:D:2166:LYS:HE3	2.01	0.85
1:A:626:LEU:O	1:A:626:LEU:HD22	1.77	0.85
1:B:2302:ARG:HB2	1:B:2323:LYS:HZ1	1.42	0.85
1:D:2443:LEU:CD2	1:D:2447:ILE:CD1	2.47	0.85
1:B:626:LEU:HD22	1:B:626:LEU:O	1.77	0.85
1:B:2167:LYS:HA	1:B:2167:LYS:HE3	1.56	0.85
1:A:2166:LYS:HE3	1:D:2128:ASP:CG	2.01	0.84
3:F:301:D12:H82	3:F:303:D12:H61	1.60	0.84
1:D:626:LEU:O	1:D:626:LEU:HD22	1.77	0.84
1:A:627:LYS:HE3	1:A:627:LYS:HA	1.60	0.84
1:D:2080:GLN:HA	1:D:2080:GLN:NE2	1.91	0.84
1:B:1515:TRP:HE3	1:B:1516:MET:HE2	1.43	0.84
1:A:2128:ASP:CG	1:B:2166:LYS:HE3	2.01	0.84
1:B:1650:LEU:HD23	1:B:1654:LEU:HD12	1.56	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1650:LEU:HD21	1:A:1654:LEU:HD12	1.59	0.83
3:C:301:D12:H82	3:C:303:D12:H61	1.60	0.83
1:A:2080:GLN:HE21	1:A:2080:GLN:CA	1.92	0.83
1:B:2358:LYS:HZ3	1:B:2383:LEU:CD2	1.92	0.83
1:D:1650:LEU:HD21	1:D:1654:LEU:HD12	1.59	0.82
1:B:2130:THR:HA	1:D:2166:LYS:O	1.80	0.82
1:B:1650:LEU:HD21	1:B:1654:LEU:HD12	1.59	0.82
1:D:2443:LEU:CD2	1:D:2443:LEU:O	2.16	0.82
3:E:301:D12:H82	3:E:303:D12:H61	1.60	0.82
1:B:627:LYS:HE3	1:B:627:LYS:HA	1.60	0.82
1:D:2213:THR:HG23	1:D:2224:THR:HG23	1.62	0.82
1:D:627:LYS:HE3	1:D:627:LYS:HA	1.60	0.82
1:A:2130:THR:HA	1:B:2166:LYS:O	1.80	0.82
1:A:2323:LYS:CB	1:A:2323:LYS:HZ2	1.79	0.82
1:B:2302:ARG:HB3	1:B:2323:LYS:HZ2	1.45	0.82
1:A:847:LYS:HD2	1:A:928:TYR:HE2	1.45	0.82
1:B:2080:GLN:HE21	1:B:2080:GLN:CA	1.92	0.82
1:D:2080:GLN:HE21	1:D:2080:GLN:CA	1.92	0.81
1:B:2468:PHE:HD2	1:D:2464:HIS:ND1	1.77	0.81
1:D:847:LYS:HD2	1:D:928:TYR:HE2	1.45	0.81
1:A:1515:TRP:HE3	1:A:1516:MET:HE2	1.43	0.81
1:A:2464:HIS:ND1	1:D:2468:PHE:HD2	1.77	0.81
1:D:1529:LEU:O	1:D:1533:THR:HG23	1.80	0.81
1:B:2167:LYS:CG	1:B:2167:LYS:O	2.29	0.81
1:A:1529:LEU:O	1:A:1533:THR:HG23	1.80	0.81
1:A:2443:LEU:C	1:A:2443:LEU:HD23	1.90	0.81
1:A:2166:LYS:O	1:D:2130:THR:HA	1.80	0.81
1:A:2167:LYS:CG	1:A:2167:LYS:O	2.29	0.81
1:A:2213:THR:HG23	1:A:2224:THR:HG23	1.61	0.81
1:B:1529:LEU:O	1:B:1533:THR:HG23	1.80	0.81
1:D:2289:LYS:HA	1:D:2292:LEU:CD1	2.11	0.81
1:A:2468:PHE:HD2	1:B:2464:HIS:ND1	1.77	0.81
1:D:2167:LYS:O	1:D:2167:LYS:CG	2.29	0.81
1:D:1650:LEU:HD23	1:D:1654:LEU:CD1	2.10	0.80
1:A:1733:ALA:HB1	1:A:1793:LEU:HD21	1.63	0.80
1:D:1733:ALA:HB1	1:D:1793:LEU:HD21	1.63	0.80
1:B:2213:THR:HG23	1:B:2224:THR:HG23	1.61	0.80
1:A:2289:LYS:HA	1:A:2292:LEU:CD1	2.11	0.80
1:B:1733:ALA:HB1	1:B:1793:LEU:HD21	1.63	0.80
1:B:2289:LYS:HA	1:B:2292:LEU:CD1	2.11	0.80
1:A:2265:ILE:HD13	1:A:2423:PHE:HA	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2358:LYS:NZ	1:D:2383:LEU:HD21	1.95	0.80
1:A:1650:LEU:HD23	1:A:1654:LEU:CD1	2.10	0.80
1:B:847:LYS:HD2	1:B:928:TYR:HE2	1.45	0.80
1:B:1650:LEU:HD23	1:B:1654:LEU:CD1	2.10	0.79
1:B:2311:LEU:HD13	1:D:2317:VAL:CG1	2.13	0.79
1:A:2311:LEU:HD13	1:B:2317:VAL:CG1	2.13	0.79
1:D:2167:LYS:HA	1:D:2167:LYS:CE	2.12	0.79
1:A:2167:LYS:HA	1:A:2167:LYS:CE	2.12	0.79
1:B:2137:MET:CE	1:D:2459:PHE:CG	2.62	0.79
1:A:2317:VAL:CG1	1:D:2311:LEU:HD13	2.13	0.79
1:A:2464:HIS:HE1	1:D:2468:PHE:HB2	1.48	0.79
1:B:2167:LYS:HA	1:B:2167:LYS:CE	2.12	0.79
1:B:2265:ILE:HD13	1:B:2423:PHE:HA	1.64	0.78
1:A:2468:PHE:HB2	1:B:2464:HIS:HE1	1.48	0.78
1:A:2507:TYR:HB2	1:B:2466:ILE:CD1	2.13	0.78
1:D:2265:ILE:HD13	1:D:2423:PHE:HA	1.64	0.78
1:B:627:LYS:HE3	1:B:627:LYS:O	1.84	0.78
1:D:2167:LYS:HE3	1:D:2167:LYS:CA	2.13	0.78
1:A:2188:TRP:CZ2	1:A:2192:LEU:HD11	2.19	0.77
1:D:2302:ARG:HB2	1:D:2323:LYS:HZ1	1.47	0.77
1:A:1943:ARG:HD3	1:A:1944:ARG:NH2	1.99	0.77
1:B:1737:THR:OG1	1:B:1790:LEU:HD13	1.84	0.77
1:D:1057:LEU:CG	1:D:1058:GLY:N	2.45	0.77
1:D:1943:ARG:HD3	1:D:1944:ARG:NH2	1.99	0.77
1:A:2137:MET:CE	1:B:2459:PHE:CG	2.62	0.77
1:D:2188:TRP:CZ2	1:D:2192:LEU:HD11	2.19	0.77
1:A:1157:MET:O	1:A:1160:VAL:HG22	1.84	0.77
1:A:2468:PHE:HD2	1:B:2464:HIS:HD1	1.29	0.77
1:B:2358:LYS:NZ	1:B:2383:LEU:HD21	1.95	0.77
1:D:1157:MET:O	1:D:1160:VAL:HG22	1.84	0.77
1:A:2302:ARG:HB3	1:A:2323:LYS:HZ2	1.48	0.77
1:B:2133:LEU:HD12	2:C:243:ILE:CD1	2.13	0.77
1:B:1157:MET:O	1:B:1160:VAL:HG22	1.84	0.77
1:B:1515:TRP:CZ3	1:B:1516:MET:CE	2.65	0.77
1:B:2468:PHE:HB2	1:D:2464:HIS:HE1	1.48	0.77
1:D:627:LYS:HE3	1:D:627:LYS:O	1.84	0.77
1:D:1737:THR:OG1	1:D:1790:LEU:HD13	1.84	0.77
1:A:2459:PHE:CG	1:D:2137:MET:CE	2.62	0.77
1:A:627:LYS:HE3	1:A:627:LYS:O	1.84	0.76
1:A:2167:LYS:CE	1:A:2167:LYS:CA	2.64	0.76
1:B:1057:LEU:CG	1:B:1058:GLY:N	2.45	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1943:ARG:HD3	1:B:1944:ARG:NH2	1.99	0.76
1:A:1737:THR:OG1	1:A:1790:LEU:HD13	1.84	0.76
1:B:2188:TRP:CZ2	1:B:2192:LEU:HD11	2.19	0.76
1:B:2507:TYR:HB2	1:D:2466:ILE:CD1	2.13	0.76
1:A:2383:LEU:HD23	1:A:2420:MET:CE	2.16	0.76
1:A:2466:ILE:CD1	1:D:2507:TYR:HB2	2.13	0.76
1:B:2383:LEU:HD23	1:B:2420:MET:CE	2.16	0.76
1:A:627:LYS:HE3	1:A:627:LYS:CA	2.16	0.76
1:B:2101:LEU:O	1:B:2105:LEU:HG	1.86	0.75
1:A:2302:ARG:CB	1:A:2323:LYS:NZ	2.50	0.75
1:A:1160:VAL:HG12	1:A:1550:LEU:HD23	1.67	0.75
1:A:2080:GLN:HA	1:A:2080:GLN:NE2	1.91	0.75
1:B:2167:LYS:O	1:B:2167:LYS:HG3	1.85	0.75
1:D:1160:VAL:HG12	1:D:1550:LEU:HD23	1.67	0.75
1:A:2167:LYS:O	1:A:2167:LYS:CD	2.35	0.75
1:B:1699:HIS:NE2	1:B:1708:LEU:CD1	2.48	0.75
1:A:2261:SER:O	1:A:2264:ASP:CB	2.34	0.75
1:A:2497:GLU:OE1	1:B:2164:GLY:N	2.20	0.75
1:B:1160:VAL:HG12	1:B:1550:LEU:HD23	1.67	0.75
1:D:1515:TRP:HE3	1:D:1516:MET:HE2	1.43	0.75
1:D:2133:LEU:HD12	2:E:243:ILE:CD1	2.14	0.75
1:D:2358:LYS:HZ2	1:D:2383:LEU:CD2	1.98	0.75
3:A:2602:D12:H62	3:E:301:D12:H72	1.68	0.75
1:D:2302:ARG:CB	1:D:2323:LYS:NZ	2.50	0.75
1:B:2167:LYS:CE	1:B:2167:LYS:CA	2.64	0.75
1:D:627:LYS:HE3	1:D:627:LYS:CA	2.16	0.75
1:D:2101:LEU:O	1:D:2105:LEU:HG	1.86	0.75
1:A:2133:LEU:HD12	2:F:243:ILE:CD1	2.13	0.74
1:A:2101:LEU:O	1:A:2105:LEU:HG	1.86	0.74
3:D:2603:D12:H62	3:C:301:D12:H72	1.68	0.74
1:A:2509:SER:HB3	1:B:2514:ILE:CD1	2.16	0.74
1:A:2514:ILE:CD1	1:D:2509:SER:HB3	2.16	0.74
1:B:2080:GLN:HA	1:B:2080:GLN:NE2	1.91	0.74
3:B:2603:D12:H62	3:F:301:D12:H72	1.68	0.74
1:D:2167:LYS:O	1:D:2167:LYS:HG3	1.85	0.74
1:A:2167:LYS:O	1:A:2167:LYS:HG3	1.85	0.74
1:D:2383:LEU:HD23	1:D:2420:MET:CE	2.16	0.74
1:B:627:LYS:HE3	1:B:627:LYS:CA	2.16	0.74
1:B:2167:LYS:O	1:B:2167:LYS:CD	2.35	0.74
1:B:2302:ARG:CB	1:B:2323:LYS:NZ	2.50	0.74
1:B:2509:SER:HB3	1:D:2514:ILE:CD1	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2167:LYS:O	1:D:2167:LYS:CD	2.35	0.74
1:B:2497:GLU:OE1	1:D:2164:GLY:N	2.20	0.74
1:D:2167:LYS:CE	1:D:2167:LYS:CA	2.64	0.74
1:D:2261:SER:O	1:D:2264:ASP:CB	2.34	0.74
1:A:1699:HIS:NE2	1:A:1708:LEU:CD1	2.48	0.73
1:A:2164:GLY:N	1:D:2497:GLU:OE1	2.20	0.73
1:A:2302:ARG:HB3	1:A:2323:LYS:NZ	2.04	0.73
1:B:2002:GLU:O	1:B:2006:VAL:CG2	2.37	0.73
1:D:2288:MET:O	1:D:2292:LEU:HG	1.88	0.73
1:B:2215:LYS:HB3	1:B:2221:PRO:HB3	1.71	0.73
1:B:2288:MET:O	1:B:2292:LEU:HG	1.88	0.73
1:A:785:ARG:HA	1:A:790:LEU:HB2	1.70	0.73
1:B:2261:SER:O	1:B:2264:ASP:CB	2.34	0.73
1:D:2002:GLU:O	1:D:2006:VAL:CG2	2.37	0.73
1:B:2358:LYS:HZ2	1:B:2383:LEU:CD2	2.02	0.73
1:B:2323:LYS:CB	1:B:2323:LYS:HZ2	1.83	0.72
1:B:2302:ARG:HB3	1:B:2323:LYS:NZ	2.04	0.72
1:A:2002:GLU:O	1:A:2006:VAL:CG2	2.37	0.72
1:B:785:ARG:HA	1:B:790:LEU:HB2	1.70	0.72
1:A:2166:LYS:CE	1:D:2128:ASP:CG	2.62	0.72
1:B:2002:GLU:O	1:B:2006:VAL:HG23	1.90	0.72
1:D:1568:LEU:C	1:D:1653:ARG:HB3	2.15	0.72
1:D:2002:GLU:O	1:D:2006:VAL:HG23	1.90	0.72
1:A:847:LYS:CD	1:A:928:TYR:HE2	2.03	0.72
1:D:2302:ARG:HB3	1:D:2323:LYS:NZ	2.04	0.72
1:A:2215:LYS:HB3	1:A:2221:PRO:HB3	1.71	0.72
1:B:847:LYS:CD	1:B:928:TYR:HE2	2.03	0.72
1:B:2089:ILE:CD1	1:B:2089:ILE:N	2.48	0.72
1:A:2167:LYS:HE3	1:A:2167:LYS:CA	2.13	0.72
1:A:2302:ARG:CB	1:A:2323:LYS:HZ1	2.02	0.72
1:B:2128:ASP:CG	1:D:2166:LYS:CE	2.62	0.72
1:A:2288:MET:O	1:A:2292:LEU:HG	1.88	0.71
1:B:1562:ARG:NE	1:B:1566:ASP:HB3	2.05	0.71
1:D:847:LYS:CD	1:D:928:TYR:HE2	2.03	0.71
1:D:1699:HIS:NE2	1:D:1708:LEU:CD1	2.48	0.71
1:D:2215:LYS:HB3	1:D:2221:PRO:HB3	1.71	0.71
1:B:1529:LEU:O	1:B:1533:THR:CG2	2.38	0.71
1:B:2214:LEU:HB2	1:B:2223:PHE:HB3	1.72	0.71
1:D:2214:LEU:HB2	1:D:2223:PHE:HB3	1.72	0.71
1:D:2383:LEU:HD23	1:D:2420:MET:HE2	1.73	0.71
1:A:2128:ASP:CG	1:B:2166:LYS:CE	2.62	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2383:LEU:HD23	1:B:2420:MET:HE2	1.73	0.71
1:D:1161:ALA:HA	1:D:1165:TYR:CD2	2.25	0.71
1:D:1529:LEU:O	1:D:1533:THR:CG2	2.38	0.71
1:A:1417:ASP:OD1	1:B:2518:ARG:NH1	2.24	0.71
1:A:2214:LEU:HB2	1:A:2223:PHE:HB3	1.72	0.71
1:B:1568:LEU:C	1:B:1653:ARG:HB3	2.15	0.71
1:D:785:ARG:HA	1:D:790:LEU:HB2	1.70	0.71
1:A:1161:ALA:HA	1:A:1165:TYR:CD2	2.25	0.71
1:A:2002:GLU:O	1:A:2006:VAL:HG23	1.90	0.71
1:A:1529:LEU:O	1:A:1533:THR:CG2	2.38	0.71
1:A:1568:LEU:C	1:A:1653:ARG:HB3	2.15	0.71
1:D:587:MET:HE2	1:D:587:MET:CA	2.21	0.71
1:A:587:MET:HE2	1:A:587:MET:CA	2.21	0.70
1:A:2253:ALA:HB1	1:A:2374:LEU:HD12	1.73	0.70
1:B:1161:ALA:HA	1:B:1165:TYR:CD2	2.25	0.70
1:B:2253:ALA:HB1	1:B:2374:LEU:HD12	1.73	0.70
1:D:1057:LEU:CG	1:D:1058:GLY:H	1.97	0.70
1:A:2518:ARG:NH1	1:D:1417:ASP:OD1	2.24	0.70
1:B:587:MET:HE2	1:B:587:MET:CA	2.21	0.70
1:B:1417:ASP:OD1	1:D:2518:ARG:NH1	2.24	0.70
1:A:626:LEU:O	1:A:630:TRP:HB2	1.91	0.70
1:A:2383:LEU:HD23	1:A:2420:MET:HE2	1.73	0.70
1:B:626:LEU:O	1:B:630:TRP:HB2	1.91	0.70
1:D:593:PHE:H	1:D:601:LYS:HE3	1.55	0.70
1:D:1562:ARG:NE	1:D:1566:ASP:HB3	2.06	0.70
1:A:593:PHE:H	1:A:601:LYS:HE3	1.56	0.70
1:D:2253:ALA:HB1	1:D:2374:LEU:HD12	1.73	0.70
1:B:2012:PHE:CE2	1:D:2184:ILE:CD1	2.69	0.69
1:B:2188:TRP:CE2	1:B:2192:LEU:HD11	2.27	0.69
1:A:1515:TRP:CZ3	1:A:1516:MET:CE	2.65	0.69
1:A:2046:PHE:C	1:A:2048:ILE:HD13	2.17	0.69
1:A:2188:TRP:CE2	1:A:2192:LEU:HD11	2.27	0.69
1:B:593:PHE:H	1:B:601:LYS:HE3	1.56	0.69
1:D:626:LEU:O	1:D:630:TRP:HB2	1.91	0.69
1:D:2046:PHE:C	1:D:2048:ILE:HD13	2.17	0.69
1:A:1562:ARG:NE	1:A:1566:ASP:HB3	2.06	0.69
1:A:2133:LEU:HB3	2:F:243:ILE:HD11	1.73	0.69
1:B:2046:PHE:C	1:B:2048:ILE:HD13	2.17	0.69
1:B:2289:LYS:HA	1:B:2292:LEU:HD12	1.75	0.69
1:A:1156:ASP:O	1:A:1160:VAL:HG13	1.93	0.69
1:D:2188:TRP:CE2	1:D:2192:LEU:HD11	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2289:LYS:HA	1:A:2292:LEU:HD11	1.75	0.69
1:A:2304:THR:HG22	1:A:2323:LYS:HZ3	1.58	0.69
1:D:1156:ASP:O	1:D:1160:VAL:HG13	1.93	0.69
1:D:2133:LEU:HB3	2:E:243:ILE:HD11	1.73	0.69
1:D:2089:ILE:CD1	1:D:2089:ILE:N	2.48	0.68
1:A:600:TYR:OH	1:A:644:VAL:CG1	2.41	0.68
1:B:2133:LEU:HB3	2:C:243:ILE:HD11	1.73	0.68
1:A:2048:ILE:CD1	1:A:2048:ILE:N	2.32	0.68
1:A:2317:VAL:HG11	1:D:2311:LEU:HD13	1.75	0.68
1:D:2048:ILE:N	1:D:2048:ILE:CD1	2.32	0.68
1:A:2304:THR:HG22	1:A:2323:LYS:NZ	2.09	0.68
1:A:2358:LYS:NZ	1:A:2383:LEU:HD22	2.08	0.68
1:B:2311:LEU:HD13	1:D:2317:VAL:HG11	1.75	0.68
1:B:2304:THR:HG22	1:B:2323:LYS:NZ	2.09	0.68
1:D:2323:LYS:CB	1:D:2323:LYS:HZ2	1.95	0.68
1:B:2046:PHE:C	1:B:2048:ILE:CD1	2.67	0.68
1:D:2358:LYS:NZ	1:D:2383:LEU:HD22	2.08	0.68
1:A:2046:PHE:C	1:A:2048:ILE:CD1	2.67	0.68
1:B:600:TYR:OH	1:B:644:VAL:CG1	2.41	0.68
1:B:1156:ASP:O	1:B:1160:VAL:HG13	1.93	0.68
1:A:679:GLU:HA	1:A:682:SER:HB2	1.76	0.67
1:A:2289:LYS:HA	1:A:2292:LEU:HD12	1.75	0.67
1:B:2302:ARG:CB	1:B:2323:LYS:HZ1	2.05	0.67
1:D:1733:ALA:CB	1:D:1793:LEU:HD21	2.24	0.67
1:D:2304:THR:HG22	1:D:2323:LYS:NZ	2.09	0.67
1:A:1057:LEU:CG	1:A:1058:GLY:H	1.97	0.67
1:B:1733:ALA:CB	1:B:1793:LEU:HD21	2.24	0.67
1:D:2046:PHE:C	1:D:2048:ILE:CD1	2.67	0.67
1:D:679:GLU:HA	1:D:682:SER:HB2	1.76	0.67
1:D:2289:LYS:HA	1:D:2292:LEU:HD12	1.75	0.67
1:A:1733:ALA:CB	1:A:1793:LEU:HD21	2.24	0.67
1:D:2289:LYS:HA	1:D:2292:LEU:HD11	1.75	0.67
1:A:2184:ILE:CD1	1:D:2012:PHE:CE2	2.70	0.67
1:A:2311:LEU:HD13	1:B:2317:VAL:HG11	1.75	0.67
1:B:847:LYS:HD2	1:B:928:TYR:CE2	2.29	0.67
1:D:600:TYR:OH	1:D:644:VAL:CG1	2.41	0.67
1:B:1515:TRP:CE3	1:B:1516:MET:HE1	2.16	0.67
1:B:2360:ILE:HA	1:B:2370:PRO:HA	1.77	0.67
1:D:1161:ALA:HA	1:D:1165:TYR:HE2	1.59	0.67
1:D:2010:ILE:HG22	1:D:2011:GLN:N	2.10	0.67
1:A:2168:LYS:HB3	1:A:2171:VAL:CG2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:847:LYS:HG3	1:D:928:TYR:CE2	2.30	0.66
1:A:847:LYS:HD2	1:A:928:TYR:CE2	2.29	0.66
1:B:2358:LYS:NZ	1:B:2383:LEU:HD22	2.08	0.66
1:D:704:PRO:HA	1:D:708:LEU:HB2	1.76	0.66
1:A:2360:ILE:HA	1:A:2370:PRO:HA	1.77	0.66
1:A:2012:PHE:CE2	1:B:2184:ILE:CD1	2.70	0.66
1:B:679:GLU:HA	1:B:682:SER:HB2	1.76	0.66
1:A:847:LYS:HG3	1:A:928:TYR:CE2	2.30	0.66
1:A:2465:SER:C	1:A:2467:MET:H	2.04	0.66
1:B:2277:LEU:HA	1:B:2402:GLU:O	1.96	0.66
1:D:1515:TRP:CE3	1:D:1516:MET:HE1	2.16	0.66
1:A:2010:ILE:HG22	1:A:2011:GLN:N	2.10	0.66
1:B:1010:ARG:HH21	1:B:1014:LEU:HB3	1.61	0.66
1:A:2137:MET:CE	1:B:2459:PHE:CE1	2.75	0.66
1:B:2289:LYS:HA	1:B:2292:LEU:HD11	1.75	0.66
1:B:2465:SER:C	1:B:2467:MET:H	2.04	0.66
1:D:1515:TRP:CZ3	1:D:1516:MET:CE	2.65	0.66
1:D:2360:ILE:HA	1:D:2370:PRO:HA	1.77	0.66
1:B:704:PRO:HA	1:B:708:LEU:HB2	1.76	0.66
1:B:1357:ILE:HG22	1:B:2495:LEU:CD2	2.26	0.66
1:D:644:VAL:HB	1:D:687:PRO:HB2	1.78	0.66
1:D:2302:ARG:HB2	1:D:2323:LYS:NZ	2.11	0.66
1:B:644:VAL:HB	1:B:687:PRO:HB2	1.78	0.66
1:B:847:LYS:HG3	1:B:928:TYR:CE2	2.30	0.66
1:B:2010:ILE:HG22	1:B:2011:GLN:N	2.09	0.66
1:B:2257:ILE:CB	1:B:2423:PHE:HE2	2.09	0.66
1:A:627:LYS:HA	1:A:627:LYS:CE	2.20	0.66
1:A:1357:ILE:HG22	1:A:2495:LEU:CD2	2.26	0.66
1:D:1357:ILE:HG22	1:D:2495:LEU:CD2	2.26	0.66
1:D:2277:LEU:HA	1:D:2402:GLU:O	1.96	0.66
1:A:704:PRO:HA	1:A:708:LEU:HB2	1.76	0.65
1:A:1010:ARG:HH21	1:A:1014:LEU:HB3	1.61	0.65
1:A:1737:THR:O	1:A:1741:VAL:CG2	2.42	0.65
1:A:2137:MET:HE2	1:B:2459:PHE:CD2	2.29	0.65
1:B:2168:LYS:HB3	1:B:2171:VAL:CG2	2.25	0.65
1:D:2465:SER:C	1:D:2467:MET:H	2.04	0.65
1:A:1357:ILE:HG22	1:A:2495:LEU:HD22	1.77	0.65
1:A:2464:HIS:CE1	1:D:2468:PHE:CD2	2.85	0.65
1:B:2302:ARG:HB2	1:B:2323:LYS:NZ	2.11	0.65
1:D:1357:ILE:HG22	1:D:2495:LEU:HD22	1.77	0.65
1:A:627:LYS:HE3	1:A:627:LYS:C	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2277:LEU:HA	1:A:2402:GLU:O	1.96	0.65
1:D:1010:ARG:HH21	1:D:1014:LEU:HB3	1.61	0.65
1:D:2257:ILE:CB	1:D:2423:PHE:HE2	2.09	0.65
1:B:1010:ARG:HD2	1:B:1098:ASN:HB3	1.79	0.65
1:B:2137:MET:CE	1:D:2459:PHE:CE1	2.75	0.65
1:B:1161:ALA:HA	1:B:1165:TYR:HE2	1.59	0.65
1:B:2304:THR:HG22	1:B:2323:LYS:HZ3	1.62	0.65
1:D:2167:LYS:O	1:D:2167:LYS:HD3	1.97	0.65
3:D:2603:D12:H71	3:C:301:D12:H81	1.79	0.65
1:D:847:LYS:HD2	1:D:928:TYR:CE2	2.29	0.64
1:D:1010:ARG:HD2	1:D:1098:ASN:HB3	1.79	0.64
1:B:627:LYS:HE3	1:B:627:LYS:C	2.22	0.64
1:A:2468:PHE:CD2	1:B:2464:HIS:CE1	2.85	0.64
1:B:1357:ILE:HG22	1:B:2495:LEU:HD22	1.77	0.64
1:B:2468:PHE:CD2	1:D:2464:HIS:CE1	2.85	0.64
1:A:644:VAL:HB	1:A:687:PRO:HB2	1.78	0.64
3:A:2602:D12:H71	3:E:301:D12:H81	1.79	0.64
1:B:624:LYS:HD2	1:B:711:MET:H	1.62	0.64
1:D:2168:LYS:HB3	1:D:2171:VAL:CG2	2.25	0.64
1:D:2358:LYS:HZ3	1:D:2383:LEU:CD2	1.96	0.64
1:A:2167:LYS:O	1:A:2167:LYS:HD3	1.97	0.64
1:A:2257:ILE:CB	1:A:2423:PHE:HE2	2.09	0.64
1:A:2514:ILE:HD11	1:D:2509:SER:HB3	1.79	0.64
1:B:2137:MET:HE2	1:D:2459:PHE:CD2	2.29	0.64
1:D:1552:GLN:CD	1:D:1552:GLN:H	2.06	0.64
1:D:624:LYS:HD2	1:D:711:MET:H	1.62	0.64
1:A:2507:TYR:CG	1:B:2466:ILE:HD11	2.33	0.64
1:D:627:LYS:HE3	1:D:627:LYS:C	2.21	0.64
1:D:2257:ILE:CA	1:D:2423:PHE:HE2	2.11	0.63
1:A:2358:LYS:NZ	1:A:2383:LEU:HD21	1.95	0.63
1:A:624:LYS:HD2	1:A:711:MET:H	1.62	0.63
1:A:2466:ILE:HD11	1:D:2507:TYR:CG	2.33	0.63
1:B:1737:THR:OG1	1:B:1790:LEU:CD1	2.47	0.63
1:B:2509:SER:HB3	1:D:2514:ILE:HD11	1.79	0.63
1:B:2167:LYS:O	1:B:2167:LYS:HD3	1.97	0.63
3:B:2603:D12:H71	3:F:301:D12:H81	1.79	0.63
1:A:853:LYS:N	1:A:853:LYS:HE2	2.13	0.63
1:A:2111:LEU:HD22	4:B:2601:L9Q:H37	1.81	0.63
1:A:2257:ILE:CA	1:A:2423:PHE:HE2	2.11	0.63
1:B:2257:ILE:CA	1:B:2423:PHE:HE2	2.11	0.63
1:D:853:LYS:HE2	1:D:853:LYS:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2509:SER:HB3	1:B:2514:ILE:HD11	1.79	0.63
1:B:853:LYS:HE2	1:B:853:LYS:N	2.13	0.62
1:D:2358:LYS:HZ2	1:D:2383:LEU:HD22	1.63	0.62
1:B:2012:PHE:O	1:B:2016:VAL:HG23	1.99	0.62
1:A:1552:GLN:CD	1:A:1552:GLN:H	2.06	0.62
1:A:2089:ILE:CD1	1:A:2089:ILE:N	2.48	0.62
1:B:1695:ILE:HD12	1:B:1714:VAL:CG2	2.29	0.62
1:B:1737:THR:O	1:B:1741:VAL:CG2	2.42	0.62
1:D:627:LYS:HA	1:D:627:LYS:CE	2.20	0.62
1:B:1552:GLN:H	1:B:1552:GLN:CD	2.06	0.62
1:B:1940:ARG:HA	1:B:1943:ARG:CD	2.29	0.62
1:D:1940:ARG:HA	1:D:1943:ARG:CD	2.29	0.62
1:A:1699:HIS:HD1	1:A:1707:SER:HB2	1.65	0.62
1:A:2253:ALA:HB1	1:A:2374:LEU:CD1	2.30	0.62
1:A:1010:ARG:HD2	1:A:1098:ASN:HB3	1.79	0.62
1:A:1737:THR:OG1	1:A:1790:LEU:CD1	2.47	0.62
1:D:1054:LEU:HA	1:D:1057:LEU:HD23	1.81	0.62
1:A:1161:ALA:HA	1:A:1165:TYR:HE2	1.59	0.62
1:A:1940:ARG:HA	1:A:1943:ARG:HD2	1.82	0.62
1:B:1054:LEU:HA	1:B:1057:LEU:HD23	1.81	0.62
1:D:1999:GLN:CB	1:D:2050:PRO:C	2.72	0.62
1:B:2253:ALA:HB1	1:B:2374:LEU:CD1	2.30	0.62
1:D:1737:THR:OG1	1:D:1790:LEU:CD1	2.47	0.62
1:A:2358:LYS:HZ2	1:A:2383:LEU:CD2	2.12	0.62
1:A:1054:LEU:HA	1:A:1057:LEU:HD23	1.81	0.62
1:A:1940:ARG:HA	1:A:1943:ARG:CD	2.29	0.62
1:A:2459:PHE:CE1	1:D:2137:MET:CE	2.75	0.62
1:B:1050:LEU:O	1:B:1054:LEU:HD13	2.00	0.62
1:A:1050:LEU:O	1:A:1054:LEU:HD13	2.00	0.61
1:A:1940:ARG:O	1:A:1944:ARG:HG2	2.00	0.61
1:B:1940:ARG:O	1:B:1944:ARG:HG2	2.00	0.61
1:B:2289:LYS:O	1:B:2292:LEU:HD12	2.00	0.61
1:D:2289:LYS:O	1:D:2292:LEU:HD12	2.00	0.61
1:D:2473:CYS:O	1:D:2473:CYS:SG	2.58	0.61
1:A:2289:LYS:O	1:A:2292:LEU:HD12	2.00	0.61
1:A:2473:CYS:O	1:A:2473:CYS:SG	2.58	0.61
1:B:1999:GLN:CB	1:B:2050:PRO:C	2.72	0.61
1:D:844:ILE:HB	1:D:848:MET:HE2	1.82	0.61
1:B:2111:LEU:HD22	4:D:2601:L9Q:H37	1.81	0.61
1:B:2473:CYS:O	1:B:2473:CYS:SG	2.58	0.61
1:D:2012:PHE:O	1:D:2016:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:844:ILE:HB	1:B:848:MET:HE2	1.82	0.61
1:B:2371:VAL:HG11	1:B:2374:LEU:HD22	1.83	0.61
1:D:2361:ARG:HG2	1:D:2371:VAL:HG22	1.83	0.61
1:D:2371:VAL:HG11	1:D:2374:LEU:HD22	1.83	0.61
1:A:683:SER:O	1:A:687:PRO:HD2	2.01	0.61
1:A:2371:VAL:HG11	1:A:2374:LEU:HD22	1.83	0.61
4:A:2603:L9Q:H37	1:D:2111:LEU:HD22	1.81	0.61
1:A:2012:PHE:O	1:A:2016:VAL:HG23	1.99	0.61
1:D:922:GLY:HA2	1:D:928:TYR:CZ	2.36	0.61
1:A:2302:ARG:HB2	1:A:2323:LYS:NZ	2.11	0.61
1:B:2361:ARG:HG2	1:B:2371:VAL:HG22	1.83	0.61
1:B:2507:TYR:CG	1:D:2466:ILE:HD11	2.33	0.61
1:D:1177:THR:HG21	1:D:1291:CYS:HB2	1.83	0.61
1:D:2253:ALA:HB1	1:D:2374:LEU:CD1	2.30	0.61
1:A:922:GLY:HA2	1:A:928:TYR:CZ	2.36	0.61
1:A:2459:PHE:CD2	1:D:2137:MET:HE2	2.29	0.61
1:B:847:LYS:CG	1:B:928:TYR:HE2	2.14	0.60
1:B:1940:ARG:HA	1:B:1943:ARG:HD2	1.82	0.60
1:D:1050:LEU:O	1:D:1054:LEU:HD13	2.00	0.60
1:D:1940:ARG:HA	1:D:1943:ARG:HD2	1.82	0.60
1:A:1177:THR:HG21	1:A:1291:CYS:HB2	1.83	0.60
1:B:2468:PHE:HB2	1:D:2464:HIS:CE1	2.34	0.60
1:D:683:SER:O	1:D:687:PRO:HD2	2.01	0.60
1:B:791:HIS:HB2	1:B:946:TYR:HE2	1.67	0.60
1:B:2048:ILE:CD1	1:B:2048:ILE:N	2.32	0.60
1:A:844:ILE:HB	1:A:848:MET:HE2	1.82	0.60
1:D:1940:ARG:O	1:D:1944:ARG:HG2	2.00	0.60
1:D:1699:HIS:HD1	1:D:1707:SER:HB2	1.65	0.60
1:D:847:LYS:CG	1:D:928:TYR:HE2	2.14	0.60
1:A:847:LYS:CG	1:A:928:TYR:HE2	2.14	0.60
1:A:2464:HIS:CE1	1:D:2468:PHE:HB2	2.34	0.60
1:B:683:SER:O	1:B:687:PRO:HD2	2.01	0.60
1:D:1737:THR:O	1:D:1741:VAL:CG2	2.42	0.60
1:A:1160:VAL:HG23	1:A:1165:TYR:OH	2.02	0.60
1:B:922:GLY:HA2	1:B:928:TYR:CZ	2.36	0.59
1:D:1943:ARG:HD3	1:D:1944:ARG:HH21	1.67	0.59
1:A:2361:ARG:HG2	1:A:2371:VAL:HG22	1.83	0.59
1:B:1699:HIS:HD1	1:B:1707:SER:HB2	1.65	0.59
1:A:791:HIS:HB2	1:A:946:TYR:HE2	1.67	0.59
1:D:2010:ILE:CG2	1:D:2011:GLN:N	2.66	0.59
1:A:1695:ILE:HD11	1:A:1714:VAL:HG21	0.69	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2443:LEU:HD22	1:D:2444:TYR:CA	2.33	0.59
1:B:1177:THR:HG21	1:B:1291:CYS:HB2	1.83	0.59
1:D:1160:VAL:HG23	1:D:1165:TYR:OH	2.02	0.59
1:D:1208:THR:HA	1:D:1302:PHE:CD1	2.38	0.59
1:D:791:HIS:HB2	1:D:946:TYR:HE2	1.67	0.59
1:A:621:LEU:HA	1:A:624:LYS:HD3	1.85	0.59
1:A:1695:ILE:HD12	1:A:1714:VAL:CG2	2.29	0.59
1:A:2468:PHE:HB2	1:B:2464:HIS:CE1	2.34	0.59
1:A:2294:ASN:O	1:A:2295:GLY:C	2.45	0.59
1:D:1654:LEU:HG	1:D:1655:ARG:NH1	2.18	0.59
1:D:2374:LEU:HD21	1:D:2423:PHE:CZ	2.38	0.59
1:A:1744:LYS:HZ3	1:A:1744:LYS:HB2	1.67	0.59
1:B:1160:VAL:HG23	1:B:1165:TYR:OH	2.02	0.59
1:B:1208:THR:HA	1:B:1302:PHE:CD1	2.38	0.59
1:D:922:GLY:HA2	1:D:928:TYR:CE2	2.38	0.59
1:A:1208:THR:HA	1:A:1302:PHE:CD1	2.38	0.59
1:B:1654:LEU:HG	1:B:1655:ARG:NH1	2.18	0.59
1:A:2374:LEU:HD21	1:A:2423:PHE:CZ	2.38	0.58
1:B:2010:ILE:CG2	1:B:2011:GLN:N	2.65	0.58
1:A:1654:LEU:HG	1:A:1655:ARG:NH1	2.18	0.58
1:A:847:LYS:HG3	1:A:928:TYR:HE2	1.68	0.58
1:A:2443:LEU:HD22	1:A:2444:TYR:CA	2.33	0.58
1:D:1744:LYS:HZ3	1:D:1744:LYS:HB2	1.68	0.58
1:A:1360:LYS:C	1:A:1362:GLU:H	2.12	0.58
1:A:922:GLY:HA2	1:A:928:TYR:CE2	2.38	0.58
1:A:922:GLY:CA	1:A:928:TYR:CE2	2.87	0.58
1:B:2443:LEU:HD22	1:B:2444:TYR:CA	2.33	0.58
1:B:621:LEU:HA	1:B:624:LYS:HD3	1.85	0.58
1:B:636:TYR:HA	1:B:639:LEU:CD1	2.34	0.58
1:B:922:GLY:HA2	1:B:928:TYR:CE2	2.38	0.58
1:B:1360:LYS:C	1:B:1362:GLU:H	2.12	0.58
1:B:2311:LEU:HD13	1:D:2317:VAL:HG13	1.85	0.58
1:D:922:GLY:CA	1:D:928:TYR:CE2	2.87	0.58
1:D:2294:ASN:O	1:D:2295:GLY:C	2.46	0.58
1:A:814:LEU:HD11	1:A:840:THR:CB	2.33	0.58
1:A:2010:ILE:CG2	1:A:2011:GLN:N	2.65	0.58
1:D:1360:LYS:C	1:D:1362:GLU:H	2.11	0.58
1:D:636:TYR:HA	1:D:639:LEU:CD1	2.34	0.58
1:D:1695:ILE:HD12	1:D:1714:VAL:CG2	2.29	0.58
1:A:1999:GLN:CB	1:A:2050:PRO:C	2.73	0.58
1:B:2374:LEU:HD21	1:B:2423:PHE:CZ	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:814:LEU:HD11	1:D:840:THR:CB	2.33	0.58
1:D:847:LYS:HG3	1:D:928:TYR:HE2	1.68	0.58
1:A:2317:VAL:HG13	1:D:2311:LEU:HD13	1.85	0.57
1:B:2133:LEU:CB	2:C:243:ILE:HD11	2.34	0.57
1:A:1160:VAL:CG1	1:A:1550:LEU:HD23	2.34	0.57
1:A:1159:LYS:O	1:A:1163:PHE:HB2	2.05	0.57
1:A:1943:ARG:HD3	1:A:1944:ARG:HH21	1.67	0.57
