



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 12:32 PM UTC

PDB ID : 7NVM / pdb_00007nvm
EMDB ID : EMD-12606
Title : Human TRiC complex in closed state with nanobody Nb18, actin and PhLP2A bound
Authors : Kelly, J.J.; Chi, G.; Bulawa, C.; Paavilainen, V.O.; Bountra, C.; Huiskonen, J.T.; Yue, W.; Structural Genomics Consortium (SGC)
Deposited on : 2021-03-15
Resolution : 3.10 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:

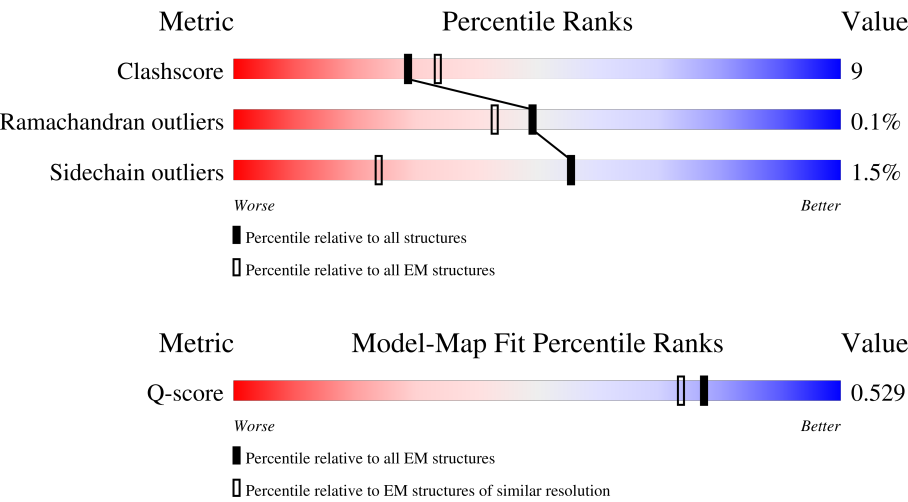
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	556	5% 73% 22% ••
1	a	556	• 75% 20% •
2	B	535	5% 75% 23% •
2	b	535	6% 77% 20% ••

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Mol	Chain	Length	Quality of chain
3	D	539	
3	d	539	
4	E	541	
4	e	541	
5	G	545	
5	g	545	
6	H	543	
6	h	543	
7	N	129	
7	n	129	
8	Q	548	
8	q	548	
9	Z	531	
9	z	531	
10	K	375	
11	P	239	

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
14	AF3	E	603	-	-	X	-
14	AF3	G	603	-	-	X	-
14	AF3	H	603	-	-	X	-
14	AF3	Q	603	-	-	X	-
14	AF3	Z	603	-	-	X	-
14	AF3	d	603	-	-	X	-
14	AF3	e	603	-	-	X	-
14	AF3	g	603	-	-	X	-
14	AF3	h	603	-	-	X	-
14	AF3	q	603	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	AF3	z	603	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 71008 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	536	Total	C	N	O	S	0	0
			4069	2548	711	787	23		
1	a	532	Total	C	N	O	S	0	0
			4041	2533	707	778	23		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	526	Total	C	N	O	S	0	0
			3952	2473	696	764	19		
2	b	525	Total	C	N	O	S	0	0
			3943	2467	694	763	19		

- Molecule 3 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	520	Total	C	N	O	S	0	0
			3923	2453	683	764	23		
3	d	520	Total	C	N	O	S	0	0
			3917	2450	680	764	23		

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	535	Total	C	N	O	S	1	0
			4132	2590	719	792	31		
4	e	540	Total	C	N	O	S	1	0
			4169	2610	724	804	31		

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	526	Total	C	N	O	S	0	0
			4089	2548	726	785	30		
5	g	538	Total	C	N	O	S	0	0
			4169	2590	740	809	30		

- Molecule 6 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	528	Total	C	N	O	S	0	0
			4054	2561	699	769	25		
6	h	525	Total	C	N	O	S	0	0
			4032	2548	696	763	25		

- Molecule 7 is a protein called Nanobody Nb18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	119	Total	C	N	O	S	0	0
			924	570	169	181	4		
7	n	119	Total	C	N	O	S	0	0
			924	570	169	181	4		

- Molecule 8 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	538	Total	C	N	O	S	0	0
			4086	2579	696	784	27		
8	q	533	Total	C	N	O	S	0	0
			4053	2558	690	778	27		

- Molecule 9 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	525	Total	C	N	O	S	0	0
			4022	2528	704	769	21		
9	z	527	Total	C	N	O	S	0	0
			4033	2534	706	772	21		

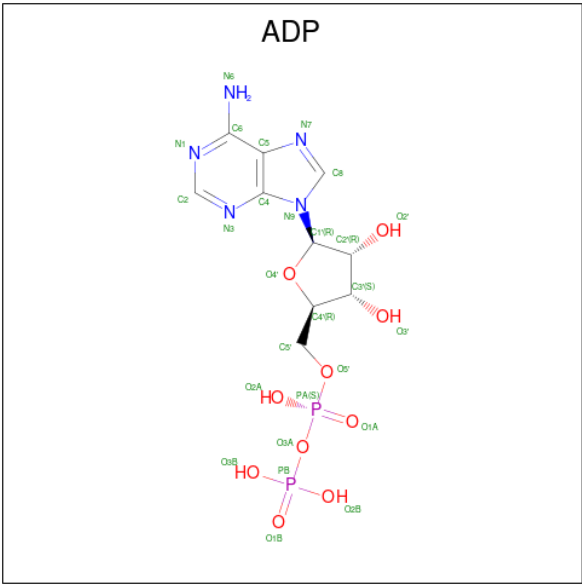
- Molecule 10 is a protein called Actin, cytoplasmic 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	317	Total	C	N	O	S	0	0
			2459	1563	409	469	18		

- Molecule 11 is a protein called Phosducin-like protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	P	190	1486	955	239	287	5	0	0

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	A	1	Total 27	10	5	10	2	0
12	B	1	Total 27	10	5	10	2	0
12	D	1	Total 27	10	5	10	2	0
12	E	1	Total 27	10	5	10	2	0
12	G	1	Total 27	10	5	10	2	0
12	H	1	Total 27	10	5	10	2	0
12	Q	1	Total 27	10	5	10	2	0
12	Z	1	Total 27	10	5	10	2	0
12	a	1	Total 27	10	5	10	2	0
12	b	1	Total 27	10	5	10	2	0

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Mol	Chain	Residues	Atoms					AltConf
12	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	e	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	g	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	h	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	q	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	z	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

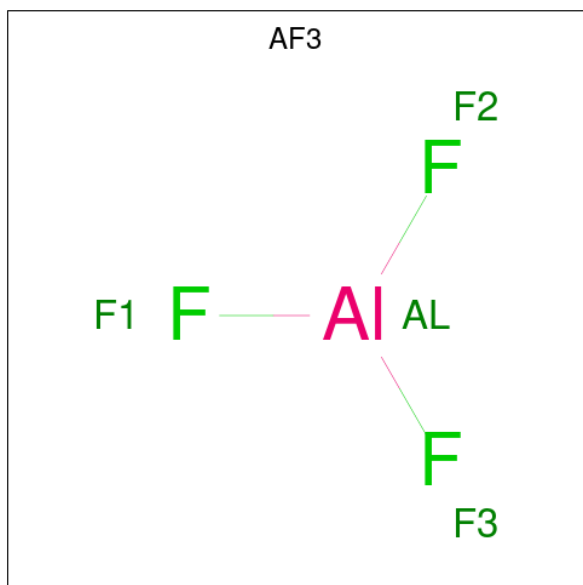
Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	Mg	0
			1	1	
13	B	1	Total	Mg	0
			1	1	
13	D	1	Total	Mg	0
			1	1	
13	E	1	Total	Mg	0
			1	1	
13	G	1	Total	Mg	0
			1	1	
13	H	1	Total	Mg	0
			1	1	
13	Q	1	Total	Mg	0
			1	1	
13	Z	1	Total	Mg	0
			1	1	
13	a	1	Total	Mg	0
			1	1	
13	b	1	Total	Mg	0
			1	1	
13	d	1	Total	Mg	0
			1	1	
13	e	1	Total	Mg	0
			1	1	
13	g	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
13	h	1	Total 1	Mg 1	0
13	q	1	Total 1	Mg 1	0
13	z	1	Total 1	Mg 1	0

- Molecule 14 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total 4	Al 1	F 3	0
14	B	1	Total 4	Al 1	F 3	0
14	D	1	Total 4	Al 1	F 3	0
14	E	1	Total 4	Al 1	F 3	0
14	G	1	Total 4	Al 1	F 3	0
14	H	1	Total 4	Al 1	F 3	0
14	Q	1	Total 4	Al 1	F 3	0
14	Z	1	Total 4	Al 1	F 3	0

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Mol	Chain	Residues	Atoms			AltConf
14	a	1	Total 4	Al 1	F 3	0
14	b	1	Total 4	Al 1	F 3	0
14	d	1	Total 4	Al 1	F 3	0
14	e	1	Total 4	Al 1	F 3	0
14	g	1	Total 4	Al 1	F 3	0
14	h	1	Total 4	Al 1	F 3	0
14	q	1	Total 4	Al 1	F 3	0
14	z	1	Total 4	Al 1	F 3	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	A	2	Total 2	O 2	0
15	B	2	Total 2	O 2	0
15	D	1	Total 1	O 1	0
15	E	1	Total 1	O 1	0
15	G	1	Total 1	O 1	0
15	H	1	Total 1	O 1	0
15	Q	1	Total 1	O 1	0
15	Z	1	Total 1	O 1	0
15	a	2	Total 2	O 2	0
15	b	1	Total 1	O 1	0
15	d	1	Total 1	O 1	0

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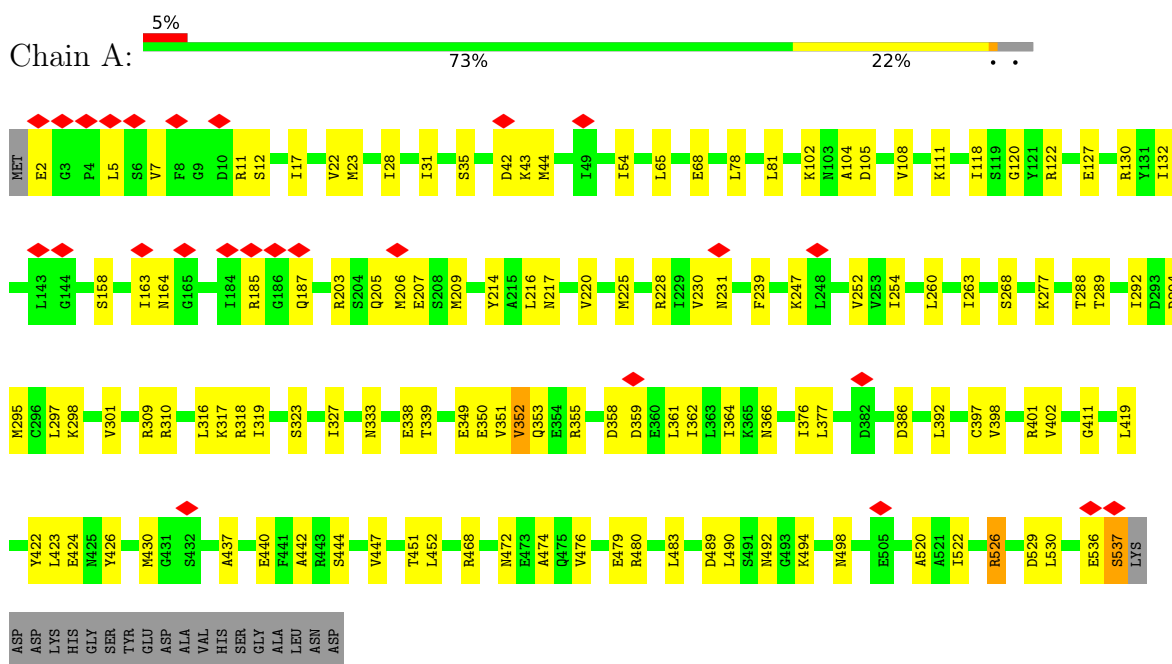
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Mol	Chain	Residues	Atoms		AltConf
15	e	1	Total 1	O 1	0
15	g	1	Total 1	O 1	0
15	h	1	Total 1	O 1	0
15	q	1	Total 1	O 1	0
15	z	1	Total 1	O 1	0

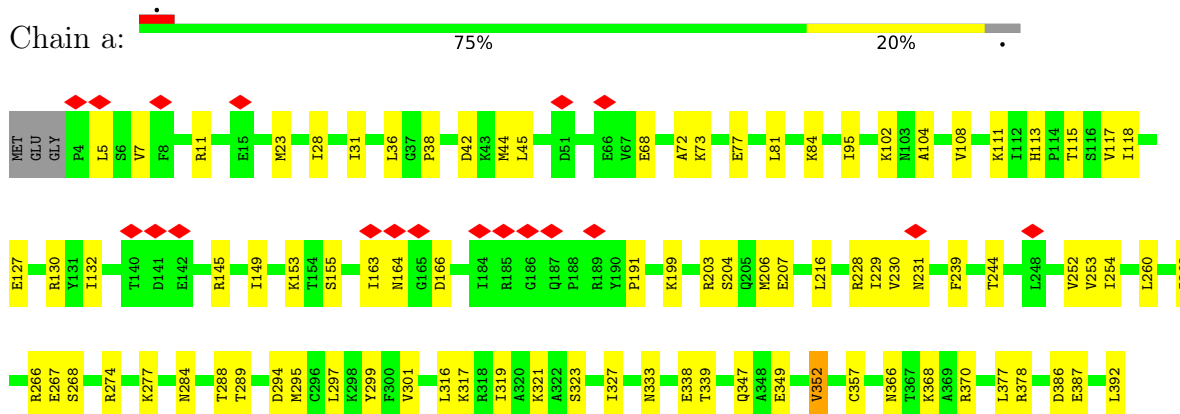
3 Residue-property plots

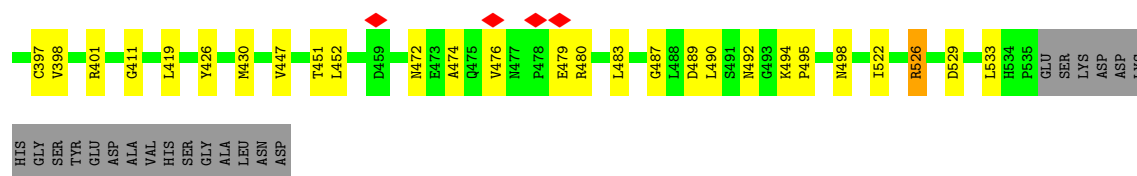
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: T-complex protein 1 subunit alpha

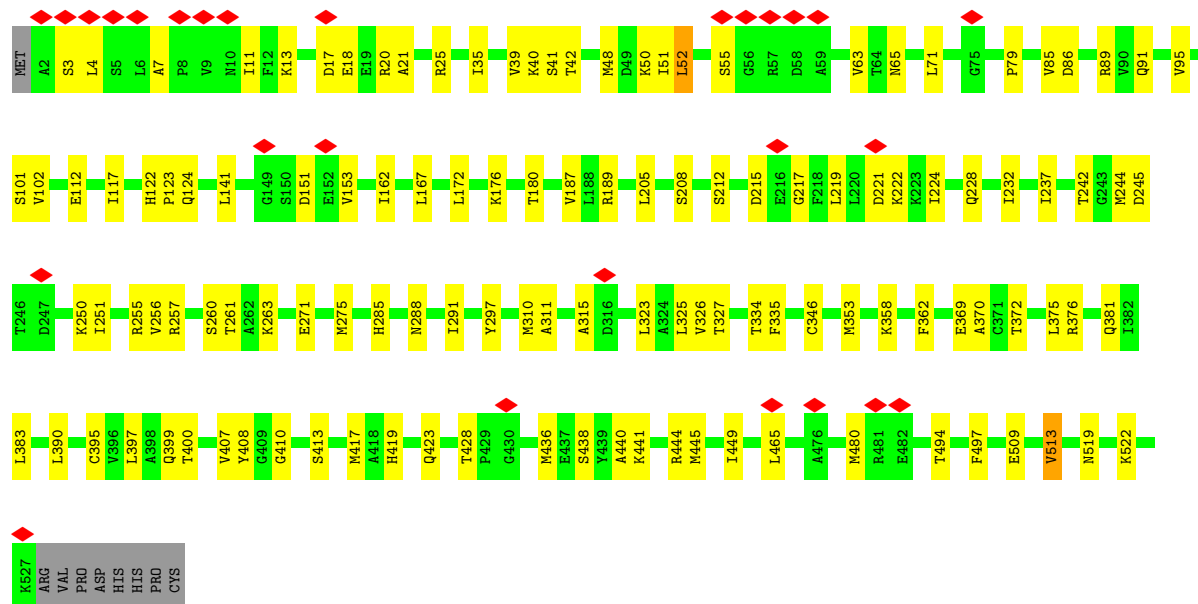
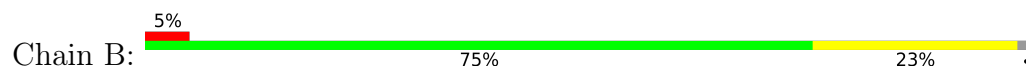