1:A:2133:LEU:CB	2:F:243:ILE:HD11	2.35	0.57
1:B:922:GLY:CA	1:B:928:TYR:CE2	2.87	0.57
1:D:621:LEU:HA	1:D:624:LYS:HD3	1.85	0.57
1:A:2277:LEU:CB	1:A:2279:ARG:HH22	2.17	0.57
1:A:2311:LEU:HD13	1:B:2317:VAL:HG13	1.85	0.57
1:B:2294:ASN:O	1:B:2295:GLY:C	2.45	0.57
1:B:814:LEU:HD11	1:B:840:THR:CB	2.34	0.57
1:B:847:LYS:HG3	1:B:928:TYR:HE2	1.68	0.57
1:B:1159:LYS:O	1:B:1163:PHE:HB2	2.05	0.57
1:B:2277:LEU:CB	1:B:2279:ARG:HH22	2.17	0.57
1:A:2276:ALA:HA	1:B:2279:ARG:HG2	1.86	0.57
1:A:2466:ILE:HD12	1:D:2507:TYR:HB2	1.87	0.57
1:B:1194:PHE:CD1	1:B:1738:GLU:HG2	2.40	0.57
1:B:2276:ALA:HA	1:D:2279:ARG:HG2	1.86	0.57
1:D:1159:LYS:O	1:D:1163:PHE:HB2	2.05	0.57
1:D:2277:LEU:CB	1:D:2279:ARG:HH22	2.17	0.57
1:A:636:TYR:HA	1:A:639:LEU:CD1	2.34	0.57
1:B:1695:ILE:CD1	1:B:1714:VAL:HG23	2.32	0.57
1:D:627:LYS:CA	1:D:627:LYS:CE	2.81	0.57
4:A:2603:L9Q:H26A	4:D:2601:L9Q:H28A	1.87	0.57
4:A:2603:L9Q:H28A	4:B:2601:L9Q:H26A	1.87	0.57
1:D:1160:VAL:CG1	1:D:1550:LEU:HD23	2.34	0.57
1:D:1568:LEU:HD13	1:D:1659:LEU:HD23	1.87	0.57
1:D:2265:ILE:HD13	1:D:2423:PHE:CA	2.35	0.57
1:B:1733:ALA:HB1	1:B:1793:LEU:CD2	2.35	0.56
1:A:2279:ARG:HG2	1:D:2276:ALA:HA	1.86	0.56
1:B:1160:VAL:CG1	1:B:1550:LEU:HD23	2.34	0.56
1:D:1733:ALA:CB	1:D:1793:LEU:CD2	2.84	0.56
1:A:2191:LEU:HB3	1:D:2005:LEU:HD21	1.88	0.56
1:A:2323:LYS:HB3	1:A:2323:LYS:HZ3	0.74	0.56
1:A:1733:ALA:CB	1:A:1793:LEU:CD2	2.84	0.56
1:A:2005:LEU:HD21	1:B:2191:LEU:HB3	1.88	0.56
1:B:2507:TYR:HB2	1:D:2466:ILE:HD12	1.87	0.56
1:B:627:LYS:CA	1:B:627:LYS:CE	2.81	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2005:LEU:HD21	1:D:2191:LEU:HB3	1.88	0.56
4:B:2601:L9Q:H28A	4:D:2601:L9Q:H26A	1.87	0.56
1:D:1194:PHE:CD1	1:D:1738:GLU:HG2	2.40	0.56
1:A:1194:PHE:CD1	1:A:1738:GLU:HG2	2.40	0.56
1:B:1943:ARG:HD3	1:B:1944:ARG:HH21	1.67	0.56
1:B:2358:LYS:HG2	1:B:2420:MET:HG3	1.88	0.56
1:D:2358:LYS:HG2	1:D:2420:MET:HG3	1.88	0.56
1:D:2133:LEU:CB	2:E:243:ILE:HD11	2.35	0.56
1:B:1733:ALA:CB	1:B:1793:LEU:CD2	2.84	0.55
1:D:2049:LEU:HD23	1:D:2049:LEU:H	1.71	0.55
1:D:2328:LEU:HD13	1:D:2335:ARG:HG3	1.88	0.55
1:A:2465:SER:C	1:A:2467:MET:N	2.64	0.55
1:A:2049:LEU:HD23	1:A:2049:LEU:H	1.71	0.55
1:B:1568:LEU:HD13	1:B:1659:LEU:HD23	1.87	0.55
1:B:2049:LEU:HD23	1:B:2049:LEU:H	1.71	0.55
1:D:2045:MET:O	1:D:2048:ILE:CD1	2.41	0.55
1:B:2208:ILE:H	1:B:2309:ARG:HA	1.72	0.55
1:A:1568:LEU:HD13	1:A:1659:LEU:HD23	1.87	0.55
1:A:2257:ILE:HA	1:A:2423:PHE:CE2	2.42	0.55
1:D:1695:ILE:CD1	1:D:1714:VAL:HG23	2.32	0.55
1:D:1733:ALA:HB1	1:D:1793:LEU:CD2	2.35	0.55
1:D:2208:ILE:H	1:D:2309:ARG:HA	1.72	0.55
1:D:2257:ILE:CB	1:D:2423:PHE:CE2	2.89	0.55
1:D:2465:SER:C	1:D:2467:MET:N	2.64	0.55
1:A:2257:ILE:CB	1:A:2423:PHE:CE2	2.89	0.55
1:A:2265:ILE:HD13	1:A:2423:PHE:CA	2.35	0.55
1:A:2358:LYS:HG2	1:A:2420:MET:HG3	1.88	0.55
1:B:778:SER:O	1:B:782:VAL:HG23	2.07	0.55
1:A:2464:HIS:CE1	1:D:2468:PHE:HD2	2.23	0.55
1:A:2507:TYR:HB2	1:B:2466:ILE:HD12	1.87	0.55
1:B:1057:LEU:CG	1:B:1058:GLY:H	1.97	0.55
1:B:2257:ILE:CB	1:B:2423:PHE:CE2	2.89	0.55
1:D:2257:ILE:HA	1:D:2423:PHE:CE2	2.42	0.55
3:F:301:D12:H82	3:F:303:D12:C6	2.36	0.55
1:A:2147:PHE:CZ	1:A:2151:CYS:SG	3.00	0.54
1:B:2147:PHE:CZ	1:B:2151:CYS:SG	3.00	0.54
1:B:2257:ILE:HA	1:B:2423:PHE:CE2	2.42	0.54
1:D:2049:LEU:H	1:D:2049:LEU:CD2	2.20	0.54
1:A:2383:LEU:HD23	1:A:2420:MET:HE3	1.89	0.54
1:B:2465:SER:C	1:B:2467:MET:N	2.64	0.54
1:D:2147:PHE:CZ	1:D:2151:CYS:SG	3.00	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2208:ILE:H	1:A:2309:ARG:HA	1.72	0.54
1:B:2363:PRO:HA	1:B:2425:ASP:HB3	1.90	0.54
1:D:1695:ILE:HD11	1:D:1714:VAL:HG21	0.69	0.54
1:B:2049:LEU:H	1:B:2049:LEU:CD2	2.20	0.54
1:A:2328:LEU:HD13	1:A:2335:ARG:HG3	1.89	0.54
1:B:2383:LEU:HD23	1:B:2420:MET:HE3	1.89	0.54
1:D:2363:PRO:HA	1:D:2425:ASP:HB3	1.90	0.54
1:A:636:TYR:HA	1:A:639:LEU:HD13	1.90	0.54
1:A:778:SER:O	1:A:782:VAL:HG23	2.07	0.54
1:D:636:TYR:HA	1:D:639:LEU:HD13	1.90	0.54
1:D:776:VAL:O	1:D:779:ARG:HG3	2.08	0.54
1:D:1010:ARG:HB3	1:D:1015:VAL:HG21	1.90	0.54
1:D:778:SER:O	1:D:782:VAL:HG23	2.07	0.54
1:D:2355:LEU:HA	1:D:2382:TYR:HD2	1.73	0.54
1:B:2328:LEU:HD13	1:B:2335:ARG:HG3	1.88	0.54
1:D:2257:ILE:CA	1:D:2423:PHE:CE2	2.91	0.54
1:D:2265:ILE:CD1	1:D:2423:PHE:CE2	2.91	0.54
1:A:776:VAL:O	1:A:779:ARG:HG3	2.08	0.53
1:A:1715:PHE:HA	1:A:1719:MET:HE2	1.90	0.53
1:B:1695:ILE:HD11	1:B:1714:VAL:HG21	0.69	0.53
1:A:1733:ALA:HB1	1:A:1793:LEU:CD2	2.35	0.53
1:B:1744:LYS:HZ3	1:B:1744:LYS:HB2	1.73	0.53
1:B:2257:ILE:CA	1:B:2423:PHE:CE2	2.91	0.53
1:A:2045:MET:O	1:A:2048:ILE:CD1	2.41	0.53
1:A:2167:LYS:HG3	1:A:2172:LYS:HG2	1.90	0.53
1:A:2465:SER:O	1:A:2467:MET:N	2.41	0.53
1:B:1336:ILE:O	1:B:1340:ARG:HG3	2.09	0.53
1:D:820:ALA:O	1:D:1046:ALA:HB1	2.09	0.53
1:B:601:LYS:HD2	1:B:848:MET:HE3	1.91	0.53
1:D:2167:LYS:HG3	1:D:2172:LYS:HG2	1.90	0.53
1:D:2465:SER:O	1:D:2467:MET:N	2.41	0.53
3:C:301:D12:H82	3:C:303:D12:C6	2.36	0.53
1:B:1568:LEU:O	1:B:1653:ARG:CB	2.44	0.53
1:B:2465:SER:O	1:B:2467:MET:N	2.41	0.53
1:D:1298:GLN:HA	1:D:1301:VAL:HG22	1.91	0.53
1:A:1298:GLN:HA	1:A:1301:VAL:HG22	1.91	0.53
1:B:2265:ILE:CD1	1:B:2423:PHE:CE2	2.91	0.53
1:B:2355:LEU:HA	1:B:2382:TYR:HD2	1.73	0.53
1:B:1010:ARG:HB3	1:B:1015:VAL:HG21	1.90	0.53
1:B:1298:GLN:HA	1:B:1301:VAL:HG22	1.91	0.53
1:B:2296:THR:HA	1:B:2330:PRO:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:587:MET:HE2	1:D:587:MET:HA	1.91	0.53
1:D:1336:ILE:O	1:D:1340:ARG:HG3	2.09	0.53
1:A:1010:ARG:HB3	1:A:1015:VAL:HG21	1.90	0.53
1:A:2191:LEU:HD13	1:D:2005:LEU:HD21	1.91	0.53
1:A:2257:ILE:CA	1:A:2423:PHE:CE2	2.91	0.53
1:A:2468:PHE:HD2	1:B:2464:HIS:CE1	2.23	0.53
1:B:820:ALA:O	1:B:1046:ALA:HB1	2.09	0.53
1:B:1160:VAL:CB	1:B:1550:LEU:HD23	2.39	0.53
1:D:1160:VAL:CB	1:D:1550:LEU:HD23	2.39	0.53
1:D:2296:THR:HA	1:D:2330:PRO:HB3	1.91	0.53
1:A:1336:ILE:O	1:A:1340:ARG:HG3	2.09	0.53
1:A:2468:PHE:CB	1:B:2464:HIS:HE1	2.21	0.53
1:B:776:VAL:O	1:B:779:ARG:HG3	2.08	0.53
1:A:820:ALA:O	1:A:1046:ALA:HB1	2.09	0.52
1:D:2383:LEU:HD23	1:D:2420:MET:HE3	1.89	0.52
1:A:1057:LEU:CG	1:A:1058:GLY:N	2.45	0.52
1:B:635:ALA:C	1:B:639:LEU:HD12	2.33	0.52
1:B:1715:PHE:HA	1:B:1719:MET:HE2	1.90	0.52
1:D:1695:ILE:HD12	1:D:1714:VAL:HG23	1.91	0.52
1:A:587:MET:HE2	1:A:587:MET:HA	1.91	0.52
4:A:2603:L9Q:H41A	1:D:2113:PRO:HD3	1.91	0.52
1:B:587:MET:HE2	1:B:587:MET:HA	1.91	0.52
1:B:1052:GLN:CB	1:B:1099:LEU:CD1	2.76	0.52
1:A:1160:VAL:CB	1:A:1550:LEU:HD23	2.39	0.52
1:A:2363:PRO:HA	1:A:2425:ASP:HB3	1.90	0.52
1:B:2468:PHE:HD2	1:D:2464:HIS:CE1	2.23	0.52
1:D:1568:LEU:HA	1:D:1657:PRO:HD2	1.91	0.52
1:B:809:SER:HA	1:B:1057:LEU:HB2	1.92	0.52
1:D:2049:LEU:HD23	1:D:2049:LEU:N	2.25	0.52
1:A:1568:LEU:HA	1:A:1657:PRO:HD2	1.91	0.52
1:A:2113:PRO:HD3	4:B:2601:L9Q:H41A	1.91	0.52
1:A:2265:ILE:CD1	1:A:2423:PHE:CE2	2.91	0.52
1:A:2296:THR:HA	1:A:2330:PRO:HB3	1.91	0.52
1:A:2355:LEU:HA	1:A:2382:TYR:HD2	1.73	0.52
1:B:2167:LYS:HG3	1:B:2172:LYS:HG2	1.90	0.52
1:D:601:LYS:HD2	1:D:848:MET:HE3	1.91	0.52
1:D:1715:PHE:HA	1:D:1719:MET:HE2	1.90	0.52
1:D:2304:THR:HG22	1:D:2323:LYS:HZ3	1.73	0.52
1:B:636:TYR:HA	1:B:639:LEU:HD13	1.90	0.52
1:B:841:CYS:O	1:B:845:VAL:HG23	2.10	0.52
1:A:601:LYS:HD2	1:A:848:MET:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1695:ILE:HD12	1:B:1714:VAL:HG23	1.91	0.52
1:B:2005:LEU:HD21	1:D:2191:LEU:HD13	1.91	0.52
1:B:2101:LEU:HD13	1:B:2105:LEU:HD11	1.92	0.52
1:D:791:HIS:HB2	1:D:946:TYR:CE2	2.45	0.52
1:D:809:SER:HA	1:D:1057:LEU:HB2	1.92	0.52
1:D:2002:GLU:O	1:D:2006:VAL:HG22	2.09	0.52
1:A:2005:LEU:HD21	1:B:2191:LEU:HD13	1.91	0.52
1:B:791:HIS:HB2	1:B:946:TYR:CE2	2.45	0.52
1:B:2046:PHE:O	1:B:2048:ILE:CD1	2.58	0.52
1:B:2265:ILE:HD13	1:B:2423:PHE:CA	2.35	0.52
1:D:2046:PHE:O	1:D:2048:ILE:CD1	2.58	0.52
1:B:1188:GLY:HA3	1:B:1221:TYR:OH	2.10	0.51
1:D:2101:LEU:HD13	1:D:2105:LEU:HD11	1.92	0.51
1:A:1208:THR:HA	1:A:1302:PHE:HD1	1.75	0.51
1:A:2275:GLY:HA3	1:B:2281:SER:HA	1.92	0.51
1:A:1188:GLY:HA3	1:A:1221:TYR:OH	2.10	0.51
1:A:2281:SER:HA	1:D:2275:GLY:HA3	1.92	0.51
1:B:2323:LYS:HB3	1:B:2323:LYS:HZ3	0.70	0.51
1:A:809:SER:HA	1:A:1057:LEU:HB2	1.92	0.51
1:A:1744:LYS:HB2	1:A:1744:LYS:NZ	2.26	0.51
1:A:2002:GLU:O	1:A:2006:VAL:HG22	2.09	0.51
1:A:2393:GLN:HG2	1:A:2400:PHE:HA	1.93	0.51
1:B:2275:GLY:HA3	1:D:2281:SER:HA	1.92	0.51
1:D:841:CYS:O	1:D:845:VAL:HG23	2.10	0.51
1:A:635:ALA:C	1:A:639:LEU:HD12	2.33	0.51
1:A:2101:LEU:HD13	1:A:2105:LEU:HD11	1.92	0.51
1:B:2113:PRO:HD3	4:D:2601:L9Q:H41A	1.91	0.51
1:D:2393:GLN:HG2	1:D:2400:PHE:HA	1.93	0.51
1:A:1052:GLN:CB	1:A:1099:LEU:CD1	2.76	0.51
1:B:2049:LEU:HD23	1:B:2049:LEU:N	2.25	0.51
1:D:1744:LYS:HB2	1:D:1744:LYS:NZ	2.26	0.51
1:A:841:CYS:O	1:A:845:VAL:HG23	2.10	0.51
1:B:2002:GLU:O	1:B:2006:VAL:HG22	2.09	0.51
1:D:1188:GLY:HA3	1:D:1221:TYR:OH	2.10	0.51
1:A:1695:ILE:CD1	1:A:1714:VAL:HG23	2.32	0.51
1:A:1695:ILE:HD12	1:A:1714:VAL:HG23	1.91	0.51
1:B:1744:LYS:HB2	1:B:1744:LYS:NZ	2.26	0.51
1:B:2449:LEU:HD22	4:B:2601:L9Q:H40	1.93	0.51
1:D:1208:THR:HA	1:D:1302:PHE:HD1	1.75	0.51
1:A:791:HIS:HB2	1:A:946:TYR:CE2	2.45	0.51
1:B:1568:LEU:HA	1:B:1657:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2315:GLY:HA2	1:D:2364:ASN:HB3	1.93	0.51
1:A:580:TRP:HZ3	1:A:701:PHE:HB2	1.76	0.51
1:A:2049:LEU:HD23	1:A:2049:LEU:N	2.25	0.50
1:A:2464:HIS:HE1	1:D:2468:PHE:CB	2.21	0.50
1:B:1208:THR:HA	1:B:1302:PHE:HD1	1.75	0.50
1:D:580:TRP:HZ3	1:D:701:PHE:HB2	1.76	0.50
1:D:1360:LYS:C	1:D:1362:GLU:N	2.69	0.50
1:D:2302:ARG:HE	1:D:2323:LYS:HZ2	1.58	0.50
1:A:2315:GLY:HA2	1:A:2364:ASN:HB3	1.93	0.50
1:A:2449:LEU:HD22	4:A:2603:L9Q:H40	1.93	0.50
1:B:2315:GLY:HA2	1:B:2364:ASN:HB3	1.93	0.50
1:B:2393:GLN:HG2	1:B:2400:PHE:HA	1.93	0.50
1:D:587:MET:CA	1:D:587:MET:CE	2.89	0.50
1:D:1568:LEU:O	1:D:1653:ARG:CB	2.44	0.50
1:D:2341:LEU:HD13	1:D:2389:LEU:HB3	1.94	0.50
1:A:1160:VAL:HA	1:A:1550:LEU:HD23	1.91	0.50
1:A:2046:PHE:O	1:A:2048:ILE:CD1	2.58	0.50
1:D:1688:GLU:OE1	1:D:1725:PRO:CD	2.60	0.50
1:D:2391:ARG:HB3	1:D:2402:GLU:HG2	1.94	0.50
1:A:1688:GLU:OE1	1:A:1725:PRO:CD	2.60	0.50
1:A:2352:ILE:HB	1:A:2385:VAL:HG13	1.94	0.50
1:B:1160:VAL:HA	1:B:1550:LEU:HD23	1.91	0.50
1:B:1704:SER:HA	1:B:2046:PHE:HE1	1.77	0.50
1:B:2352:ILE:HB	1:B:2385:VAL:HG13	1.94	0.50
1:A:2511:GLU:OE2	1:D:2509:SER:HB2	2.12	0.50
1:B:1360:LYS:C	1:B:1362:GLU:N	2.69	0.50
1:B:2010:ILE:HG22	1:B:2011:GLN:H	1.77	0.50
1:B:2391:ARG:HB3	1:B:2402:GLU:HG2	1.94	0.50
1:A:602:ILE:HG23	1:A:845:VAL:HG22	1.93	0.49
1:A:2135:SER:HB3	1:A:2500:TYR:OH	2.12	0.49
1:B:602:ILE:HG23	1:B:845:VAL:HG22	1.93	0.49
1:B:1562:ARG:HD2	1:B:1566:ASP:HB2	1.94	0.49
1:B:2135:SER:HB3	1:B:2500:TYR:OH	2.12	0.49
1:D:602:ILE:HG23	1:D:845:VAL:HG22	1.93	0.49
1:D:922:GLY:HA3	1:D:928:TYR:CE2	2.47	0.49
1:D:949:GLN:HA	1:D:952:TYR:HB2	1.94	0.49
1:D:2352:ILE:HB	1:D:2385:VAL:HG13	1.94	0.49
1:A:2046:PHE:O	1:A:2048:ILE:HD13	2.12	0.49
1:A:922:GLY:HA3	1:A:928:TYR:CE2	2.47	0.49
1:B:1688:GLU:OE1	1:B:1725:PRO:CD	2.60	0.49
1:B:2358:LYS:HZ2	1:B:2383:LEU:HD22	1.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1704:SER:HA	1:A:2046:PHE:HE1	1.77	0.49
1:A:2010:ILE:HG22	1:A:2011:GLN:H	1.77	0.49
1:B:580:TRP:HZ3	1:B:701:PHE:HB2	1.76	0.49
1:B:644:VAL:HG12	1:B:683:SER:HB2	1.94	0.49
1:B:922:GLY:HA3	1:B:928:TYR:CE2	2.47	0.49
1:B:949:GLN:HA	1:B:952:TYR:HB2	1.94	0.49
1:B:2509:SER:HB2	1:D:2511:GLU:OE2	2.12	0.49
1:D:644:VAL:HG12	1:D:683:SER:HB2	1.94	0.49
1:D:2449:LEU:HD22	4:D:2601:L9Q:H40	1.93	0.49
1:A:949:GLN:HA	1:A:952:TYR:HB2	1.94	0.49
1:B:2274:SER:CB	1:B:2404:TRP:H	2.25	0.49
1:D:2135:SER:HB3	1:D:2500:TYR:OH	2.12	0.49
1:D:2274:SER:CB	1:D:2404:TRP:H	2.25	0.49
1:D:2277:LEU:CB	1:D:2279:ARG:NH2	2.76	0.49
1:A:2274:SER:CB	1:A:2404:TRP:H	2.25	0.49
1:A:2391:ARG:HB3	1:A:2402:GLU:HG2	1.94	0.49
1:D:635:ALA:C	1:D:639:LEU:HD12	2.33	0.49
3:E:301:D12:H82	3:E:303:D12:C6	2.36	0.49
1:A:2509:SER:HB2	1:B:2511:GLU:OE2	2.12	0.49
1:D:950:GLU:HB3	1:D:954:ARG:HH21	1.78	0.49
1:A:950:GLU:HB3	1:A:954:ARG:HH21	1.78	0.49
1:B:2277:LEU:CB	1:B:2279:ARG:NH2	2.76	0.49
1:B:2497:GLU:OE1	1:D:2164:GLY:CA	2.61	0.49
3:C:301:D12:H61	3:C:301:D12:H32	1.52	0.49
1:B:1028:ARG:HB3	1:B:1034:ILE:HG12	1.95	0.49
1:B:2293:TYR:HB2	1:B:2294:ASN:OD1	2.13	0.49
1:D:2046:PHE:O	1:D:2048:ILE:HD13	2.12	0.49
1:A:1028:ARG:HB3	1:A:1034:ILE:HG12	1.95	0.49
1:A:2289:LYS:CA	1:A:2292:LEU:HD12	2.42	0.49
1:A:2341:LEU:HD13	1:A:2389:LEU:HB3	1.94	0.49
1:B:2030:LYS:HD2	1:B:2030:LYS:HA	1.58	0.49
1:D:2010:ILE:HG22	1:D:2011:GLN:H	1.77	0.49
1:A:2277:LEU:CB	1:A:2279:ARG:NH2	2.76	0.48
1:A:2358:LYS:HZ2	1:A:2383:LEU:HD22	1.77	0.48
1:B:2046:PHE:O	1:B:2048:ILE:HD13	2.12	0.48
1:B:2289:LYS:CA	1:B:2292:LEU:HD12	2.42	0.48
1:A:596:ARG:HD2	1:A:596:ARG:HA	1.63	0.48
1:A:785:ARG:HG2	1:A:790:LEU:HG	1.95	0.48
1:B:1160:VAL:HG12	1:B:1550:LEU:CD2	2.41	0.48
1:B:2341:LEU:HD13	1:B:2389:LEU:HB3	1.94	0.48
1:B:1313:ASP:HA	1:B:1547:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2164:GLY:CA	1:D:2497:GLU:OE1	2.61	0.48
1:A:2459:PHE:CD1	1:D:2137:MET:SD	3.06	0.48
1:B:1420:LEU:HD13	1:B:2502:LYS:HG2	1.96	0.48
1:B:1555:LEU:H	1:B:1555:LEU:HG	1.48	0.48
1:B:2128:ASP:CG	1:D:2166:LYS:HE2	2.39	0.48
1:D:1562:ARG:NE	1:D:1566:ASP:CB	2.77	0.48
1:A:644:VAL:HG12	1:A:683:SER:HB2	1.94	0.48
1:A:1562:ARG:HD2	1:A:1566:ASP:HB2	1.94	0.48
1:A:2265:ILE:HD13	1:A:2423:PHE:CB	2.44	0.48
1:A:2497:GLU:OE1	1:B:2164:GLY:CA	2.61	0.48
1:B:950:GLU:HB3	1:B:954:ARG:HH21	1.78	0.48
1:B:2045:MET:O	1:B:2048:ILE:CD1	2.41	0.48
1:B:2137:MET:SD	1:D:2459:PHE:CD1	3.06	0.48
1:B:2185:ALA:HA	1:B:2189:PHE:HB2	1.96	0.48
3:E:303:D12:H21	3:E:303:D12:H51	1.54	0.48
1:A:984:LYS:HA	1:A:984:LYS:HD2	1.47	0.48
1:A:1420:LEU:HD13	1:A:2502:LYS:HG2	1.96	0.48
1:A:2137:MET:SD	1:B:2459:PHE:CD1	3.06	0.48
1:A:2293:TYR:HB2	1:A:2294:ASN:OD1	2.13	0.48
1:D:1704:SER:HA	1:D:2046:PHE:HE1	1.77	0.48
1:A:2281:SER:HA	1:D:2275:GLY:CA	2.44	0.48
1:B:1208:THR:HB	1:B:1311:ARG:HE	1.79	0.48
1:D:1028:ARG:HB3	1:D:1034:ILE:HG12	1.95	0.48
1:D:2010:ILE:O	1:D:2011:GLN:C	2.57	0.48
1:D:2289:LYS:CA	1:D:2292:LEU:HD12	2.42	0.48
1:A:978:ASP:HA	1:A:1155:LEU:HG	1.96	0.48
1:A:1313:ASP:HA	1:A:1547:ARG:HH21	1.78	0.48
1:A:1710:LEU:HD23	1:A:1710:LEU:HA	1.76	0.48
1:A:2166:LYS:HE2	1:D:2128:ASP:CG	2.39	0.48
1:B:978:ASP:HA	1:B:1155:LEU:HG	1.96	0.48
1:B:2010:ILE:O	1:B:2011:GLN:C	2.57	0.48
1:D:2153:ARG:HA	1:D:2153:ARG:HD3	1.61	0.48
1:A:1206:ARG:O	1:A:1210:ALA:HB3	2.13	0.48
1:A:1360:LYS:C	1:A:1362:GLU:N	2.69	0.48
1:A:2185:ALA:HA	1:A:2189:PHE:HB2	1.96	0.48
1:B:785:ARG:HG2	1:B:790:LEU:HG	1.95	0.48
1:B:2323:LYS:H	1:B:2323:LYS:HG2	1.40	0.48
1:D:2293:TYR:HB2	1:D:2294:ASN:OD1	2.13	0.48
1:A:1728:ARG:H	1:A:1728:ARG:HG3	1.37	0.48
1:D:1562:ARG:HD2	1:D:1566:ASP:HB2	1.94	0.48
1:A:2275:GLY:CA	1:B:2281:SER:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2292:LEU:HD22	1:A:2338:LEU:HB3	1.95	0.47
1:B:688:GLY:O	1:B:692:LEU:HG	2.14	0.47
1:D:1206:ARG:O	1:D:1210:ALA:HB3	2.13	0.47
1:D:1699:HIS:CG	1:D:1707:SER:HB2	2.49	0.47
1:D:2294:ASN:OD1	1:D:2294:ASN:N	2.47	0.47
1:A:1208:THR:HB	1:A:1311:ARG:HE	1.79	0.47
1:B:1656:ILE:H	1:B:1656:ILE:HG12	1.51	0.47
1:D:682:SER:O	1:D:683:SER:C	2.57	0.47
1:D:688:GLY:O	1:D:692:LEU:HG	2.14	0.47
1:D:2185:ALA:HA	1:D:2189:PHE:HB2	1.96	0.47
1:D:2292:LEU:HD22	1:D:2338:LEU:HB3	1.95	0.47
1:A:1953:LYS:HB2	1:A:1954:TYR:H	1.47	0.47
1:A:2188:TRP:CZ3	1:D:2009:LEU:HG	2.50	0.47
1:A:2468:PHE:CB	1:B:2464:HIS:CE1	2.98	0.47
1:B:602:ILE:H	1:B:602:ILE:HG13	1.47	0.47
1:D:978:ASP:HA	1:D:1155:LEU:HG	1.96	0.47
1:A:688:GLY:O	1:A:692:LEU:HG	2.14	0.47
1:B:2009:LEU:HG	1:D:2188:TRP:CZ3	2.50	0.47
1:B:2292:LEU:HD22	1:B:2338:LEU:HB3	1.95	0.47
1:B:2293:TYR:CB	1:B:2294:ASN:OD1	2.63	0.47
1:B:2468:PHE:CB	1:D:2464:HIS:HE1	2.21	0.47
1:D:785:ARG:HG2	1:D:790:LEU:HG	1.95	0.47
1:D:1313:ASP:HA	1:D:1547:ARG:HH21	1.78	0.47
1:D:1420:LEU:HD13	1:D:2502:LYS:HG2	1.96	0.47
1:D:2265:ILE:HD13	1:D:2423:PHE:CB	2.44	0.47
1:A:573:LYS:HA	1:A:573:LYS:HD3	1.51	0.47
1:A:806:LYS:HA	1:A:806:LYS:HD3	1.64	0.47
1:A:1568:LEU:O	1:A:1653:ARG:CB	2.44	0.47
1:B:2294:ASN:OD1	1:B:2294:ASN:N	2.47	0.47
1:B:2341:LEU:HG	1:B:2348:GLN:HB2	1.97	0.47
1:D:2341:LEU:HG	1:D:2348:GLN:HB2	1.97	0.47
1:A:2302:ARG:HB3	1:A:2302:ARG:HE	1.42	0.47
1:B:1206:ARG:O	1:B:1210:ALA:HB3	2.13	0.47
1:B:2289:LYS:CA	1:B:2292:LEU:CD1	2.90	0.47
1:D:1203:LEU:O	1:D:1207:ASP:HB2	2.15	0.47
1:D:2307:PHE:HE2	1:D:2360:ILE:HG21	1.80	0.47
1:A:1160:VAL:HG12	1:A:1550:LEU:CD2	2.41	0.47
1:A:2009:LEU:HG	1:B:2188:TRP:CZ3	2.50	0.47
1:B:2101:LEU:HD22	1:B:2101:LEU:HA	1.72	0.47
1:B:2275:GLY:CA	1:D:2281:SER:HA	2.44	0.47
1:D:572:VAL:HA	1:D:575:VAL:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:984:LYS:HD2	1:D:984:LYS:HA	1.47	0.47
1:D:1160:VAL:HA	1:D:1550:LEU:HD23	1.91	0.47
1:D:1160:VAL:HG12	1:D:1550:LEU:CD2	2.41	0.47
1:D:1208:THR:HB	1:D:1311:ARG:HE	1.79	0.47
1:A:2099:ASN:HB3	1:A:2100:HIS:H	1.57	0.47
1:A:2157:LYS:HE2	1:A:2157:LYS:HB2	1.56	0.47
1:B:572:VAL:HA	1:B:575:VAL:HB	1.97	0.47
1:B:1203:LEU:O	1:B:1207:ASP:HB2	2.15	0.47
1:B:1316:ALA:HA	1:B:1319:LEU:HB2	1.97	0.47
1:A:682:SER:O	1:A:683:SER:C	2.57	0.47
1:A:1744:LYS:NZ	1:A:1744:LYS:CB	2.78	0.47
1:A:2341:LEU:HG	1:A:2348:GLN:HB2	1.97	0.47
1:D:1171:LEU:HD13	1:D:1171:LEU:HA	1.56	0.47
1:D:2222:LEU:HG	1:D:2278:TRP:HB3	1.96	0.47
3:C:303:D12:H21	3:C:303:D12:H51	1.54	0.47
1:A:2147:PHE:CE1	1:A:2151:CYS:SG	3.08	0.47
1:A:2294:ASN:OD1	1:A:2294:ASN:N	2.47	0.47
1:B:682:SER:O	1:B:683:SER:C	2.57	0.47
1:B:1515:TRP:HE3	1:B:1516:MET:CE	2.08	0.47
1:B:2354:ASN:HA	1:B:2384:GLY:HA2	1.97	0.47
1:D:1316:ALA:HA	1:D:1319:LEU:HB2	1.97	0.47
1:D:2503:LEU:HA	1:D:2503:LEU:HD23	1.82	0.47
1:A:1744:LYS:HD2	1:A:1782:TYR:HB2	1.97	0.46
1:B:2225:MET:HB2	1:B:2406:ILE:HD11	1.96	0.46
1:B:2307:PHE:HE2	1:B:2360:ILE:HG21	1.80	0.46
1:D:786:ARG:HE	1:D:786:ARG:HB3	1.55	0.46
1:D:1710:LEU:HD23	1:D:1710:LEU:HA	1.76	0.46
1:D:2256:PHE:CD2	1:D:2371:VAL:HG13	2.51	0.46
1:D:2293:TYR:CB	1:D:2294:ASN:OD1	2.63	0.46
1:A:2208:ILE:HG23	1:A:2229:GLN:HG2	1.97	0.46
1:A:2225:MET:HB2	1:A:2406:ILE:HD11	1.96	0.46
1:A:2401:LEU:HD22	1:A:2403:TRP:CH2	2.51	0.46
1:B:814:LEU:HD23	1:B:814:LEU:HA	1.68	0.46
1:B:2208:ILE:HG23	1:B:2229:GLN:HG2	1.97	0.46
1:A:1553:GLU:HB2	1:A:1554:LEU:H	1.58	0.46
1:A:1744:LYS:HZ3	1:A:1744:LYS:CB	2.28	0.46
1:A:2010:ILE:HD12	1:A:2010:ILE:HA	1.63	0.46
1:A:2222:LEU:HG	1:A:2278:TRP:HB3	1.96	0.46
1:A:2464:HIS:CE1	1:D:2468:PHE:CB	2.98	0.46
1:B:2292:LEU:HG	1:B:2292:LEU:H	1.41	0.46
1:B:2308:GLN:HG3	1:B:2319:TYR:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1157:MET:HA	1:D:1160:VAL:HG22	1.98	0.46
1:D:1214:LEU:HD22	1:D:1214:LEU:HA	1.74	0.46
1:D:1649:LEU:H	1:D:1649:LEU:HG	1.58	0.46
1:D:2099:ASN:HB3	1:D:2100:HIS:H	1.57	0.46
1:D:2308:GLN:HG3	1:D:2319:TYR:HD2	1.80	0.46
1:A:635:ALA:O	1:A:639:LEU:CD1	2.45	0.46
1:A:1559:GLU:H	1:A:1559:GLU:HG3	1.51	0.46
1:A:2293:TYR:CB	1:A:2294:ASN:OD1	2.63	0.46
1:A:2502:LYS:HB3	1:A:2502:LYS:HE3	1.39	0.46
1:B:1157:MET:HA	1:B:1160:VAL:HG22	1.98	0.46
1:B:2302:ARG:H	1:B:2302:ARG:HG2	1.35	0.46
1:B:2408:LEU:H	1:B:2411:CYS:HB2	1.81	0.46
1:B:2513:MET:HE2	1:B:2513:MET:HB2	1.67	0.46
1:D:2208:ILE:HG23	1:D:2229:GLN:HG2	1.97	0.46
1:A:1203:LEU:O	1:A:1207:ASP:HB2	2.15	0.46
1:A:1316:ALA:HA	1:A:1319:LEU:HB2	1.97	0.46
1:A:2184:ILE:HD11	1:D:2012:PHE:CD2	2.43	0.46
1:A:2308:GLN:HG3	1:A:2319:TYR:HD2	1.80	0.46
1:A:2434:PHE:HD1	1:A:2435:LEU:N	2.14	0.46
1:B:596:ARG:HD2	1:B:596:ARG:HA	1.64	0.46
1:B:1037:LEU:HD23	1:B:1037:LEU:HA	1.73	0.46
1:B:2222:LEU:HG	1:B:2278:TRP:HB3	1.96	0.46
3:C:302:D12:H41	3:C:302:D12:H71	1.58	0.46
1:A:587:MET:CA	1:A:587:MET:CE	2.89	0.46
1:A:627:LYS:CA	1:A:627:LYS:CE	2.81	0.46
1:A:2167:LYS:HA	1:A:2167:LYS:HE2	1.95	0.46
1:B:1649:LEU:H	1:B:1649:LEU:HG	1.58	0.46
1:B:2147:PHE:CE1	1:B:2151:CYS:SG	3.09	0.46
1:B:2153:ARG:HA	1:B:2153:ARG:HD3	1.61	0.46
1:D:1014:LEU:HD12	1:D:1014:LEU:HA	1.73	0.46
1:D:1949:ILE:HD12	1:D:1949:ILE:HA	1.80	0.46
1:D:2225:MET:HB2	1:D:2406:ILE:HD11	1.96	0.46
1:D:2377:ASN:CB	1:D:2380:ALA:HB3	2.45	0.46
1:D:2434:PHE:CD1	1:D:2435:LEU:N	2.84	0.46
1:A:1157:MET:HA	1:A:1160:VAL:HG22	1.98	0.46
1:A:2128:ASP:CG	1:B:2166:LYS:HE2	2.39	0.46
1:A:2189:PHE:HD1	1:A:2189:PHE:HA	1.63	0.46
1:A:2307:PHE:HE2	1:A:2360:ILE:HG21	1.80	0.46
1:D:695:ILE:HD12	1:D:695:ILE:HA	1.78	0.46
1:D:2401:LEU:HD22	1:D:2403:TRP:CH2	2.51	0.46
3:E:301:D12:H61	3:E:301:D12:H32	1.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:THR:HG23	1:A:815:LEU:HD21	1.98	0.46
1:A:853:LYS:H	1:A:853:LYS:CE	2.29	0.46
1:A:2434:PHE:CD1	1:A:2435:LEU:N	2.84	0.46
1:B:1649:LEU:HB2	1:B:1650:LEU:H	1.59	0.46
1:B:2434:PHE:HD1	1:B:2435:LEU:N	2.14	0.46
1:D:1220:LEU:HD13	1:D:1220:LEU:HA	1.76	0.46
1:D:1744:LYS:NZ	1:D:1744:LYS:CB	2.78	0.46
1:D:2147:PHE:CE1	1:D:2151:CYS:SG	3.08	0.46
1:D:2189:PHE:HD1	1:D:2189:PHE:HA	1.63	0.46
1:A:1554:LEU:HB3	1:A:1555:LEU:H	1.51	0.46
1:A:2010:ILE:O	1:A:2011:GLN:C	2.57	0.46
1:A:2012:PHE:CD2	1:B:2184:ILE:HD11	2.43	0.46
1:A:2377:ASN:CB	1:A:2380:ALA:HB3	2.45	0.46
1:B:800:THR:HG23	1:B:815:LEU:HD21	1.98	0.46
1:B:1555:LEU:HB2	1:B:1556:GLN:H	1.45	0.46
1:D:587:MET:HA	1:D:587:MET:CE	2.45	0.46
1:D:2434:PHE:HD1	1:D:2435:LEU:N	2.14	0.46
1:D:2513:MET:HE2	1:D:2513:MET:HB2	1.67	0.46
1:A:602:ILE:H	1:A:602:ILE:HG13	1.47	0.46
1:A:768:GLU:HB2	1:A:769:LEU:H	1.64	0.46
1:B:2166:LYS:HB3	1:B:2167:LYS:H	1.52	0.46
1:D:800:THR:HG23	1:D:815:LEU:HD21	1.98	0.46
1:D:1052:GLN:CB	1:D:1099:LEU:CD1	2.76	0.46
1:D:2302:ARG:H	1:D:2302:ARG:HG2	1.35	0.46
1:A:1214:LEU:HD22	1:A:1214:LEU:HA	1.74	0.45
1:A:1365:ARG:HA	1:A:1368:ARG:HE	1.80	0.45
1:A:1699:HIS:CG	1:A:1707:SER:HB2	2.49	0.45
1:A:2466:ILE:O	1:D:2508:ARG:HG2	2.17	0.45
1:B:1358:ARG:HE	1:B:1358:ARG:HB2	1.46	0.45
1:B:1360:LYS:HB2	1:B:1360:LYS:HE2	1.52	0.45
1:B:1744:LYS:NZ	1:B:1744:LYS:CB	2.78	0.45
1:B:2302:ARG:HE	1:B:2323:LYS:HZ2	1.63	0.45
1:B:2401:LEU:HD22	1:B:2403:TRP:CH2	2.51	0.45
1:D:1555:LEU:H	1:D:1555:LEU:HG	1.47	0.45
1:D:1744:LYS:HD2	1:D:1782:TYR:HB2	1.97	0.45
1:D:2222:LEU:HB3	1:D:2223:PHE:H	1.50	0.45
1:A:572:VAL:HA	1:A:575:VAL:HB	1.97	0.45
1:A:2256:PHE:CD2	1:A:2371:VAL:HG13	2.51	0.45
1:A:2289:LYS:CA	1:A:2292:LEU:CD1	2.90	0.45
1:B:1650:LEU:HD23	1:B:1654:LEU:HD11	1.94	0.45
1:B:1710:LEU:HD23	1:B:1710:LEU:HA	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2377:ASN:CB	1:B:2380:ALA:HB3	2.45	0.45
1:D:1515:TRP:HE3	1:D:1516:MET:CE	2.08	0.45
1:D:2167:LYS:HA	1:D:2167:LYS:HE2	1.95	0.45
1:D:2313:LYS:H	1:D:2313:LYS:HG3	1.51	0.45
1:D:2354:ASN:HA	1:D:2384:GLY:HA2	1.97	0.45
1:D:2408:LEU:H	1:D:2411:CYS:HB2	1.81	0.45
3:E:302:D12:H41	3:E:302:D12:H71	1.58	0.45
1:A:2137:MET:HB3	1:B:2462:ILE:CD1	2.47	0.45
1:B:785:ARG:HB3	1:B:945:VAL:HG21	1.99	0.45
1:B:984:LYS:HD2	1:B:984:LYS:HA	1.47	0.45
1:B:2434:PHE:CD1	1:B:2435:LEU:N	2.84	0.45
1:A:1219:ILE:HG13	1:A:1295:LEU:HB3	1.98	0.45
1:A:1562:ARG:HD2	1:A:1562:ARG:HA	1.36	0.45
1:A:2354:ASN:HA	1:A:2384:GLY:HA2	1.97	0.45
1:A:2408:LEU:H	1:A:2411:CYS:HB2	1.81	0.45
1:B:635:ALA:O	1:B:639:LEU:CD1	2.45	0.45
1:B:1568:LEU:HD13	1:B:1659:LEU:CD2	2.47	0.45
1:B:2468:PHE:CB	1:D:2464:HIS:CE1	2.98	0.45
1:D:1365:ARG:HA	1:D:1368:ARG:HE	1.81	0.45
1:D:1940:ARG:N	1:D:1941:PRO:HD3	2.32	0.45
1:D:2010:ILE:HD12	1:D:2010:ILE:HA	1.63	0.45
1:A:1568:LEU:HD13	1:A:1659:LEU:CD2	2.47	0.45
1:B:2222:LEU:HD13	1:B:2222:LEU:HA	1.77	0.45
1:D:1360:LYS:HB2	1:D:1360:LYS:HE2	1.52	0.45
1:D:1555:LEU:HB2	1:D:1556:GLN:H	1.45	0.45
1:A:684:ILE:O	1:A:685:LEU:C	2.60	0.45
3:A:2601:D12:H62	3:A:2601:D12:H92	1.51	0.45
1:B:1219:ILE:HG13	1:B:1295:LEU:HB3	1.98	0.45
1:B:1554:LEU:HB3	1:B:1555:LEU:H	1.51	0.45
1:B:1699:HIS:CG	1:B:1707:SER:HB2	2.49	0.45
1:B:1744:LYS:HD2	1:B:1782:TYR:HB2	1.97	0.45
1:A:798:LEU:HD13	1:A:798:LEU:HA	1.68	0.45
1:B:622:TRP:HB2	1:B:711:MET:HE2	1.99	0.45
1:B:2157:LYS:HB2	1:B:2157:LYS:HE2	1.56	0.45
3:C:302:D12:H112	3:C:302:D12:H82	1.34	0.45
1:A:678:SER:O	1:A:682:SER:N	2.50	0.45
1:A:1568:LEU:C	1:A:1653:ARG:CB	2.88	0.45
1:B:2137:MET:HB3	1:D:2462:ILE:CD1	2.47	0.45
1:B:2256:PHE:CD2	1:B:2371:VAL:HG13	2.51	0.45
1:B:2508:ARG:HG2	1:D:2466:ILE:O	2.17	0.45
1:D:1218:LEU:HD22	1:D:1218:LEU:HA	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2374:LEU:HD12	1:D:2374:LEU:HA	1.78	0.45
1:A:1649:LEU:HB2	1:A:1650:LEU:H	1.59	0.45
1:A:1940:ARG:N	1:A:1941:PRO:HD3	2.32	0.45
1:A:2222:LEU:HB3	1:A:2223:PHE:H	1.50	0.45
1:A:2248:ASP:HA	1:A:2254:MET:HB2	1.99	0.45
1:A:2508:ARG:HG2	1:B:2466:ILE:O	2.17	0.45
1:B:2265:ILE:HD13	1:B:2423:PHE:CB	2.44	0.45
1:D:847:LYS:HA	1:D:847:LYS:HD3	1.56	0.45
1:A:2374:LEU:HD12	1:A:2374:LEU:HA	1.78	0.45
1:A:2462:ILE:CD1	1:D:2137:MET:HB3	2.47	0.45
1:B:853:LYS:CE	1:B:853:LYS:H	2.29	0.45
1:B:1365:ARG:HA	1:B:1368:ARG:HE	1.80	0.45
1:D:678:SER:O	1:D:682:SER:N	2.50	0.45
1:D:806:LYS:HA	1:D:806:LYS:HD3	1.64	0.45
1:D:1219:ILE:HG13	1:D:1295:LEU:HB3	1.98	0.45
1:D:1656:ILE:HB	1:D:1657:PRO:HD3	1.99	0.45
1:D:2292:LEU:HG	1:D:2292:LEU:H	1.41	0.45
1:D:2341:LEU:HB3	1:D:2389:LEU:HD23	2.00	0.45
1:A:607:LEU:HD23	1:A:607:LEU:HA	1.84	0.44
1:A:1656:ILE:HB	1:A:1657:PRO:HD3	1.99	0.44
1:A:2065:LEU:HD13	1:A:2065:LEU:HA	1.71	0.44
1:B:2222:LEU:HB3	1:B:2223:PHE:H	1.50	0.44
1:D:785:ARG:HB3	1:D:945:VAL:HG21	1.99	0.44
1:D:1953:LYS:HB2	1:D:1954:TYR:H	1.47	0.44
1:D:2011:GLN:HE21	1:D:2011:GLN:HB2	1.44	0.44
1:A:786:ARG:HE	1:A:786:ARG:HB3	1.55	0.44
1:A:2198:ARG:HE	1:A:2198:ARG:HB2	1.57	0.44
1:B:1187:LEU:HD23	1:B:1187:LEU:HA	1.87	0.44
1:B:1220:LEU:HD13	1:B:1220:LEU:HA	1.76	0.44
1:B:1562:ARG:NE	1:B:1566:ASP:CB	2.77	0.44
1:D:2157:LYS:HB2	1:D:2157:LYS:HE2	1.56	0.44
1:D:2288:MET:O	1:D:2292:LEU:CG	2.64	0.44
1:A:1345:LYS:HB2	1:A:1345:LYS:HE2	1.81	0.44
1:B:1656:ILE:HB	1:B:1657:PRO:HD3	1.99	0.44
1:D:622:TRP:HB2	1:D:711:MET:HE2	1.99	0.44
1:D:1650:LEU:HD23	1:D:1654:LEU:HD11	1.94	0.44
3:F:301:D12:H122	3:F:301:D12:H91	1.69	0.44
1:B:1546:GLU:H	1:B:1546:GLU:HG3	1.67	0.44
1:B:1552:GLN:OE1	1:B:1552:GLN:N	2.45	0.44
1:B:1744:LYS:O	1:B:1747:PHE:CD1	2.71	0.44
1:B:1940:ARG:N	1:B:1941:PRO:HD3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1744:LYS:O	1:D:1747:PHE:CD1	2.71	0.44
1:D:2325:MET:HB3	1:D:2325:MET:HE3	1.65	0.44
1:A:807:GLU:H	1:A:807:GLU:HG2	1.44	0.44
1:A:1744:LYS:O	1:A:1747:PHE:CD1	2.71	0.44
1:B:684:ILE:O	1:B:685:LEU:C	2.60	0.44
1:B:2248:ASP:HA	1:B:2254:MET:HB2	1.99	0.44
1:B:2432:LEU:H	1:B:2432:LEU:HG	1.62	0.44
1:D:609:LEU:HD12	1:D:609:LEU:HA	1.80	0.44
1:D:635:ALA:O	1:D:639:LEU:CD1	2.45	0.44
1:D:1037:LEU:HD23	1:D:1037:LEU:HA	1.73	0.44
1:A:847:LYS:HA	1:A:847:LYS:HD3	1.56	0.44
1:A:1043:LEU:HD23	1:A:1043:LEU:HA	1.77	0.44
1:A:2341:LEU:HB3	1:A:2389:LEU:HD23	2.00	0.44
1:D:853:LYS:CE	1:D:853:LYS:H	2.29	0.44
1:A:785:ARG:HB3	1:A:945:VAL:HG21	1.99	0.44
1:A:814:LEU:HD23	1:A:814:LEU:HA	1.68	0.44
1:A:1360:LYS:HB2	1:A:1360:LYS:HE2	1.52	0.44
1:A:1562:ARG:NE	1:A:1566:ASP:CB	2.77	0.44
1:B:587:MET:CA	1:B:587:MET:CE	2.89	0.44
1:B:2220:GLU:HB2	1:B:2280:ILE:HG23	2.00	0.44
1:D:2101:LEU:HD22	1:D:2101:LEU:HA	1.72	0.44
1:A:2220:GLU:HB2	1:A:2280:ILE:HG23	2.00	0.44
1:B:683:SER:O	1:B:684:ILE:C	2.61	0.44
1:B:807:GLU:H	1:B:807:GLU:HG2	1.44	0.44
1:B:2341:LEU:HB3	1:B:2389:LEU:HD23	2.00	0.44
1:D:1562:ARG:HD2	1:D:1562:ARG:HA	1.36	0.44
1:D:1568:LEU:C	1:D:1653:ARG:CB	2.88	0.44
1:D:2248:ASP:HA	1:D:2254:MET:HB2	1.99	0.44
1:B:708:LEU:HD23	1:B:708:LEU:HA	1.85	0.44
1:B:2175:MET:SD	2:F:239:GLU:HB2	2.58	0.44
1:D:1112:GLN:O	1:D:1116:PHE:HB2	2.18	0.44
1:D:1674:ARG:HE	1:D:1674:ARG:HB3	1.53	0.44
1:A:827:ARG:H	1:A:827:ARG:HG2	1.45	0.43
1:A:2467:MET:HA	1:D:2508:ARG:HG2	2.00	0.43
1:B:573:LYS:HA	1:B:573:LYS:HD3	1.51	0.43
1:B:587:MET:HA	1:B:587:MET:CE	2.45	0.43
1:B:703:ARG:H	1:B:703:ARG:HG3	1.51	0.43
1:B:2291:GLU:HB3	1:B:2335:ARG:NH2	2.33	0.43
1:D:683:SER:O	1:D:684:ILE:C	2.61	0.43
1:D:1554:LEU:HB3	1:D:1555:LEU:H	1.51	0.43
1:D:2254:MET:HE3	1:D:2254:MET:HB3	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2302:ARG:HB3	1:D:2302:ARG:HE	1.42	0.43
1:D:2341:LEU:HD23	1:D:2341:LEU:HA	1.90	0.43
1:D:2418:LEU:HA	1:D:2419:PRO:HD3	1.88	0.43
4:D:2601:L9Q:H24	4:D:2601:L9Q:H27	1.73	0.43
1:A:1357:ILE:CG2	1:A:2495:LEU:HD22	2.47	0.43
1:A:2153:ARG:HA	1:A:2153:ARG:HD3	1.61	0.43
1:A:2383:LEU:HD12	1:A:2383:LEU:HA	1.84	0.43
1:B:2502:LYS:HE3	1:B:2502:LYS:HB3	1.39	0.43
1:D:1656:ILE:H	1:D:1656:ILE:HG12	1.51	0.43
1:D:2220:GLU:HB2	1:D:2280:ILE:HG23	2.00	0.43
1:D:2309:ARG:H	1:D:2318:GLU:HB2	1.83	0.43
1:A:1104:LEU:HD13	1:A:1104:LEU:HA	1.73	0.43
1:A:1733:ALA:HB3	1:A:1793:LEU:CD2	2.48	0.43
1:A:2213:THR:CG2	1:A:2224:THR:HG23	2.42	0.43
1:A:2223:PHE:CE1	1:A:2406:ILE:HG12	2.54	0.43
1:A:2309:ARG:H	1:A:2318:GLU:HB2	1.83	0.43
1:B:1568:LEU:C	1:B:1653:ARG:CB	2.88	0.43
1:B:2252:LEU:H	1:B:2252:LEU:HG	1.39	0.43
1:D:1744:LYS:HZ3	1:D:1744:LYS:CB	2.29	0.43
3:D:2602:D12:H62	3:D:2602:D12:H92	1.51	0.43
1:A:1654:LEU:HB3	1:A:1655:ARG:H	1.60	0.43
1:A:1674:ARG:HE	1:A:1674:ARG:HB3	1.53	0.43
1:A:2101:LEU:HD22	1:A:2101:LEU:HA	1.72	0.43
1:B:1112:GLN:O	1:B:1116:PHE:HB2	2.18	0.43
1:B:2167:LYS:HA	1:B:2167:LYS:HE2	1.95	0.43
1:B:2384:GLY:O	1:B:2408:LEU:HG	2.19	0.43
3:B:2602:D12:H21	3:B:2602:D12:H51	1.90	0.43
1:D:1351:LYS:HD2	1:D:1351:LYS:HA	1.28	0.43
1:D:1568:LEU:HD13	1:D:1659:LEU:CD2	2.47	0.43
1:D:2302:ARG:CB	1:D:2323:LYS:HZ1	2.13	0.43
4:D:2601:L9Q:H45	4:D:2601:L9Q:H42	1.69	0.43
1:A:622:TRP:HB2	1:A:711:MET:HE2	1.99	0.43
1:A:853:LYS:N	1:A:853:LYS:CE	2.81	0.43
1:A:2009:LEU:HG	1:B:2188:TRP:CH2	2.54	0.43
1:A:2222:LEU:HD13	1:A:2222:LEU:HA	1.77	0.43
1:B:587:MET:N	1:B:587:MET:CE	2.66	0.43
1:B:2099:ASN:HB3	1:B:2100:HIS:H	1.57	0.43
1:B:2110:ARG:NH1	4:D:2601:L9Q:C4	2.82	0.43
1:B:2417:LEU:HD23	1:B:2417:LEU:HA	1.79	0.43
1:B:2507:TYR:HB3	1:D:2466:ILE:CG1	2.46	0.43
1:D:787:LEU:HD22	1:D:787:LEU:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2175:MET:SD	2:C:239:GLU:HB2	2.58	0.43
1:D:2223:PHE:CE1	1:D:2406:ILE:HG12	2.53	0.43
1:A:623:ARG:HE	1:A:623:ARG:HB2	1.48	0.43
1:A:2175:MET:SD	2:E:239:GLU:HB2	2.58	0.43
1:A:2292:LEU:HG	1:A:2292:LEU:H	1.41	0.43
1:A:2313:LYS:H	1:A:2313:LYS:HG3	1.51	0.43
1:A:2508:ARG:HG2	1:B:2467:MET:HA	2.00	0.43
1:B:571:LEU:H	1:B:571:LEU:HG	1.65	0.43
1:B:787:LEU:HD22	1:B:787:LEU:HA	1.77	0.43
1:D:623:ARG:HE	1:D:623:ARG:HB2	1.48	0.43
3:E:301:D12:H12	3:E:301:D12:H41	1.84	0.43
1:A:1112:GLN:O	1:A:1116:PHE:HB2	2.18	0.43
1:A:1358:ARG:HE	1:A:1358:ARG:HB2	1.46	0.43
1:A:1360:LYS:O	1:A:1362:GLU:N	2.52	0.43
1:A:2019:ARG:HE	1:A:2023:LEU:CD2	2.32	0.43
1:B:678:SER:O	1:B:682:SER:N	2.50	0.43
1:B:1043:LEU:HD23	1:B:1043:LEU:HA	1.77	0.43
1:B:1214:LEU:HA	1:B:1214:LEU:HD22	1.74	0.43
1:B:1697:LEU:HD22	1:B:1697:LEU:HA	1.81	0.43
1:B:2019:ARG:HE	1:B:2023:LEU:HD22	1.84	0.43
1:B:2223:PHE:CE1	1:B:2406:ILE:HG12	2.54	0.43
1:B:2254:MET:HE3	1:B:2254:MET:HB3	1.58	0.43
1:D:587:MET:N	1:D:587:MET:CE	2.66	0.43
1:D:1319:LEU:HD12	1:D:1319:LEU:HA	1.85	0.43
1:D:2166:LYS:HB3	1:D:2167:LYS:H	1.52	0.43
1:D:2291:GLU:HB3	1:D:2335:ARG:NH2	2.33	0.43
1:A:2110:ARG:NH1	4:B:2601:L9Q:C4	2.82	0.43
1:A:2188:TRP:CH2	1:D:2009:LEU:HG	2.54	0.43
1:B:636:TYR:HA	1:B:639:LEU:HD12	2.01	0.43
1:B:768:GLU:HB2	1:B:769:LEU:H	1.64	0.43
1:D:2037:LEU:HD23	1:D:2037:LEU:HA	1.79	0.43
3:F:302:D12:H61	3:F:302:D12:H91	1.86	0.43
3:F:303:D12:H21	3:F:303:D12:H51	1.54	0.43
1:A:2168:LYS:HD3	1:A:2168:LYS:HA	1.81	0.43
1:A:2169:LYS:HZ3	1:A:2169:LYS:HG2	1.70	0.43
1:B:1733:ALA:HB3	1:B:1793:LEU:CD2	2.48	0.43
1:B:2309:ARG:H	1:B:2318:GLU:HB2	1.83	0.43
3:B:2602:D12:H62	3:B:2602:D12:H92	1.51	0.43
1:D:2019:ARG:HE	1:D:2023:LEU:HD22	1.84	0.43
1:A:597:LEU:HD23	1:A:848:MET:O	2.19	0.43
1:A:1949:ILE:HD12	1:A:1949:ILE:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:LEU:HD12	1:B:610:LEU:HA	1.77	0.43
1:B:2107:GLN:HB3	2:F:245:PHE:CZ	2.54	0.43
1:B:2443:LEU:HD22	1:B:2444:TYR:HA	2.01	0.43
1:D:636:TYR:HA	1:D:639:LEU:HD12	2.01	0.43
1:D:1722:ILE:H	1:D:1722:ILE:HG13	1.23	0.43
1:D:1733:ALA:HB3	1:D:1793:LEU:CD2	2.48	0.43
3:E:302:D12:H82	3:E:302:D12:H112	1.34	0.43
1:A:2137:MET:HG2	1:B:2459:PHE:CD1	2.54	0.42
1:A:2462:ILE:HD13	1:D:2137:MET:HB3	2.01	0.42
4:A:2603:L9Q:C4	1:D:2110:ARG:NH1	2.82	0.42
1:B:847:LYS:HD3	1:B:847:LYS:HA	1.56	0.42
1:B:1719:MET:HE2	1:B:1719:MET:HB2	1.64	0.42
1:D:1975:ILE:HD13	1:D:1975:ILE:HA	1.91	0.42
1:A:787:LEU:HD22	1:A:787:LEU:HA	1.77	0.42
1:A:2302:ARG:H	1:A:2302:ARG:HG2	1.35	0.42
1:B:2010:ILE:HA	1:B:2010:ILE:HD12	1.63	0.42
1:B:2019:ARG:HE	1:B:2023:LEU:CD2	2.32	0.42
1:B:2313:LYS:H	1:B:2313:LYS:HG3	1.51	0.42
1:D:951:HIS:HA	1:D:954:ARG:HB2	2.01	0.42
1:D:1552:GLN:OE1	1:D:1552:GLN:N	2.45	0.42
1:A:785:ARG:HA	1:A:790:LEU:CB	2.46	0.42
1:A:951:HIS:HA	1:A:954:ARG:HB2	2.01	0.42
1:A:1351:LYS:HA	1:A:1351:LYS:HD2	1.28	0.42
1:A:2037:LEU:HD23	1:A:2037:LEU:HA	1.79	0.42
1:A:2265:ILE:HD11	1:A:2423:PHE:CE2	2.51	0.42
1:D:684:ILE:O	1:D:685:LEU:C	2.60	0.42
1:D:710:ASP:HB2	1:D:712:GLU:OE1	2.20	0.42
1:A:710:ASP:HB2	1:A:712:GLU:OE1	2.20	0.42
1:A:1719:MET:HE2	1:A:1719:MET:HB2	1.64	0.42
1:B:1218:LEU:HD22	1:B:1218:LEU:HA	1.68	0.42
1:D:827:ARG:H	1:D:827:ARG:HG2	1.45	0.42
1:D:1345:LYS:HB2	1:D:1345:LYS:HE2	1.81	0.42
1:D:1549:LEU:HD13	1:D:1549:LEU:HA	1.84	0.42
1:D:1719:MET:HE2	1:D:1719:MET:HB2	1.64	0.42
1:D:2107:GLN:HB3	2:C:245:PHE:CZ	2.54	0.42
1:A:2459:PHE:CD1	1:D:2137:MET:HG2	2.54	0.42
1:B:849:LEU:O	1:B:850:TYR:C	2.63	0.42
1:B:2116:VAL:HG21	1:D:2456:ARG:NH2	2.35	0.42
4:B:2601:L9Q:H27	4:B:2601:L9Q:H24	1.73	0.42
2:E:246:PRO:O	2:E:247:SER:C	2.63	0.42
1:A:683:SER:O	1:A:684:ILE:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2025:LYS:HD2	1:A:2085:TYR:HB3	2.02	0.42
1:A:2030:LYS:HD2	1:A:2030:LYS:HA	1.58	0.42
1:A:2291:GLU:HB3	1:A:2335:ARG:NH2	2.34	0.42
1:A:2432:LEU:H	1:A:2432:LEU:HG	1.62	0.42
1:B:710:ASP:HB2	1:B:712:GLU:OE1	2.20	0.42
1:B:1674:ARG:HE	1:B:1674:ARG:HB3	1.53	0.42
1:B:2015:MET:HE2	1:B:2015:MET:HB2	1.86	0.42
1:B:2288:MET:O	1:B:2292:LEU:CG	2.64	0.42
4:B:2601:L9Q:H39	4:B:2601:L9Q:H42	1.93	0.42
1:D:2019:ARG:HE	1:D:2023:LEU:CD2	2.32	0.42
1:D:2314:GLY:HA3	1:D:2427:VAL:HG11	2.02	0.42
1:A:1943:ARG:H	1:A:1943:ARG:HG3	1.47	0.42
1:A:2305:TRP:HE3	1:A:2307:PHE:HZ	1.68	0.42
1:A:2456:ARG:NH2	1:D:2116:VAL:HG21	2.35	0.42
4:A:2603:L9Q:H45	4:A:2603:L9Q:H42	1.69	0.42
1:B:951:HIS:HA	1:B:954:ARG:HB2	2.01	0.42
1:B:1363:LYS:HB3	1:B:1363:LYS:HE3	1.28	0.42
1:B:2025:LYS:HD2	1:B:2085:TYR:HB3	2.02	0.42
1:D:1102:ASP:OD1	1:D:1102:ASP:O	2.38	0.42
1:D:1408:ASP:HB2	1:D:1411:THR:HG23	2.01	0.42
1:D:1722:ILE:O	1:D:1723:PRO:C	2.63	0.42
1:A:2107:GLN:HB3	2:E:245:PHE:CZ	2.54	0.42
1:A:2384:GLY:O	1:A:2408:LEU:HG	2.19	0.42
4:A:2603:L9Q:H24	4:A:2603:L9Q:H27	1.73	0.42
1:B:627:LYS:HA	1:B:627:LYS:CE	2.20	0.42
1:B:806:LYS:HA	1:B:806:LYS:HD3	1.64	0.42
1:B:1102:ASP:OD1	1:B:1102:ASP:O	2.38	0.42
1:B:2009:LEU:HG	1:D:2188:TRP:CH2	2.54	0.42
1:B:2012:PHE:CD2	1:D:2184:ILE:HD11	2.43	0.42
1:B:2305:TRP:HE3	1:B:2307:PHE:HZ	1.68	0.42
1:D:1360:LYS:O	1:D:1362:GLU:N	2.52	0.42
2:C:246:PRO:O	2:C:247:SER:C	2.63	0.42
3:F:302:D12:H71	3:F:302:D12:H41	1.58	0.42
1:A:2019:ARG:HE	1:A:2023:LEU:HD22	1.84	0.42
1:A:2302:ARG:HE	1:A:2323:LYS:HZ2	1.66	0.42
1:A:2418:LEU:HA	1:A:2419:PRO:HD3	1.88	0.42
1:B:2114:PHE:CE1	1:D:2452:GLY:HA2	2.55	0.42
1:D:597:LEU:HD23	1:D:848:MET:O	2.19	0.42
1:D:947:ARG:HA	1:D:950:GLU:HB2	2.02	0.42
1:A:610:LEU:HD12	1:A:610:LEU:HA	1.77	0.42
1:A:1658:GLU:HB3	1:A:1661:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2511:GLU:HG3	1:D:1418:TYR:OH	2.19	0.42
1:A:2520:LYS:HB3	1:A:2520:LYS:HE3	1.71	0.42
1:B:1360:LYS:O	1:B:1362:GLU:N	2.52	0.42
1:B:2309:ARG:HB2	1:B:2310:ASP:H	1.60	0.42
1:D:1728:ARG:H	1:D:1728:ARG:HG3	1.37	0.42
1:D:2170:ILE:H	1:D:2170:ILE:HG12	1.32	0.42
1:D:2309:ARG:HB2	1:D:2310:ASP:H	1.60	0.42
1:A:852:LEU:H	1:A:852:LEU:HG	1.66	0.41
1:A:1418:TYR:OH	1:B:2511:GLU:HG3	2.20	0.41
1:B:597:LEU:HD23	1:B:848:MET:O	2.19	0.41
1:B:2508:ARG:HG2	1:D:2467:MET:HA	2.00	0.41
1:D:2025:LYS:HD2	1:D:2085:TYR:HB3	2.02	0.41
1:A:1186:GLY:HA3	1:A:1745:TYR:OH	2.20	0.41
1:A:1649:LEU:H	1:A:1649:LEU:HG	1.58	0.41
1:A:2137:MET:HB3	1:B:2462:ILE:HD13	2.01	0.41
1:A:2146:ILE:HG23	1:A:2474:VAL:HB	2.02	0.41
1:A:2341:LEU:HD23	1:A:2341:LEU:HA	1.90	0.41
1:A:2452:GLY:HA2	1:D:2114:PHE:CE1	2.55	0.41
1:B:1722:ILE:O	1:B:1723:PRO:C	2.63	0.41
1:D:607:LEU:HD23	1:D:607:LEU:HA	1.84	0.41
1:D:768:GLU:HB2	1:D:769:LEU:H	1.64	0.41
1:D:1658:GLU:HB3	1:D:1661:GLU:HB2	2.02	0.41
1:D:2133:LEU:HB3	2:E:243:ILE:CD1	2.47	0.41
2:F:246:PRO:O	2:F:247:SER:C	2.63	0.41
1:A:1697:LEU:HA	1:A:1697:LEU:HD22	1.81	0.41
1:A:2116:VAL:HG21	1:B:2456:ARG:NH2	2.35	0.41
1:A:2252:LEU:H	1:A:2252:LEU:HG	1.39	0.41
1:A:2325:MET:HE3	1:A:2325:MET:HB3	1.65	0.41
1:A:2509:SER:CB	1:B:2511:GLU:OE2	2.68	0.41
1:D:806:LYS:HB3	1:D:807:GLU:H	1.55	0.41
1:D:807:GLU:H	1:D:807:GLU:HG2	1.44	0.41
1:D:849:LEU:O	1:D:850:TYR:C	2.63	0.41
1:D:1099:LEU:HD12	1:D:1099:LEU:HA	1.84	0.41
1:D:1559:GLU:H	1:D:1559:GLU:HG3	1.51	0.41
1:D:1943:ARG:H	1:D:1943:ARG:HG3	1.47	0.41
1:D:2384:GLY:O	1:D:2408:LEU:HG	2.19	0.41
1:D:2443:LEU:HD22	1:D:2444:TYR:HA	2.01	0.41
3:D:2602:D12:H21	3:D:2602:D12:H51	1.91	0.41
1:A:1408:ASP:HB2	1:A:1411:THR:HG23	2.01	0.41
1:A:1650:LEU:HD23	1:A:1654:LEU:HD11	1.94	0.41
1:B:1186:GLY:HA3	1:B:1745:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1357:ILE:CG2	1:B:2495:LEU:HD22	2.46	0.41
1:D:955:GLN:O	1:D:956:HIS:C	2.63	0.41
1:A:614:LEU:HD23	1:A:614:LEU:HA	1.89	0.41
1:A:777:LEU:O	1:A:778:SER:C	2.62	0.41
1:A:955:GLN:O	1:A:956:HIS:C	2.63	0.41
1:A:2167:LYS:HE3	1:A:2167:LYS:HB2	1.80	0.41
1:A:2443:LEU:HD22	1:A:2444:TYR:HA	2.01	0.41
1:A:2471:LEU:HA	1:A:2472:PRO:HD3	1.96	0.41
1:B:786:ARG:HE	1:B:786:ARG:HB3	1.55	0.41
1:B:827:ARG:H	1:B:827:ARG:HG2	1.45	0.41
1:B:947:ARG:HA	1:B:950:GLU:HB2	2.02	0.41
1:B:1418:TYR:OH	1:D:2511:GLU:HG3	2.20	0.41
1:B:2137:MET:HG2	1:D:2459:PHE:CD1	2.54	0.41
1:D:1186:GLY:HA3	1:D:1745:TYR:OH	2.20	0.41
1:D:2030:LYS:HA	1:D:2030:LYS:HD2	1.58	0.41
1:D:2417:LEU:HD23	1:D:2417:LEU:HA	1.79	0.41
1:A:849:LEU:O	1:A:850:TYR:C	2.63	0.41
1:A:1549:LEU:HD13	1:A:1549:LEU:HA	1.84	0.41
1:A:2117:GLU:OE2	1:B:2456:ARG:HD3	2.21	0.41
1:A:2503:LEU:HD23	1:A:2503:LEU:HA	1.82	0.41
1:B:615:PHE:HB2	1:B:621:LEU:O	2.21	0.41
1:B:955:GLN:O	1:B:956:HIS:C	2.63	0.41
1:B:1296:LEU:HD12	1:B:1296:LEU:HA	1.94	0.41
1:B:1797:ARG:HE	1:B:1797:ARG:HB3	1.40	0.41
1:B:2137:MET:HB3	1:D:2462:ILE:HD13	2.01	0.41
1:B:2418:LEU:HA	1:B:2419:PRO:HD3	1.88	0.41
1:D:1724:ARG:O	1:D:1725:PRO:C	2.64	0.41
1:D:1797:ARG:HE	1:D:1797:ARG:HB3	1.40	0.41
1:D:1940:ARG:HA	1:D:1943:ARG:NE	2.35	0.41
1:D:2305:TRP:HE3	1:D:2307:PHE:HZ	1.68	0.41
1:A:587:MET:HA	1:A:587:MET:CE	2.45	0.41
1:A:2114:PHE:CE1	1:B:2452:GLY:HA2	2.55	0.41
1:A:2497:GLU:OE1	1:B:2164:GLY:HA2	2.21	0.41
1:B:777:LEU:O	1:B:778:SER:C	2.62	0.41
1:B:2117:GLU:OE2	1:D:2456:ARG:HD3	2.21	0.41
1:B:2497:GLU:OE1	1:D:2164:GLY:HA2	2.21	0.41
1:D:2146:ILE:HG23	1:D:2474:VAL:HB	2.02	0.41
3:E:301:D12:H122	3:E:301:D12:H91	1.69	0.41
1:A:615:PHE:HB2	1:A:621:LEU:O	2.21	0.41
1:A:636:TYR:HA	1:A:639:LEU:HD12	2.01	0.41
1:A:636:TYR:N	1:A:636:TYR:CD1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:ARG:HA	1:A:950:GLU:HB2	2.02	0.41
1:A:1550:LEU:O	1:A:1550:LEU:HG	2.21	0.41
1:A:1722:ILE:O	1:A:1723:PRO:C	2.63	0.41
1:B:577:ALA:HB1	1:B:701:PHE:HB3	2.03	0.41
1:B:1724:ARG:O	1:B:1725:PRO:C	2.64	0.41
1:B:2037:LEU:HD23	1:B:2037:LEU:HA	1.79	0.41
1:D:614:LEU:HD23	1:D:614:LEU:HA	1.89	0.41
1:A:626:LEU:O	1:A:630:TRP:N	2.53	0.41
1:A:626:LEU:HD22	1:A:626:LEU:C	2.41	0.41
1:A:691:LEU:HD22	1:A:691:LEU:HA	1.83	0.41
1:A:1102:ASP:O	1:A:1102:ASP:OD1	2.38	0.41
1:A:1327:LEU:HD12	1:A:1539:MET:HG2	2.03	0.41
1:A:2121:VAL:O	1:A:2125:VAL:HG23	2.21	0.41
1:A:2270:ILE:HD13	1:A:2418:LEU:HD13	2.03	0.41
1:A:2323:LYS:H	1:A:2323:LYS:HG2	1.40	0.41
1:A:2507:TYR:HB3	1:B:2466:ILE:CG1	2.46	0.41
1:B:596:ARG:O	1:B:600:TYR:HB2	2.21	0.41
1:B:1327:LEU:HD12	1:B:1539:MET:HG2	2.03	0.41
1:B:1408:ASP:HB2	1:B:1411:THR:HG23	2.01	0.41
1:B:2146:ILE:HG23	1:B:2474:VAL:HB	2.02	0.41
1:B:2167:LYS:HE3	1:B:2167:LYS:HB2	1.80	0.41
1:B:2213:THR:CG2	1:B:2224:THR:HG23	2.42	0.41
1:B:2371:VAL:CG1	1:B:2374:LEU:HD22	2.50	0.41
1:B:2407:GLU:HB3	1:B:2415:CYS:SG	2.61	0.41
1:B:2509:SER:CB	1:D:2511:GLU:OE2	2.68	0.41
4:B:2601:L9Q:H42	4:B:2601:L9Q:H45	1.69	0.41
1:D:849:LEU:H	1:D:849:LEU:HG	1.58	0.41
1:D:2015:MET:HE2	1:D:2015:MET:HB2	1.86	0.41
1:D:2289:LYS:CA	1:D:2292:LEU:CD1	2.90	0.41
1:A:823:LEU:HD12	1:A:823:LEU:HA	1.91	0.41
1:B:607:LEU:HD23	1:B:607:LEU:HA	1.84	0.41
1:B:1940:ARG:HA	1:B:1943:ARG:NE	2.35	0.41
1:B:1943:ARG:H	1:B:1943:ARG:HG3	1.48	0.41
1:B:2168:LYS:HD3	1:B:2168:LYS:HA	1.81	0.41
1:B:2268:ALA:HB2	1:B:2422:ILE:HG13	2.03	0.41
1:D:818:LEU:HD23	1:D:818:LEU:HA	1.90	0.41
1:D:1357:ILE:CG2	1:D:2495:LEU:HD22	2.46	0.41
1:D:2023:LEU:HD13	1:D:2023:LEU:HA	1.83	0.41
1:D:2213:THR:CG2	1:D:2224:THR:HG23	2.42	0.41
1:A:577:ALA:HB1	1:A:701:PHE:HB3	2.03	0.40
1:A:806:LYS:HB3	1:A:807:GLU:H	1.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1940:ARG:HA	1:A:1943:ARG:NE	2.35	0.40
1:A:2323:LYS:HZ2	1:A:2323:LYS:HB2	1.76	0.40
1:B:1182:ILE:H	1:B:1182:ILE:HG12	1.73	0.40
1:B:2314:GLY:HA3	1:B:2427:VAL:HG11	2.02	0.40
1:D:596:ARG:O	1:D:600:TYR:HB2	2.21	0.40
1:D:1550:LEU:O	1:D:1550:LEU:HG	2.21	0.40
1:A:2274:SER:HB3	1:A:2403:TRP:HB3	2.02	0.40
1:A:2407:GLU:HB3	1:A:2415:CYS:SG	2.61	0.40
1:A:2511:GLU:OE2	1:D:2509:SER:CB	2.68	0.40
1:B:578:LYS:HE3	1:B:578:LYS:HB2	1.58	0.40
1:B:1658:GLU:HB3	1:B:1661:GLU:HB2	2.02	0.40
1:D:624:LYS:HA	1:D:706:MET:O	2.22	0.40
1:D:924:PRO:HG2	1:D:928:TYR:CB	2.40	0.40
1:D:1546:GLU:H	1:D:1546:GLU:HG3	1.67	0.40
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.85	0.40
1:A:1797:ARG:HE	1:A:1797:ARG:HB3	1.40	0.40
1:A:2049:LEU:H	1:A:2049:LEU:CD2	2.20	0.40
1:A:2360:ILE:HG21	1:A:2360:ILE:HD12	1.88	0.40
1:A:2513:MET:HE2	1:A:2513:MET:HB2	1.67	0.40
1:B:624:LYS:HA	1:B:706:MET:O	2.22	0.40
1:B:686:VAL:CB	1:B:687:PRO:HD3	2.52	0.40
1:B:1565:LEU:H	1:B:1565:LEU:HG	1.67	0.40
1:B:2011:GLN:HE21	1:B:2011:GLN:HB2	1.44	0.40
1:B:2130:THR:HG23	1:B:2493:LEU:HB3	2.03	0.40
1:D:777:LEU:O	1:D:778:SER:C	2.62	0.40
1:D:853:LYS:N	1:D:853:LYS:CE	2.81	0.40
1:D:1363:LYS:HE3	1:D:1363:LYS:HB3	1.28	0.40
1:D:2121:VAL:O	1:D:2125:VAL:HG23	2.21	0.40
1:D:2383:LEU:HD12	1:D:2383:LEU:HA	1.84	0.40
1:D:2407:GLU:HB3	1:D:2415:CYS:SG	2.61	0.40
1:A:1656:ILE:H	1:A:1656:ILE:HG12	1.51	0.40
1:A:1724:ARG:O	1:A:1725:PRO:C	2.64	0.40
1:B:1327:LEU:HD22	1:B:1327:LEU:HA	1.90	0.40
1:B:1975:ILE:HD13	1:B:1975:ILE:HA	1.91	0.40
1:B:2121:VAL:O	1:B:2125:VAL:HG23	2.21	0.40
1:B:2274:SER:HB3	1:B:2403:TRP:HB3	2.02	0.40
1:B:2471:LEU:HA	1:B:2472:PRO:HD3	1.96	0.40
1:D:577:ALA:HB1	1:D:701:PHE:HB3	2.03	0.40
1:D:615:PHE:HB2	1:D:621:LEU:O	2.21	0.40
1:D:697:GLN:H	1:D:697:GLN:HG3	1.73	0.40
1:D:2361:ARG:H	1:D:2361:ARG:HG3	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:ARG:O	1:A:600:TYR:HB2	2.21	0.40
1:A:1546:GLU:H	1:A:1546:GLU:HG3	1.67	0.40
1:A:1555:LEU:HB2	1:A:1556:GLN:H	1.45	0.40
1:A:2207:PRO:HB3	1:A:2307:PHE:HB3	2.04	0.40
1:A:2371:VAL:HB	1:A:2374:LEU:HB2	2.04	0.40
1:A:2407:GLU:HA	1:A:2415:CYS:HA	2.04	0.40
1:B:1161:ALA:CA	1:B:1165:TYR:CE2	2.88	0.40
1:B:1547:ARG:HB3	1:B:1548:TYR:H	1.75	0.40
1:B:2503:LEU:HD23	1:B:2503:LEU:HA	1.82	0.40
1:D:814:LEU:HD23	1:D:814:LEU:HA	1.68	0.40
1:D:1327:LEU:HD12	1:D:1539:MET:HG2	2.03	0.40
1:D:2210:VAL:HG21	1:D:2268:ALA:HB1	2.04	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 PDB entries followed by that with respect to all EM entries.