- Molecule 1: T-complex protein 1 subunit alpha

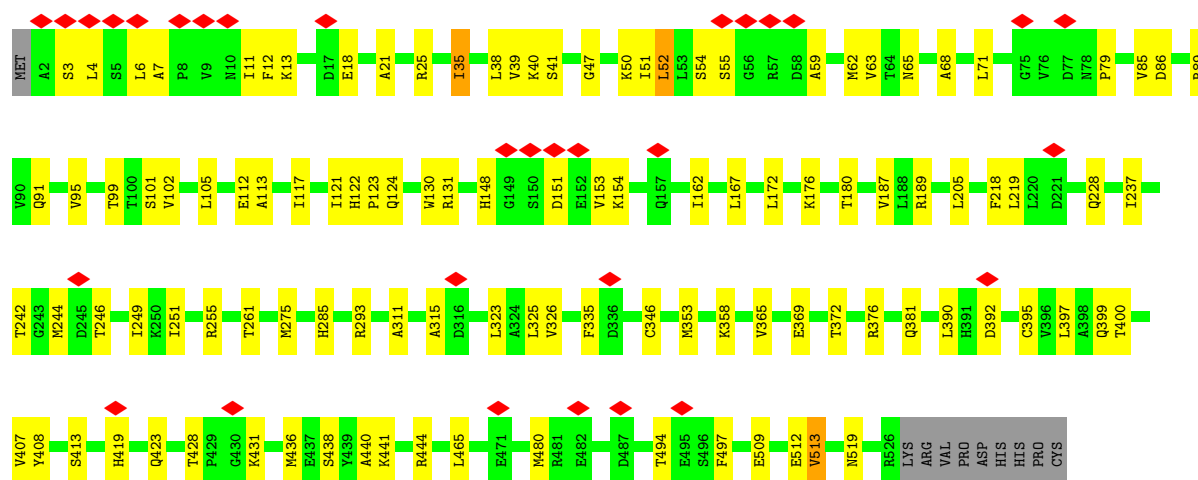




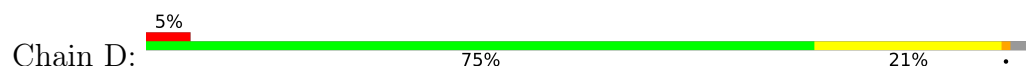
• Molecule 2: T-complex protein 1 subunit beta

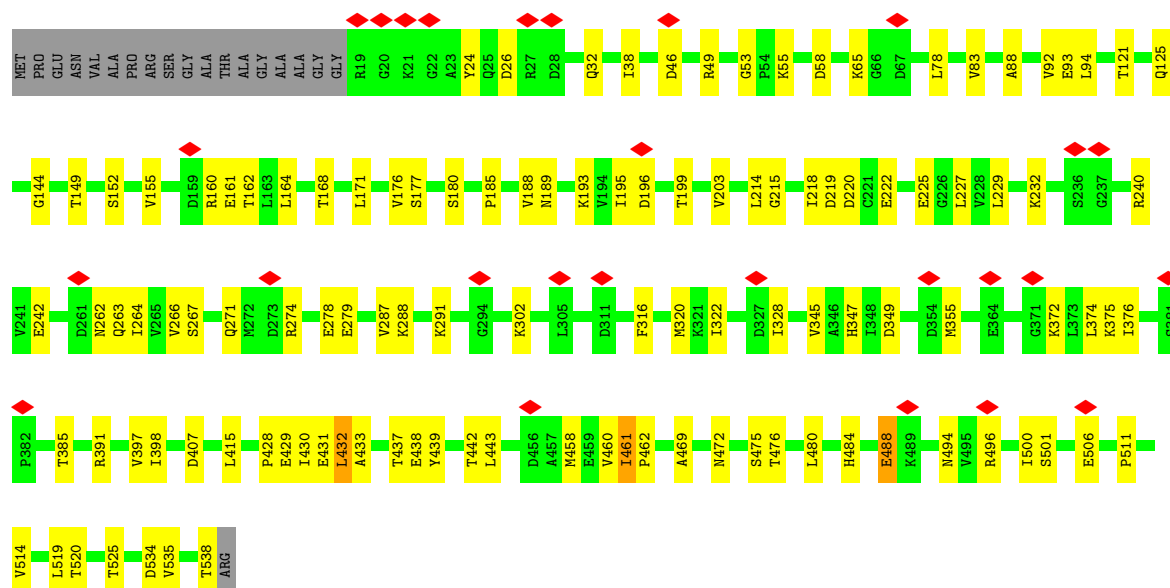


• Molecule 2: T-complex protein 1 subunit beta

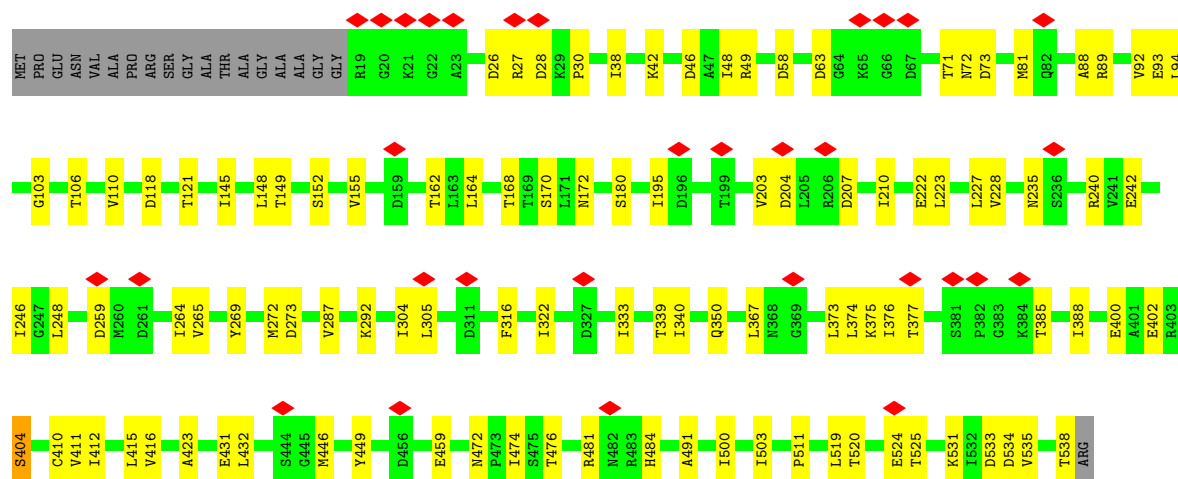
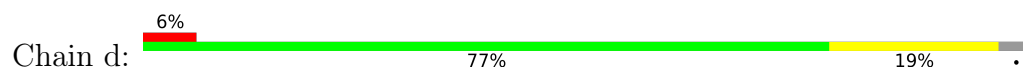


• Molecule 3: T-complex protein 1 subunit delta

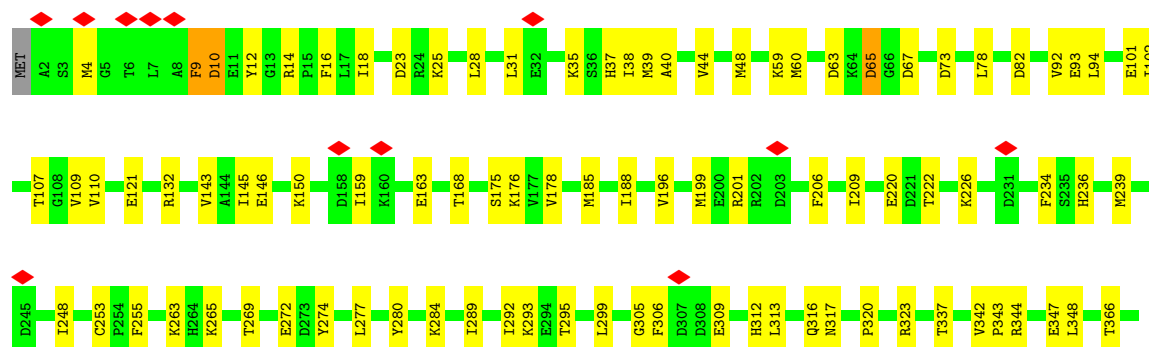


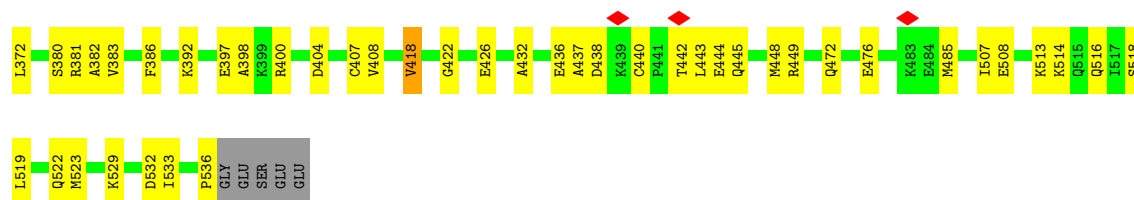


• Molecule 3: T-complex protein 1 subunit delta

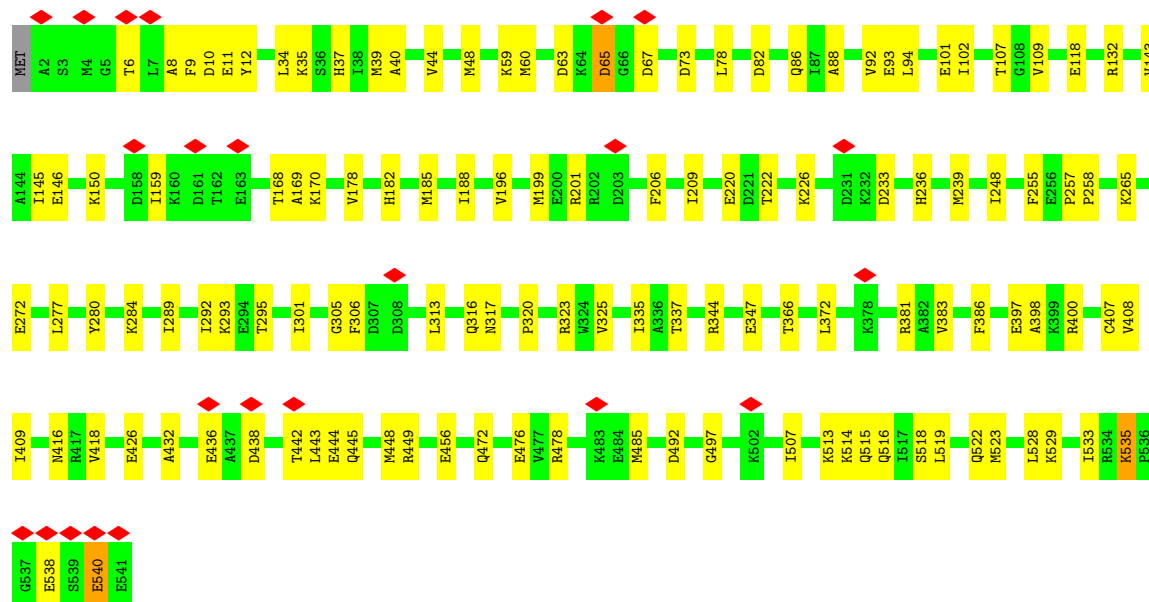
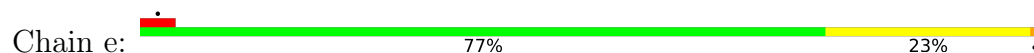


• Molecule 4: T-complex protein 1 subunit epsilon

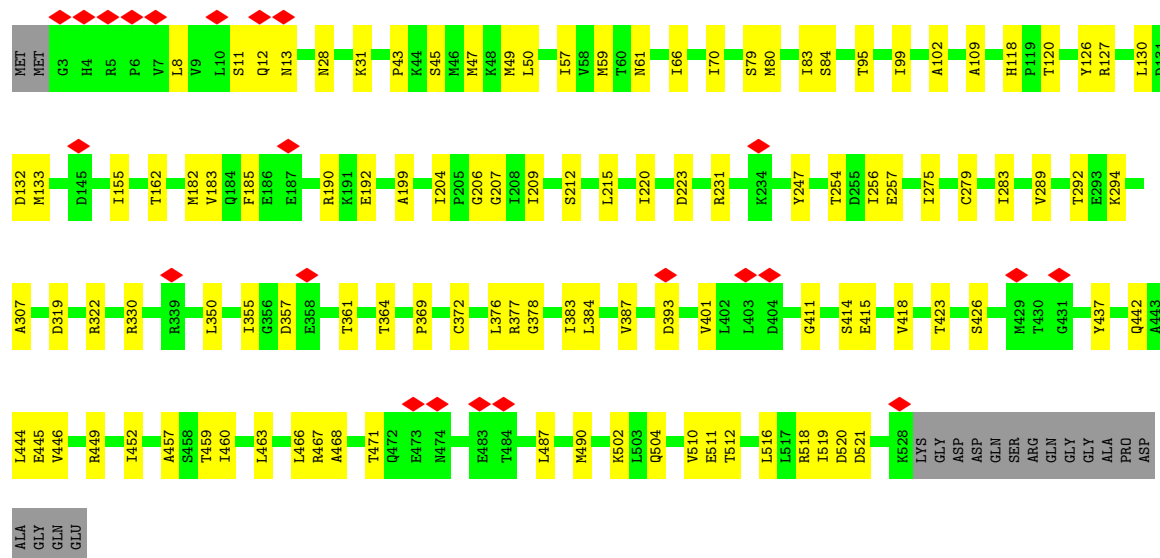
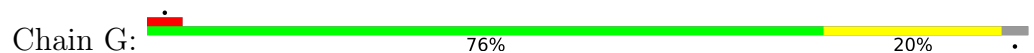




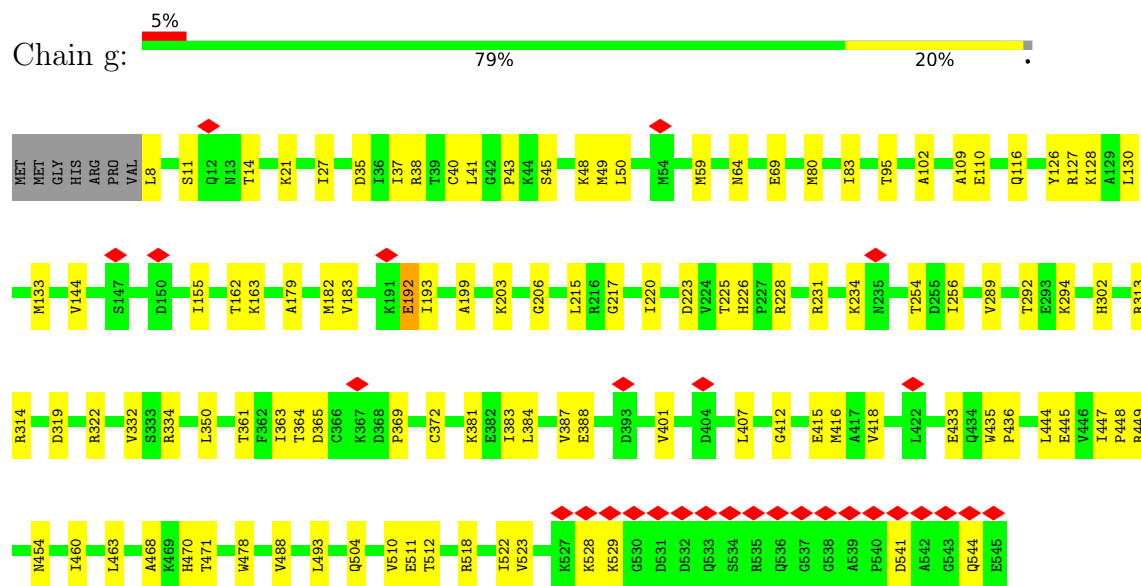
• Molecule 4: T-complex protein 1 subunit epsilon



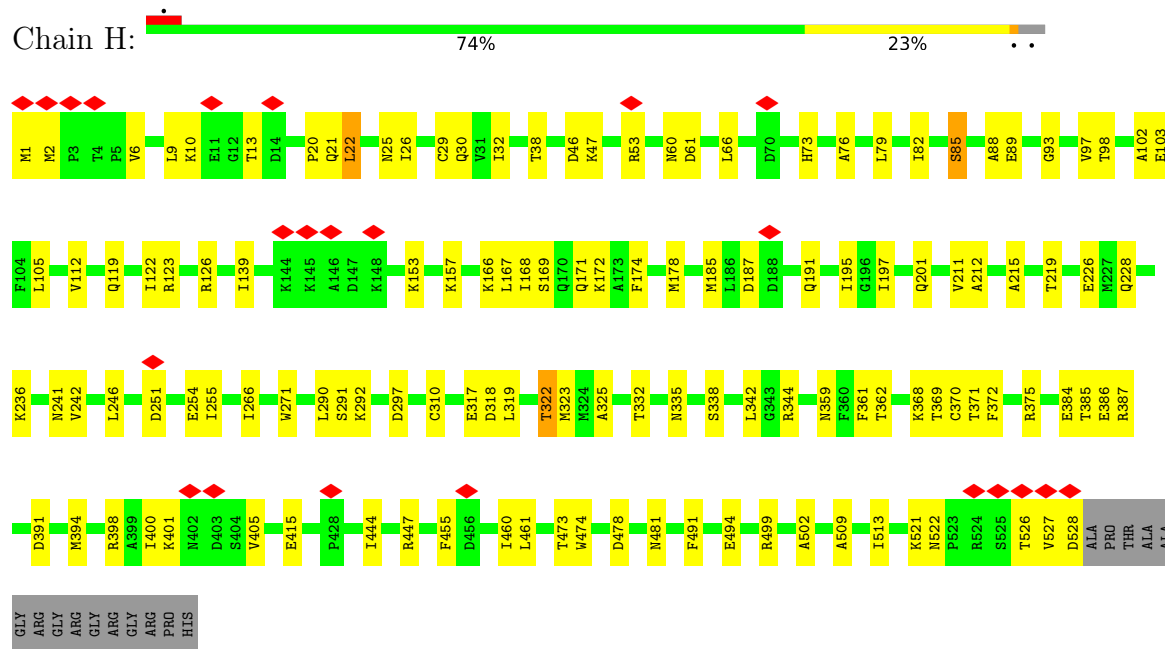
• Molecule 5: T-complex protein 1 subunit gamma



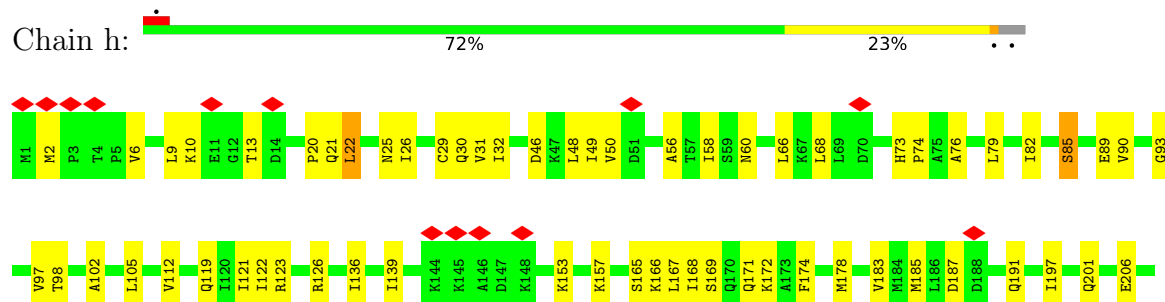
- Molecule 5: T-complex protein 1 subunit gamma

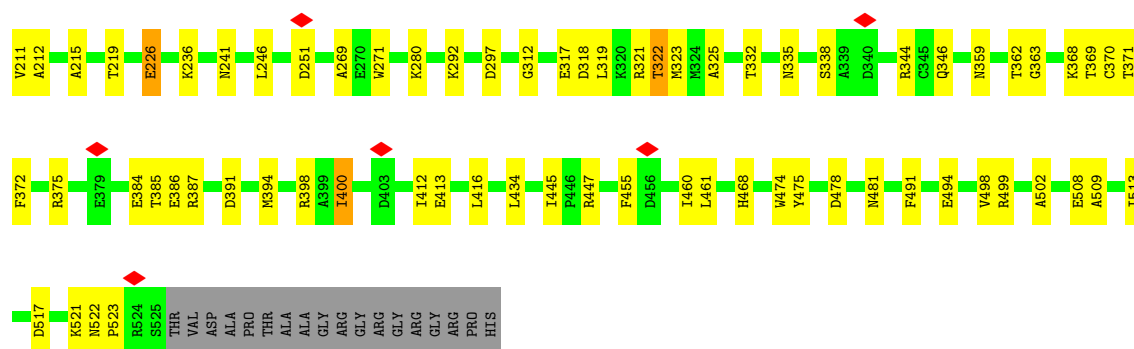


- Molecule 6: T-complex protein 1 subunit eta

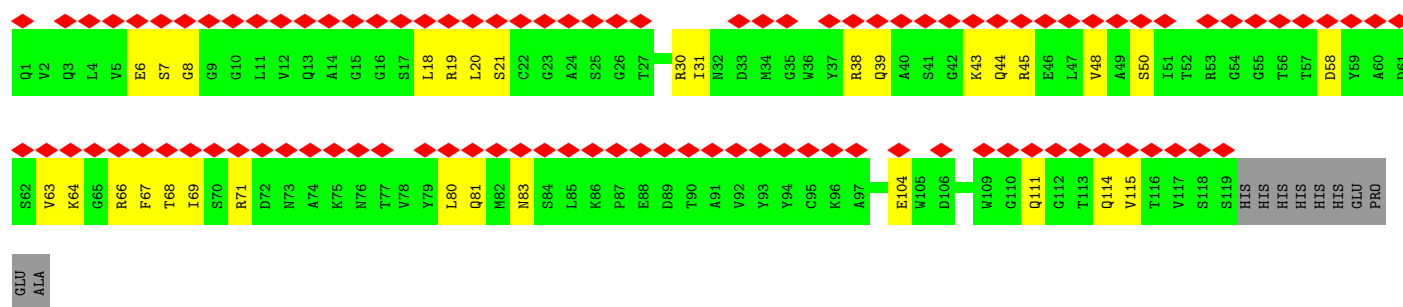
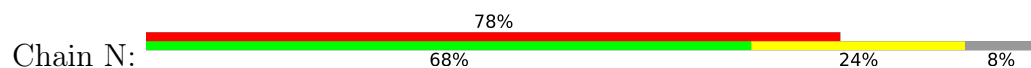


- Molecule 6: T-complex protein 1 subunit eta

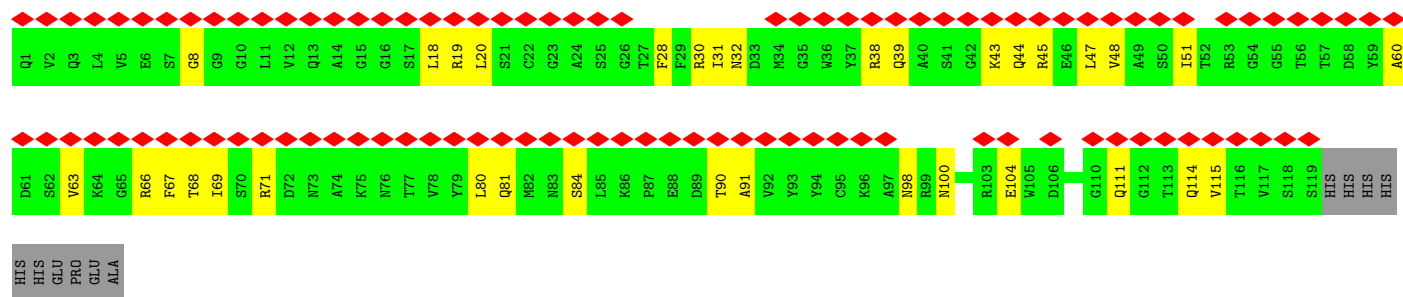
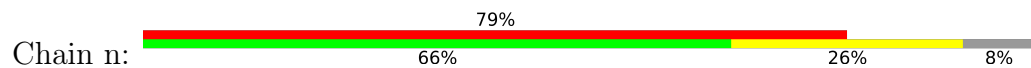




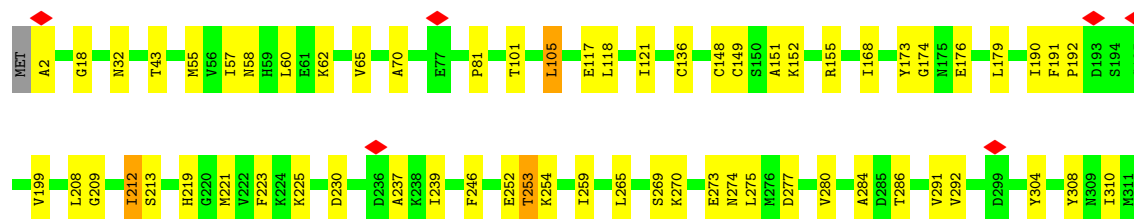
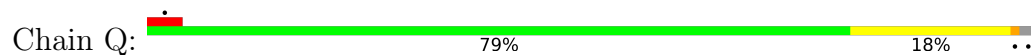
• Molecule 7: Nanobody Nb18

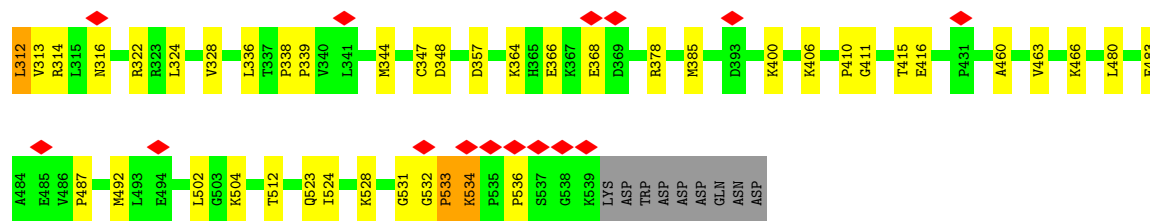


• Molecule 7: Nanobody Nb18



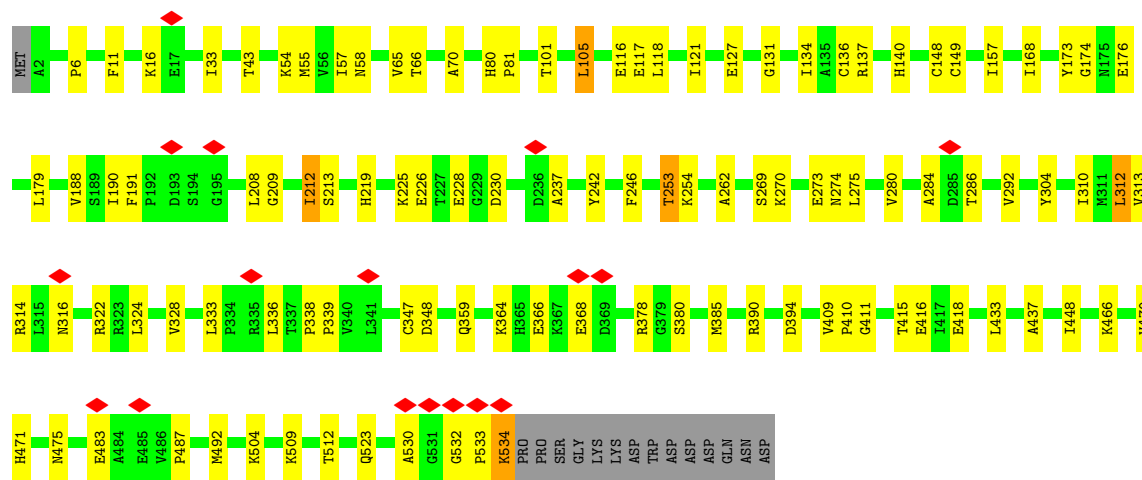
• Molecule 8: T-complex protein 1 subunit theta





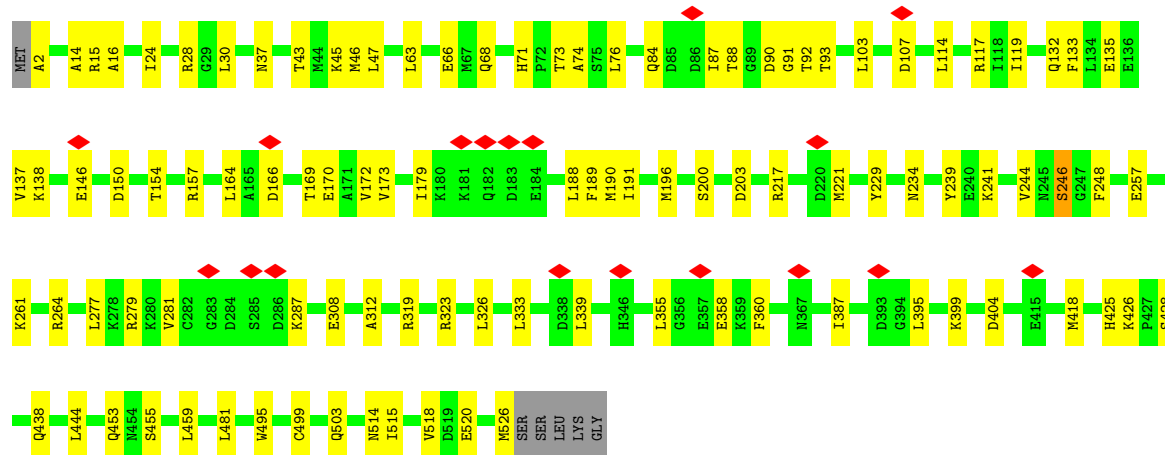
• Molecule 8: T-complex protein 1 subunit theta

Chain q: 77% 19%



• Molecule 9: T-complex protein 1 subunit zeta

Chain Z: 80% 19%



• Molecule 9: T-complex protein 1 subunit zeta

Chain z: 80% 19%

F184	G185	G186	M187	N188	L189	T190	R191	D192	E193	L194	E195	V196	K197	L198	S199	E200	S201	G202	A203	I204	M205	T206	D207	L208	E209	E210	N211	P212	LYS	PRO	ILE	GLU	ASP	VAL	LEU	LEU	SER	SER	VAL	ARG	ARG	SER	VAL	LEU	MET	LYS	ARG	ASP	SER	ASP	SER	GLU	GLY	ASP				
G123	I124	P125	L126	C127	A128	L129	I130	N131	Q132	H133	L134	S135	G136	L137	A138	R139	K140	F141	P142	D143	V144	K145	F146	I147	K148	A149	I150	S151	T152	T153	C154	N157	Y158	P159	D160	R161	N162	L163	P164	T165	I166	F167	V168	Y169	L170	E171	G172	D173	I174	K175	A176	Q177	F178	I179	G180	P181	L182	V183
E62	F63	N64	E65	E66	D67	E68	R69	A70	I71	E72	M73	Y74	R75	R76	L79	A80	E81	W82	K83	A84	T85	K86	L87	K88	N89	K90	F91	G92	E93	V94	L95	E96	I97	S98	G99	K100	D101	Y102	V103	Q104	E105	V106	T107	K108	A109	G110	E111	G112	L113	W114	V115	I116	L117	H118	L119	Y120	K121	Q122

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63082	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: MG, ADP, AF3

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	0.26	0/4109	0.43	0/5548
1	a	0.24	0/4081	0.41	0/5510
2	B	0.23	0/3995	0.42	0/5386
2	b	0.24	0/3986	0.43	0/5375
3	D	0.22	0/3955	0.37	0/5338
3	d	0.24	0/3949	0.42	0/5331
4	E	0.26	0/4183	0.45	0/5635
4	e	0.28	0/4220	0.48	0/5684
5	G	0.24	0/4136	0.42	0/5579
5	g	0.24	0/4215	0.40	0/5683
6	H	0.28	0/4111	0.44	0/5550
6	h	0.26	0/4089	0.42	0/5519
7	N	0.14	0/941	0.42	0/1270
7	n	0.16	0/941	0.43	0/1270
8	Q	0.26	0/4147	0.45	0/5606
8	q	0.24	0/4112	0.42	0/5558
9	Z	0.25	0/4069	0.43	0/5486
9	z	0.24	0/4080	0.43	0/5501
10	K	0.23	0/2510	0.50	1/3401 (0.0%)
11	P	0.15	0/1518	0.36	0/2062
All	All	0.24	0/71347	0.43	1/96292 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	e	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	332	PRO	N-CA-C	5.07	116.89	110.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	e	8	ALA	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4069	0	4224	82	0
1	a	4041	0	4205	77	0
2	B	3952	0	4070	84	0
2	b	3943	0	4057	77	0
3	D	3923	0	4131	83	0
3	d	3917	0	4120	73	0
4	E	4132	0	4246	95	0
4	e	4169	0	4272	93	0
5	G	4089	0	4224	83	0
5	g	4169	0	4287	80	0
6	H	4054	0	4160	90	0
6	h	4032	0	4140	95	0
7	N	924	0	884	24	0
7	n	924	0	884	26	0
8	Q	4086	0	4160	85	0
8	q	4053	0	4125	79	0
9	Z	4022	0	4161	73	0
9	z	4033	0	4171	70	0
10	K	2459	0	2419	105	0
11	P	1486	0	1429	49	0
12	A	27	0	12	1	0
12	B	27	0	12	4	0
12	D	27	0	12	2	0
12	E	27	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	G	27	0	12	1	0
12	H	27	0	12	1	0
12	Q	27	0	12	1	0
12	Z	27	0	12	2	0
12	a	27	0	12	1	0
12	b	27	0	12	3	0
12	d	27	0	12	2	0
12	e	27	0	12	2	0
12	g	27	0	12	3	0
12	h	27	0	12	2	0
12	q	27	0	12	2	0
12	z	27	0	12	2	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	D	1	0	0	0	0
13	E	1	0	0	0	0
13	G	1	0	0	0	0
13	H	1	0	0	0	0
13	Q	1	0	0	0	0
13	Z	1	0	0	0	0
13	a	1	0	0	0	0
13	b	1	0	0	0	0
13	d	1	0	0	0	0
13	e	1	0	0	0	0
13	g	1	0	0	0	0
13	h	1	0	0	0	0
13	q	1	0	0	0	0
13	z	1	0	0	0	0
14	A	4	0	0	0	0
14	B	4	0	0	1	0
14	D	4	0	0	0	0
14	E	4	0	0	3	0
14	G	4	0	0	2	0
14	H	4	0	0	2	0
14	Q	4	0	0	2	0
14	Z	4	0	0	2	0
14	a	4	0	0	0	0
14	b	4	0	0	1	0
14	d	4	0	0	3	0
14	e	4	0	0	2	0
14	g	4	0	0	2	0
14	h	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	q	4	0	0	2	0
14	z	4	0	0	2	0
15	A	2	0	0	1	0
15	B	2	0	0	0	0
15	D	1	0	0	1	0
15	E	1	0	0	1	0
15	G	1	0	0	1	0
15	H	1	0	0	2	0
15	Q	1	0	0	0	0
15	Z	1	0	0	0	0
15	a	2	0	0	0	0
15	b	1	0	0	1	0
15	d	1	0	0	1	0
15	e	1	0	0	0	0
15	g	1	0	0	0	0
15	h	1	0	0	1	0
15	q	1	0	0	1	0
15	z	1	0	0	0	0
All	All	71008	0	72561	1354	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 9.