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	1248/2521 (50%)	1069 (86%)	145 (12%)	34 (3%)	4	25
1	B	1248/2521 (50%)	1069 (86%)	145 (12%)	34 (3%)	4	25
1	D	1248/2521 (50%)	1069 (86%)	145 (12%)	34 (3%)	4	25
2	C	19/246 (8%)	17 (90%)	2 (10%)	0	100	100
2	E	19/246 (8%)	17 (90%)	2 (10%)	0	100	100
2	F	19/246 (8%)	17 (90%)	2 (10%)	0	100	100
All	All	3801/8301 (46%)	3258 (86%)	441 (12%)	102 (3%)	6	25

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1723	PRO

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Mol	Chain	Res	Type
1	A	1725	PRO
1	A	1953	LYS
1	A	2316	THR
1	A	2379	GLU
1	B	1723	PRO
1	B	1725	PRO
1	B	1953	LYS
1	B	2316	THR
1	B	2379	GLU
1	D	1723	PRO
1	D	1725	PRO
1	D	1953	LYS
1	D	2316	THR
1	D	2379	GLU
1	A	1029	ARG
1	A	1941	PRO
1	A	2295	GLY
1	A	2363	PRO
1	A	2382	TYR
1	B	1029	ARG
1	B	1941	PRO
1	B	2295	GLY
1	B	2363	PRO
1	B	2382	TYR
1	D	1029	ARG
1	D	1941	PRO
1	D	2295	GLY
1	D	2363	PRO
1	D	2382	TYR
1	A	850	TYR
1	A	921	LYS
1	A	1164	ARG
1	A	1555	LEU
1	A	1672	ALA
1	A	1726	SER
1	B	850	TYR
1	B	921	LYS
1	B	1164	ARG
1	B	1555	LEU
1	B	1672	ALA
1	B	1726	SER
1	D	850	TYR

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Mol	Chain	Res	Type
1	D	921	LYS
1	D	1164	ARG
1	D	1555	LEU
1	D	1672	ALA
1	D	1726	SER
1	A	620	SER
1	A	684	ILE
1	A	1200	GLY
1	A	1658	GLU
1	A	2168	LYS
1	A	2466	ILE
1	B	620	SER
1	B	684	ILE
1	B	1200	GLY
1	B	1658	GLU
1	B	2168	LYS
1	B	2466	ILE
1	D	620	SER
1	D	684	ILE
1	D	1200	GLY
1	D	1658	GLU
1	D	2168	LYS
1	D	2466	ILE
1	A	851	GLN
1	A	971	THR
1	A	1361	GLN
1	A	2113	PRO
1	B	851	GLN
1	B	971	THR
1	B	1361	GLN
1	B	2113	PRO
1	D	851	GLN
1	D	971	THR
1	D	1361	GLN
1	D	2113	PRO
1	A	1954	TYR
1	A	2419	PRO
1	B	1954	TYR
1	B	2419	PRO
1	D	1954	TYR
1	D	2419	PRO
1	A	599	VAL

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Mol	Chain	Res	Type
1	A	808	VAL
1	A	2353	PRO
1	B	599	VAL
1	B	808	VAL
1	B	2353	PRO
1	D	599	VAL
1	D	808	VAL
1	D	2353	PRO
1	A	2344	GLY
1	B	2344	GLY
1	D	2344	GLY
1	A	598	VAL
1	A	854	VAL
1	B	598	VAL
1	B	854	VAL
1	D	598	VAL
1	D	854	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 PDB entries followed by that with respect to all EM entries.