All (1354) 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)
8:Q:531:GLY:HA3	11:P:10:TRP:HB2	1.40	1.03
8:Q:532:GLY:HA3	10:K:351:THR:HG21	1.44	0.99
8:Q:531:GLY:HA3	11:P:10:TRP:CB	1.92	0.97
10:K:332:PRO:HD2	10:K:333:PRO:CD	1.97	0.94
7:N:68:THR:HB	7:N:81:GLN:HB3	1.50	0.92
7:n:68:THR:HB	7:n:81:GLN:HB3	1.48	0.92
9:Z:154:THR:HG21	9:Z:495:TRP:H	1.37	0.89
9:z:154:THR:HG21	9:z:495:TRP:H	1.38	0.88
5:G:206:GLY:HA3	9:Z:87:ILE:HG13	1.57	0.87
10:K:332:PRO:HD2	10:K:333:PRO:HD2	1.58	0.85
10:K:332:PRO:CD	10:K:333:PRO:HD2	2.07	0.83
8:q:280:VAL:HG21	8:q:304:TYR:HB3	1.58	0.83
5:g:83:ILE:HD11	5:g:512:THR:HG21	1.58	0.83
9:Z:217:ARG:NH2	10:K:375:PHE:C	2.36	0.83
4:e:94:LEU:HD13	4:e:523:MET:HG3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:189:LEU:HD21	11:P:194:LEU:HB2	1.59	0.82
1:A:44:MET:HE3	5:G:519:ILE:HD13	1.61	0.81
5:g:206:GLY:HA3	9:z:87:ILE:HG13	1.62	0.81
10:K:332:PRO:N	10:K:333:PRO:HD2	1.96	0.79
10:K:365:SER:HB2	10:K:369:ILE:HB	1.63	0.79
10:K:332:PRO:CD	10:K:333:PRO:CD	2.60	0.78
10:K:332:PRO:HD2	10:K:333:PRO:HD3	1.64	0.78
2:b:381:GLN:HE22	3:d:93:GLU:HG3	1.50	0.77
2:b:91:GLN:HG3	2:b:102:VAL:HG11	1.68	0.76
10:K:62:ARG:HA	10:K:65:LEU:HD12	1.66	0.76
4:e:418:VAL:CG1	4:e:507:ILE:HG23	2.14	0.76
3:D:53:GLY:HA2	12:D:601:ADP:H5'2	1.66	0.76
5:g:183:VAL:HG21	5:g:199:ALA:HB2	1.68	0.76
4:e:438:ASP:OD1	4:e:449:ARG:NH2	2.19	0.75
4:E:94:LEU:HD13	4:E:523:MET:HG3	1.67	0.75
6:h:197:ILE:HG21	6:h:386:GLU:HG3	1.69	0.75
4:e:538:GLU:HG3	4:e:540:GLU:HB2	1.68	0.75
9:z:8:ASN:HD21	9:z:526:MET:HG2	1.50	0.75
1:a:474:ALA:HB2	1:a:483:LEU:HB2	1.70	0.74
1:a:42:ASP:OD1	5:g:518:ARG:NH1	2.21	0.73
1:A:349:GLU:HB2	1:A:366:ASN:HB2	1.71	0.73
8:Q:280:VAL:HG21	8:Q:304:TYR:HB3	1.70	0.72
3:D:430:ILE:HG13	3:D:480:LEU:HD13	1.70	0.72
3:D:24:TYR:OH	2:b:25:ARG:NH1	2.22	0.72
3:d:195:ILE:HG21	3:d:203:VAL:HG22	1.71	0.72
6:H:82:ILE:HG21	6:H:509:ALA:HB2	1.72	0.71
4:E:445:GLN:HE21	4:E:449:ARG:HH12	1.39	0.71
1:A:122:ARG:NH2	3:D:219:ASP:OD2	2.24	0.71
1:A:333:ASN:HD22	1:A:339:THR:HG22	1.54	0.71
1:a:349:GLU:HB2	1:a:366:ASN:HB2	1.73	0.71
5:G:223:ASP:OD1	5:G:231:ARG:NH1	2.24	0.71
7:n:32:ASN:N	7:n:98:ASN:O	2.24	0.70
1:A:23:MET:HG2	4:e:11:GLU:HG2	1.73	0.70
2:B:228:GLN:NE2	2:B:311:ALA:H	1.89	0.70
2:B:219:LEU:HB2	2:B:372:THR:HG21	1.73	0.70
4:e:78:LEU:HB3	4:e:92:VAL:HG22	1.71	0.70
2:b:50:LYS:HD2	3:d:534:ASP:HB3	1.73	0.70
10:K:164:PRO:HD2	10:K:175:ILE:HD13	1.71	0.70
5:g:40:CYS:SG	5:g:48:LYS:NZ	2.65	0.70
1:A:474:ALA:HB2	1:A:483:LEU:HB2	1.74	0.69
6:H:197:ILE:HG21	6:H:386:GLU:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:GLU:HG3	1:A:480:ARG:HG2	1.75	0.69
2:b:438:SER:HA	2:b:441:LYS:HE2	1.73	0.69
3:D:480:LEU:HG	3:D:500:ILE:HD12	1.74	0.69
6:H:478:ASP:OD2	6:H:481:ASN:ND2	2.26	0.69
5:G:256:ILE:HB	9:Z:246:SER:HA	1.74	0.69
8:Q:531:GLY:CA	11:P:10:TRP:HB2	2.21	0.69
2:b:63:VAL:HG22	2:b:381:GLN:HB3	1.75	0.69
12:z:601:ADP:O1B	14:z:603:AF3:F1	2.01	0.69
10:K:70:PRO:HG3	10:K:81:ASP:HB3	1.74	0.69
3:d:287:VAL:HG21	3:d:316:PHE:HB3	1.75	0.69
3:D:432:LEU:HD11	3:D:519:LEU:HD11	1.73	0.68
4:E:9[C]:PHE:O	4:E:10:ASP:HB2	1.92	0.68
5:G:449:ARG:HG2	5:G:463:LEU:HD11	1.74	0.68
6:H:53:ARG:NH1	10:K:321:ALA:O	2.26	0.68
10:K:262:PHE:HE2	10:K:313:MET:HG2	1.56	0.68
8:q:270:LYS:O	8:q:274:ASN:ND2	2.20	0.68
2:B:438:SER:HA	2:B:441:LYS:HE2	1.76	0.68
5:G:516:LEU:HA	5:G:519:ILE:HD12	1.75	0.68
7:N:31:ILE:O	7:N:71:ARG:NH2	2.26	0.68
4:e:305:GLY:HA2	4:e:323:ARG:HB2	1.73	0.68
3:D:26:ASP:O	2:b:25:ARG:NH2	2.27	0.68
9:Z:217:ARG:HH22	10:K:375:PHE:C	2.00	0.68
3:d:227:LEU:HB3	3:d:339:THR:HG21	1.75	0.68
1:A:526:ARG:NH1	3:D:58:ASP:OD1	2.27	0.68
5:g:217:GLY:HA3	5:g:363:ILE:O	1.93	0.68
6:H:53:ARG:NH1	10:K:318:THR:O	2.27	0.67
3:d:170:SER:HB3	3:d:411:VAL:HG21	1.75	0.67
6:h:82:ILE:HG21	6:h:509:ALA:HB2	1.76	0.67
5:g:45:SER:O	9:z:117:ARG:NH2	2.27	0.67
4:e:101:GLU:OE1	6:h:375:ARG:NH2	2.27	0.67
8:q:225:LYS:NZ	8:q:314:ARG:O	2.27	0.67
3:D:488:GLU:N	3:D:488:GLU:OE1	2.27	0.67
4:E:305:GLY:HA2	4:E:323:ARG:HB2	1.76	0.67
11:P:120:TYR:HA	11:P:163:LEU:HD13	1.77	0.67
10:K:31:PHE:HB3	10:K:32:PRO:HD3	1.75	0.67
3:d:431:GLU:OE1	3:d:431:GLU:HA	1.94	0.67
5:G:8:LEU:CD2	4:e:9[B]:PHE:CD2	2.78	0.67
3:D:240:ARG:NH1	3:D:242:GLU:OE2	2.28	0.66
8:Q:523:GLN:HB2	9:Z:45:LYS:HD2	1.78	0.66
8:q:219:HIS:NE2	8:q:368:GLU:OE1	2.28	0.66
7:N:63:VAL:HG23	7:N:66:ARG:HH21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:292:THR:HG22	5:G:294:LYS:H	1.60	0.66
4:E:438:ASP:OD1	4:E:449:ARG:NH2	2.28	0.66
6:H:335:ASN:ND2	8:Q:273:GLU:OE1	2.28	0.66
1:a:479:GLU:HG3	1:a:480:ARG:HG2	1.78	0.66
1:A:289:THR:HG23	1:A:316:LEU:HD22	1.77	0.66
8:q:523:GLN:HB2	9:z:45:LYS:HD2	1.77	0.65
4:e:418:VAL:HG13	4:e:507:ILE:HG23	1.76	0.65
7:n:18:LEU:HD13	7:n:20:LEU:HD13	1.79	0.65
1:a:164:ASN:ND2	1:a:206:MET:SD	2.70	0.65
9:z:15:ARG:HH21	9:z:15:ARG:H	1.45	0.65
10:K:219:VAL:HG11	10:K:309:ILE:HA	1.79	0.64
5:G:279:CYS:O	5:G:283:ILE:HG13	1.96	0.64
6:h:478:ASP:OD2	6:h:481:ASN:ND2	2.30	0.64
8:Q:314:ARG:NH2	8:Q:316:ASN:OD1	2.30	0.64
2:B:255:ARG:HD3	4:E:265:LYS:HD2	1.78	0.64
4:e:418:VAL:HG11	4:e:507:ILE:HG23	1.78	0.64
8:Q:531:GLY:HA3	11:P:10:TRP:HB3	1.77	0.64
6:H:38:THR:HG1	6:H:47:LYS:HZ1	1.45	0.63
10:K:296:ASN:ND2	11:P:2:GLN:OE1	2.31	0.63
2:b:228:GLN:NE2	2:b:311:ALA:H	1.96	0.63
7:N:38:ARG:O	7:N:45:ARG:HA	1.97	0.63
5:G:8:LEU:HD21	4:e:9[A]:PHE:HD2	1.63	0.63
8:Q:292:VAL:HG22	8:Q:313:VAL:HB	1.80	0.63
2:B:63:VAL:HG22	2:B:381:GLN:HB3	1.80	0.63
7:n:63:VAL:HG23	7:n:66:ARG:HH21	1.64	0.63
1:A:164:ASN:ND2	1:A:206:MET:SD	2.72	0.63
3:D:195:ILE:HG21	3:D:203:VAL:HG22	1.81	0.63
1:a:266:ARG:NH2	3:d:273:ASP:OD2	2.32	0.62
8:q:410:PRO:O	8:q:415:THR:OG1	2.16	0.62
10:K:331:ALA:N	10:K:332:PRO:HD3	2.15	0.62
5:G:446:VAL:HA	5:G:449:ARG:HD3	1.80	0.62
10:K:147:ARG:HD3	10:K:296:ASN:OD1	2.00	0.62
6:h:157:LYS:HD3	6:h:491:PHE:HB3	1.82	0.62
8:q:328:VAL:HG12	8:q:347:CYS:SG	2.40	0.62
5:g:128:LYS:NZ	5:g:433:GLU:OE1	2.32	0.62
8:q:314:ARG:NH2	8:q:316:ASN:OD1	2.32	0.62
10:K:285:CYS:HB3	10:K:289:ILE:HD11	1.82	0.62
2:b:219:LEU:HB2	2:b:372:THR:HG21	1.82	0.62
1:a:289:THR:HG23	1:a:316:LEU:HD22	1.81	0.61
6:h:335:ASN:ND2	8:q:273:GLU:OE1	2.33	0.61
2:b:13:LYS:HE2	4:e:82:ASP:OD1	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:601:ADP:O2B	14:b:603:AF3:F3	2.08	0.61
7:n:38:ARG:HG3	7:n:48:VAL:CG2	2.30	0.61
10:K:371:HIS:CE1	10:K:373:LYS:HA	2.35	0.61
11:P:196:TRP:CD1	11:P:210:GLU:HB2	2.34	0.61
3:D:287:VAL:HG21	3:D:316:PHE:HB3	1.83	0.61
5:G:45:SER:O	9:Z:117:ARG:NH2	2.30	0.61
8:Q:270:LYS:O	8:Q:274:ASN:ND2	2.26	0.61
8:Q:328:VAL:HG12	8:Q:347:CYS:SG	2.40	0.61
5:g:130:LEU:HB2	5:g:510:VAL:HG11	1.82	0.61
6:h:494:GLU:OE1	6:h:499:ARG:NH2	2.34	0.61
5:g:155:ILE:HG21	5:g:401:VAL:HG21	1.82	0.61
8:Q:190:ILE:HG22	8:Q:191:PHE:H	1.65	0.61
2:b:255:ARG:HD3	4:e:265:LYS:HD2	1.83	0.61
5:g:203:LYS:NZ	5:g:388:GLU:OE1	2.30	0.61
10:K:285:CYS:O	10:K:290:ARG:NH2	2.30	0.61
8:Q:466:LYS:NZ	8:Q:487:PRO:O	2.31	0.61
9:Z:47:LEU:HD13	9:Z:66:GLU:HB2	1.81	0.61
2:B:11:ILE:HD11	4:E:40:ALA:HA	1.83	0.61
2:B:112:GLU:HB3	2:B:438:SER:HB3	1.83	0.61
8:Q:151:ALA:HB3	8:Q:406:LYS:HE2	1.80	0.61
5:g:41:LEU:O	5:g:454:ASN:ND2	2.31	0.61
7:N:39:GLN:NE2	7:N:43:LYS:O	2.34	0.61
1:a:533:LEU:HD12	3:d:63:ASP:HA	1.83	0.61
3:d:423:ALA:HB1	3:d:503:ILE:HD11	1.82	0.61
6:h:166:LYS:NZ	14:h:603:AF3:F1	2.23	0.61
8:q:190:ILE:HG22	8:q:191:PHE:H	1.65	0.61
1:A:11:ARG:NH2	1:A:529:ASP:OD2	2.33	0.61
1:A:203:ARG:HA	5:G:504:GLN:HE22	1.65	0.61
2:B:91:GLN:HG3	2:B:102:VAL:HG11	1.82	0.61
11:P:126:LEU:HG	11:P:187:MET:HE2	1.83	0.61
8:Q:410:PRO:O	8:Q:415:THR:OG1	2.18	0.60
6:H:292:LYS:HB2	6:H:319:LEU:HD12	1.82	0.60
1:a:319:ILE:O	1:a:323:SER:OG	2.18	0.60
10:K:68:LYS:NZ	10:K:72:GLU:OE1	2.30	0.60
1:A:132:ILE:HD11	1:A:419:LEU:HD11	1.83	0.60
3:D:171:LEU:O	3:D:177:SER:OG	2.18	0.60
5:G:468:ALA:O	5:G:471:THR:OG1	2.18	0.60
1:A:353:GLN:O	5:G:190:ARG:NH2	2.33	0.60
5:G:393:ASP:OD1	15:G:701:HOH:O	2.16	0.60
1:a:377:LEU:HD21	1:a:392:LEU:HD22	1.82	0.60
2:b:11:ILE:HD11	4:e:40:ALA:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:307:PRO:HG2	10:K:309:ILE:HG22	1.84	0.60
11:P:89:ASN:HB3	11:P:142:PRO:HB2	1.84	0.60
4:E:25:LYS:HG3	4:E:536:PRO:HA	1.84	0.60
5:g:223:ASP:OD1	5:g:231:ARG:NH1	2.34	0.60
7:n:69:ILE:HB	7:n:80:LEU:HD13	1.83	0.60
1:a:266:ARG:HG3	3:d:269:TYR:HB2	1.83	0.60
1:A:220:VAL:HB	1:A:225:MET:HE3	1.84	0.60
1:a:333:ASN:HD22	1:a:339:THR:HG22	1.67	0.60
10:K:367:PRO:HA	10:K:370:VAL:HG13	1.84	0.60
3:D:214:LEU:O	3:D:391:ARG:NH1	2.35	0.60
4:E:236:HIS:HB3	4:E:239:MET:HG3	1.83	0.59
4:E:255:PHE:HB2	4:E:306:PHE:HB3	1.84	0.59
5:G:283:ILE:HD13	5:G:307:ALA:HB2	1.84	0.59
1:a:317:LYS:HA	1:a:327:ILE:HD11	1.83	0.59
9:z:418:MET:HE3	9:z:444:LEU:HD13	1.84	0.59
5:G:155:ILE:HG21	5:G:401:VAL:HG21	1.83	0.59
2:B:189:ARG:NH2	2:B:370:ALA:O	2.35	0.59
12:Z:601:ADP:O1B	14:Z:603:AF3:F1	2.10	0.59
1:A:111:LYS:NZ	6:h:455:PHE:O	2.29	0.59
3:D:155:VAL:HG21	3:D:162:THR:HG21	1.83	0.59
5:G:8:LEU:HD22	4:e:9[B]:PHE:HD2	1.68	0.59
8:Q:253:THR:HG1	9:Z:239:TYR:HH	1.48	0.59
4:e:426:GLU:OE2	4:e:513:LYS:NZ	2.25	0.59
6:h:292:LYS:HB2	6:h:319:LEU:HD12	1.83	0.59
1:a:411:GLY:O	1:a:498:ASN:ND2	2.29	0.59
3:d:235:ASN:ND2	3:d:322:ILE:O	2.36	0.59
9:z:188:LEU:HD11	9:z:399:LYS:HD2	1.85	0.59
11:P:85:THR:O	11:P:89:ASN:ND2	2.34	0.59
8:Q:536:PRO:HB3	10:K:355:MET:HG2	1.83	0.59
2:b:40:LYS:O	2:b:41:SER:OG	2.15	0.59
6:h:280:LYS:NZ	6:h:335:ASN:OD1	2.31	0.59
9:z:103:LEU:HD21	9:z:515:ILE:HG21	1.85	0.59
1:a:203:ARG:HA	5:g:504:GLN:HE22	1.68	0.58
2:b:408:TYR:O	2:b:413:SER:OG	2.20	0.58
11:P:92:GLY:HA2	11:P:142:PRO:HA	1.84	0.58
9:Z:132:GLN:O	9:Z:135:GLU:HG3	2.04	0.58
1:a:526:ARG:HD3	3:d:58:ASP:OD2	2.03	0.58