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	1121/2172 (52%)	642 (57%)	479 (43%)	0	0
1	B	1121/2172 (52%)	642 (57%)	479 (43%)	0	0
1	D	1121/2172 (52%)	642 (57%)	479 (43%)	0	0
2	C	20/203 (10%)	17 (85%)	3 (15%)	3	15
2	E	20/203 (10%)	17 (85%)	3 (15%)	3	15
2	F	20/203 (10%)	17 (85%)	3 (15%)	3	15
All	All	3423/7125 (48%)	1977 (58%)	1446 (42%)	0	0

All (1446) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	570	GLU

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Mol	Chain	Res	Type
1	A	571	LEU
1	A	572	VAL
1	A	573	LYS
1	A	578	LYS
1	A	579	TYR
1	A	580	TRP
1	A	581	ILE
1	A	583	VAL
1	A	587	MET
1	A	589	ILE
1	A	591	VAL
1	A	592	SER
1	A	593	PHE
1	A	596	ARG
1	A	597	LEU
1	A	598	VAL
1	A	602	ILE
1	A	608	PHE
1	A	609	LEU
1	A	610	LEU
1	A	611	CYS
1	A	612	LEU
1	A	617	VAL
1	A	621	LEU
1	A	623	ARG
1	A	626	LEU
1	A	627	LYS
1	A	631	TRP
1	A	638	MET
1	A	644	VAL
1	A	679	GLU
1	A	680	LEU
1	A	682	SER
1	A	685	LEU
1	A	687	PRO
1	A	691	LEU
1	A	694	CYS
1	A	695	ILE
1	A	696	LEU
1	A	700	TYR
1	A	703	ARG
1	A	706	MET

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Mol	Chain	Res	Type
1	A	707	GLN
1	A	708	LEU
1	A	709	THR
1	A	768	GLU
1	A	769	LEU
1	A	781	GLN
1	A	784	LEU
1	A	786	ARG
1	A	787	LEU
1	A	788	LEU
1	A	792	VAL
1	A	794	LYS
1	A	798	LEU
1	A	799	TYR
1	A	805	LEU
1	A	806	LYS
1	A	807	GLU
1	A	808	VAL
1	A	809	SER
1	A	813	LEU
1	A	817	VAL
1	A	823	LEU
1	A	827	ARG
1	A	828	PHE
1	A	831	MET
1	A	833	SER
1	A	836	SER
1	A	837	THR
1	A	839	TRP
1	A	841	CYS
1	A	843	ILE
1	A	844	ILE
1	A	848	MET
1	A	849	LEU
1	A	851	GLN
1	A	852	LEU
1	A	853	LYS
1	A	854	VAL
1	A	855	VAL
1	A	856	ASN
1	A	917	PHE
1	A	919	VAL

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Mol	Chain	Res	Type
1	A	920	ARG
1	A	921	LYS
1	A	925	ASN
1	A	930	GLN
1	A	932	HIS
1	A	933	LEU
1	A	935	VAL
1	A	936	LEU
1	A	938	LEU
1	A	946	TYR
1	A	949	GLN
1	A	953	ARG
1	A	954	ARG
1	A	971	THR
1	A	973	GLN
1	A	974	GLN
1	A	975	LEU
1	A	976	ASP
1	A	978	ASP
1	A	979	LEU
1	A	980	LEU
1	A	983	LEU
1	A	984	LYS
1	A	990	PHE
1	A	993	LYS
1	A	999	CYS
1	A	1002	MET
1	A	1007	ILE
1	A	1010	ARG
1	A	1014	LEU
1	A	1015	VAL
1	A	1025	ILE
1	A	1026	LEU
1	A	1028	ARG
1	A	1030	HIS
1	A	1031	ARG
1	A	1032	GLN
1	A	1034	ILE
1	A	1036	ARG
1	A	1037	LEU
1	A	1043	LEU
1	A	1048	PHE

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Mol	Chain	Res	Type
1	A	1050	LEU
1	A	1052	GLN
1	A	1055	LEU
1	A	1057	LEU
1	A	1097	THR
1	A	1099	LEU
1	A	1100	ILE
1	A	1101	SER
1	A	1103	PHE
1	A	1104	LEU
1	A	1112	GLN
1	A	1116	PHE
1	A	1119	GLU
1	A	1155	LEU
1	A	1156	ASP
1	A	1158	LEU
1	A	1162	VAL
1	A	1165	TYR
1	A	1171	LEU
1	A	1175	PHE
1	A	1181	ARG
1	A	1182	ILE
1	A	1184	ILE
1	A	1187	LEU
1	A	1191	LEU
1	A	1198	LEU
1	A	1201	THR
1	A	1203	LEU
1	A	1204	LEU
1	A	1205	GLN
1	A	1206	ARG
1	A	1208	THR
1	A	1209	ARG
1	A	1211	ARG
1	A	1212	LEU
1	A	1214	LEU
1	A	1216	ASP
1	A	1217	CYS
1	A	1218	LEU
1	A	1219	ILE
1	A	1220	LEU
1	A	1227	ILE

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Mol	Chain	Res	Type
1	A	1231	MET
1	A	1232	LEU
1	A	1233	SER
1	A	1285	ILE
1	A	1286	ILE
1	A	1296	LEU
1	A	1299	ARG
1	A	1300	ARG
1	A	1303	LEU
1	A	1304	SER
1	A	1307	TYR
1	A	1308	LEU
1	A	1310	VAL
1	A	1319	LEU
1	A	1322	SER
1	A	1323	ARG
1	A	1327	LEU
1	A	1328	TYR
1	A	1333	LEU
1	A	1336	ILE
1	A	1340	ARG
1	A	1343	GLU
1	A	1344	GLU
1	A	1345	LYS
1	A	1347	LEU
1	A	1349	GLN
1	A	1351	LYS
1	A	1355	GLU
1	A	1356	ARG
1	A	1358	ARG
1	A	1360	LYS
1	A	1362	GLU
1	A	1363	LYS
1	A	1365	ARG
1	A	1366	GLN
1	A	1411	THR
1	A	1423	SER
1	A	1424	ASP
1	A	1426	GLU
1	A	1427	GLU
1	A	1514	LEU
1	A	1524	GLU

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Mol	Chain	Res	Type
1	A	1533	THR
1	A	1534	ARG
1	A	1536	HIS
1	A	1539	MET
1	A	1543	LEU
1	A	1544	ARG
1	A	1546	GLU
1	A	1547	ARG
1	A	1549	LEU
1	A	1551	THR
1	A	1553	GLU
1	A	1554	LEU
1	A	1555	LEU
1	A	1556	GLN
1	A	1559	GLU
1	A	1560	VAL
1	A	1562	ARG
1	A	1564	VAL
1	A	1565	LEU
1	A	1566	ASP
1	A	1567	GLN
1	A	1646	SER
1	A	1647	GLU
1	A	1649	LEU
1	A	1650	LEU
1	A	1651	ASP
1	A	1653	ARG
1	A	1654	LEU
1	A	1655	ARG
1	A	1656	ILE
1	A	1659	LEU
1	A	1660	GLU
1	A	1663	GLU
1	A	1665	PHE
1	A	1667	GLU
1	A	1669	GLN
1	A	1673	LEU
1	A	1674	ARG
1	A	1675	LEU
1	A	1676	LEU
1	A	1677	ARG
1	A	1681	GLN

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Mol	Chain	Res	Type
1	A	1687	SER
1	A	1689	LEU
1	A	1690	LEU
1	A	1695	ILE
1	A	1696	ILE
1	A	1697	LEU
1	A	1699	HIS
1	A	1707	SER
1	A	1708	LEU
1	A	1722	ILE
1	A	1724	ARG
1	A	1727	LYS
1	A	1728	ARG
1	A	1731	MET
1	A	1741	VAL
1	A	1744	LYS
1	A	1779	THR
1	A	1780	ASP
1	A	1783	ILE
1	A	1786	ASP
1	A	1787	LEU
1	A	1793	LEU
1	A	1797	ARG
1	A	1801	LEU
1	A	1802	CYS
1	A	1803	TYR
1	A	1940	ARG
1	A	1942	LEU
1	A	1943	ARG
1	A	1949	ILE
1	A	1950	LEU
1	A	1953	LYS
1	A	1954	TYR
1	A	1955	ARG
1	A	1958	THR
1	A	1960	VAL
1	A	1972	PHE
1	A	1974	ILE
1	A	1976	ILE
1	A	1977	PHE
1	A	1979	PHE
1	A	1980	TRP

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Mol	Chain	Res	Type
1	A	1999	GLN
1	A	2000	VAL
1	A	2004	PHE
1	A	2006	VAL
1	A	2007	MET
1	A	2008	LEU
1	A	2009	LEU
1	A	2010	ILE
1	A	2011	GLN
1	A	2023	LEU
1	A	2026	THR
1	A	2027	VAL
1	A	2028	LEU
1	A	2030	LYS
1	A	2031	LEU
1	A	2037	LEU
1	A	2043	LEU
1	A	2045	MET
1	A	2048	ILE
1	A	2049	LEU
1	A	2061	VAL
1	A	2065	LEU
1	A	2066	TRP
1	A	2070	LYS
1	A	2077	SER
1	A	2080	GLN
1	A	2082	ARG
1	A	2083	CYS
1	A	2087	THR
1	A	2088	ARG
1	A	2089	ILE
1	A	2090	LEU
1	A	2094	LEU
1	A	2096	LYS
1	A	2097	LYS
1	A	2100	HIS
1	A	2101	LEU
1	A	2103	LEU
1	A	2115	LEU
1	A	2116	VAL
1	A	2117	GLU
1	A	2122	MET

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Mol	Chain	Res	Type
1	A	2129	THR
1	A	2133	LEU
1	A	2134	SER
1	A	2135	SER
1	A	2137	MET
1	A	2140	GLU
1	A	2152	SER
1	A	2153	ARG
1	A	2154	GLU
1	A	2159	TYR
1	A	2161	GLN
1	A	2163	LYS
1	A	2165	GLN
1	A	2166	LYS
1	A	2167	LYS
1	A	2169	LYS
1	A	2170	ILE
1	A	2171	VAL
1	A	2184	ILE
1	A	2187	ILE
1	A	2189	PHE
1	A	2198	ARG
1	A	2201	VAL
1	A	2204	VAL
1	A	2205	ASN
1	A	2210	VAL
1	A	2211	THR
1	A	2215	LYS
1	A	2216	LEU
1	A	2220	GLU
1	A	2222	LEU
1	A	2223	PHE
1	A	2224	THR
1	A	2228	GLN
1	A	2229	GLN
1	A	2231	SER
1	A	2232	ILE
1	A	2236	THR
1	A	2238	GLN
1	A	2242	GLU
1	A	2243	LEU
1	A	2244	SER

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Mol	Chain	Res	Type
1	A	2248	ASP
1	A	2250	GLN
1	A	2252	LEU
1	A	2254	MET
1	A	2259	GLN
1	A	2263	GLU
1	A	2265	ILE
1	A	2266	VAL
1	A	2269	GLN
1	A	2270	ILE
1	A	2271	GLU
1	A	2278	TRP
1	A	2279	ARG
1	A	2280	ILE
1	A	2281	SER
1	A	2287	GLN
1	A	2291	GLU
1	A	2292	LEU
1	A	2294	ASN
1	A	2302	ARG
1	A	2306	ASN
1	A	2309	ARG
1	A	2310	ASP
1	A	2313	LYS
1	A	2316	THR
1	A	2317	VAL
1	A	2318	GLU
1	A	2319	TYR
1	A	2321	ASN
1	A	2323	LYS
1	A	2325	MET
1	A	2326	LEU
1	A	2331	ASN
1	A	2340	SER
1	A	2342	LEU
1	A	2343	GLU
1	A	2345	THR
1	A	2346	SER
1	A	2347	ASP
1	A	2351	VAL
1	A	2354	ASN
1	A	2355	LEU

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Mol	Chain	Res	Type
1	A	2356	PHE
1	A	2358	LYS
1	A	2360	ILE
1	A	2361	ARG
1	A	2364	ASN
1	A	2372	LYS
1	A	2374	LEU
1	A	2375	GLN
1	A	2381	ASP
1	A	2387	ILE
1	A	2389	LEU
1	A	2390	ARG
1	A	2400	PHE
1	A	2405	VAL
1	A	2406	ILE
1	A	2407	GLU
1	A	2408	LEU
1	A	2410	GLU
1	A	2412	ARG
1	A	2413	THR
1	A	2414	ASP
1	A	2420	MET
1	A	2421	VAL
1	A	2424	SER
1	A	2426	LYS
1	A	2427	VAL
1	A	2431	SER
1	A	2432	LEU
1	A	2435	LEU
1	A	2441	MET
1	A	2443	LEU
1	A	2446	SER
1	A	2453	LYS
1	A	2456	ARG
1	A	2462	ILE
1	A	2465	SER
1	A	2469	GLU
1	A	2470	GLU
1	A	2473	CYS
1	A	2477	ILE
1	A	2480	LEU
1	A	2486	LEU

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Mol	Chain	Res	Type
1	A	2487	VAL
1	A	2489	GLU
1	A	2491	ARG
1	A	2492	GLU
1	A	2494	GLU
1	A	2498	GLU
1	A	2502	LYS
1	A	2504	ILE
1	A	2506	LEU
1	A	2509	SER
1	A	2511	GLU
1	A	2512	THR
1	A	2513	MET
1	A	2516	TRP
1	A	2520	LYS
1	A	2521	GLU
1	B	570	GLU
1	B	571	LEU
1	B	572	VAL
1	B	573	LYS
1	B	578	LYS
1	B	579	TYR
1	B	580	TRP
1	B	581	ILE
1	B	583	VAL
1	B	587	MET
1	B	589	ILE
1	B	591	VAL
1	B	592	SER
1	B	593	PHE
1	B	596	ARG
1	B	597	LEU
1	B	598	VAL
1	B	602	ILE
1	B	608	PHE
1	B	609	LEU
1	B	610	LEU
1	B	611	CYS
1	B	612	LEU
1	B	617	VAL
1	B	621	LEU
1	B	623	ARG

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Mol	Chain	Res	Type
1	B	626	LEU
1	B	627	LYS
1	B	631	TRP
1	B	638	MET
1	B	644	VAL
1	B	679	GLU
1	B	680	LEU
1	B	682	SER
1	B	685	LEU
1	B	687	PRO
1	B	691	LEU
1	B	694	CYS
1	B	695	ILE
1	B	696	LEU
1	B	700	TYR
1	B	703	ARG
1	B	706	MET
1	B	707	GLN
1	B	708	LEU
1	B	709	THR
1	B	768	GLU
1	B	769	LEU
1	B	781	GLN
1	B	784	LEU
1	B	786	ARG
1	B	787	LEU
1	B	788	LEU
1	B	792	VAL
1	B	794	LYS
1	B	798	LEU
1	B	799	TYR
1	B	805	LEU
1	B	806	LYS
1	B	807	GLU
1	B	808	VAL
1	B	809	SER
1	B	813	LEU
1	B	817	VAL
1	B	823	LEU
1	B	827	ARG
1	B	828	PHE
1	B	831	MET

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Mol	Chain	Res	Type
1	B	833	SER
1	B	836	SER
1	B	837	THR
1	B	839	TRP
1	B	841	CYS
1	B	843	ILE
1	B	844	ILE
1	B	848	MET
1	B	849	LEU
1	B	851	GLN
1	B	852	LEU
1	B	853	LYS
1	B	854	VAL
1	B	855	VAL
1	B	856	ASN
1	B	917	PHE
1	B	919	VAL
1	B	920	ARG
1	B	921	LYS
1	B	925	ASN
1	B	930	GLN
1	B	932	HIS
1	B	933	LEU
1	B	935	VAL
1	B	936	LEU
1	B	938	LEU
1	B	946	TYR
1	B	949	GLN
1	B	953	ARG
1	B	954	ARG
1	B	971	THR
1	B	973	GLN
1	B	974	GLN
1	B	975	LEU
1	B	976	ASP
1	B	978	ASP
1	B	979	LEU
1	B	980	LEU
1	B	983	LEU
1	B	984	LYS
1	B	990	PHE
1	B	993	LYS

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Mol	Chain	Res	Type
1	B	999	CYS
1	B	1002	MET
1	B	1007	ILE
1	B	1010	ARG
1	B	1014	LEU
1	B	1015	VAL
1	B	1025	ILE
1	B	1026	LEU
1	B	1028	ARG
1	B	1030	HIS
1	B	1031	ARG
1	B	1032	GLN
1	B	1034	ILE
1	B	1036	ARG
1	B	1037	LEU
1	B	1043	LEU
1	B	1048	PHE
1	B	1050	LEU
1	B	1052	GLN
1	B	1055	LEU
1	B	1057	LEU
1	B	1097	THR
1	B	1099	LEU
1	B	1100	ILE
1	B	1101	SER
1	B	1103	PHE
1	B	1104	LEU
1	B	1112	GLN
1	B	1116	PHE
1	B	1119	GLU
1	B	1155	LEU
1	B	1156	ASP
1	B	1158	LEU
1	B	1162	VAL
1	B	1165	TYR
1	B	1171	LEU
1	B	1175	PHE
1	B	1181	ARG
1	B	1182	ILE
1	B	1184	ILE
1	B	1187	LEU
1	B	1191	LEU

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Mol	Chain	Res	Type
1	B	1198	LEU
1	B	1201	THR
1	B	1203	LEU
1	B	1204	LEU
1	B	1205	GLN
1	B	1206	ARG
1	B	1208	THR
1	B	1209	ARG
1	B	1211	ARG
1	B	1212	LEU
1	B	1214	LEU
1	B	1216	ASP
1	B	1217	CYS
1	B	1218	LEU
1	B	1219	ILE
1	B	1220	LEU
1	B	1227	ILE
1	B	1231	MET
1	B	1232	LEU
1	B	1233	SER
1	B	1285	ILE
1	B	1286	ILE
1	B	1296	LEU
1	B	1299	ARG
1	B	1300	ARG
1	B	1303	LEU
1	B	1304	SER
1	B	1307	TYR
1	B	1308	LEU
1	B	1310	VAL
1	B	1319	LEU
1	B	1322	SER
1	B	1323	ARG
1	B	1327	LEU
1	B	1328	TYR
1	B	1333	LEU
1	B	1336	ILE
1	B	1340	ARG
1	B	1343	GLU
1	B	1344	GLU
1	B	1345	LYS
1	B	1347	LEU

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Mol	Chain	Res	Type
1	B	1349	GLN
1	B	1351	LYS
1	B	1355	GLU
1	B	1356	ARG
1	B	1358	ARG
1	B	1360	LYS
1	B	1362	GLU
1	B	1363	LYS
1	B	1365	ARG
1	B	1366	GLN
1	B	1411	THR
1	B	1423	SER
1	B	1424	ASP
1	B	1426	GLU
1	B	1427	GLU
1	B	1514	LEU
1	B	1524	GLU
1	B	1533	THR
1	B	1534	ARG
1	B	1536	HIS
1	B	1539	MET
1	B	1543	LEU
1	B	1544	ARG
1	B	1546	GLU
1	B	1547	ARG
1	B	1549	LEU
1	B	1551	THR
1	B	1553	GLU
1	B	1554	LEU
1	B	1555	LEU
1	B	1556	GLN
1	B	1559	GLU
1	B	1560	VAL
1	B	1562	ARG
1	B	1564	VAL
1	B	1565	LEU
1	B	1566	ASP
1	B	1567	GLN
1	B	1646	SER
1	B	1647	GLU
1	B	1649	LEU
1	B	1650	LEU

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Mol	Chain	Res	Type
1	B	1651	ASP
1	B	1653	ARG
1	B	1654	LEU
1	B	1655	ARG
1	B	1656	ILE
1	B	1659	LEU
1	B	1660	GLU
1	B	1663	GLU
1	B	1665	PHE
1	B	1667	GLU
1	B	1669	GLN
1	B	1673	LEU
1	B	1674	ARG
1	B	1675	LEU
1	B	1676	LEU
1	B	1677	ARG
1	B	1681	GLN
1	B	1687	SER
1	B	1689	LEU
1	B	1690	LEU
1	B	1695	ILE
1	B	1696	ILE
1	B	1697	LEU
1	B	1699	HIS
1	B	1707	SER
1	B	1708	LEU
1	B	1722	ILE
1	B	1724	ARG
1	B	1727	LYS
1	B	1728	ARG
1	B	1731	MET
1	B	1741	VAL
1	B	1744	LYS
1	B	1779	THR
1	B	1780	ASP
1	B	1783	ILE
1	B	1786	ASP
1	B	1787	LEU
1	B	1793	LEU
1	B	1797	ARG
1	B	1801	LEU
1	B	1802	CYS

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Mol	Chain	Res	Type
1	B	1803	TYR
1	B	1940	ARG
1	B	1942	LEU
1	B	1943	ARG
1	B	1949	ILE
1	B	1950	LEU
1	B	1953	LYS
1	B	1954	TYR
1	B	1955	ARG
1	B	1958	THR
1	B	1960	VAL
1	B	1972	PHE
1	B	1974	ILE
1	B	1976	ILE
1	B	1977	PHE
1	B	1979	PHE
1	B	1980	TRP
1	B	1999	GLN
1	B	2000	VAL
1	B	2004	PHE
1	B	2006	VAL
1	B	2007	MET
1	B	2008	LEU
1	B	2009	LEU
1	B	2010	ILE
1	B	2011	GLN
1	B	2023	LEU
1	B	2026	THR
1	B	2027	VAL
1	B	2028	LEU
1	B	2030	LYS
1	B	2031	LEU
1	B	2037	LEU
1	B	2043	LEU
1	B	2045	MET
1	B	2048	ILE
1	B	2049	LEU
1	B	2061	VAL
1	B	2065	LEU
1	B	2066	TRP
1	B	2070	LYS
1	B	2077	SER

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Mol	Chain	Res	Type
1	B	2080	GLN
1	B	2082	ARG
1	B	2083	CYS
1	B	2087	THR
1	B	2088	ARG
1	B	2089	ILE
1	B	2090	LEU
1	B	2094	LEU
1	B	2096	LYS
1	B	2097	LYS
1	B	2100	HIS
1	B	2101	LEU
1	B	2103	LEU
1	B	2115	LEU
1	B	2116	VAL
1	B	2117	GLU
1	B	2122	MET
1	B	2129	THR
1	B	2133	LEU
1	B	2134	SER
1	B	2135	SER
1	B	2137	MET
1	B	2140	GLU
1	B	2152	SER
1	B	2153	ARG
1	B	2154	GLU
1	B	2159	TYR
1	B	2161	GLN
1	B	2163	LYS
1	B	2165	GLN
1	B	2166	LYS
1	B	2167	LYS
1	B	2169	LYS
1	B	2170	ILE
1	B	2171	VAL
1	B	2184	ILE
1	B	2187	ILE
1	B	2189	PHE
1	B	2198	ARG
1	B	2201	VAL
1	B	2204	VAL
1	B	2205	ASN

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Mol	Chain	Res	Type
1	B	2210	VAL
1	B	2211	THR
1	B	2215	LYS
1	B	2216	LEU
1	B	2220	GLU
1	B	2222	LEU
1	B	2223	PHE
1	B	2224	THR
1	B	2228	GLN
1	B	2229	GLN
1	B	2231	SER
1	B	2232	ILE
1	B	2236	THR
1	B	2238	GLN
1	B	2242	GLU
1	B	2243	LEU
1	B	2244	SER
1	B	2248	ASP
1	B	2250	GLN
1	B	2252	LEU
1	B	2254	MET
1	B	2259	GLN
1	B	2263	GLU
1	B	2265	ILE
1	B	2266	VAL
1	B	2269	GLN
1	B	2270	ILE
1	B	2271	GLU
1	B	2278	TRP
1	B	2279	ARG
1	B	2280	ILE
1	B	2281	SER
1	B	2287	GLN
1	B	2291	GLU
1	B	2292	LEU
1	B	2294	ASN
1	B	2302	ARG
1	B	2306	ASN
1	B	2309	ARG
1	B	2310	ASP
1	B	2313	LYS
1	B	2316	THR

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Mol	Chain	Res	Type
1	B	2317	VAL
1	B	2318	GLU
1	B	2319	TYR
1	B	2321	ASN
1	B	2323	LYS
1	B	2325	MET
1	B	2326	LEU
1	B	2331	ASN
1	B	2340	SER
1	B	2342	LEU
1	B	2343	GLU
1	B	2345	THR
1	B	2346	SER
1	B	2347	ASP
1	B	2351	VAL
1	B	2354	ASN
1	B	2355	LEU
1	B	2356	PHE
1	B	2358	LYS
1	B	2360	ILE
1	B	2361	ARG
1	B	2364	ASN
1	B	2372	LYS
1	B	2374	LEU
1	B	2375	GLN
1	B	2381	ASP
1	B	2387	ILE
1	B	2389	LEU
1	B	2390	ARG
1	B	2400	PHE
1	B	2405	VAL
1	B	2406	ILE
1	B	2407	GLU
1	B	2408	LEU
1	B	2410	GLU
1	B	2412	ARG
1	B	2413	THR
1	B	2414	ASP
1	B	2420	MET
1	B	2421	VAL
1	B	2424	SER
1	B	2426	LYS

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Mol	Chain	Res	Type
1	B	2427	VAL
1	B	2431	SER
1	B	2432	LEU
1	B	2435	LEU
1	B	2441	MET
1	B	2443	LEU
1	B	2446	SER
1	B	2453	LYS
1	B	2456	ARG
1	B	2462	ILE
1	B	2465	SER
1	B	2469	GLU
1	B	2470	GLU
1	B	2473	CYS
1	B	2477	ILE
1	B	2480	LEU
1	B	2486	LEU
1	B	2487	VAL
1	B	2489	GLU
1	B	2491	ARG
1	B	2492	GLU
1	B	2494	GLU
1	B	2498	GLU
1	B	2502	LYS
1	B	2504	ILE
1	B	2506	LEU
1	B	2509	SER
1	B	2511	GLU
1	B	2512	THR
1	B	2513	MET
1	B	2516	TRP
1	B	2520	LYS
1	B	2521	GLU
1	D	570	GLU
1	D	571	LEU
1	D	572	VAL
1	D	573	LYS
1	D	578	LYS
1	D	579	TYR
1	D	580	TRP
1	D	581	ILE
1	D	583	VAL

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Mol	Chain	Res	Type
1	D	587	MET
1	D	589	ILE
1	D	591	VAL
1	D	592	SER
1	D	593	PHE
1	D	596	ARG
1	D	597	LEU
1	D	598	VAL
1	D	602	ILE
1	D	608	PHE
1	D	609	LEU
1	D	610	LEU
1	D	611	CYS
1	D	612	LEU
1	D	617	VAL
1	D	621	LEU
1	D	623	ARG
1	D	626	LEU
1	D	627	LYS
1	D	631	TRP
1	D	638	MET
1	D	644	VAL
1	D	679	GLU
1	D	680	LEU
1	D	682	SER
1	D	685	LEU
1	D	687	PRO
1	D	691	LEU
1	D	694	CYS
1	D	695	ILE
1	D	696	LEU
1	D	700	TYR
1	D	703	ARG
1	D	706	MET
1	D	707	GLN
1	D	708	LEU
1	D	709	THR
1	D	768	GLU
1	D	769	LEU
1	D	781	GLN
1	D	784	LEU
1	D	786	ARG

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Mol	Chain	Res	Type
1	D	787	LEU
1	D	788	LEU
1	D	792	VAL
1	D	794	LYS
1	D	798	LEU
1	D	799	TYR
1	D	805	LEU
1	D	806	LYS
1	D	807	GLU
1	D	808	VAL
1	D	809	SER
1	D	813	LEU
1	D	817	VAL
1	D	823	LEU
1	D	827	ARG
1	D	828	PHE
1	D	831	MET
1	D	833	SER
1	D	836	SER
1	D	837	THR
1	D	839	TRP
1	D	841	CYS
1	D	843	ILE
1	D	844	ILE
1	D	848	MET
1	D	849	LEU
1	D	851	GLN
1	D	852	LEU
1	D	853	LYS
1	D	854	VAL
1	D	855	VAL
1	D	856	ASN
1	D	917	PHE
1	D	919	VAL
1	D	920	ARG
1	D	921	LYS
1	D	925	ASN
1	D	930	GLN
1	D	932	HIS
1	D	933	LEU
1	D	935	VAL
1	D	936	LEU

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Mol	Chain	Res	Type
1	D	938	LEU
1	D	946	TYR
1	D	949	GLN
1	D	953	ARG
1	D	954	ARG
1	D	971	THR
1	D	973	GLN
1	D	974	GLN
1	D	975	LEU
1	D	976	ASP
1	D	978	ASP
1	D	979	LEU
1	D	980	LEU
1	D	983	LEU
1	D	984	LYS
1	D	990	PHE
1	D	993	LYS
1	D	999	CYS
1	D	1002	MET
1	D	1007	ILE
1	D	1010	ARG
1	D	1014	LEU
1	D	1015	VAL
1	D	1025	ILE
1	D	1026	LEU
1	D	1028	ARG
1	D	1030	HIS
1	D	1031	ARG
1	D	1032	GLN
1	D	1034	ILE
1	D	1036	ARG
1	D	1037	LEU
1	D	1043	LEU
1	D	1048	PHE
1	D	1050	LEU
1	D	1052	GLN
1	D	1055	LEU
1	D	1057	LEU
1	D	1097	THR
1	D	1099	LEU
1	D	1100	ILE
1	D	1101	SER

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Mol	Chain	Res	Type
1	D	1103	PHE
1	D	1104	LEU
1	D	1112	GLN
1	D	1116	PHE
1	D	1119	GLU
1	D	1155	LEU
1	D	1156	ASP
1	D	1158	LEU
1	D	1162	VAL
1	D	1165	TYR
1	D	1171	LEU
1	D	1175	PHE
1	D	1181	ARG
1	D	1182	ILE
1	D	1184	ILE
1	D	1187	LEU
1	D	1191	LEU
1	D	1198	LEU
1	D	1201	THR
1	D	1203	LEU
1	D	1204	LEU
1	D	1205	GLN
1	D	1206	ARG
1	D	1208	THR
1	D	1209	ARG
1	D	1211	ARG
1	D	1212	LEU
1	D	1214	LEU
1	D	1216	ASP
1	D	1217	CYS
1	D	1218	LEU
1	D	1219	ILE
1	D	1220	LEU
1	D	1227	ILE
1	D	1231	MET
1	D	1232	LEU
1	D	1233	SER
1	D	1285	ILE
1	D	1286	ILE
1	D	1296	LEU
1	D	1299	ARG
1	D	1300	ARG