10:K:185:LEU:HD23	10:K:213:LYS:HE2	1.84	0.58
2:B:20:ARG:NH2	3:d:28:ASP:OD2	2.37	0.58
2:B:250:LYS:NZ	4:E:309:GLU:OE1	2.36	0.58
3:D:214:LEU:HD12	3:D:398:ILE:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:445:GLN:HE21	4:e:449:ARG:HH12	1.51	0.58
3:D:78:LEU:HB3	3:D:92:VAL:HG22	1.85	0.58
6:H:166:LYS:NZ	14:H:603:AF3:F1	2.27	0.58
4:e:535:LYS:HA	6:h:50:VAL:HB	1.86	0.58
2:b:167:LEU:HD22	2:b:172:LEU:HD12	1.86	0.58
4:e:236:HIS:HB3	4:e:239:MET:HG3	1.84	0.58
6:H:93:GLY:O	6:H:97:VAL:HG23	2.04	0.58
10:K:362:TYR:HA	10:K:369:ILE:HG21	1.86	0.58
4:E:101:GLU:OE1	6:H:375:ARG:NH2	2.37	0.57
9:Z:189:PHE:O	9:Z:323:ARG:NH2	2.36	0.57
2:b:285:HIS:HE1	2:b:335:PHE:HB3	1.67	0.57
6:h:32:ILE:HG13	6:h:76:ALA:HB1	1.84	0.57
6:h:391:ASP:OD1	15:h:701:HOH:O	2.17	0.57
9:z:132:GLN:O	9:z:135:GLU:HG3	2.04	0.57
5:G:182:MET:HE3	5:G:369:PRO:HG2	1.86	0.57
4:e:185:MET:HE1	4:e:222:THR:HB	1.86	0.57
5:g:289:VAL:HG21	5:g:350:LEU:HD13	1.86	0.57
8:q:55:MET:HG2	8:q:65:VAL:HG22	1.87	0.57
9:z:24:ILE:HD13	9:z:107:ASP:HB2	1.86	0.57
2:B:285:HIS:HE1	2:B:335:PHE:HB3	1.70	0.57
9:z:37:ASN:OD1	9:z:45:LYS:NZ	2.21	0.57
9:z:459:LEU:H	9:z:459:LEU:HD12	1.68	0.57
2:B:13:LYS:HE2	4:E:82:ASP:OD1	2.05	0.57
5:G:319:ASP:OD1	5:G:322:ARG:NH1	2.37	0.57
9:Z:459:LEU:HD12	9:Z:459:LEU:H	1.70	0.57
9:z:150:ASP:O	9:z:154:THR:HG23	2.04	0.57
4:E:255:PHE:HB2	4:E:306:PHE:CB	2.34	0.57
4:E:293:LYS:HD2	4:E:317:ASN:HB3	1.85	0.57
3:D:38:ILE:HG21	3:D:121:THR:OG1	2.05	0.57
2:B:86:ASP:OD1	2:B:89:ARG:NH2	2.29	0.57
3:D:125:GLN:NE2	4:e:118:GLU:OE2	2.32	0.57
5:g:319:ASP:OD1	5:g:322:ARG:NH1	2.37	0.57
8:Q:219:HIS:NE2	8:Q:368:GLU:OE1	2.37	0.57
2:b:187:VAL:HG21	2:b:397:LEU:HB2	1.87	0.57
7:n:19:ARG:HA	7:n:80:LEU:O	2.05	0.57
4:E:9[C]:PHE:O	4:E:16:PHE:HB2	2.04	0.56
5:G:132:ASP:OD2	5:G:437:TYR:OH	2.21	0.56
2:b:162:ILE:HD13	2:b:400:THR:HG21	1.87	0.56
5:g:470:HIS:NE2	5:g:478:TRP:O	2.30	0.56
4:e:132:ARG:NH1	4:e:443:LEU:HD23	2.19	0.56
8:q:253:THR:HG22	8:q:254:LYS:N	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LEU:HD23	2:B:18:GLU:HG3	1.87	0.56
4:E:175:SER:OG	12:E:601:ADP:O1A	2.11	0.56
6:H:89:GLU:OE1	8:Q:378:ARG:NH2	2.38	0.56
6:H:167:LEU:H	6:H:167:LEU:HD23	1.69	0.56
9:Z:418:MET:HE3	9:Z:444:LEU:HD13	1.86	0.56
2:b:121:ILE:HG12	2:b:431:LYS:HD3	1.86	0.56
2:b:353:MET:SD	2:b:358:LYS:HG3	2.45	0.56
2:b:18:GLU:OE2	2:b:519:ASN:ND2	2.38	0.56
6:h:21:GLN:OE1	6:h:25:ASN:ND2	2.34	0.56
7:n:63:VAL:HG22	7:n:67:PHE:HE1	1.70	0.56
8:q:157:ILE:HG13	8:q:188:VAL:HG21	1.87	0.56
4:E:404:ASP:OD1	15:E:701:HOH:O	2.18	0.56
4:E:426:GLU:OE1	4:E:426:GLU:N	2.33	0.56
8:Q:225:LYS:NZ	8:Q:314:ARG:O	2.39	0.56
9:z:47:LEU:HD13	9:z:66:GLU:HB2	1.88	0.56
8:q:466:LYS:NZ	8:q:487:PRO:O	2.37	0.56
10:K:12:ASN:HD21	10:K:86:TRP:HZ2	1.53	0.56
11:P:194:LEU:O	11:P:198:LEU:HG	2.06	0.56
7:n:31:ILE:O	7:n:71:ARG:NH2	2.34	0.56
1:A:377:LEU:HD21	1:A:392:LEU:HD22	1.87	0.56
2:B:50:LYS:HD2	3:D:534:ASP:HB3	1.88	0.56
2:B:51:ILE:HD12	3:D:535:VAL:HG22	1.88	0.56
6:H:97:VAL:HG22	6:H:502:ALA:HA	1.87	0.56
1:a:11:ARG:NH2	1:a:529:ASP:OD2	2.38	0.56
3:d:210:ILE:HG21	3:d:402:GLU:HG3	1.88	0.56
4:e:432:ALA:O	4:e:436:GLU:HG2	2.06	0.56
10:K:332:PRO:N	10:K:333:PRO:CD	2.67	0.56
8:Q:533:PRO:O	10:K:169:TYR:CE2	2.59	0.55
6:H:22:LEU:HD22	6:H:112:VAL:HG11	1.89	0.55
6:h:30:GLN:NE2	6:h:102:ALA:O	2.28	0.55
2:b:47:GLY:O	3:d:531:LYS:NZ	2.39	0.55
2:B:353:MET:SD	2:B:358:LYS:HG3	2.47	0.55
5:G:59:MET:HE3	9:Z:514:ASN:HB3	1.88	0.55
4:e:63:ASP:OD1	4:e:67:ASP:N	2.39	0.55
1:A:203:ARG:HE	1:A:207:GLU:HG2	1.71	0.55
6:h:178:MET:HE2	6:h:372:PHE:HE1	1.70	0.55
8:q:280:VAL:HG21	8:q:304:TYR:CB	2.34	0.55
8:Q:60:LEU:HB3	10:K:288:ASP:HB3	1.87	0.55
1:a:266:ARG:HB2	3:d:272:MET:HE3	1.88	0.55
3:d:415:LEU:HD13	3:d:511:PRO:HB3	1.88	0.55
3:d:534:ASP:OD1	3:d:535:VAL:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:z:15:ARG:H	9:z:15:ARG:NH2	2.04	0.55
4:E:93:GLU:OE1	6:H:201:GLN:NE2	2.40	0.55
8:Q:533:PRO:O	10:K:169:TYR:HE2	1.90	0.55
6:H:153:LYS:O	6:H:157:LYS:HG3	2.07	0.55
2:b:79:PRO:HB2	4:e:60:MET:SD	2.46	0.55
6:h:73:HIS:HB3	6:h:76:ALA:HB3	1.89	0.55
5:G:8:LEU:HD21	4:e:9[B]:PHE:CD2	2.42	0.55
6:H:169:SER:HA	6:H:172:LYS:HB3	1.89	0.55
6:H:241:ASN:HB3	6:H:332:THR:HG22	1.87	0.55
2:b:509:GLU:O	2:b:513:VAL:HG13	2.07	0.55
3:d:46:ASP:HA	3:d:49:ARG:HD3	1.88	0.55
6:h:219:THR:O	6:h:219:THR:OG1	2.25	0.55
12:q:601:ADP:O1B	14:q:603:AF3:F1	2.15	0.55
9:z:84:GLN:HE21	9:z:91:GLY:HA3	1.72	0.55
8:Q:168:ILE:HD13	8:Q:179:LEU:HB2	1.89	0.54
11:P:126:LEU:HD12	11:P:126:LEU:H	1.72	0.54
3:D:430:ILE:HG12	3:D:462:PRO:HG2	1.89	0.54
12:Q:601:ADP:O1B	14:Q:603:AF3:F1	2.15	0.54
6:h:167:LEU:H	6:h:167:LEU:HD23	1.71	0.54
1:A:228:ARG:HG3	1:A:352:VAL:HG13	1.88	0.54
5:G:520:ASP:OD1	5:G:521:ASP:N	2.34	0.54
8:Q:136:CYS:HB2	8:Q:512:THR:HG21	1.89	0.54
3:d:375:LYS:HE3	3:d:377:THR:HG22	1.89	0.54
8:q:190:ILE:HG22	8:q:191:PHE:N	2.22	0.54
11:P:82:TRP:CD1	11:P:86:LYS:HD2	2.43	0.54
1:A:217:ASN:ND2	10:K:54:VAL:HA	2.22	0.54
3:D:55:LYS:HG3	3:D:469:ALA:HA	1.88	0.54
8:Q:55:MET:HG2	8:Q:65:VAL:HG22	1.88	0.54
9:Z:103:LEU:HD21	9:Z:515:ILE:HG21	1.89	0.54
9:Z:150:ASP:O	9:Z:154:THR:HG23	2.06	0.54
8:q:286:THR:HG21	8:q:338:PRO:HB2	1.88	0.54
9:z:14:ALA:O	9:z:520:GLU:HA	2.08	0.54
10:K:111:ASN:HD21	10:K:115:ASN:HB2	1.73	0.54
10:K:294:TYR:HB3	10:K:327:ILE:HG22	1.89	0.54
5:g:179:ALA:O	5:g:183:VAL:HG23	2.08	0.54
2:B:408:TYR:O	2:B:413:SER:OG	2.21	0.54
5:G:8:LEU:HD22	4:e:9[B]:PHE:CD2	2.42	0.54
9:Z:279:ARG:NH1	9:Z:308:GLU:OE2	2.32	0.54
4:e:248:ILE:HD12	4:e:337:THR:HG21	1.90	0.54
5:g:43:PRO:HG3	12:g:601:ADP:C6	2.43	0.54
6:h:241:ASN:HB3	6:h:332:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:601:ADP:O3B	14:E:603:AF3:F3	2.15	0.54
2:b:519:ASN:HB3	4:e:59:LYS:HD3	1.89	0.54
10:K:262:PHE:CE2	10:K:313:MET:HG2	2.42	0.54
2:B:117:ILE:HD11	2:B:123:PRO:HB3	1.90	0.54
12:d:601:ADP:O2B	14:d:603:AF3:F1	2.15	0.54
5:g:203:LYS:HB2	5:g:384:LEU:HD13	1.90	0.54
7:N:19:ARG:HA	7:N:80:LEU:O	2.08	0.54
8:Q:62:LYS:HB2	10:K:288:ASP:OD2	2.08	0.54
10:K:314:GLN:O	10:K:327:ILE:HD11	2.07	0.54
1:A:28:ILE:HA	1:A:31:ILE:HD12	1.90	0.53
2:B:162:ILE:HD13	2:B:400:THR:HG21	1.88	0.53
3:D:193:LYS:NZ	3:D:225:GLU:OE2	2.41	0.53
9:z:172:VAL:HG13	9:z:395:LEU:HD23	1.89	0.53
1:A:359:ASP:HB3	10:K:54:VAL:HG12	1.89	0.53
6:H:236:LYS:HG2	6:H:344:ARG:HE	1.73	0.53
1:a:132:ILE:HD11	1:a:419:LEU:HD11	1.89	0.53
3:d:304:ILE:HD12	3:d:305:LEU:HD13	1.90	0.53
6:h:97:VAL:HG22	6:h:502:ALA:HA	1.88	0.53
10:K:278:THR:HG21	10:K:313:MET:HE1	1.90	0.53
11:P:68:GLU:HA	11:P:71:ILE:HD12	1.89	0.53
12:B:601:ADP:O2B	14:B:603:AF3:F3	2.16	0.53
3:D:439:TYR:O	3:D:443:LEU:HG	2.08	0.53
4:E:73:ASP:OD1	14:E:603:AF3:F2	2.17	0.53
9:Z:93:THR:HB	12:Z:601:ADP:O2B	2.08	0.53
4:E:63:ASP:OD1	4:E:67:ASP:N	2.41	0.53
6:H:455:PHE:O	1:a:111:LYS:NZ	2.38	0.53
10:K:124:PHE:CZ	10:K:132:MET:HG2	2.43	0.53
1:a:299:TYR:OH	5:g:334:ARG:NH1	2.42	0.53
2:b:112:GLU:HB3	2:b:438:SER:HB3	1.89	0.53
8:q:418:GLU:OE1	8:q:471:HIS:ND1	2.33	0.53
1:A:268:SER:HB2	1:A:295:MET:SD	2.49	0.53
2:B:509:GLU:O	2:B:513:VAL:HG13	2.08	0.53
4:E:78:LEU:HB3	4:E:92:VAL:HG22	1.89	0.53
8:Q:190:ILE:HG22	8:Q:191:PHE:N	2.22	0.53
1:A:317:LYS:HA	1:A:327:ILE:HD11	1.90	0.53
5:G:133:MET:HE2	5:G:444:LEU:HD11	1.89	0.53
6:H:66:LEU:HD11	6:H:98:THR:HG21	1.91	0.53
6:H:157:LYS:HD3	6:H:491:PHE:HB3	1.90	0.53
2:b:101:SER:N	12:b:601:ADP:O3B	2.35	0.53
4:e:145:ILE:HG23	4:e:514:LYS:HD2	1.90	0.53
2:B:381:GLN:HE22	3:D:93:GLU:HG3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:z:189:PHE:O	9:z:323:ARG:NH2	2.41	0.53
2:B:162:ILE:HG13	2:B:494:THR:HG23	1.91	0.53
2:B:519:ASN:HB3	4:E:59:LYS:HD3	1.91	0.53
6:h:10:LYS:HE3	6:h:523:PRO:HG2	1.91	0.53
10:K:153:MET:HB3	10:K:299:LEU:HD22	1.90	0.53
5:G:289:VAL:HG21	5:G:350:LEU:HD13	1.91	0.53
6:H:10:LYS:O	6:H:13:THR:OG1	2.26	0.53
2:b:480:MET:HG3	12:b:601:ADP:C2	2.44	0.53
4:e:344:ARG:NE	4:e:347:GLU:OE2	2.38	0.53
5:g:468:ALA:O	5:g:471:THR:OG1	2.26	0.53
9:z:455:SER:OG	9:z:481:LEU:O	2.27	0.53
10:K:117:GLU:CD	10:K:367:PRO:HB3	2.34	0.53
9:Z:319:ARG:HG3	10:K:364:GLU:HA	1.91	0.52
1:a:426:TYR:OH	1:a:430:MET:HE2	2.09	0.52
2:b:52:LEU:HB2	2:b:62:MET:HB2	1.91	0.52
4:e:426:GLU:OE1	4:e:426:GLU:N	2.36	0.52
5:g:144:VAL:HG21	5:g:407:LEU:HD22	1.90	0.52
1:A:54:ILE:HD13	5:G:519:ILE:HD11	1.92	0.52
3:D:476:THR:HG22	3:D:500:ILE:HD11	1.91	0.52
2:b:65:ASN:O	2:b:65:ASN:ND2	2.42	0.52
10:K:312:ARG:HE	10:K:316:GLU:CD	2.18	0.52
6:H:219:THR:O	6:H:219:THR:OG1	2.25	0.52
5:g:80:MET:HA	5:g:83:ILE:HD12	1.91	0.52
8:q:416:GLU:OE2	8:q:416:GLU:N	2.40	0.52
9:z:164:LEU:HD21	9:z:387:ILE:HG12	1.91	0.52
9:Z:455:SER:OG	9:Z:481:LEU:O	2.27	0.52
6:h:171:GLN:O	6:h:174:PHE:HB3	2.10	0.52
2:B:65:ASN:O	2:B:65:ASN:ND2	2.43	0.52
2:B:176:LYS:O	2:B:180:THR:OG1	2.26	0.52
8:Q:253:THR:HG22	8:Q:254:LYS:N	2.23	0.52
8:Q:280:VAL:HG21	8:Q:304:TYR:CB	2.39	0.52
2:b:218:PHE:HB2	2:b:326:VAL:HG21	1.91	0.52
4:E:10:ASP:HB2	4:E:14:ARG:O	2.09	0.52
5:G:445:GLU:OE2	5:G:467:ARG:NH2	2.33	0.52
6:H:394:MET:O	6:H:398:ARG:HG2	2.10	0.52
8:Q:253:THR:OG1	9:Z:239:TYR:OH	2.23	0.52
2:b:86:ASP:OD1	2:b:89:ARG:NH2	2.36	0.52
2:B:251:ILE:HG13	4:E:277:LEU:HD11	1.90	0.52
6:h:93:GLY:O	6:h:97:VAL:HG23	2.08	0.52
3:D:439:TYR:CE2	3:D:443:LEU:HD11	2.45	0.52
6:H:236:LYS:HE2	6:H:342:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:526:THR:HB	11:P:2:GLN:NE2	2.25	0.52
7:N:18:LEU:HD13	7:N:20:LEU:HD13	1.91	0.52
8:Q:364:LYS:NZ	8:Q:366:GLU:OE2	2.33	0.52
4:e:65:ASP:OD1	4:e:65:ASP:N	2.43	0.52
4:e:255:PHE:HB2	4:e:306:PHE:CB	2.40	0.52
12:e:601:ADP:O3B	14:e:603:AF3:F3	2.17	0.52
4:e:206:PHE:HD1	4:e:209:ILE:HD12	1.75	0.52
6:h:66:LEU:HD11	6:h:98:THR:HG21	1.91	0.52
7:n:38:ARG:HG3	7:n:48:VAL:HG22	1.92	0.52
9:z:313:LEU:HD11	9:z:361:THR:HG21	1.92	0.52
1:A:319:ILE:O	1:A:323:SER:OG	2.21	0.51
5:g:27:ILE:HG21	5:g:110:GLU:HB2	1.92	0.51
6:h:10:LYS:O	6:h:13:THR:OG1	2.26	0.51
1:A:254:ILE:HG13	1:A:260:LEU:HD13	1.93	0.51
8:Q:284:ALA:HB2	8:Q:310:ILE:HD11	1.91	0.51
9:Z:37:ASN:HD21	9:Z:63:LEU:HD22	1.74	0.51
5:g:416:MET:SD	5:g:445:GLU:HG2	2.51	0.51
11:P:48:TYR:CG	11:P:71:ILE:HG12	2.46	0.51
1:A:424:GLU:OE1	1:A:468:ARG:NH2	2.30	0.51
2:B:40:LYS:O	2:B:41:SER:OG	2.14	0.51
4:E:432:ALA:O	4:E:436:GLU:HG2	2.11	0.51
10:K:309:ILE:HD11	10:K:313:MET:HG3	1.92	0.51
1:A:536:GLU:HG2	1:A:537:SER:N	2.25	0.51
1:a:5:LEU:HB3	1:a:7:VAL:HG23	1.91	0.51
1:a:447:VAL:O	1:a:451:THR:OG1	2.23	0.51
4:e:35:LYS:O	4:e:39:MET:HG3	2.10	0.51
7:n:63:VAL:HG22	7:n:67:PHE:CE1	2.46	0.51
10:K:178:LEU:HD22	10:K:277:THR:HG21	1.92	0.51
4:E:18:ILE:HA	6:H:73:HIS:HB2	1.92	0.51
8:Q:70:ALA:HB2	8:Q:101:THR:HG21	1.92	0.51
1:a:277:LYS:NZ	1:a:338:GLU:HG2	2.26	0.51
2:b:242:THR:HG21	2:b:335:PHE:CE2	2.44	0.51
5:g:11:SER:O	5:g:14:THR:OG1	2.29	0.51
8:q:394:ASP:OD1	15:q:701:HOH:O	2.19	0.51
10:K:275:HIS:H	10:K:275:HIS:CD2	2.27	0.51
5:G:130:LEU:HB2	5:G:510:VAL:HG11	1.92	0.51
4:e:34:LEU:HD21	4:e:528:LEU:HA	1.92	0.51
3:D:32:GLN:HB3	2:b:6:LEU:HD23	1.92	0.51
8:q:532:GLY:HA3	9:z:51:ALA:HA	1.93	0.51
5:G:8:LEU:CD2	4:e:9[B]:PHE:HD2	2.19	0.51
6:H:185:MET:HE1	6:H:212:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:200:SER:OG	9:Z:203:ASP:OD2	2.25	0.51
3:D:26:ASP:OD1	3:D:26:ASP:N	2.43	0.51
8:Q:411:GLY:O	8:Q:492:MET:HG3	2.11	0.51
2:b:293:ARG:HA	2:b:315:ALA:O	2.11	0.51
3:d:248:LEU:HD21	3:d:333:ILE:HG23	1.92	0.51
4:e:472:GLN:O	4:e:476:GLU:HG2	2.11	0.51
7:n:28:PHE:HA	7:n:100:ASN:HD21	1.76	0.51
2:B:101:SER:N	12:B:601:ADP:O3B	2.40	0.51
5:G:204:ILE:HG21	5:G:355:ILE:HG21	1.92	0.51
1:a:216:LEU:HD11	1:a:319:ILE:HD11	1.93	0.51
2:b:4:LEU:HD23	2:b:18:GLU:HG3	1.93	0.51
2:b:71:LEU:HB3	2:b:85:VAL:HG22	1.93	0.51
10:K:280:ASN:O	10:K:284:LYS:HG3	2.11	0.51
1:A:411:GLY:O	1:A:498:ASN:ND2	2.34	0.50
2:B:232:ILE:HD13	2:B:288:ASN:HB3	1.91	0.50
8:q:532:GLY:N	8:q:533:PRO:HD3	2.26	0.50
8:Q:173:TYR:OH	8:Q:483:GLU:OE1	2.29	0.50
6:h:153:LYS:O	6:h:157:LYS:HG3	2.10	0.50
7:n:39:GLN:NE2	7:n:43:LYS:O	2.44	0.50
6:H:178:MET:HE2	6:H:372:PHE:HE1	1.76	0.50
4:e:196:VAL:HG12	4:e:381:ARG:O	2.11	0.50
9:Z:28:ARG:HB3	9:Z:28:ARG:HH21	1.75	0.50
7:n:114:GLN:OE1	7:n:115:VAL:N	2.45	0.50
10:K:297:THR:HB	10:K:329:ILE:HG12	1.94	0.50
5:G:414:SER:O	5:G:418:VAL:HG12	2.11	0.50
6:H:73:HIS:HB3	6:H:76:ALA:HB3	1.94	0.50
8:Q:532:GLY:HA3	10:K:351:THR:CG2	2.31	0.50
5:g:215:LEU:HB3	5:g:364:THR:HG22	1.92	0.50
9:z:114:LEU:HD23	9:z:119:ILE:HD11	1.92	0.50
1:A:310:ARG:HB2	10:K:59:GLN:HG3	1.94	0.50
4:E:4:MET:HE1	4:E:23:ASP:O	2.12	0.50
4:E:185:MET:HE1	4:E:222:THR:HB	1.92	0.50
3:d:484:HIS:NE2	3:d:491:ALA:O	2.33	0.50
1:A:440:GLU:O	1:A:444:SER:OG	2.30	0.50
2:B:323:LEU:O	2:B:327:THR:OG1	2.27	0.50
4:E:65:ASP:OD1	4:E:65:ASP:N	2.42	0.50
5:G:207:GLY:O	9:Z:503:GLN:NE2	2.26	0.50
6:H:323:MET:HE1	8:Q:230:ASP:OD2	2.12	0.50
4:e:397:GLU:OE1	4:e:400:ARG:HD2	2.12	0.50
3:D:232:LYS:NZ	3:D:372:LYS:HB2	2.26	0.50
4:E:206:PHE:HD1	4:E:209:ILE:HD12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:222:THR:HA	4:E:386:PHE:O	2.12	0.50
6:H:527:VAL:HG23	6:H:528:ASP:H	1.76	0.50
6:h:318:ASP:OD1	6:h:321:ARG:NH1	2.45	0.50
6:H:88:ALA:HB1	8:Q:357:ASP:HB2	1.93	0.50
8:Q:43:THR:OG1	8:Q:105:LEU:HD23	2.12	0.50
1:a:153:LYS:NZ	1:a:166:ASP:OD1	2.23	0.50
3:d:350:GLN:OE1	3:d:350:GLN:N	2.44	0.50
3:d:520:THR:O	3:d:524:GLU:HG2	2.11	0.50
9:Z:90:ASP:OD1	9:Z:91:GLY:N	2.45	0.49
1:a:229:ILE:HD13	1:a:284:ASN:HB3	1.94	0.49
3:d:240:ARG:NE	3:d:242:GLU:OE2	2.44	0.49
4:e:280:TYR:O	4:e:284:LYS:HG2	2.12	0.49
10:K:31:PHE:CE2	10:K:64:ILE:HG21	2.47	0.49
10:K:282:ILE:HG12	10:K:293:LEU:HB3	1.94	0.49
1:a:268:SER:HB2	1:a:295:MET:SD	2.52	0.49
2:b:38:LEU:O	2:b:50:LYS:NZ	2.39	0.49
3:d:73:ASP:OD1	14:d:603:AF3:F2	2.19	0.49
5:g:447:ILE:HB	5:g:448:PRO:HD3	1.93	0.49
4:E:263:LYS:HD2	6:H:254:GLU:HG2	1.95	0.49
1:a:155:SER:HB3	1:a:398:VAL:HG21	1.93	0.49
1:a:489:ASP:OD2	1:a:492:ASN:ND2	2.39	0.49
2:b:122:HIS:CD2	2:b:124:GLN:HB2	2.48	0.49
3:d:27:ARG:HH11	3:d:27:ARG:HG3	1.78	0.49
3:d:42:LYS:HG2	3:d:118:ASP:OD2	2.12	0.49
6:h:447:ARG:HB2	6:h:461:LEU:HD11	1.94	0.49
9:z:30:LEU:HD11	9:z:74:ALA:HA	1.94	0.49
10:K:155:SER:O	10:K:303:THR:HB	2.12	0.49
2:B:242:THR:HG21	2:B:335:PHE:CE2	2.47	0.49
6:H:32:ILE:HG13	6:H:76:ALA:HB1	1.93	0.49
9:Z:66:GLU:O	9:Z:68:GLN:NE2	2.46	0.49
9:Z:169:THR:O	9:Z:173:VAL:HG12	2.13	0.49
5:g:449:ARG:HB2	5:g:463:LEU:HD11	1.93	0.49
9:z:93:THR:HB	12:z:601:ADP:O2B	2.12	0.49
3:D:94:LEU:HD13	3:D:525:THR:OG1	2.12	0.49
9:Z:172:VAL:HG13	9:Z:395:LEU:HD23	1.95	0.49
5:g:182:MET:HE3	5:g:369:PRO:HG2	1.95	0.49
6:h:46:ASP:OD1	6:h:60:ASN:HB2	2.13	0.49
2:B:18:GLU:OE2	2:B:519:ASN:ND2	2.46	0.49
6:H:494:GLU:OE1	6:H:499:ARG:NH2	2.45	0.49
8:Q:18:GLY:HA3	8:Q:528:LYS:HG3	1.95	0.49
8:Q:275:LEU:HD21	9:Z:257:GLU:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:297:LEU:O	1:a:301:VAL:HG23	2.12	0.49
5:G:8:LEU:HD21	4:e:9[A]:PHE:CD2	2.46	0.49
7:N:63:VAL:HG22	7:N:67:PHE:CE1	2.48	0.49
3:d:30:PRO:HB3	3:d:533:ASP:HB2	1.94	0.49
4:e:196:VAL:O	4:e:196:VAL:HG23	2.13	0.49
4:e:222:THR:HA	4:e:386:PHE:O	2.12	0.49
6:h:236:LYS:HG2	6:h:344:ARG:HE	1.77	0.49
8:q:416:GLU:HG2	8:q:448:ILE:HG13	1.94	0.49
9:z:169:THR:O	9:z:173:VAL:HG12	2.12	0.49
9:z:453:GLN:OE1	9:z:459:LEU:HD11	2.12	0.49
1:A:492:ASN:HB2	1:A:494:LYS:HG2	1.94	0.49
2:B:189:ARG:O	2:B:369:GLU:HA	2.13	0.49
7:N:19:ARG:HB2	7:N:81:GLN:NE2	2.27	0.49
8:Q:416:GLU:OE2	8:Q:416:GLU:N	2.42	0.49
1:A:489:ASP:HB3	1:A:494:LYS:O	2.13	0.49
5:g:292:THR:HG22	5:g:294:LYS:H	1.78	0.49
4:E:529:LYS:HB3	6:H:46:ASP:OD2	2.12	0.49
5:G:423:THR:O	5:G:426:SER:OG	2.28	0.49
9:Z:47:LEU:HD13	9:Z:66:GLU:CB	2.43	0.49
1:a:254:ILE:HG13	1:a:260:LEU:HD13	1.94	0.49
5:g:256:ILE:HB	9:z:246:SER:HA	1.94	0.49
10:K:31:PHE:HZ	10:K:88:HIS:HD2	1.61	0.49
2:B:79:PRO:HB2	4:E:60:MET:SD	2.52	0.48
3:D:53:GLY:CA	12:D:601:ADP:H5'2	2.39	0.48
4:E:35:LYS:O	4:E:39:MET:HG3	2.12	0.48
4:E:37:HIS:NE2	4:E:533:ILE:HD11	2.28	0.48
4:e:196:VAL:HG21	4:e:209:ILE:HG13	1.95	0.48
6:h:168:ILE:HG21	6:h:385:THR:HG23	1.94	0.48
1:A:247:LYS:NZ	3:D:279:GLU:OE1	2.42	0.48
1:A:292:ILE:O	1:A:309:ARG:NH1	2.46	0.48
3:D:432:LEU:HD13	3:D:458:MET:HE2	1.94	0.48
4:E:518:SER:O	4:E:522:GLN:HG2	2.13	0.48
1:a:263:ILE:HG23	3:d:272:MET:HE1	1.96	0.48
2:b:3:SER:O	2:b:7:ALA:HB2	2.14	0.48
3:d:223:LEU:HD12	3:d:388:ILE:HG12	1.94	0.48
9:z:196:MET:HE2	9:z:355:LEU:HD12	1.95	0.48
11:P:130:ILE:HD11	11:P:184:PHE:HD2	1.78	0.48
1:A:361:LEU:HD23	10:K:54:VAL:HG22	1.95	0.48
4:E:196:VAL:O	4:E:196:VAL:HG23	2.13	0.48
4:E:472:GLN:O	4:E:476:GLU:HG2	2.13	0.48
6:H:30:GLN:NE2	6:H:102:ALA:O	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:109:VAL:HG13	4:e:516:GLN:HG2	1.95	0.48
10:K:152:VAL:HA	10:K:298:VAL:O	2.13	0.48
6:H:521:LYS:HG2	8:Q:57:ILE:HD12	1.93	0.48
8:Q:348:ASP:CB	8:Q:366:GLU:HG2	2.43	0.48
3:d:228:VAL:HG11	3:d:373:LEU:HD13	1.95	0.48
4:e:293:LYS:HD2	4:e:317:ASN:HB3	1.96	0.48
9:z:179:ILE:HD13	9:z:191:ILE:HG13	1.95	0.48
9:z:418:MET:HE1	9:z:505:LEU:HD21	1.94	0.48
11:P:120:TYR:O	11:P:150:ILE:HA	2.13	0.48
1:A:12:SER:HB3	1:A:17:ILE:HB	1.96	0.48
9:Z:24:ILE:HD13	9:Z:107:ASP:HB2	1.95	0.48
4:e:168:THR:HG23	4:e:507:ILE:HG22	1.95	0.48
8:q:136:CYS:HB2	8:q:512:THR:HG21	1.96	0.48
1:A:355:ARG:NH2	1:A:358:ASP:HA	2.28	0.48
4:E:422:GLY:HA2	12:E:601:ADP:N3	2.29	0.48
6:H:46:ASP:OD1	6:H:60:ASN:HB2	2.13	0.48
6:H:522:ASN:HD22	8:Q:58:ASN:HA	1.78	0.48
9:Z:2:ALA:HB1	9:Z:15:ARG:HH21	1.77	0.48
9:Z:43:THR:O	9:Z:45:LYS:NZ	2.45	0.48
11:P:121:LYS:HD2	11:P:163:LEU:HD12	1.94	0.48
4:E:132:ARG:HH12	4:E:443:LEU:HD23	1.78	0.48
5:G:449:ARG:CG	5:G:463:LEU:HD11	2.40	0.48
8:Q:324:LEU:O	8:Q:328:VAL:HG22	2.14	0.48
8:Q:460:ALA:H	5:g:116:GLN:HE22	1.60	0.48
1:a:68:GLU:OE2	5:g:11:SER:HA	2.13	0.48
1:a:230:VAL:HG23	1:a:231:ASN:H	1.78	0.48
8:q:43:THR:OG1	8:q:105:LEU:HD23	2.12	0.48
8:q:269:SER:O	8:q:273:GLU:HG2	2.13	0.48
10:K:156:GLY:O	10:K:303:THR:OG1	2.18	0.48
2:B:17:ASP:OD1	2:B:522:LYS:HB2	2.13	0.48
3:D:291:LYS:HD3	3:D:322:ILE:HD11	1.95	0.48
3:D:407:ASP:OD1	15:D:701:HOH:O	2.20	0.48
5:G:83:ILE:HD13	5:G:512:THR:HG21	1.96	0.48
5:G:415:GLU:OE1	5:G:415:GLU:N	2.44	0.48
9:Z:425:HIS:O	9:Z:428:SER:OG	2.32	0.48
9:Z:453:GLN:OE1	9:Z:459:LEU:HD11	2.14	0.48
1:a:492:ASN:HB2	1:a:494:LYS:HG2	1.96	0.48
5:G:383:ILE:O	5:G:387:VAL:HG23	2.14	0.48
2:b:95:VAL:HG12	2:b:399:GLN:HG3	1.95	0.48
2:b:323:LEU:HA	2:b:326:VAL:HG12	1.94	0.48
3:d:164:LEU:O	3:d:168:THR:OG1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:412:ILE:O	3:d:416:VAL:HG23	2.14	0.48
6:h:119:GLN:HA	6:h:122:ILE:HG12	1.96	0.48
7:n:19:ARG:HB2	7:n:81:GLN:NE2	2.29	0.48
9:z:47:LEU:HD13	9:z:66:GLU:CB	2.44	0.48
10:K:303:THR:O	10:K:307:PRO:HD2	2.14	0.48
2:B:237:ILE:HD11	2:B:346:CYS:SG	2.54	0.48
2:B:419:HIS:O	2:B:423:GLN:HG2	2.14	0.48
3:D:160:ARG:HG2	3:D:164:LEU:HD23	1.95	0.48
4:E:380:SER:OG	4:E:382:ALA:O	2.31	0.48
4:E:485:MET:O	7:N:30:ARG:HD3	2.13	0.48
8:Q:190:ILE:CG2	8:Q:191:PHE:H	2.27	0.48
8:Q:277:ASP:OD1	8:Q:308:TYR:OH	2.21	0.48
9:Z:188:LEU:HD11	9:Z:399:LYS:HD2	1.96	0.48
1:a:252:VAL:HB	5:g:254:THR:HA	1.95	0.48
1:a:294:ASP:HA	1:a:297:LEU:HD12	1.95	0.48
4:e:272:GLU:CD	4:e:272:GLU:H	2.22	0.48
5:g:415:GLU:OE1	5:g:415:GLU:N	2.46	0.48
8:q:226:GLU:OE2	8:q:359:GLN:NE2	2.47	0.48
1:A:127:GLU:HG3	1:A:426:TYR:CZ	2.48	0.47
6:H:171:GLN:O	6:H:174:PHE:HB3	2.14	0.47
6:H:415:GLU:HG2	6:H:473:THR:HG23	1.96	0.47
7:N:8:GLY:HA3	7:N:20:LEU:HG	1.96	0.47
1:a:254:ILE:HD11	1:a:263:ILE:HD12	1.96	0.47
5:g:488:VAL:HG21	5:g:493:LEU:HD22	1.94	0.47
6:h:508:GLU:OE1	8:q:380:SER:OG	2.30	0.47