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Mol	Chain	Res	Type
1	D	1303	LEU
1	D	1304	SER
1	D	1307	TYR
1	D	1308	LEU
1	D	1310	VAL
1	D	1319	LEU
1	D	1322	SER
1	D	1323	ARG
1	D	1327	LEU
1	D	1328	TYR
1	D	1333	LEU
1	D	1336	ILE
1	D	1340	ARG
1	D	1343	GLU
1	D	1344	GLU
1	D	1345	LYS
1	D	1347	LEU
1	D	1349	GLN
1	D	1351	LYS
1	D	1355	GLU
1	D	1356	ARG
1	D	1358	ARG
1	D	1360	LYS
1	D	1362	GLU
1	D	1363	LYS
1	D	1365	ARG
1	D	1366	GLN
1	D	1411	THR
1	D	1423	SER
1	D	1424	ASP
1	D	1426	GLU
1	D	1427	GLU
1	D	1514	LEU
1	D	1524	GLU
1	D	1533	THR
1	D	1534	ARG
1	D	1536	HIS
1	D	1539	MET
1	D	1543	LEU
1	D	1544	ARG
1	D	1546	GLU
1	D	1547	ARG

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Mol	Chain	Res	Type
1	D	1549	LEU
1	D	1551	THR
1	D	1553	GLU
1	D	1554	LEU
1	D	1555	LEU
1	D	1556	GLN
1	D	1559	GLU
1	D	1560	VAL
1	D	1562	ARG
1	D	1564	VAL
1	D	1565	LEU
1	D	1566	ASP
1	D	1567	GLN
1	D	1646	SER
1	D	1647	GLU
1	D	1649	LEU
1	D	1650	LEU
1	D	1651	ASP
1	D	1653	ARG
1	D	1654	LEU
1	D	1655	ARG
1	D	1656	ILE
1	D	1659	LEU
1	D	1660	GLU
1	D	1663	GLU
1	D	1665	PHE
1	D	1667	GLU
1	D	1669	GLN
1	D	1673	LEU
1	D	1674	ARG
1	D	1675	LEU
1	D	1676	LEU
1	D	1677	ARG
1	D	1681	GLN
1	D	1687	SER
1	D	1689	LEU
1	D	1690	LEU
1	D	1695	ILE
1	D	1696	ILE
1	D	1697	LEU
1	D	1699	HIS
1	D	1707	SER

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Mol	Chain	Res	Type
1	D	1708	LEU
1	D	1722	ILE
1	D	1724	ARG
1	D	1727	LYS
1	D	1728	ARG
1	D	1731	MET
1	D	1741	VAL
1	D	1744	LYS
1	D	1779	THR
1	D	1780	ASP
1	D	1783	ILE
1	D	1786	ASP
1	D	1787	LEU
1	D	1793	LEU
1	D	1797	ARG
1	D	1801	LEU
1	D	1802	CYS
1	D	1803	TYR
1	D	1940	ARG
1	D	1942	LEU
1	D	1943	ARG
1	D	1949	ILE
1	D	1950	LEU
1	D	1953	LYS
1	D	1954	TYR
1	D	1955	ARG
1	D	1958	THR
1	D	1960	VAL
1	D	1972	PHE
1	D	1974	ILE
1	D	1976	ILE
1	D	1977	PHE
1	D	1979	PHE
1	D	1980	TRP
1	D	1999	GLN
1	D	2000	VAL
1	D	2004	PHE
1	D	2006	VAL
1	D	2007	MET
1	D	2008	LEU
1	D	2009	LEU
1	D	2010	ILE

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Mol	Chain	Res	Type
1	D	2011	GLN
1	D	2023	LEU
1	D	2026	THR
1	D	2027	VAL
1	D	2028	LEU
1	D	2030	LYS
1	D	2031	LEU
1	D	2037	LEU
1	D	2043	LEU
1	D	2045	MET
1	D	2048	ILE
1	D	2049	LEU
1	D	2061	VAL
1	D	2065	LEU
1	D	2066	TRP
1	D	2070	LYS
1	D	2077	SER
1	D	2080	GLN
1	D	2082	ARG
1	D	2083	CYS
1	D	2087	THR
1	D	2088	ARG
1	D	2089	ILE
1	D	2090	LEU
1	D	2094	LEU
1	D	2096	LYS
1	D	2097	LYS
1	D	2100	HIS
1	D	2101	LEU
1	D	2103	LEU
1	D	2115	LEU
1	D	2116	VAL
1	D	2117	GLU
1	D	2122	MET
1	D	2129	THR
1	D	2133	LEU
1	D	2134	SER
1	D	2135	SER
1	D	2137	MET
1	D	2140	GLU
1	D	2152	SER
1	D	2153	ARG

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Mol	Chain	Res	Type
1	D	2154	GLU
1	D	2159	TYR
1	D	2161	GLN
1	D	2163	LYS
1	D	2165	GLN
1	D	2166	LYS
1	D	2167	LYS
1	D	2169	LYS
1	D	2170	ILE
1	D	2171	VAL
1	D	2184	ILE
1	D	2187	ILE
1	D	2189	PHE
1	D	2198	ARG
1	D	2201	VAL
1	D	2204	VAL
1	D	2205	ASN
1	D	2210	VAL
1	D	2211	THR
1	D	2215	LYS
1	D	2216	LEU
1	D	2220	GLU
1	D	2222	LEU
1	D	2223	PHE
1	D	2224	THR
1	D	2228	GLN
1	D	2229	GLN
1	D	2231	SER
1	D	2232	ILE
1	D	2236	THR
1	D	2238	GLN
1	D	2242	GLU
1	D	2243	LEU
1	D	2244	SER
1	D	2248	ASP
1	D	2250	GLN
1	D	2252	LEU
1	D	2254	MET
1	D	2259	GLN
1	D	2263	GLU
1	D	2265	ILE
1	D	2266	VAL

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Mol	Chain	Res	Type
1	D	2269	GLN
1	D	2270	ILE
1	D	2271	GLU
1	D	2278	TRP
1	D	2279	ARG
1	D	2280	ILE
1	D	2281	SER
1	D	2287	GLN
1	D	2291	GLU
1	D	2292	LEU
1	D	2294	ASN
1	D	2302	ARG
1	D	2306	ASN
1	D	2309	ARG
1	D	2310	ASP
1	D	2313	LYS
1	D	2316	THR
1	D	2317	VAL
1	D	2318	GLU
1	D	2319	TYR
1	D	2321	ASN
1	D	2323	LYS
1	D	2325	MET
1	D	2326	LEU
1	D	2331	ASN
1	D	2340	SER
1	D	2342	LEU
1	D	2343	GLU
1	D	2345	THR
1	D	2346	SER
1	D	2347	ASP
1	D	2351	VAL
1	D	2354	ASN
1	D	2355	LEU
1	D	2356	PHE
1	D	2358	LYS
1	D	2360	ILE
1	D	2361	ARG
1	D	2364	ASN
1	D	2372	LYS
1	D	2374	LEU
1	D	2375	GLN

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Mol	Chain	Res	Type
1	D	2381	ASP
1	D	2387	ILE
1	D	2389	LEU
1	D	2390	ARG
1	D	2400	PHE
1	D	2405	VAL
1	D	2406	ILE
1	D	2407	GLU
1	D	2408	LEU
1	D	2410	GLU
1	D	2412	ARG
1	D	2413	THR
1	D	2414	ASP
1	D	2420	MET
1	D	2421	VAL
1	D	2424	SER
1	D	2426	LYS
1	D	2427	VAL
1	D	2431	SER
1	D	2432	LEU
1	D	2435	LEU
1	D	2441	MET
1	D	2443	LEU
1	D	2446	SER
1	D	2453	LYS
1	D	2456	ARG
1	D	2462	ILE
1	D	2465	SER
1	D	2469	GLU
1	D	2470	GLU
1	D	2473	CYS
1	D	2477	ILE
1	D	2480	LEU
1	D	2486	LEU
1	D	2487	VAL
1	D	2489	GLU
1	D	2491	ARG
1	D	2492	GLU
1	D	2494	GLU
1	D	2498	GLU
1	D	2502	LYS
1	D	2504	ILE

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Mol	Chain	Res	Type
1	D	2506	LEU
1	D	2509	SER
1	D	2511	GLU
1	D	2512	THR
1	D	2513	MET
1	D	2516	TRP
1	D	2520	LYS
1	D	2521	GLU
2	C	229	GLU
2	C	243	ILE
2	C	247	SER
2	E	229	GLU
2	E	243	ILE
2	E	247	SER
2	F	229	GLU
2	F	243	ILE
2	F	247	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	699	HIS
1	A	702	HIS
1	A	851	GLN
1	A	925	ASN
1	A	1040	ASN
1	A	1052	GLN
1	A	1222	ASN
1	A	1305	HIS
1	A	1309	HIS
1	A	1536	HIS
1	A	1561	HIS
1	A	1698	ASN
1	A	1796	HIS
1	A	1999	GLN
1	A	2080	GLN
1	A	2102	ASN
1	A	2161	GLN
1	A	2206	GLN
1	A	2229	GLN
1	A	2331	ASN
1	A	2354	ASN

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Mol	Chain	Res	Type
1	A	2364	ASN
1	B	699	HIS
1	B	702	HIS
1	B	851	GLN
1	B	925	ASN
1	B	1040	ASN
1	B	1222	ASN
1	B	1305	HIS
1	B	1309	HIS
1	B	1536	HIS
1	B	1561	HIS
1	B	1698	ASN
1	B	1796	HIS
1	B	1999	GLN
1	B	2080	GLN
1	B	2102	ASN
1	B	2161	GLN
1	B	2206	GLN
1	B	2229	GLN
1	B	2331	ASN
1	B	2354	ASN
1	B	2364	ASN
1	D	699	HIS
1	D	702	HIS
1	D	851	GLN
1	D	925	ASN
1	D	1040	ASN
1	D	1052	GLN
1	D	1222	ASN
1	D	1305	HIS
1	D	1309	HIS
1	D	1536	HIS
1	D	1561	HIS
1	D	1698	ASN
1	D	1796	HIS
1	D	1999	GLN
1	D	2080	GLN
1	D	2102	ASN
1	D	2161	GLN
1	D	2229	GLN
1	D	2331	ASN
1	D	2348	GLN

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Mol	Chain	Res	Type
1	D	2354	ASN
1	D	2364	ASN

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 ⓘ

18 ligands are 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	D12	A	2601	-	11,11,11	0.26	0	10,10,10	0.42	0
3	D12	D	2603	-	11,11,11	0.27	0	10,10,10	0.39	0
3	D12	C	301	-	11,11,11	0.30	0	10,10,10	0.40	0
3	D12	F	303	-	11,11,11	0.29	0	10,10,10	0.35	0
3	D12	C	303	-	11,11,11	0.29	0	10,10,10	0.35	0
4	L9Q	B	2601	-	50,50,50	1.06	3 (6%)	53,55,55	1.08	3 (5%)
3	D12	B	2602	-	11,11,11	0.26	0	10,10,10	0.42	0
3	D12	C	302	-	11,11,11	0.26	0	10,10,10	0.45	0
4	L9Q	D	2601	-	50,50,50	1.06	3 (6%)	53,55,55	1.08	3 (5%)
3	D12	E	302	-	11,11,11	0.26	0	10,10,10	0.45	0
3	D12	E	303	-	11,11,11	0.29	0	10,10,10	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	L9Q	A	2603	-	50,50,50	1.06	3 (6%)	53,55,55	1.08	3 (5%)
3	D12	D	2602	-	11,11,11	0.26	0	10,10,10	0.42	0
3	D12	A	2602	-	11,11,11	0.27	0	10,10,10	0.39	0
3	D12	F	302	-	11,11,11	0.26	0	10,10,10	0.45	0
3	D12	F	301	-	11,11,11	0.30	0	10,10,10	0.40	0
3	D12	B	2603	-	11,11,11	0.27	0	10,10,10	0.39	0
3	D12	E	301	-	11,11,11	0.29	0	10,10,10	0.40	0

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	D12	A	2601	-	-	7/9/9/9	-
3	D12	D	2603	-	-	6/9/9/9	-
3	D12	C	301	-	-	7/9/9/9	-
3	D12	F	303	-	-	5/9/9/9	-
3	D12	C	303	-	-	5/9/9/9	-
4	L9Q	B	2601	-	-	30/54/54/54	-
3	D12	B	2602	-	-	7/9/9/9	-
3	D12	C	302	-	-	8/9/9/9	-
4	L9Q	D	2601	-	-	30/54/54/54	-
3	D12	E	302	-	-	8/9/9/9	-
3	D12	E	303	-	-	5/9/9/9	-
4	L9Q	A	2603	-	-	30/54/54/54	-
3	D12	D	2602	-	-	7/9/9/9	-
3	D12	A	2602	-	-	6/9/9/9	-
3	D12	F	302	-	-	8/9/9/9	-
3	D12	F	301	-	-	7/9/9/9	-
3	D12	B	2603	-	-	6/9/9/9	-
3	D12	E	301	-	-	7/9/9/9	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2603	L9Q	O3-C11	4.24	1.45	1.33
4	B	2601	L9Q	O3-C11	4.23	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2601	L9Q	O3-C11	4.23	1.45	1.33
4	B	2601	L9Q	O2-C31	4.05	1.45	1.34
4	A	2603	L9Q	O2-C31	4.05	1.45	1.34
4	D	2601	L9Q	O2-C31	4.03	1.45	1.34
4	D	2601	L9Q	C40-C39	3.70	1.52	1.31
4	B	2601	L9Q	C40-C39	3.69	1.52	1.31
4	A	2603	L9Q	C40-C39	3.69	1.52	1.31

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2601	L9Q	O2-C31-C32	3.86	119.82	111.48
4	D	2601	L9Q	O2-C31-C32	3.85	119.81	111.48
4	A	2603	L9Q	O2-C31-C32	3.84	119.80	111.48
4	D	2601	L9Q	O3-C11-C12	2.85	120.51	111.83
4	A	2603	L9Q	O3-C11-C12	2.84	120.50	111.83
4	B	2601	L9Q	O3-C11-C12	2.84	120.48	111.83
4	A	2603	L9Q	C2-O2-C31	-2.41	112.03	117.80
4	B	2601	L9Q	C2-O2-C31	-2.41	112.04	117.80
4	D	2601	L9Q	C2-O2-C31	-2.40	112.05	117.80

There are no chirality outliers.

All (189) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2603	L9Q	C1-O3P-P-O1P
4	A	2603	L9Q	C1-O3P-P-O2P
4	A	2603	L9Q	C1-O3P-P-O4P
4	A	2603	L9Q	O4P-C4-C5-N
4	B	2601	L9Q	C1-O3P-P-O1P
4	B	2601	L9Q	C1-O3P-P-O2P
4	B	2601	L9Q	C1-O3P-P-O4P
4	B	2601	L9Q	O4P-C4-C5-N
4	D	2601	L9Q	C1-O3P-P-O1P
4	D	2601	L9Q	C1-O3P-P-O2P
4	D	2601	L9Q	C1-O3P-P-O4P
4	D	2601	L9Q	O4P-C4-C5-N
4	A	2603	L9Q	O11-C11-O3-C3
4	B	2601	L9Q	O11-C11-O3-C3
4	D	2601	L9Q	O11-C11-O3-C3
4	A	2603	L9Q	C12-C11-O3-C3
4	B	2601	L9Q	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
4	D	2601	L9Q	C12-C11-O3-C3
3	F	302	D12	C11-C10-C9-C8
3	C	302	D12	C11-C10-C9-C8
3	E	302	D12	C11-C10-C9-C8
3	A	2601	D12	C2-C3-C4-C5
3	A	2601	D12	C6-C7-C8-C9
3	B	2602	D12	C2-C3-C4-C5
3	B	2602	D12	C6-C7-C8-C9
3	D	2602	D12	C2-C3-C4-C5
3	D	2602	D12	C6-C7-C8-C9
3	C	303	D12	C2-C3-C4-C5
3	E	303	D12	C2-C3-C4-C5
3	F	303	D12	C2-C3-C4-C5
4	A	2603	L9Q	C24-C25-C26-C27
4	B	2601	L9Q	C24-C25-C26-C27
4	D	2601	L9Q	C24-C25-C26-C27
4	A	2603	L9Q	C31-C32-C33-C34
4	B	2601	L9Q	C31-C32-C33-C34
4	D	2601	L9Q	C31-C32-C33-C34
3	C	301	D12	C3-C4-C5-C6
3	E	301	D12	C3-C4-C5-C6
3	F	301	D12	C3-C4-C5-C6
3	C	301	D12	C9-C10-C11-C12
3	E	301	D12	C9-C10-C11-C12
3	F	301	D12	C9-C10-C11-C12
4	A	2603	L9Q	C42-C43-C44-C45
4	B	2601	L9Q	C42-C43-C44-C45
4	D	2601	L9Q	C42-C43-C44-C45
3	C	302	D12	C4-C5-C6-C7
3	E	302	D12	C4-C5-C6-C7
3	F	302	D12	C4-C5-C6-C7
3	B	2603	D12	C3-C4-C5-C6
3	D	2603	D12	C3-C4-C5-C6
3	A	2602	D12	C3-C4-C5-C6
3	E	302	D12	C2-C3-C4-C5
3	C	302	D12	C2-C3-C4-C5
3	C	302	D12	C3-C4-C5-C6
3	C	302	D12	C6-C7-C8-C9
3	E	302	D12	C3-C4-C5-C6
3	E	302	D12	C6-C7-C8-C9
3	F	302	D12	C2-C3-C4-C5
3	F	302	D12	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	F	302	D12	C6-C7-C8-C9
4	D	2601	L9Q	C41-C42-C43-C44
4	A	2603	L9Q	C32-C33-C34-C35
4	A	2603	L9Q	C41-C42-C43-C44
4	B	2601	L9Q	C32-C33-C34-C35
4	B	2601	L9Q	C41-C42-C43-C44
4	D	2601	L9Q	C32-C33-C34-C35
4	A	2603	L9Q	C13-C14-C15-C16
4	B	2601	L9Q	C13-C14-C15-C16
4	D	2601	L9Q	C13-C14-C15-C16
4	D	2601	L9Q	C14-C15-C16-C17
4	A	2603	L9Q	C14-C15-C16-C17
4	B	2601	L9Q	C14-C15-C16-C17
4	A	2603	L9Q	C39-C40-C41-C42
4	B	2601	L9Q	C39-C40-C41-C42
4	D	2601	L9Q	C39-C40-C41-C42
4	A	2603	L9Q	C16-C17-C18-C19
4	D	2601	L9Q	C16-C17-C18-C19
4	B	2601	L9Q	C16-C17-C18-C19
3	A	2602	D12	C2-C3-C4-C5
3	B	2603	D12	C2-C3-C4-C5
3	D	2603	D12	C2-C3-C4-C5
3	C	302	D12	C7-C8-C9-C10
3	E	302	D12	C7-C8-C9-C10
3	F	302	D12	C7-C8-C9-C10
4	A	2603	L9Q	C15-C16-C17-C18
4	B	2601	L9Q	C15-C16-C17-C18
4	D	2601	L9Q	C15-C16-C17-C18
3	A	2601	D12	C3-C4-C5-C6
3	B	2602	D12	C3-C4-C5-C6
3	D	2602	D12	C3-C4-C5-C6
4	A	2603	L9Q	C35-C36-C37-C38
4	B	2601	L9Q	C35-C36-C37-C38
4	D	2601	L9Q	C35-C36-C37-C38
3	C	301	D12	C1-C2-C3-C4
3	E	301	D12	C1-C2-C3-C4
3	F	301	D12	C1-C2-C3-C4
3	A	2601	D12	C11-C10-C9-C8
3	B	2602	D12	C11-C10-C9-C8
3	D	2602	D12	C11-C10-C9-C8
4	A	2603	L9Q	C17-C18-C19-C20
4	B	2601	L9Q	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
4	D	2601	L9Q	C17-C18-C19-C20
4	A	2603	L9Q	O3P-C1-C2-C3
4	B	2601	L9Q	O3P-C1-C2-C3
4	D	2601	L9Q	O3P-C1-C2-C3
3	C	301	D12	C6-C7-C8-C9
3	E	301	D12	C6-C7-C8-C9
3	F	301	D12	C6-C7-C8-C9
3	C	301	D12	C4-C5-C6-C7
3	E	301	D12	C4-C5-C6-C7
3	F	301	D12	C4-C5-C6-C7
3	A	2601	D12	C7-C8-C9-C10
3	B	2602	D12	C7-C8-C9-C10
3	D	2602	D12	C7-C8-C9-C10
3	A	2602	D12	C1-C2-C3-C4
3	B	2603	D12	C1-C2-C3-C4
3	D	2603	D12	C1-C2-C3-C4
3	A	2602	D12	C6-C7-C8-C9
3	B	2603	D12	C6-C7-C8-C9
3	D	2603	D12	C6-C7-C8-C9
3	C	302	D12	C1-C2-C3-C4
3	E	302	D12	C1-C2-C3-C4
3	F	302	D12	C1-C2-C3-C4
3	C	302	D12	C9-C10-C11-C12
3	E	302	D12	C9-C10-C11-C12
3	F	302	D12	C9-C10-C11-C12
3	A	2602	D12	C4-C5-C6-C7
3	D	2603	D12	C4-C5-C6-C7
3	B	2603	D12	C4-C5-C6-C7
3	C	301	D12	C5-C6-C7-C8
3	E	301	D12	C5-C6-C7-C8
3	F	301	D12	C5-C6-C7-C8
3	A	2601	D12	C5-C6-C7-C8
3	D	2602	D12	C5-C6-C7-C8
3	B	2602	D12	C5-C6-C7-C8
4	B	2601	L9Q	C22-C23-C24-C25
4	A	2603	L9Q	C22-C23-C24-C25
4	D	2601	L9Q	C22-C23-C24-C25
3	C	303	D12	C7-C8-C9-C10
3	E	303	D12	C7-C8-C9-C10
3	F	303	D12	C7-C8-C9-C10
3	C	303	D12	C3-C4-C5-C6
3	E	303	D12	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	F	303	D12	C3-C4-C5-C6
4	A	2603	L9Q	C36-C37-C38-C39
4	B	2601	L9Q	C36-C37-C38-C39
4	D	2601	L9Q	C36-C37-C38-C39
4	D	2601	L9Q	C21-C22-C23-C24
4	A	2603	L9Q	C21-C22-C23-C24
4	B	2601	L9Q	C21-C22-C23-C24
3	C	303	D12	C9-C10-C11-C12
3	F	303	D12	C9-C10-C11-C12
3	E	303	D12	C9-C10-C11-C12
4	A	2603	L9Q	C2-C1-O3P-P
4	B	2601	L9Q	C2-C1-O3P-P
4	D	2601	L9Q	C2-C1-O3P-P
4	A	2603	L9Q	O3P-C1-C2-O2
4	B	2601	L9Q	O3P-C1-C2-O2
4	D	2601	L9Q	O3P-C1-C2-O2
4	A	2603	L9Q	C4-O4P-P-O1P
4	B	2601	L9Q	C4-O4P-P-O1P
4	D	2601	L9Q	C4-O4P-P-O1P
4	A	2603	L9Q	O2-C31-C32-C33
4	B	2601	L9Q	O2-C31-C32-C33
4	D	2601	L9Q	O2-C31-C32-C33
3	A	2601	D12	C9-C10-C11-C12
3	B	2602	D12	C9-C10-C11-C12
3	D	2602	D12	C9-C10-C11-C12
3	C	303	D12	C6-C7-C8-C9
3	E	303	D12	C6-C7-C8-C9
3	F	303	D12	C6-C7-C8-C9
4	D	2601	L9Q	C23-C24-C25-C26
3	A	2602	D12	C9-C10-C11-C12
3	B	2603	D12	C9-C10-C11-C12
3	D	2603	D12	C9-C10-C11-C12
4	A	2603	L9Q	C23-C24-C25-C26
4	B	2601	L9Q	C23-C24-C25-C26
3	C	301	D12	C11-C10-C9-C8
3	E	301	D12	C11-C10-C9-C8
3	F	301	D12	C11-C10-C9-C8
4	A	2603	L9Q	C37-C38-C39-C40
4	B	2601	L9Q	C37-C38-C39-C40
4	D	2601	L9Q	C37-C38-C39-C40
4	A	2603	L9Q	C19-C20-C21-C22
4	B	2601	L9Q	C19-C20-C21-C22

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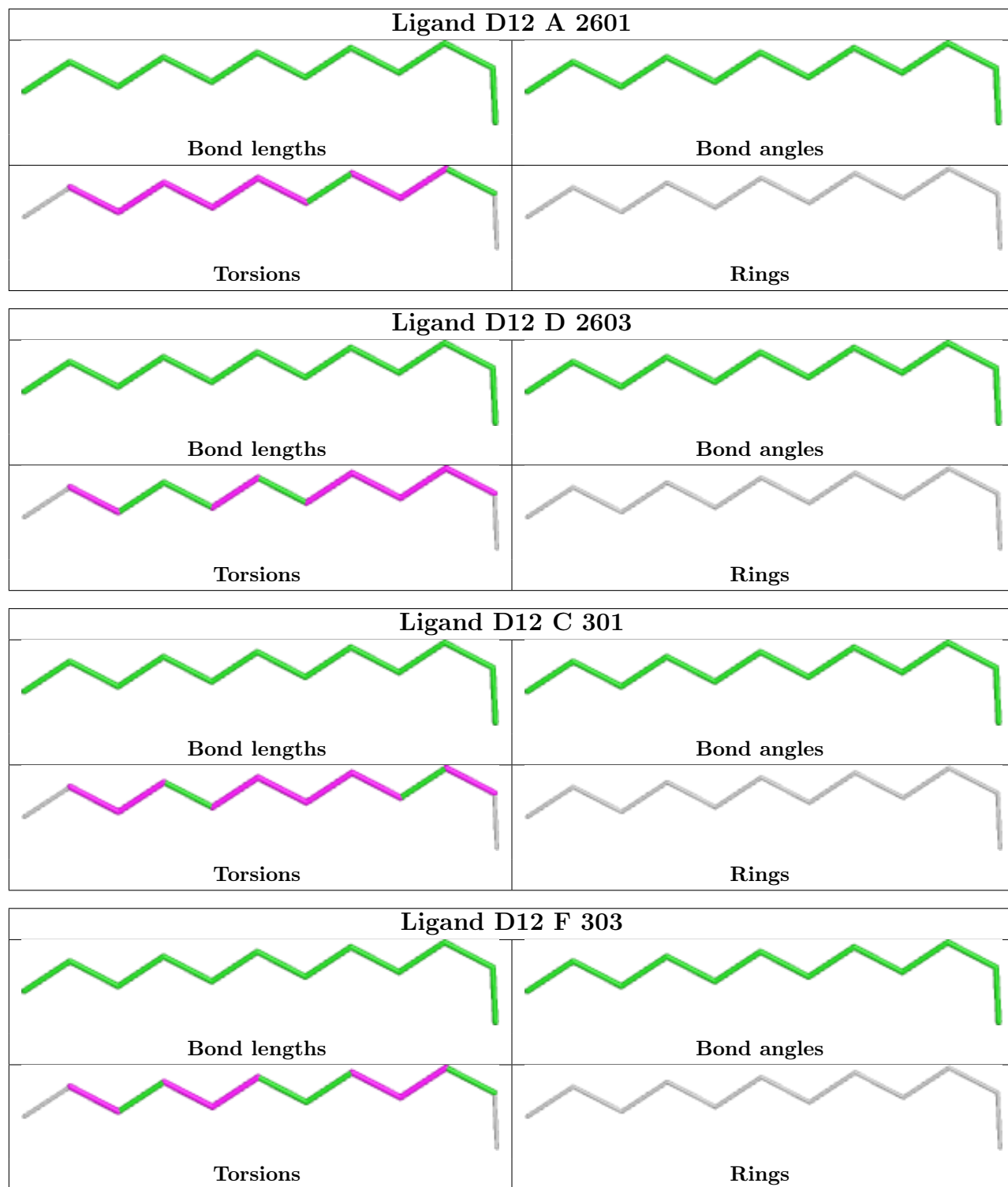
Mol	Chain	Res	Type	Atoms
4	D	2601	L9Q	C19-C20-C21-C22
4	D	2601	L9Q	C20-C21-C22-C23
4	A	2603	L9Q	C20-C21-C22-C23
4	B	2601	L9Q	C20-C21-C22-C23

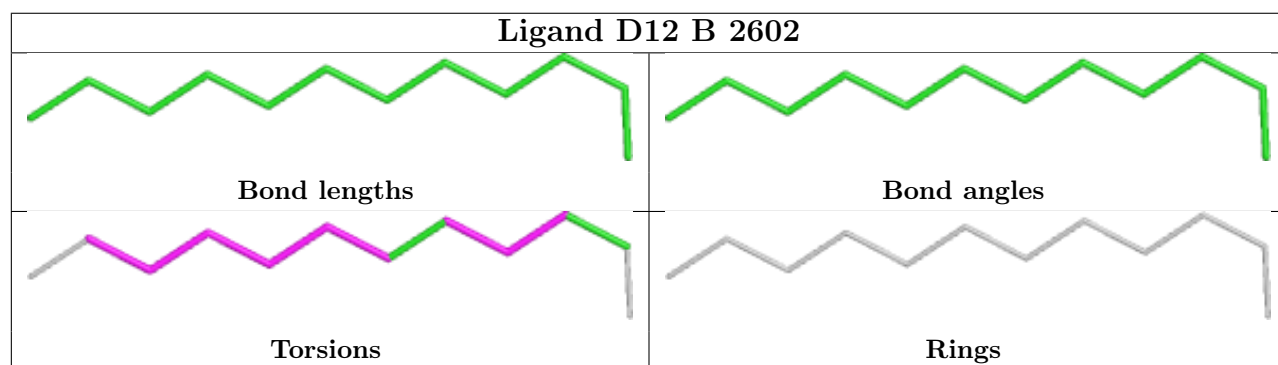
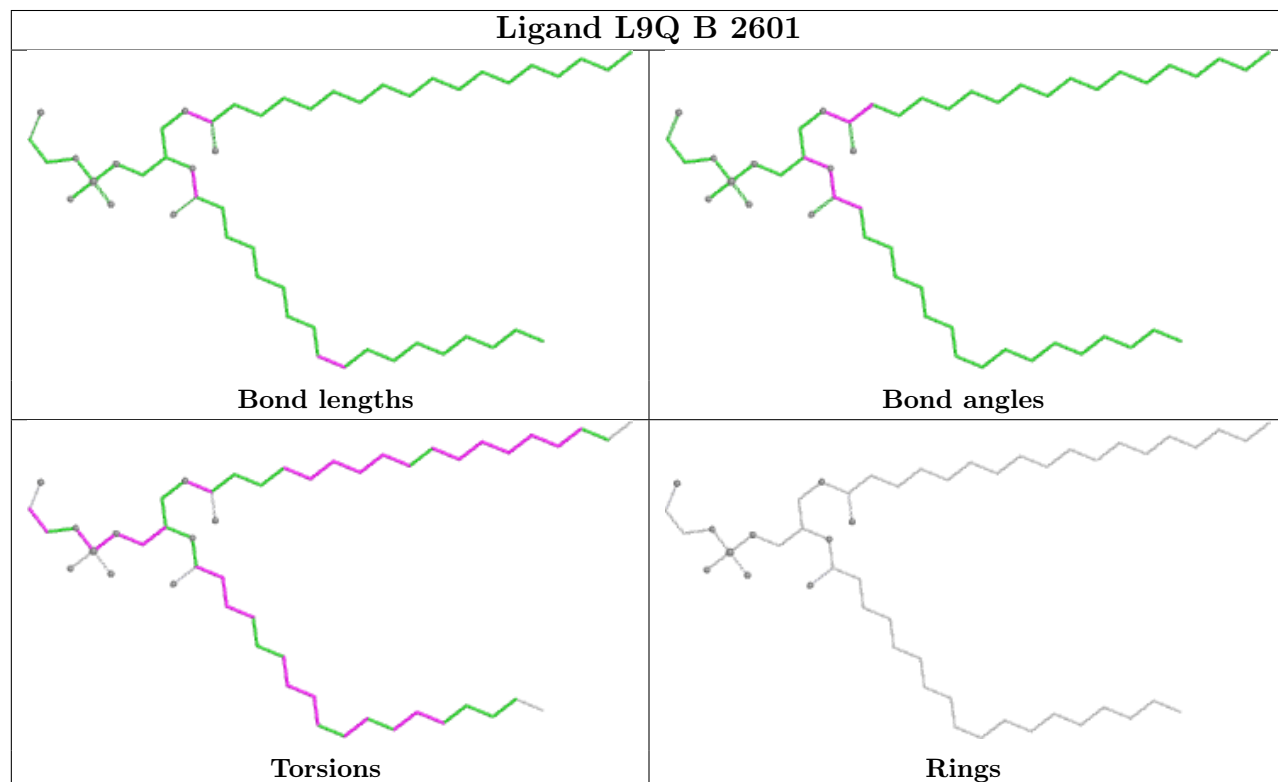
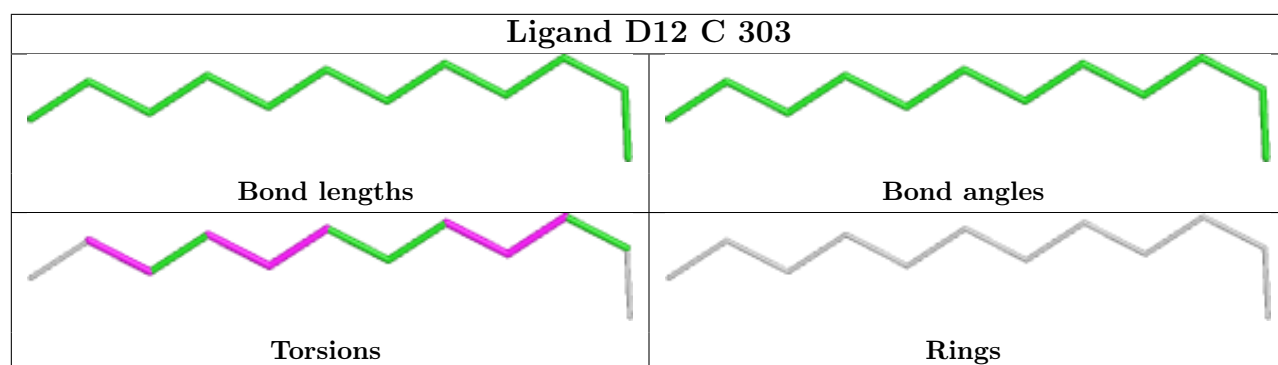
There are no ring outliers.