2:B:261:THR:HG22	3:D:264:ILE:HD13	1.96	0.47
4:E:292:ILE:O	4:E:295:THR:HG22	2.14	0.47
5:G:79:SER:O	5:G:83:ILE:HG23	2.14	0.47
6:H:398:ARG:HA	6:H:401:LYS:HE2	1.96	0.47
9:Z:92:THR:N	14:Z:603:AF3:F3	2.36	0.47
3:d:446:MET:HA	3:d:449:TYR:HD2	1.79	0.47
4:e:88:ALA:O	4:e:92:VAL:HG23	2.14	0.47
4:e:529:LYS:HB3	6:h:46:ASP:OD2	2.14	0.47
5:g:80:MET:O	5:g:83:ILE:HB	2.14	0.47
3:D:429:GLU:HG2	3:D:461:ILE:HB	1.97	0.47
7:N:50:SER:OG	7:N:58:ASP:OD1	2.22	0.47
8:Q:532:GLY:HA2	10:K:349:LEU:CD1	2.45	0.47
2:b:189:ARG:O	2:b:369:GLU:HA	2.14	0.47
3:d:94:LEU:HD13	3:d:525:THR:OG1	2.15	0.47
9:z:71:HIS:HD2	9:z:73:THR:H	1.62	0.47
1:A:397:CYS:O	1:A:401:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ARG:HH11	3:D:263:GLN:CD	2.22	0.47
4:E:196:VAL:HG12	4:E:381:ARG:O	2.14	0.47
8:q:140:HIS:NE2	8:q:509:LYS:HE3	2.29	0.47
8:q:348:ASP:CB	8:q:366:GLU:HG2	2.44	0.47
3:D:185:PRO:HA	3:D:188:VAL:HG12	1.95	0.47
1:a:397:CYS:O	1:a:401:ARG:HG2	2.15	0.47
5:g:332:VAL:HG12	5:g:334:ARG:H	1.80	0.47
6:h:22:LEU:HD22	6:h:112:VAL:HG11	1.96	0.47
6:h:26:ILE:HG23	6:h:105:LEU:HB3	1.96	0.47
6:h:413:GLU:HG3	6:h:445:ILE:HB	1.96	0.47
10:K:274:ILE:O	10:K:278:THR:HG23	2.14	0.47
1:A:42:ASP:OD1	5:G:518:ARG:NH2	2.42	0.47
3:D:196:ASP:OD1	3:D:196:ASP:N	2.46	0.47
3:D:199:THR:O	3:D:199:THR:HG22	2.15	0.47
6:H:211:VAL:CG2	6:H:371:THR:HB	2.45	0.47
4:e:220:GLU:CD	4:e:220:GLU:H	2.23	0.47
8:q:190:ILE:CG2	8:q:191:PHE:H	2.26	0.47
9:z:90:ASP:OD1	9:z:91:GLY:N	2.48	0.47
1:A:43:LYS:HG2	5:G:521:ASP:O	2.14	0.47
1:A:230:VAL:HG23	1:A:231:ASN:H	1.78	0.47
2:B:334:THR:OG1	4:E:312:HIS:ND1	2.39	0.47
3:D:168:THR:HG23	3:D:180:SER:OG	2.15	0.47
3:D:433:ALA:O	3:D:437:THR:OG1	2.33	0.47
4:E:344:ARG:NE	4:E:347:GLU:OE2	2.40	0.47
6:H:246:LEU:HD11	6:H:271:TRP:CZ2	2.50	0.47
2:b:428:THR:HG21	2:b:436:MET:HE1	1.97	0.47
4:e:143:VAL:O	4:e:146:GLU:HG3	2.14	0.47
12:q:601:ADP:O1B	14:q:603:AF3:F2	2.22	0.47
11:P:137:LEU:HD22	11:P:141:PHE:HE2	1.80	0.47
2:B:122:HIS:CD2	2:B:124:GLN:HB2	2.50	0.47
3:D:266:VAL:HG13	3:D:271:GLN:HB2	1.95	0.47
4:E:107:THR:HB	12:E:601:ADP:O2B	2.15	0.47
4:E:272:GLU:CD	4:E:272:GLU:H	2.23	0.47
7:N:69:ILE:HB	7:N:80:LEU:HD13	1.97	0.47
3:d:38:ILE:HG21	3:d:121:THR:OG1	2.14	0.47
3:d:246:ILE:HD12	3:d:340:ILE:HG21	1.95	0.47
10:K:75:ILE:HD11	10:K:112:PRO:HD2	1.96	0.47
10:K:147:ARG:HB3	11:P:2:GLN:HB2	1.97	0.47
10:K:331:ALA:N	10:K:332:PRO:CD	2.78	0.47
3:D:302:LYS:N	3:D:328:ILE:O	2.46	0.47
4:E:38:ILE:HG21	4:E:121:GLU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:319:LEU:HD23	6:H:319:LEU:HA	1.75	0.47
8:Q:101:THR:N	14:Q:603:AF3:F1	2.37	0.47
8:Q:252:GLU:HG3	9:Z:264:ARG:HH12	1.79	0.47
2:b:59:ALA:O	3:d:89:ARG:NH2	2.37	0.47
2:b:261:THR:HG22	3:d:264:ILE:HD13	1.97	0.47
6:h:251:ASP:OD1	6:h:251:ASP:N	2.48	0.47
8:q:324:LEU:O	8:q:328:VAL:HG22	2.15	0.47
10:K:31:PHE:CE2	10:K:88:HIS:HB3	2.50	0.47
3:D:267:SER:H	3:D:271:GLN:NE2	2.12	0.47
4:E:145:ILE:HG23	4:E:514:LYS:HD2	1.97	0.47
6:H:318:ASP:O	6:H:322:THR:OG1	2.31	0.47
3:d:484:HIS:CD2	3:d:491:ALA:HB3	2.50	0.47
6:h:297:ASP:OD1	6:h:297:ASP:N	2.48	0.47
1:A:68:GLU:OE2	5:G:11:SER:HA	2.16	0.46
1:A:277:LYS:NZ	1:A:338:GLU:HG2	2.30	0.46
2:B:407:VAL:HG23	2:B:497:PHE:HB2	1.97	0.46
12:G:601:ADP:O1B	14:G:603:AF3:F3	2.23	0.46
8:Q:155:ARG:NH1	8:Q:192:PRO:O	2.49	0.46
9:Z:114:LEU:HD23	9:Z:119:ILE:HD11	1.96	0.46
1:a:203:ARG:HE	1:a:207:GLU:HG2	1.80	0.46
2:b:395:CYS:HB3	4:e:366:THR:HG21	1.97	0.46
3:d:103:GLY:HA3	3:d:410:CYS:HB3	1.96	0.46
4:e:107:THR:HB	12:e:601:ADP:O2B	2.15	0.46
6:h:178:MET:HE2	6:h:372:PHE:CE1	2.50	0.46
8:q:411:GLY:O	8:q:492:MET:HG3	2.15	0.46
2:B:71:LEU:HB3	2:B:85:VAL:HG22	1.96	0.46
4:E:168:THR:HG23	4:E:507:ILE:HG22	1.97	0.46
5:G:452:ILE:HG23	5:G:457:ALA:HB3	1.97	0.46
8:Q:463:VAL:HG11	8:Q:480:LEU:HD22	1.97	0.46
6:h:187:ASP:HB3	6:h:368:LYS:HD3	1.96	0.46
8:q:168:ILE:HD13	8:q:179:LEU:HB2	1.96	0.46
9:z:28:ARG:HB3	9:z:28:ARG:HH21	1.80	0.46
11:P:68:GLU:HA	11:P:71:ILE:HB	1.96	0.46
12:H:601:ADP:O3B	14:H:603:AF3:F2	2.23	0.46
3:d:400:GLU:O	3:d:404:SER:OG	2.28	0.46
4:e:12:TYR:CD1	6:h:20:PRO:HB3	2.50	0.46
5:g:412:GLY:HA3	5:g:448:PRO:HG3	1.97	0.46
8:q:131:GLY:HA3	8:q:437:ALA:HB3	1.96	0.46
9:z:143:MET:HG3	9:z:402:ILE:HA	1.98	0.46
10:K:10:ILE:HB	10:K:105:LEU:HD23	1.98	0.46
10:K:353:GLN:HA	10:K:356:TRP:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:45:VAL:HG23	11:P:45:VAL:O	2.15	0.46
11:P:120:TYR:HB2	11:P:127:CYS:HB3	1.96	0.46
5:G:185:PHE:HB3	5:G:192:GLU:HG2	1.98	0.46
6:H:126:ARG:NE	8:Q:174:GLY:HA3	2.30	0.46
7:N:43:LYS:HG2	7:N:44:GLN:H	1.80	0.46
8:Q:246:PHE:CD1	8:Q:336:LEU:HD11	2.51	0.46
9:Z:190:MET:SD	9:Z:326:LEU:HD12	2.56	0.46
1:A:297:LEU:O	1:A:301:VAL:HG23	2.16	0.46
2:B:205:LEU:HA	2:B:383:LEU:HD11	1.96	0.46
2:B:221:ASP:OD1	2:B:221:ASP:N	2.46	0.46
3:D:345:VAL:HG22	3:D:355:MET:HE3	1.98	0.46
4:E:143:VAL:O	4:E:146:GLU:HG3	2.15	0.46
4:E:397:GLU:OE1	4:E:400:ARG:HD2	2.15	0.46
5:G:84:SER:HB2	5:G:99:ILE:HD11	1.97	0.46
5:G:414:SER:HB3	5:G:502:LYS:NZ	2.31	0.46
6:H:85:SER:OG	8:Q:209:GLY:HA2	2.16	0.46
6:H:139:ILE:HD12	6:H:474:TRP:CH2	2.50	0.46
8:Q:254:LYS:O	9:Z:248:PHE:HB2	2.16	0.46
1:a:23:MET:HE3	1:a:23:MET:HB3	1.86	0.46
2:b:113:ALA:HB2	2:b:130:TRP:CH2	2.50	0.46
7:n:43:LYS:HG2	7:n:44:GLN:H	1.80	0.46
10:K:93:GLU:O	10:K:93:GLU:HG3	2.15	0.46
6:h:93:GLY:HA2	12:h:601:ADP:O2B	2.15	0.46
2:B:323:LEU:HA	2:B:326:VAL:HG12	1.96	0.46
6:H:297:ASP:OD1	6:H:297:ASP:N	2.49	0.46
9:Z:426:LYS:NZ	9:Z:438:GLN:HE21	2.13	0.46
1:a:228:ARG:HG3	1:a:352:VAL:HG13	1.96	0.46
4:e:93:GLU:OE1	6:h:201:GLN:NE2	2.48	0.46
4:e:255:PHE:HB2	4:e:306:PHE:HB3	1.98	0.46
4:e:492:ASP:OD2	4:e:497:GLY:N	2.47	0.46
10:K:162:THR:HG22	10:K:176:LEU:O	2.16	0.46
10:K:213:LYS:NZ	10:K:306:TYR:HD2	2.13	0.46
3:D:494:ASN:HB2	3:D:501:SER:OG	2.16	0.46
2:b:176:LYS:O	2:b:180:THR:OG1	2.30	0.46
3:d:227:LEU:HD21	3:d:376:ILE:HD12	1.96	0.46
10:K:27:PRO:HD3	10:K:340:TRP:CD1	2.51	0.46
4:E:220:GLU:CD	4:E:220:GLU:H	2.23	0.46
1:a:28:ILE:HA	1:a:31:ILE:HD12	1.97	0.46
1:a:44:MET:HB2	5:g:522:ILE:HG12	1.98	0.46
4:e:444:GLU:O	4:e:448:MET:HG3	2.16	0.46
6:h:74:PRO:HB2	8:q:55:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:121:LYS:HD2	11:P:163:LEU:CD1	2.46	0.46
11:P:165:THR:OG1	11:P:179:ILE:HG22	2.16	0.46
1:A:214:TYR:OH	1:A:318:ARG:HD2	2.16	0.46
5:g:83:ILE:HD11	5:g:512:THR:CG2	2.37	0.46
8:q:208:LEU:HD12	8:q:385:MET:HE2	1.98	0.46
1:A:81:LEU:HD11	3:D:215:GLY:HA2	1.96	0.45
2:B:3:SER:O	2:B:7:ALA:HB2	2.16	0.45
3:D:415:LEU:HD12	3:D:415:LEU:HA	1.80	0.45
4:E:280:TYR:O	4:E:284:LYS:HG2	2.16	0.45
4:E:444:GLU:O	4:E:448:MET:HG3	2.16	0.45
5:G:215:LEU:HB3	5:G:364:THR:HG22	1.98	0.45
6:H:29:CYS:SG	6:H:513:ILE:HD13	2.56	0.45
6:H:187:ASP:HB3	6:H:368:LYS:HD3	1.98	0.45
1:a:73:LYS:O	1:a:77:GLU:HG2	2.16	0.45
5:g:182:MET:HE2	5:g:372:CYS:HB3	1.98	0.45
6:h:185:MET:HE1	6:h:212:ALA:HA	1.98	0.45
10:K:50:LYS:HG3	10:K:51:ASP:H	1.82	0.45
3:D:431:GLU:OE2	3:D:484:HIS:ND1	2.37	0.45
1:a:81:LEU:HA	1:a:84:LYS:NZ	2.32	0.45
1:a:472:ASN:O	1:a:476:VAL:HG22	2.16	0.45
2:b:251:ILE:HG13	4:e:277:LEU:HD11	1.98	0.45
8:q:168:ILE:HD11	8:q:176:GLU:O	2.16	0.45
1:A:5:LEU:HB3	1:A:7:VAL:HG23	1.98	0.45
7:N:114:GLN:OE1	7:N:115:VAL:N	2.50	0.45
6:h:187:ASP:OD1	6:h:187:ASP:N	2.42	0.45
10:K:19:ALA:HB3	10:K:29:ALA:HB3	1.98	0.45
10:K:133:TYR:HB3	10:K:352:PHE:HE1	1.81	0.45
1:A:5:LEU:HD23	1:A:5:LEU:HA	1.86	0.45
2:B:257:ARG:O	4:E:269:THR:HG22	2.16	0.45
2:B:428:THR:HG21	2:B:436:MET:HE1	1.97	0.45
5:G:43:PRO:HA	5:G:162:THR:HA	1.97	0.45
6:H:317:GLU:H	6:H:317:GLU:CD	2.23	0.45
1:a:127:GLU:HG3	1:a:426:TYR:CE2	2.51	0.45
5:G:49:MET:HE2	9:Z:76:LEU:HD11	1.98	0.45
9:Z:426:LYS:HZ2	9:Z:438:GLN:HE21	1.62	0.45
2:b:68:ALA:HB2	2:b:99:THR:HG21	1.98	0.45
2:b:407:VAL:HG23	2:b:497:PHE:HB2	1.99	0.45
5:g:35:ASP:OD1	5:g:38:ARG:NH1	2.48	0.45
7:n:51:ILE:HD13	7:n:71:ARG:HB2	1.99	0.45
8:q:246:PHE:CD1	8:q:336:LEU:HD11	2.52	0.45
9:z:303:ASP:O	9:z:307:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:269:SER:O	8:Q:273:GLU:HG2	2.16	0.45
1:a:489:ASP:HB3	1:a:494:LYS:O	2.16	0.45
3:d:415:LEU:HD12	3:d:415:LEU:HA	1.80	0.45
5:g:40:CYS:HG	5:g:48:LYS:NZ	2.12	0.45
10:K:16:MET:HB3	10:K:32:PRO:HD2	1.97	0.45
4:E:196:VAL:HG21	4:E:209:ILE:HG13	1.98	0.45
9:Z:234:ASN:N	9:Z:333:LEU:O	2.43	0.45
3:d:73:ASP:OD2	15:d:701:HOH:O	2.20	0.45
5:g:21:LYS:HD3	5:g:21:LYS:HA	1.71	0.45
6:h:121:ILE:HA	6:h:434:LEU:HD13	1.98	0.45
1:A:216:LEU:HB2	1:A:362:ILE:HB	1.99	0.45
6:H:21:GLN:OE1	6:H:25:ASN:ND2	2.41	0.45
9:Z:146:GLU:CD	9:Z:146:GLU:H	2.25	0.45
1:a:113:HIS:HD2	1:a:115:THR:H	1.65	0.45
4:e:292:ILE:O	4:e:295:THR:HG22	2.16	0.45
4:e:485:MET:O	7:n:30:ARG:HD3	2.16	0.45
5:g:416:MET:SD	5:g:448:PRO:HG2	2.56	0.45
11:P:83:LYS:HA	11:P:86:LYS:HD3	1.98	0.45
3:D:229:LEU:HD12	3:D:374:LEU:HD12	1.98	0.45
4:E:9[C]:PHE:C	4:E:16:PHE:HB2	2.42	0.45
4:E:12:TYR:CG	6:H:20:PRO:HB3	2.52	0.45
4:E:94:LEU:HD11	4:E:519:LEU:HB3	1.97	0.45
4:E:201:ARG:HA	4:E:201:ARG:NE	2.31	0.45
8:Q:168:ILE:HD11	8:Q:176:GLU:O	2.16	0.45
9:Z:164:LEU:HD21	9:Z:387:ILE:HG12	1.99	0.45
1:a:274:ARG:HG2	1:a:338:GLU:OE2	2.17	0.45
6:h:325:ALA:HB2	6:h:369:THR:OG1	2.17	0.45
9:z:146:GLU:H	9:z:146:GLU:CD	2.25	0.45
10:K:31:PHE:HB3	10:K:32:PRO:CD	2.46	0.45
11:P:170:LEU:HB3	11:P:175:LYS:HE3	1.99	0.45
1:A:120:GLY:HA3	1:A:437:ALA:HB3	1.98	0.45
3:D:46:ASP:HA	3:D:49:ARG:HD3	1.99	0.45
8:Q:212:ILE:HG13	8:Q:213:SER:N	2.32	0.45
8:Q:532:GLY:HA2	10:K:349:LEU:HD13	1.99	0.45
6:h:2:MET:HB3	6:h:2:MET:HE2	1.72	0.45
5:G:28:ASN:HA	5:G:31:LYS:HG2	1.97	0.44
8:Q:339:PRO:HG2	8:Q:344:MET:HE3	1.99	0.44
5:g:48:LYS:O	5:g:59:MET:HA	2.16	0.44
5:g:50:LEU:HD22	5:g:69:GLU:HB2	1.99	0.44
6:h:318:ASP:O	6:h:322:THR:OG1	2.35	0.44
7:n:91:ALA:O	7:n:115:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:z:264:ARG:NH2	9:z:298:ASP:OD2	2.47	0.44