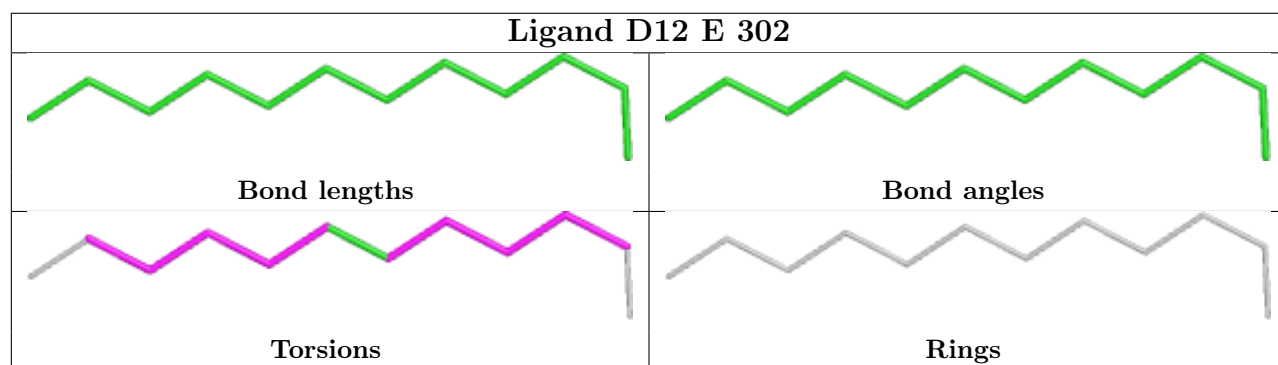
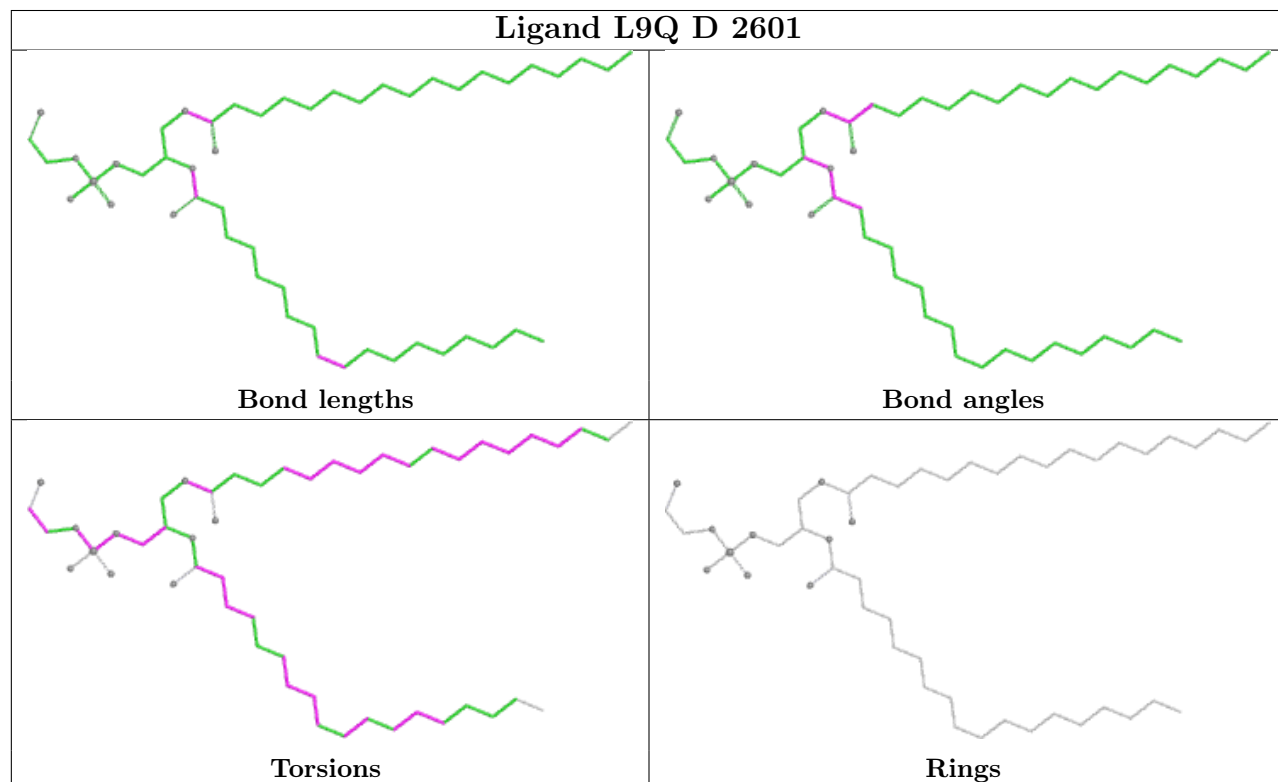
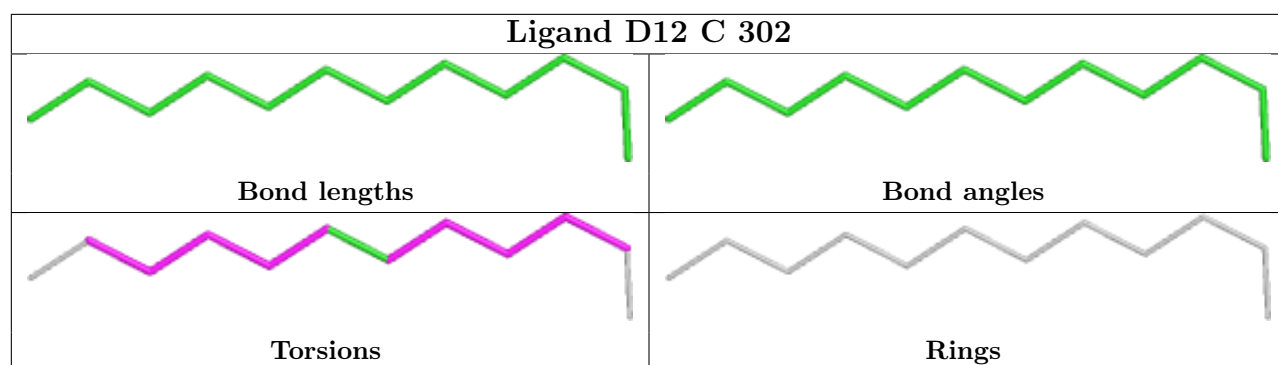
18 monomers are involved in 53 short contacts:

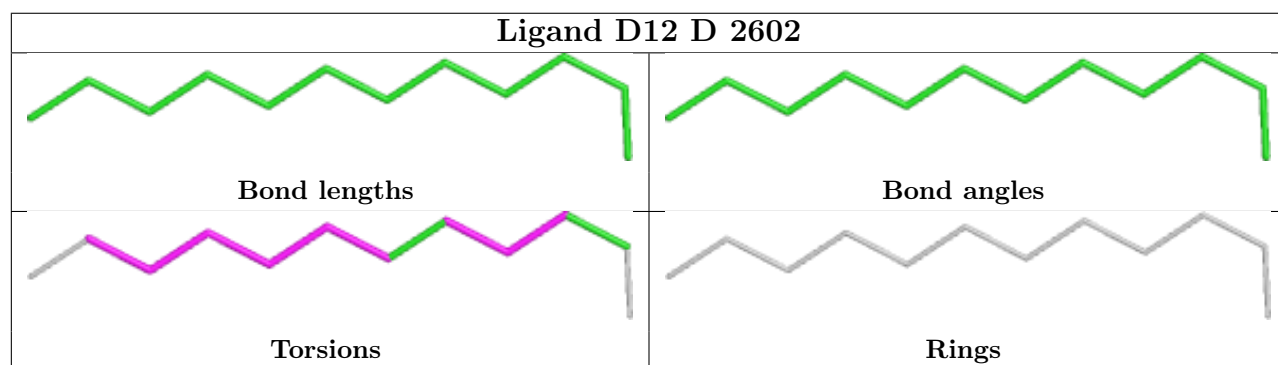
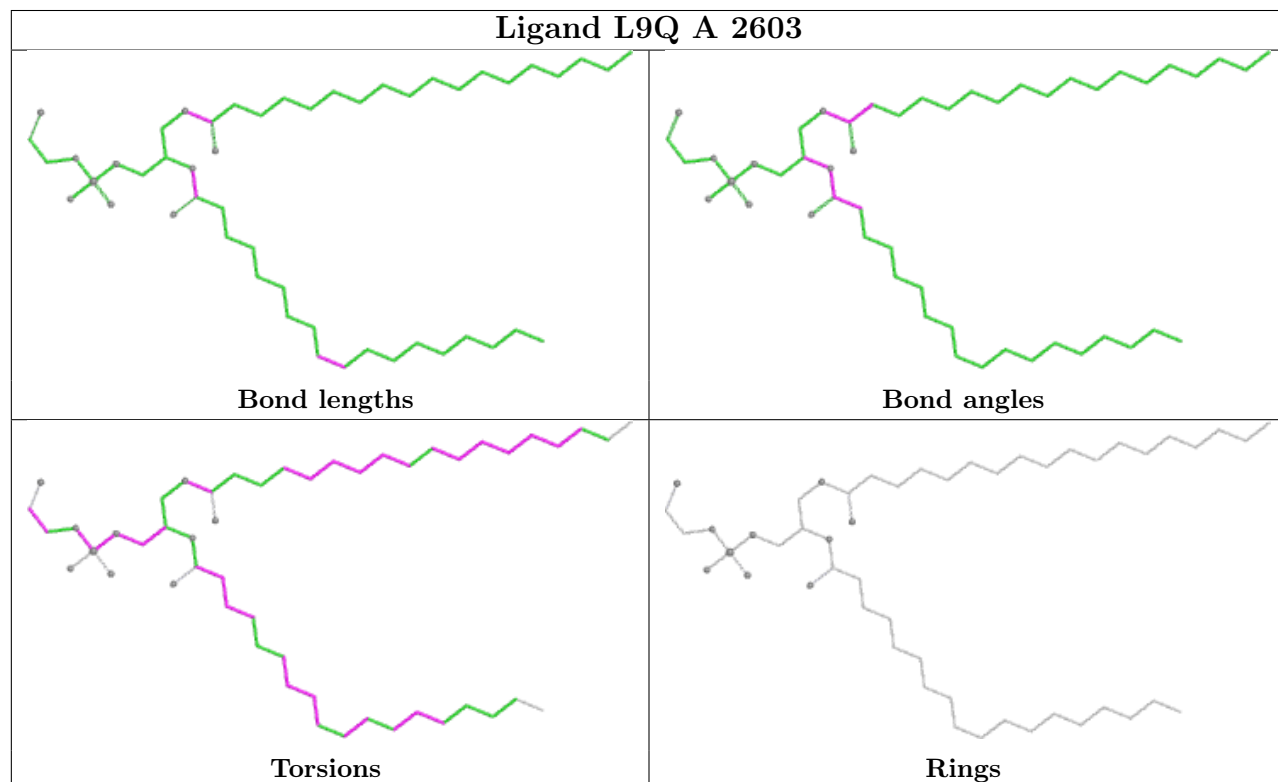
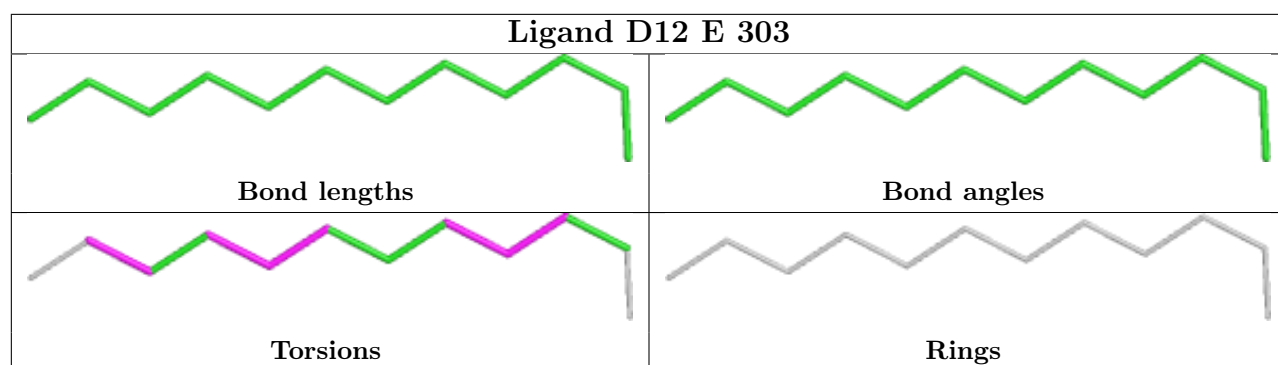
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2601	D12	1	0
3	D	2603	D12	2	0
3	C	301	D12	5	0
3	F	303	D12	3	0
3	C	303	D12	3	0
4	B	2601	L9Q	9	0
3	B	2602	D12	2	0
3	C	302	D12	2	0
4	D	2601	L9Q	8	0
3	E	302	D12	2	0
3	E	303	D12	3	0
4	A	2603	L9Q	8	0
3	D	2602	D12	2	0
3	A	2602	D12	2	0
3	F	302	D12	2	0
3	F	301	D12	5	0
3	B	2603	D12	2	0
3	E	301	D12	7	0

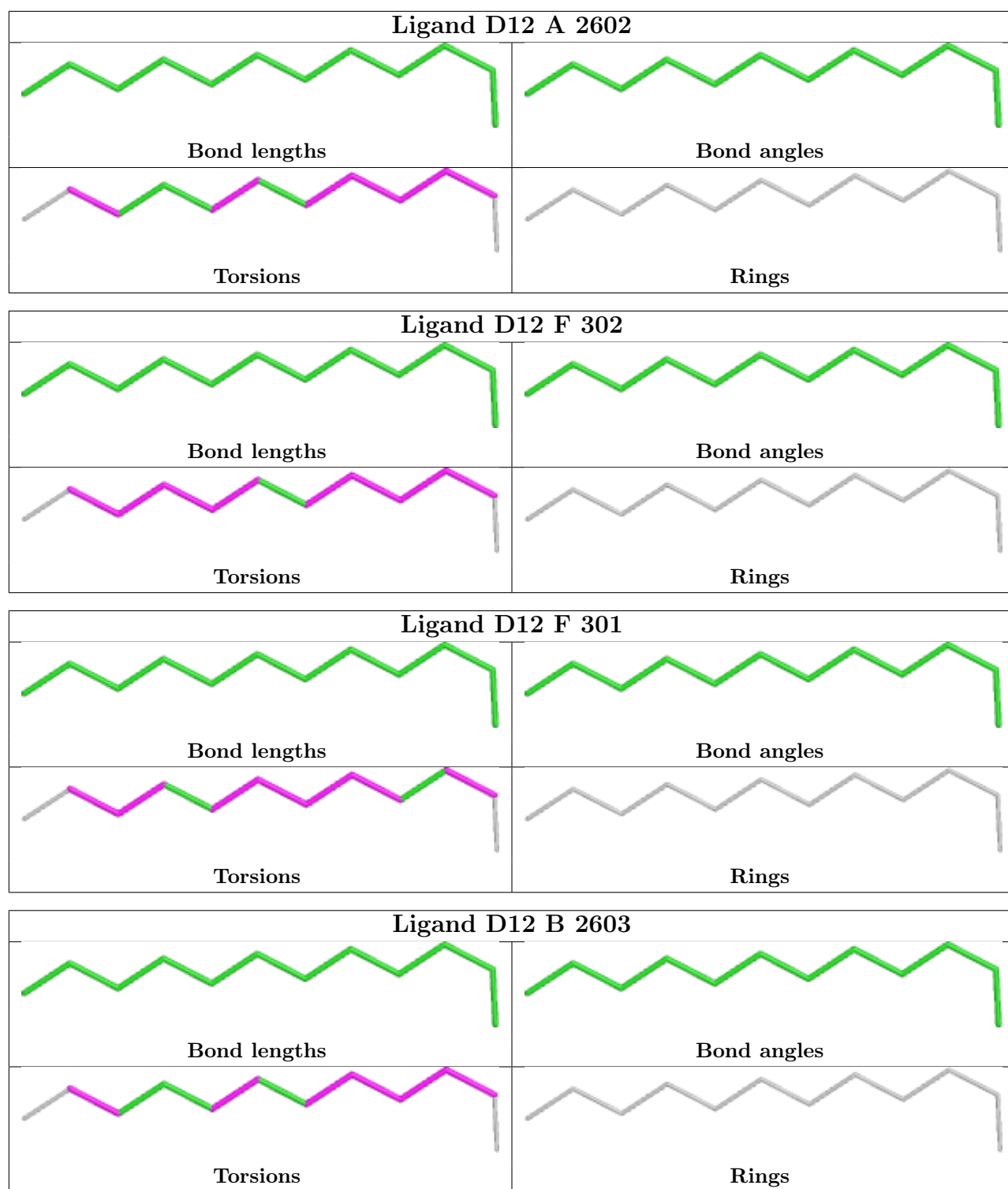
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

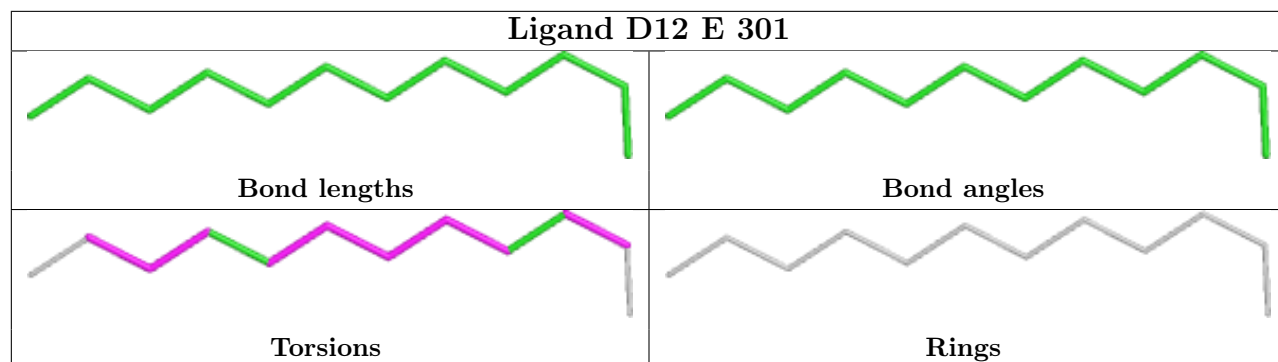












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

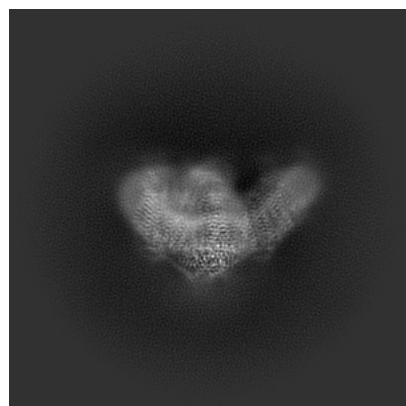
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39219. These allow visual inspection of the internal detail of the map and identification of artifacts.

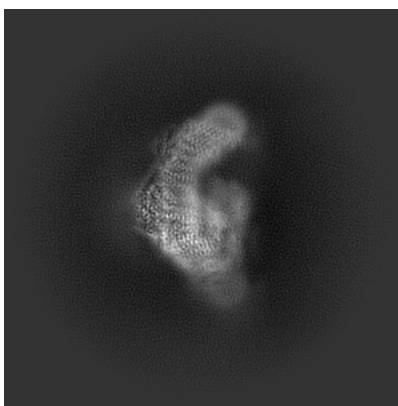
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

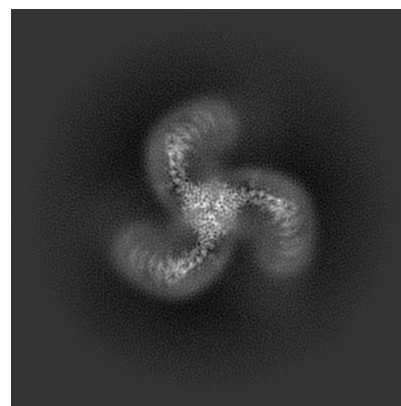
6.1.1 Primary map



X

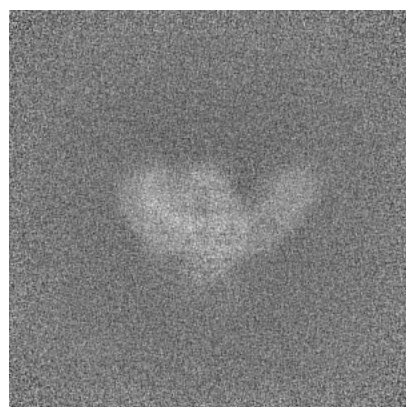


Y

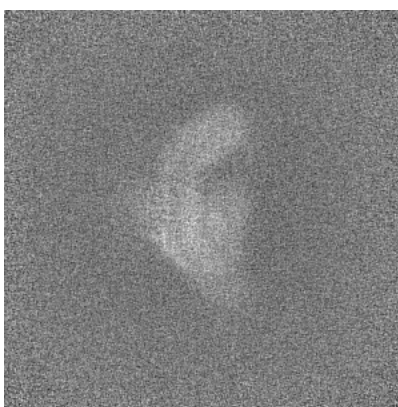


Z

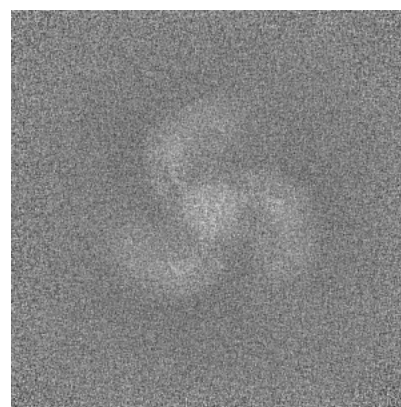
6.1.2 Raw map



X



Y



Z

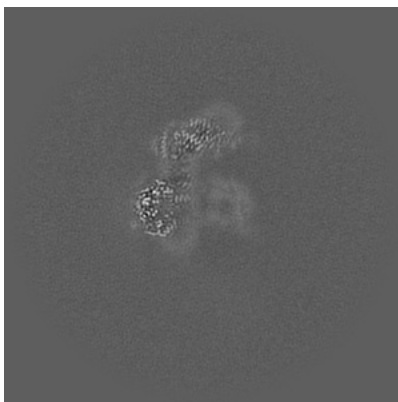
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

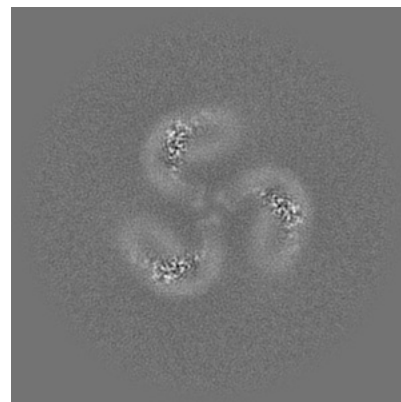
6.2.1 Primary map



X Index: 400

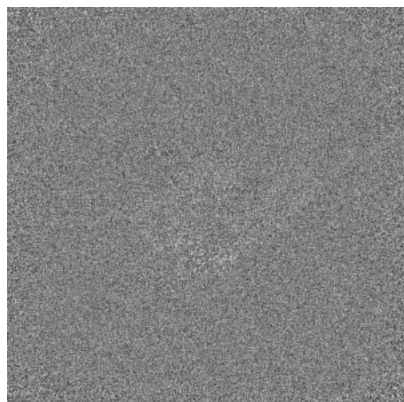


Y Index: 400

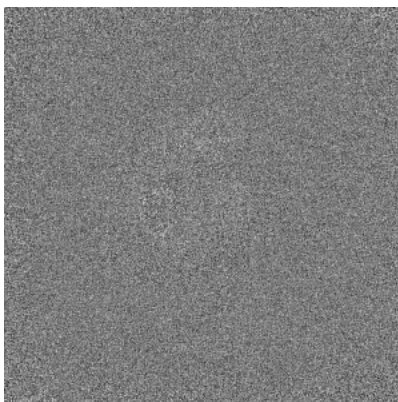


Z Index: 400

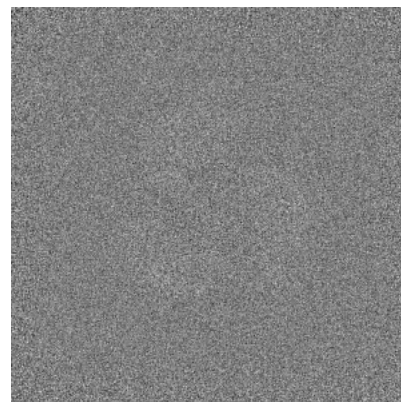
6.2.2 Raw map



X Index: 400



Y Index: 400

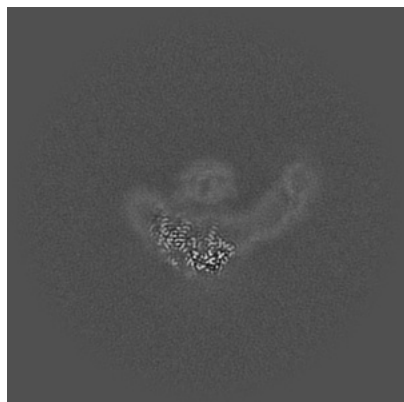


Z Index: 400

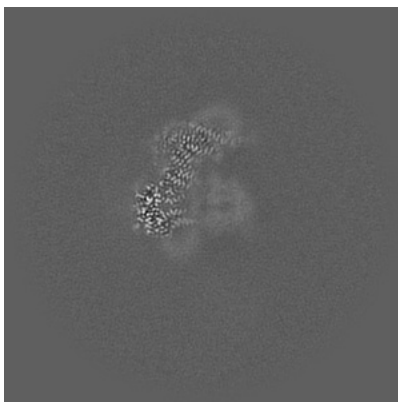
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

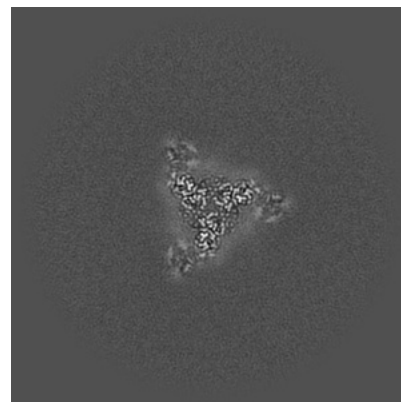
6.3.1 Primary map



X Index: 386

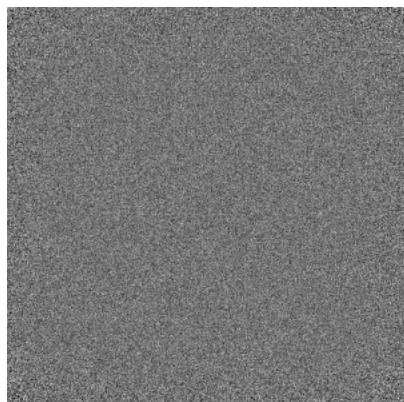


Y Index: 409

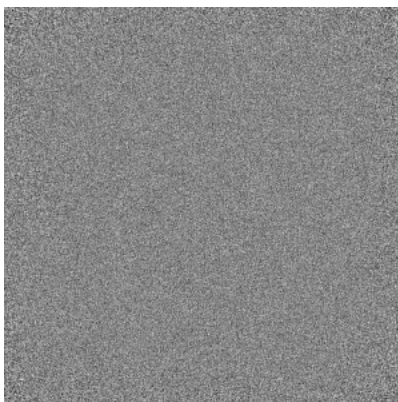


Z Index: 326

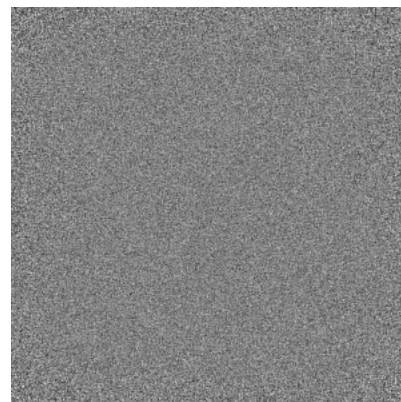
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

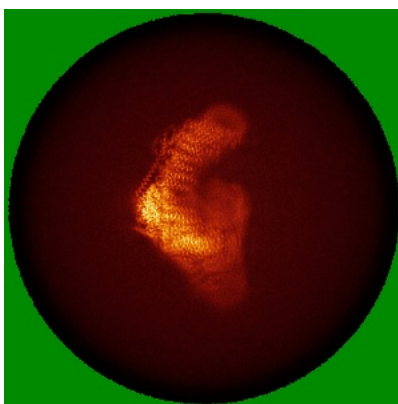
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

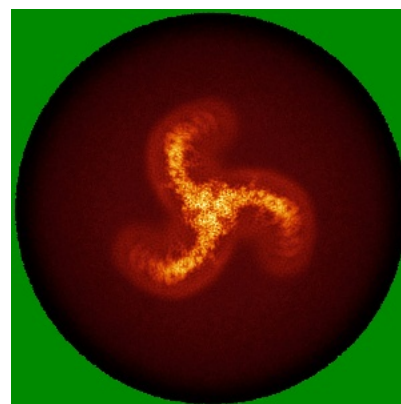
6.4.1 Primary map



X

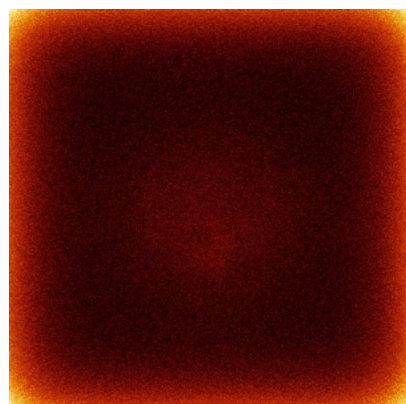


Y

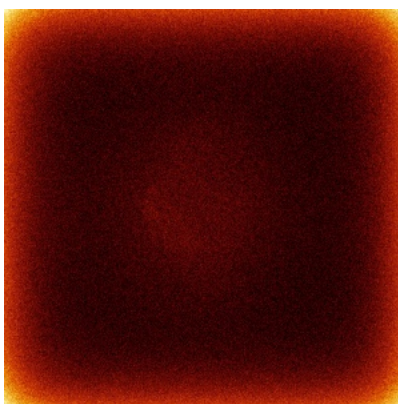


Z

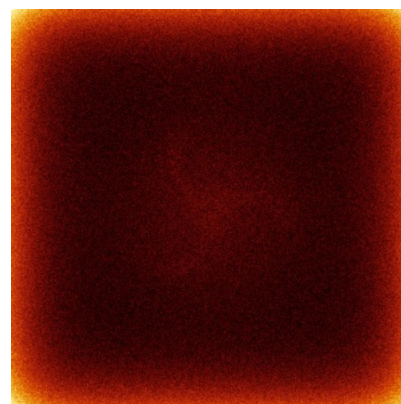
6.4.2 Raw map



X



Y

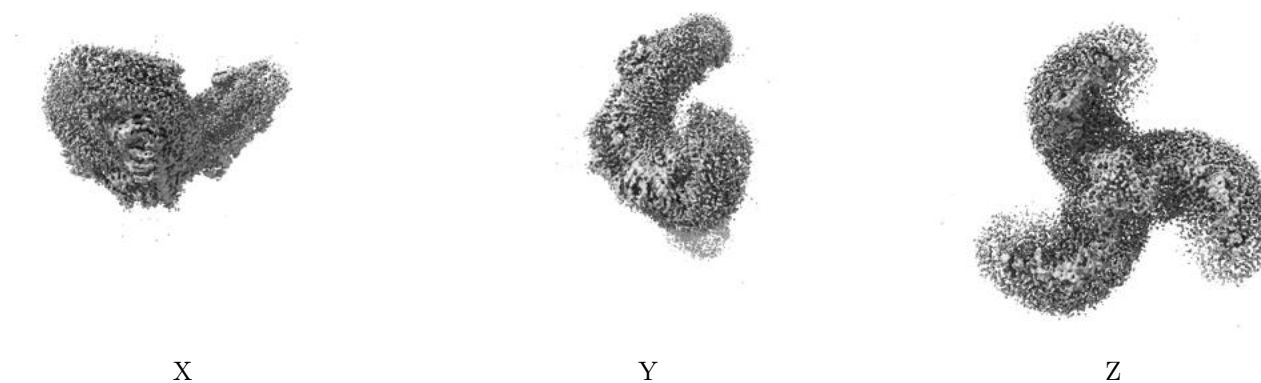


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

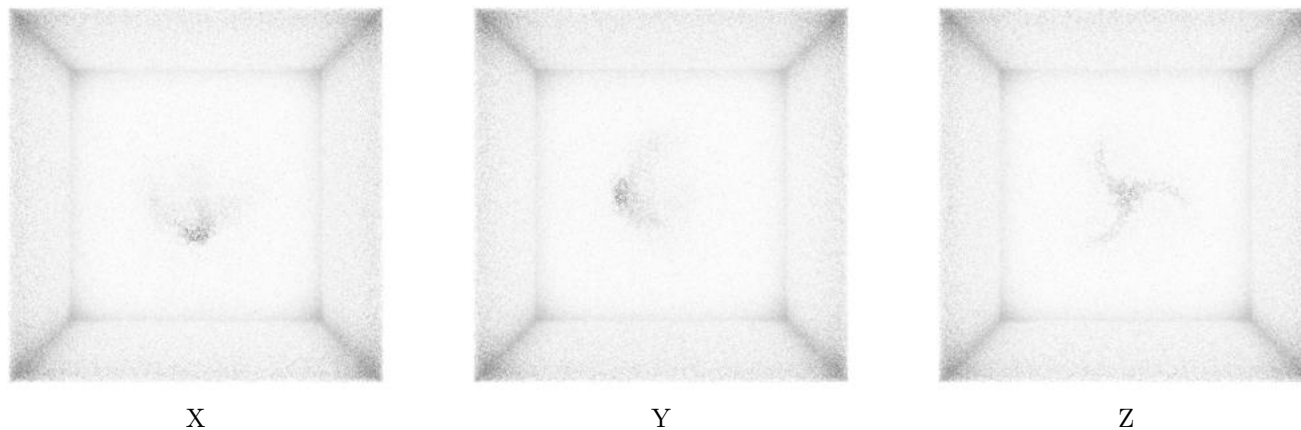
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

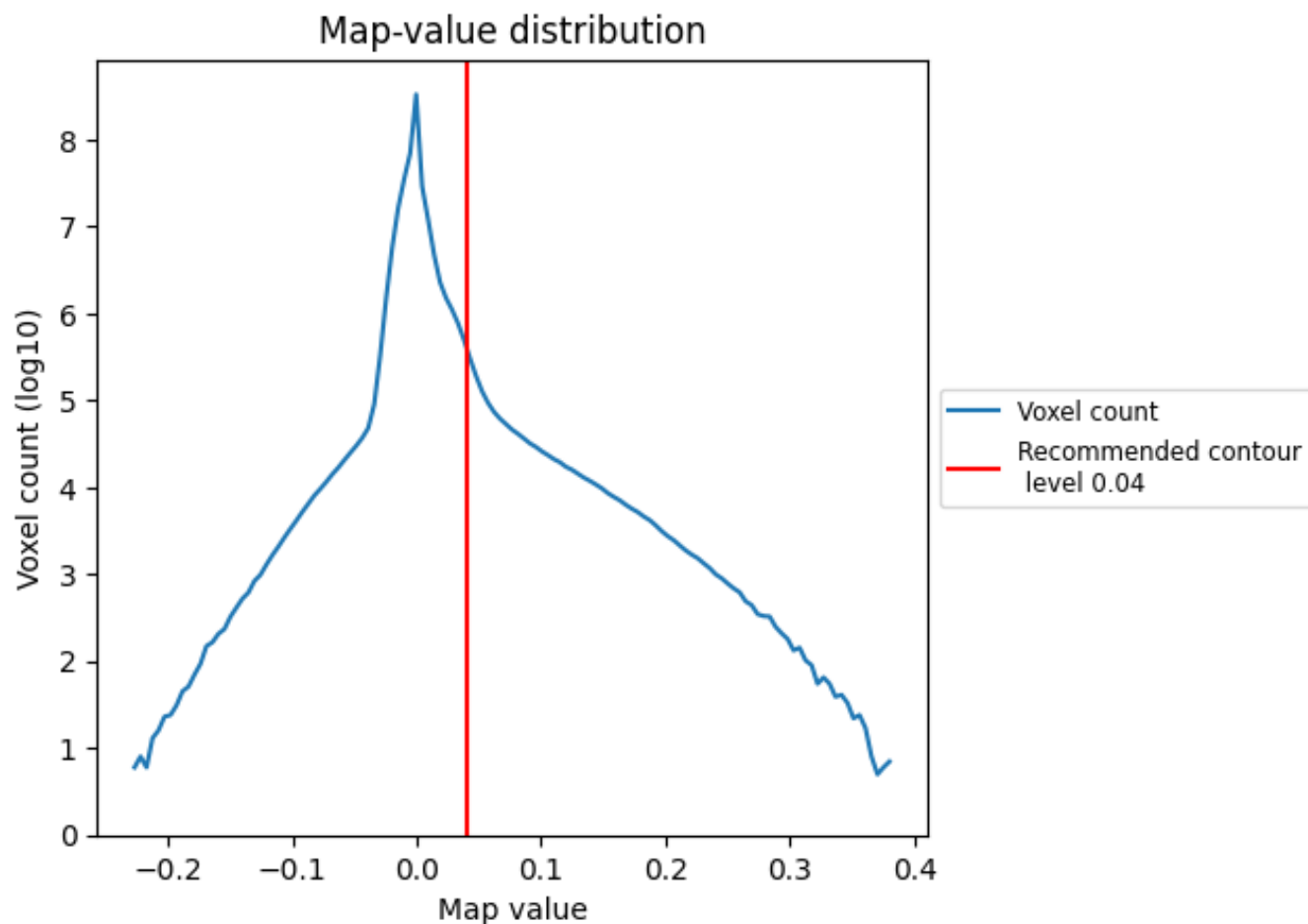
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

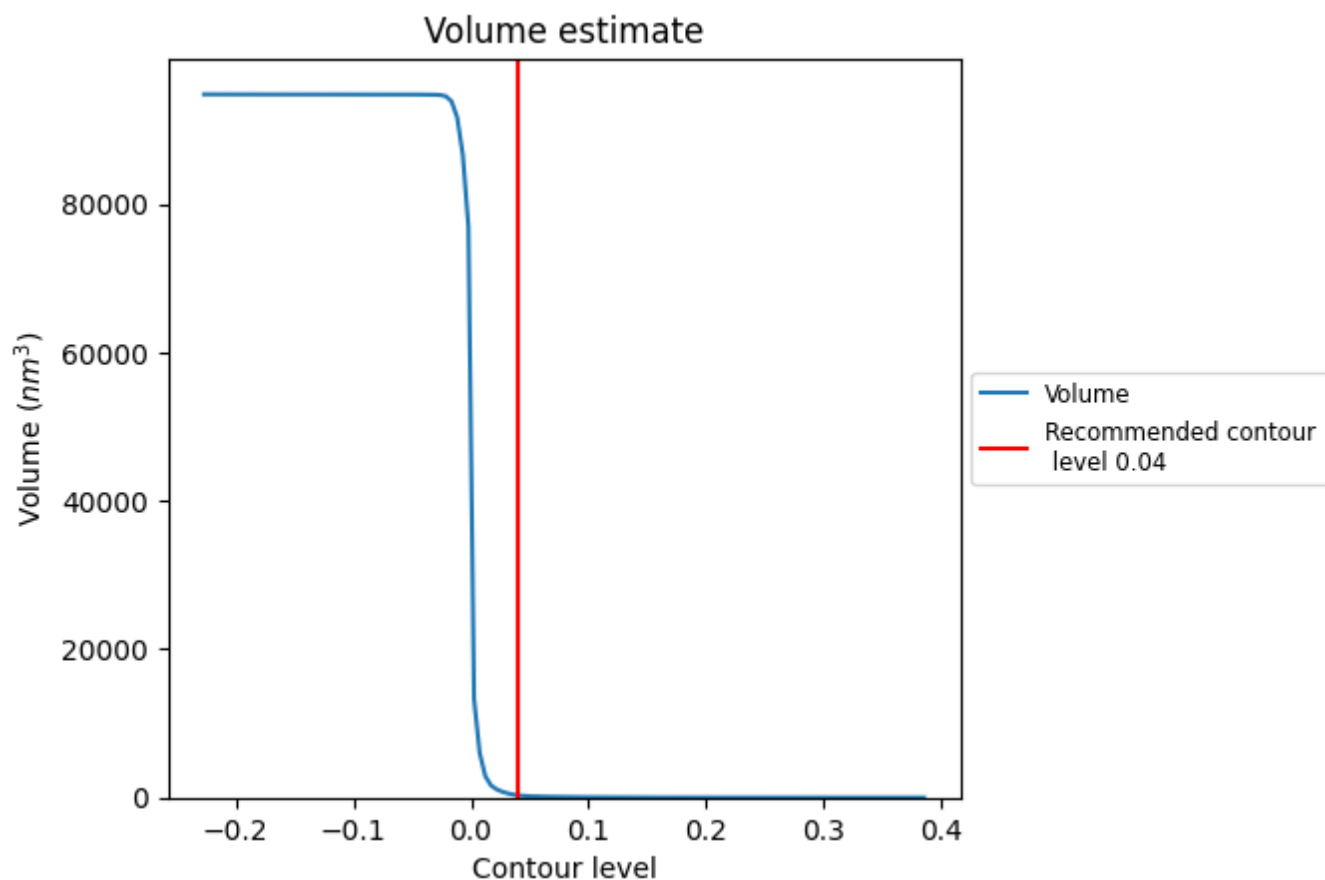
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

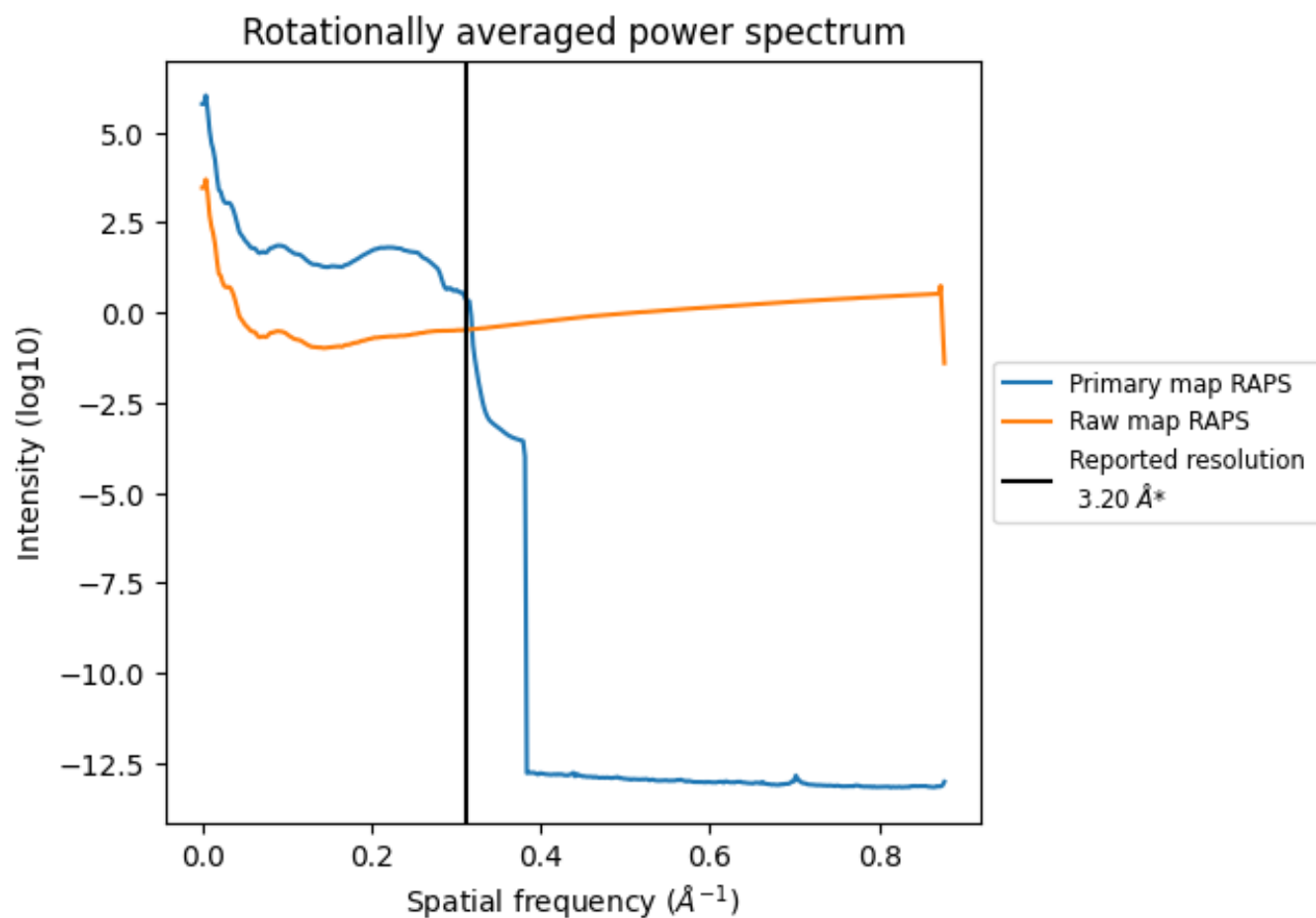
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm³; this corresponds to an approximate mass of 275 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

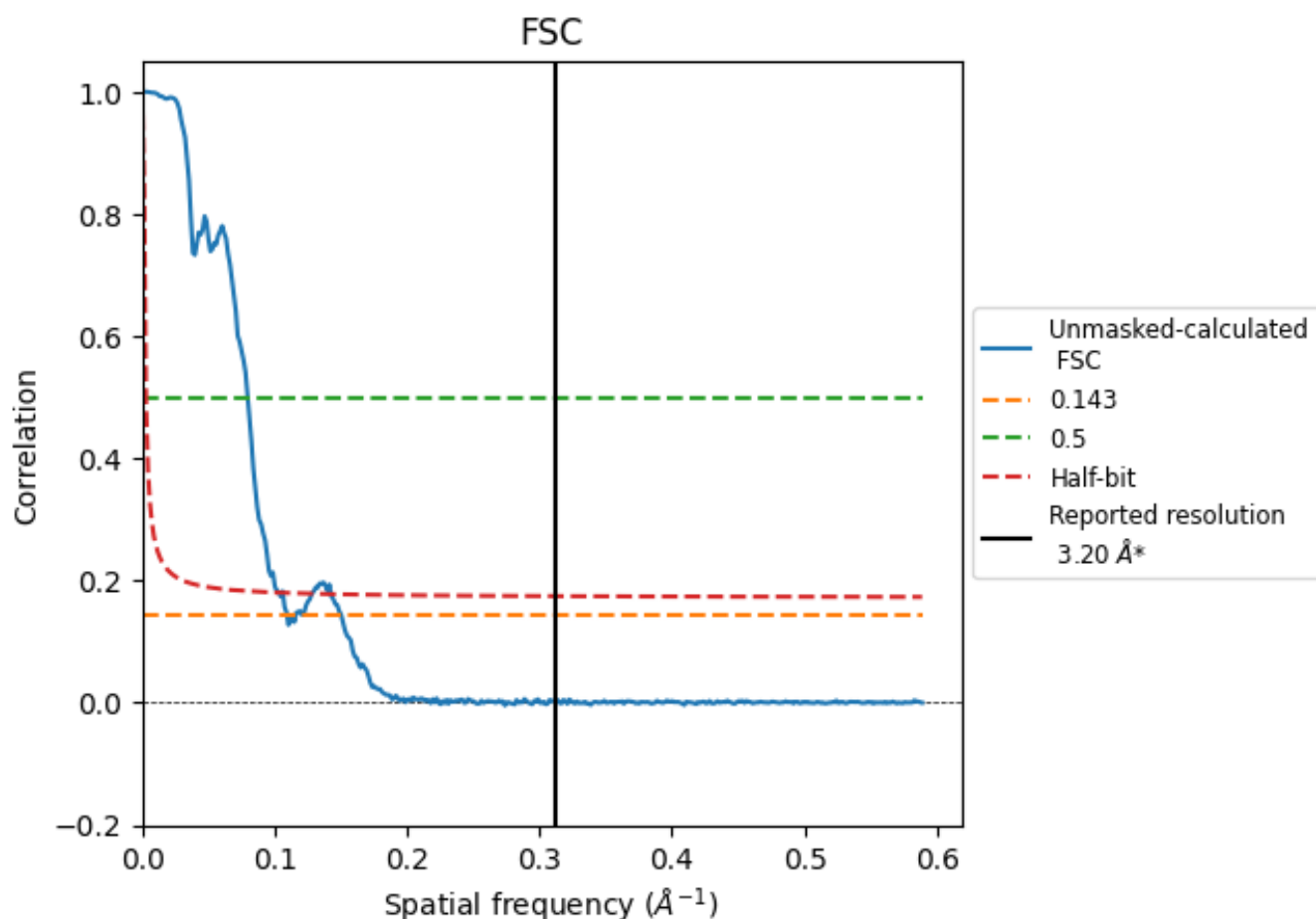


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

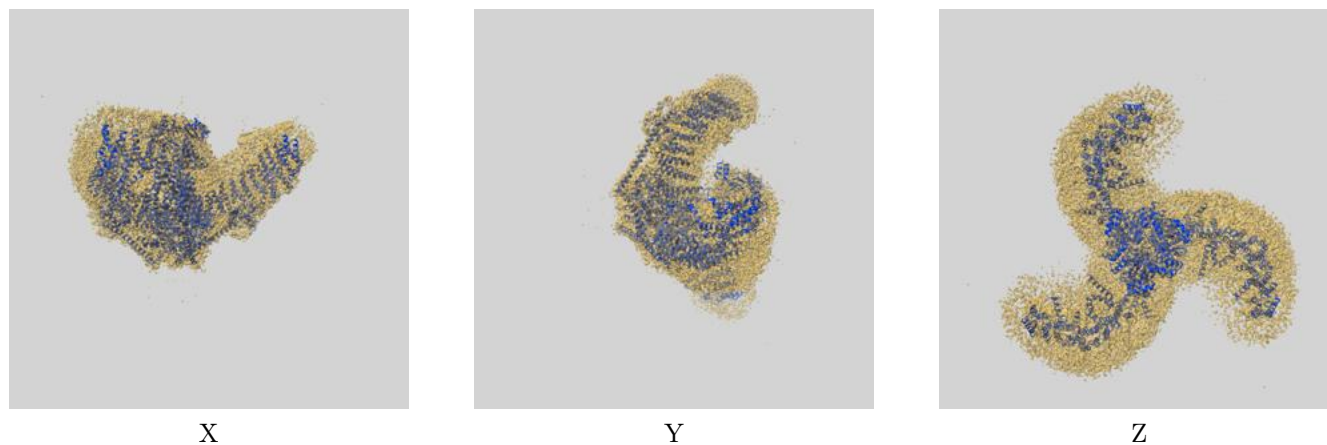
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.15	12.56	9.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.15 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

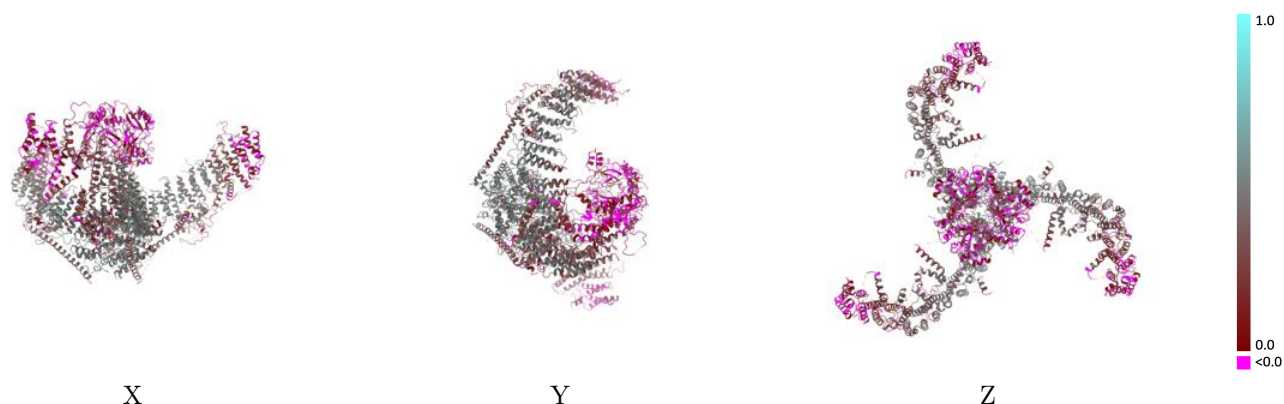
This section contains information regarding the fit between EMDB map EMD-39219 and PDB model 8YFC. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



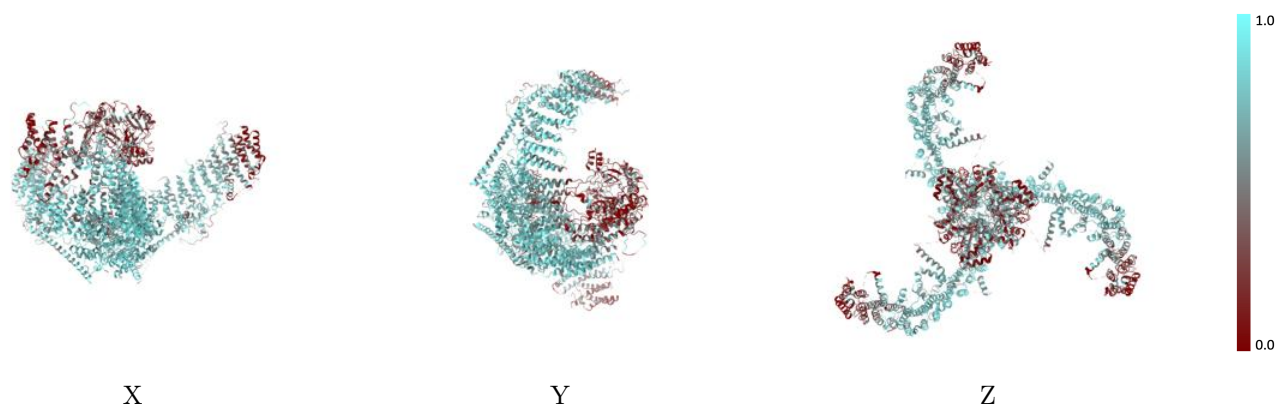
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



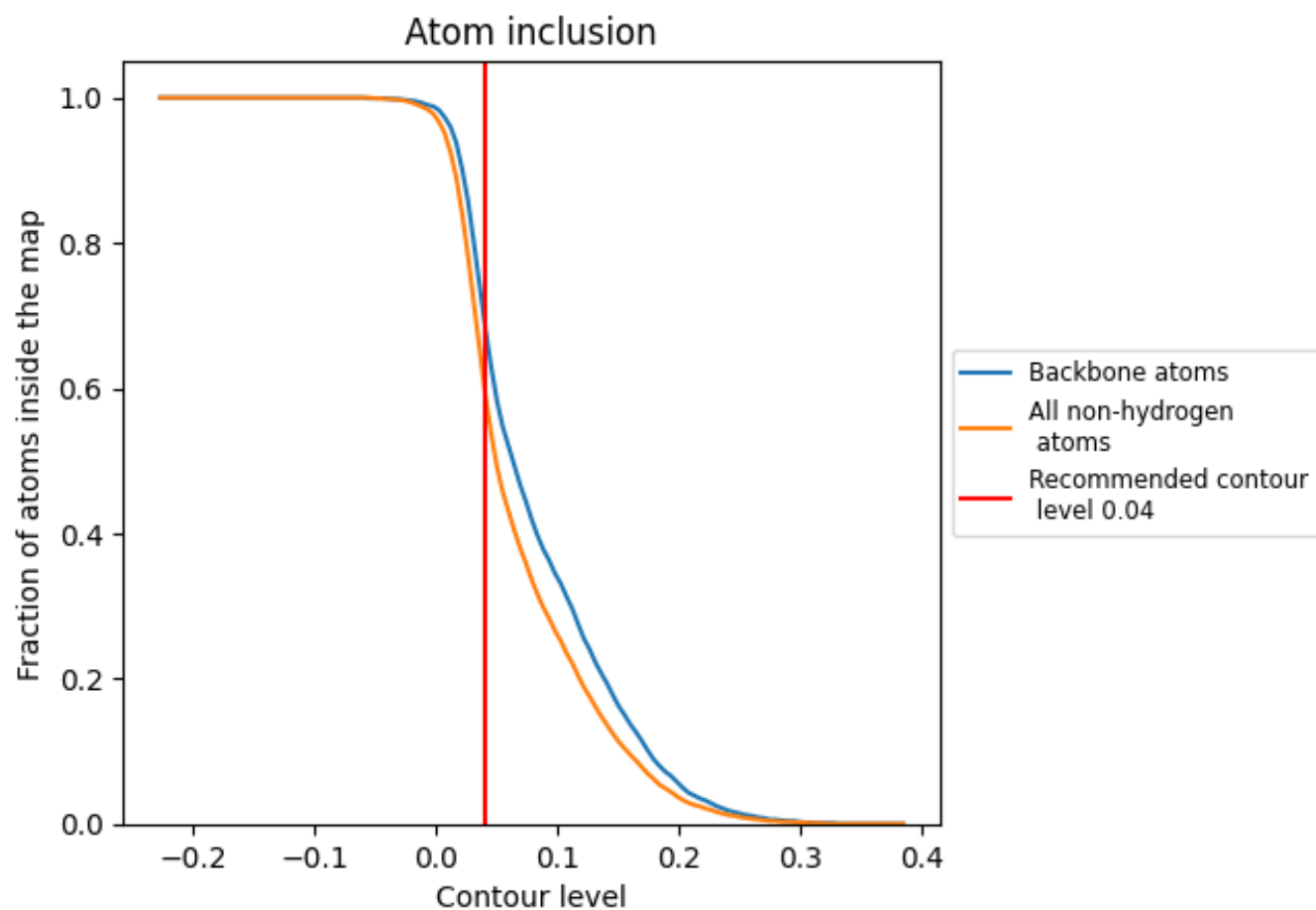
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6020	0.2880
A	0.6010	0.2850
B	0.6000	0.2860
C	0.6830	0.3720
D	0.6010	0.2870
E	0.6940	0.3760
F	0.6770	0.3770

1.0

0.0

<0.0