9:z:523:ARG:CZ	9:z:526:MET:HE1	2.47	0.44
1:A:78:LEU:HD13	1:A:520:ALA:HB2	2.00	0.44
1:A:447:VAL:O	1:A:451:THR:OG1	2.21	0.44
2:B:395:CYS:HB3	4:E:366:THR:HG21	1.99	0.44
4:E:176:LYS:NZ	14:E:603:AF3:F1	2.27	0.44
4:E:239:MET:HE2	4:E:320:PRO:HA	1.99	0.44
1:a:102:LYS:NZ	1:a:102:LYS:HB3	2.33	0.44
1:a:104:ALA:O	1:a:108:VAL:HG23	2.17	0.44
3:d:58:ASP:OD1	3:d:72:ASN:HB2	2.17	0.44
3:d:367:LEU:HD11	3:d:373:LEU:HG	1.98	0.44
11:P:124:ILE:H	11:P:124:ILE:HG13	1.62	0.44
4:E:44:VAL:O	4:E:48:MET:HG2	2.18	0.44
7:N:64:LYS:HA	7:N:67:PHE:CE1	2.52	0.44
9:Z:157:ARG:NH1	9:Z:166:ASP:OD1	2.43	0.44
2:b:440:ALA:O	2:b:444:ARG:HG3	2.17	0.44
4:e:178:VAL:HG11	4:e:398:ALA:HA	1.98	0.44
6:h:126:ARG:HE	8:q:174:GLY:HA3	1.83	0.44
6:h:319:LEU:HD23	6:h:319:LEU:HA	1.77	0.44
7:n:111:GLN:CD	7:n:111:GLN:H	2.24	0.44
10:K:7:ALA:HB3	10:K:347:ALA:HB1	1.99	0.44
2:B:189:ARG:NH1	2:B:215:ASP:O	2.51	0.44
6:H:391:ASP:OD1	15:H:701:HOH:O	2.20	0.44
2:b:285:HIS:CE1	2:b:335:PHE:HB3	2.49	0.44
5:g:407:LEU:HD12	5:g:407:LEU:HA	1.85	0.44
5:g:541:ASP:HB2	5:g:544:GLN:NE2	2.33	0.44
6:h:29:CYS:SG	6:h:513:ILE:HD13	2.57	0.44
7:n:38:ARG:O	7:n:45:ARG:HA	2.17	0.44
11:P:166:ILE:HB	11:P:178:PHE:HD2	1.82	0.44
6:H:195:ILE:HG12	6:H:370:CYS:SG	2.58	0.44
8:Q:259:ILE:HG21	8:Q:265:LEU:HB2	1.98	0.44
9:Z:179:ILE:HD13	9:Z:191:ILE:HG13	2.00	0.44
4:e:9[B]:PHE:CG	4:e:9[B]:PHE:O	2.70	0.44
9:z:234:ASN:N	9:z:333:LEU:O	2.45	0.44
10:K:107:GLU:OE1	10:K:111:ASN:HB3	2.17	0.44
11:P:81:GLU:O	11:P:85:THR:HG23	2.17	0.44
1:A:472:ASN:O	1:A:476:VAL:HG22	2.17	0.44
2:B:480:MET:HG3	12:B:601:ADP:C2	2.53	0.44
4:E:437:ALA:HA	4:E:440:CYS:SG	2.58	0.44
1:a:28:ILE:HG13	1:a:72:ALA:HB1	2.00	0.44
2:b:465:LEU:HD23	2:b:465:LEU:HA	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:239:MET:HE2	4:e:320:PRO:HA	2.00	0.44
6:h:211:VAL:CG2	6:h:371:THR:HB	2.48	0.44
6:h:521:LYS:HG2	8:q:57:ILE:HD12	2.00	0.44
10:K:349:LEU:HD23	10:K:349:LEU:HA	1.87	0.44
6:H:79:LEU:HA	6:H:82:ILE:HG12	2.00	0.44
6:H:168:ILE:HG21	6:H:385:THR:HG23	1.99	0.44
5:g:109:ALA:HB2	5:g:126:TYR:OH	2.17	0.44
12:h:601:ADP:O1B	14:h:603:AF3:F3	2.26	0.44
8:q:237:ALA:HB3	8:q:347:CYS:HB2	1.99	0.44
1:A:130:ARG:NH2	1:A:422:TYR:OH	2.46	0.44
1:A:254:ILE:HD11	1:A:263:ILE:HD12	2.00	0.44
5:G:414:SER:HB3	5:G:502:LYS:HZ3	1.82	0.44
6:H:1:MET:HG3	6:H:2:MET:H	1.83	0.44
6:H:344:ARG:HB2	6:H:344:ARG:CZ	2.48	0.44
7:N:63:VAL:HG22	7:N:67:PHE:HE1	1.82	0.44
8:Q:152:LYS:HE2	8:Q:152:LYS:HB2	1.73	0.44
1:a:452:LEU:HB3	1:a:490:LEU:HD11	2.00	0.44
3:d:155:VAL:HG21	3:d:162:THR:HG21	2.00	0.44
4:e:73:ASP:OD1	14:e:603:AF3:F2	2.26	0.44
4:e:94:LEU:HD11	4:e:519:LEU:HB3	2.00	0.44
9:z:133:PHE:O	9:z:137:VAL:HG22	2.18	0.44
10:K:327:ILE:HG13	10:K:327:ILE:O	2.17	0.44
1:A:252:VAL:HB	5:G:254:THR:HA	2.00	0.44
1:A:277:LYS:HZ2	1:A:338:GLU:HG2	1.83	0.44
4:E:16:PHE:CE2	4:E:18:ILE:HD11	2.53	0.44
7:N:48:VAL:HG12	7:N:67:PHE:HE2	1.83	0.44
4:e:150:LYS:HB2	4:e:150:LYS:HE3	1.80	0.44
5:g:226:HIS:HD2	5:g:228:ARG:H	1.64	0.44
6:h:89:GLU:OE1	8:q:378:ARG:NH2	2.46	0.44
6:h:126:ARG:NE	8:q:174:GLY:HA3	2.32	0.44
8:q:284:ALA:HB2	8:q:310:ILE:HD11	1.98	0.44
2:B:141:LEU:HD22	2:B:417:MET:HE3	2.00	0.43
2:B:167:LEU:HD22	2:B:172:LEU:HD12	2.00	0.43
5:G:247:TYR:HB2	5:G:275:ILE:HD11	2.00	0.43
6:H:178:MET:HE2	6:H:372:PHE:CE1	2.53	0.43
6:H:251:ASP:OD1	6:H:251:ASP:N	2.51	0.43
8:Q:286:THR:HG21	8:Q:338:PRO:HB2	2.00	0.43
1:a:191:PRO:HB2	5:g:544:GLN:HA	2.00	0.43
3:d:81:MET:O	3:d:81:MET:HG3	2.18	0.43
3:d:106:THR:OG1	14:d:603:AF3:F3	2.23	0.43
5:g:43:PRO:HA	5:g:162:THR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:80:MET:HE1	5:g:102:ALA:HB3	1.99	0.43
8:q:148:CYS:SG	8:q:149:CYS:N	2.91	0.43
1:A:228:ARG:NE	1:A:350:GLU:OE2	2.31	0.43
5:G:212:SER:HB2	5:G:376:LEU:HA	2.00	0.43
9:Z:244:VAL:HG12	9:Z:244:VAL:O	2.17	0.43
1:a:253:VAL:HB	3:d:265:VAL:HG13	2.00	0.43
8:q:134:ILE:HD12	8:q:137:ARG:HH11	1.83	0.43
9:z:170:GLU:OE1	9:z:170:GLU:N	2.51	0.43
4:E:102:ILE:O	4:E:407:CYS:HB3	2.17	0.43
5:G:12:GLN:O	5:G:13:ASN:CG	2.62	0.43
8:Q:237:ALA:HB3	8:Q:347:CYS:HB2	2.01	0.43
9:Z:133:PHE:O	9:Z:137:VAL:HG22	2.18	0.43
6:h:206:GLU:H	6:h:206:GLU:CD	2.26	0.43
8:q:333:LEU:HD11	8:q:339:PRO:HB3	2.00	0.43
3:D:288:LYS:HG2	3:D:320:MET:HE1	2.00	0.43
6:H:32:ILE:CG1	6:H:76:ALA:HB1	2.48	0.43
1:a:239:PHE:O	1:a:288:THR:OG1	2.36	0.43
2:b:117:ILE:HD11	2:b:123:PRO:HB3	2.00	0.43
2:b:122:HIS:HD2	2:b:124:GLN:HB2	1.82	0.43
2:b:131:ARG:NH2	2:b:512:GLU:OE2	2.44	0.43
3:d:204:ASP:HB3	3:d:207:ASP:OD2	2.18	0.43
6:h:136:ILE:HG12	6:h:412:ILE:HD11	1.99	0.43
6:h:139:ILE:HD12	6:h:474:TRP:CH2	2.53	0.43
8:q:117:GLU:O	8:q:121:ILE:HG23	2.18	0.43
1:A:11:ARG:HA	1:A:530:LEU:O	2.18	0.43
6:H:122:ILE:HG13	6:H:123:ARG:N	2.33	0.43
7:N:111:GLN:H	7:N:111:GLN:CD	2.25	0.43
2:b:51:ILE:HD12	3:d:535:VAL:HG22	2.00	0.43
3:d:172:ASN:HD22	12:d:601:ADP:HN61	1.66	0.43
7:n:8:GLY:HA3	7:n:20:LEU:HG	2.00	0.43
8:q:275:LEU:HD21	9:z:257:GLU:HG3	2.00	0.43
9:z:28:ARG:HB3	9:z:28:ARG:NH2	2.33	0.43
9:z:59:ASP:OD1	14:z:603:AF3:F2	2.26	0.43
3:D:472:ASN:O	3:D:476:THR:OG1	2.29	0.43
7:N:6:GLU:OE2	7:N:111:GLN:NE2	2.51	0.43
5:g:182:MET:CE	5:g:372:CYS:HB3	2.49	0.43
8:q:16:LYS:HE3	9:z:70:GLN:HG2	2.00	0.43
8:q:322:ARG:CZ	8:q:322:ARG:HB3	2.49	0.43
10:K:162:THR:HG21	10:K:277:THR:HG22	2.01	0.43
11:P:162:ASN:O	11:P:163:LEU:HD23	2.19	0.43
1:A:351:VAL:HG22	1:A:364:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:VAL:HG12	2:B:399:GLN:HG3	2.00	0.43
5:G:66:ILE:O	5:G:70:ILE:HG23	2.19	0.43
5:G:209:ILE:HA	5:G:377:ARG:O	2.18	0.43
6:H:26:ILE:O	6:H:30:GLN:HG2	2.19	0.43
6:H:185:MET:CE	6:H:370:CYS:HB3	2.48	0.43
6:H:384:GLU:OE1	6:H:387:ARG:HD2	2.19	0.43
8:Q:322:ARG:CZ	8:Q:322:ARG:HB3	2.49	0.43
8:Q:416:GLU:OE1	8:Q:504:LYS:HE3	2.18	0.43
9:Z:277:LEU:HD22	9:Z:339:LEU:HG	2.00	0.43
1:a:45:LEU:HA	5:g:523:VAL:O	2.19	0.43
6:h:49:ILE:HD13	6:h:68:LEU:HD12	2.01	0.43
6:h:323:MET:HE1	8:q:230:ASP:CG	2.44	0.43
2:B:217:GLY:HA3	2:B:362:PHE:O	2.19	0.43
4:E:31:LEU:HD12	4:E:31:LEU:HA	1.81	0.43
5:G:109:ALA:HB2	5:G:126:TYR:OH	2.19	0.43
5:G:118:HIS:ND1	5:G:120:THR:HG23	2.33	0.43
6:H:187:ASP:OD1	6:H:187:ASP:N	2.41	0.43
8:Q:208:LEU:HD12	8:Q:385:MET:HE2	2.00	0.43
3:d:48:ILE:HD11	3:d:110:VAL:HG11	2.00	0.43
4:e:301:ILE:HG23	4:e:325:VAL:HG21	2.00	0.43
6:h:79:LEU:HA	6:h:82:ILE:HG12	2.01	0.43
6:h:90:VAL:HG11	6:h:498:VAL:HG22	2.01	0.43
6:h:169:SER:HA	6:h:172:LYS:HB3	2.00	0.43
8:q:409:VAL:HG21	8:q:504:LYS:HG3	2.00	0.43
9:z:190:MET:SD	9:z:326:LEU:HD12	2.59	0.43
1:A:35:SER:O	15:A:701:HOH:O	2.21	0.43
1:A:294:ASP:O	1:A:298:LYS:HG2	2.19	0.43
6:H:119:GLN:HA	6:H:122:ILE:HG12	2.00	0.43
6:H:494:GLU:OE2	6:H:499:ARG:HG2	2.19	0.43
8:Q:502:LEU:HD23	8:Q:502:LEU:HA	1.88	0.43
1:a:118:ILE:HG23	1:a:522:ILE:HG12	2.01	0.43
1:a:199:LYS:NZ	1:a:386:ASP:OD1	2.41	0.43
6:h:317:GLU:H	6:h:317:GLU:CD	2.27	0.43
6:h:384:GLU:OE1	6:h:387:ARG:HD2	2.19	0.43
6:h:394:MET:O	6:h:398:ARG:HG2	2.19	0.43
8:q:81:PRO:HB2	9:z:46:MET:SD	2.58	0.43
8:q:533:PRO:HD2	8:q:534:LYS:HZ2	1.84	0.43
10:K:71:ILE:HG12	10:K:76:VAL:HG22	2.00	0.43
1:A:398:VAL:O	1:A:402:VAL:HG23	2.19	0.43
5:G:357:ASP:HB2	10:K:360:GLN:HE22	1.82	0.43
5:G:459:THR:O	5:G:463:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:2:ALA:HB2	9:z:75:SER:OG	2.18	0.43
8:Q:117:GLU:O	8:Q:121:ILE:HG23	2.19	0.43
2:b:11:ILE:O	2:b:12:PHE:CG	2.71	0.43
2:b:148:HIS:HB3	2:b:154:LYS:HG2	2.00	0.43
4:e:199:MET:HE3	4:e:199:MET:HB2	1.97	0.43
6:h:136:ILE:HD11	6:h:416:LEU:HD11	1.99	0.43
6:h:522:ASN:HD22	8:q:58:ASN:HA	1.84	0.43
8:q:292:VAL:HG22	8:q:313:VAL:HB	2.01	0.43
1:A:22:VAL:HG21	1:A:105:ASP:CB	2.49	0.42
1:A:426:TYR:OH	1:A:430:MET:HE2	2.17	0.42
6:H:103:GLU:HG2	6:H:444:ILE:HB	2.01	0.42
1:a:321:LYS:HD2	1:a:370:ARG:NH2	2.34	0.42
2:b:35:ILE:HD13	2:b:35:ILE:HA	1.86	0.42
2:b:419:HIS:O	2:b:423:GLN:HG2	2.19	0.42
4:e:233:ASP:OD1	4:e:233:ASP:N	2.52	0.42
5:g:11:SER:HB2	5:g:14:THR:HG23	2.00	0.42
5:g:381:LYS:HA	5:g:381:LYS:HD3	1.86	0.42
6:h:122:ILE:HG13	6:h:123:ARG:N	2.34	0.42
8:q:364:LYS:NZ	8:q:366:GLU:OE2	2.39	0.42
9:z:114:LEU:HD22	9:z:435:LEU:HD12	2.00	0.42
2:B:151:ASP:OD1	2:B:153:VAL:HG12	2.19	0.42
2:B:256:VAL:O	3:D:262:ASN:HA	2.19	0.42
3:D:176:VAL:O	3:D:176:VAL:HG23	2.19	0.42
5:G:47:MET:SD	5:G:61:ASN:ND2	2.92	0.42
5:G:378:GLY:HA3	5:G:384:LEU:HD21	2.01	0.42
6:H:228:GLN:NE2	6:H:310:CYS:SG	2.78	0.42
2:b:392:ASP:OD1	15:b:701:HOH:O	2.21	0.42
8:q:253:THR:HA	9:z:241:LYS:HE2	2.01	0.42
10:K:64:ILE:HD13	10:K:67:LEU:HD22	2.02	0.42
3:D:176:VAL:HG12	3:D:218:ILE:HD13	2.00	0.42
5:G:247:TYR:HB2	5:G:275:ILE:CD1	2.49	0.42
7:N:104:GLU:CD	7:N:104:GLU:H	2.28	0.42
8:Q:32:ASN:HD21	8:Q:524:ILE:HD11	1.84	0.42
2:b:249:ILE:HG21	4:e:277:LEU:HG	2.01	0.42
4:e:44:VAL:O	4:e:48:MET:HG2	2.19	0.42
4:e:518:SER:O	4:e:522:GLN:HG2	2.19	0.42
8:q:173:TYR:OH	8:q:483:GLU:OE1	2.36	0.42
9:z:355:LEU:O	9:z:358:GLU:HG2	2.19	0.42
1:A:423:LEU:HB2	1:A:442:ALA:HB2	2.00	0.42
2:B:260:SER:OG	2:B:263:LYS:HG3	2.20	0.42
4:E:253:CYS:HB3	4:E:343:PRO:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:445:GLN:HE21	4:E:449:ARG:NH1	2.11	0.42
9:Z:30:LEU:HD11	9:Z:74:ALA:HA	2.02	0.42
9:Z:71:HIS:HD2	9:Z:73:THR:H	1.68	0.42
4:e:86:GLN:NE2	6:h:56:ALA:HB2	2.35	0.42
4:e:257:PRO:HA	4:e:258:PRO:HD3	1.97	0.42
5:g:64:ASN:HB2	5:g:95:THR:HG21	2.02	0.42
12:g:601:ADP:O1B	14:g:603:AF3:F1	2.27	0.42
6:h:32:ILE:CG1	6:h:76:ALA:HB1	2.48	0.42
6:h:246:LEU:HD11	6:h:271:TRP:CZ2	2.54	0.42
6:h:517:ASP:OD1	8:q:54:LYS:NZ	2.52	0.42
8:q:254:LYS:O	9:z:248:PHE:HB2	2.19	0.42
1:A:205:GLN:HG3	5:G:511:GLU:OE2	2.20	0.42
2:B:325:LEU:HB3	2:B:369:GLU:O	2.20	0.42
3:D:375:LYS:HE2	3:D:375:LYS:HB3	1.73	0.42
4:E:426:GLU:OE2	4:E:513:LYS:NZ	2.36	0.42
6:H:126:ARG:HE	8:Q:174:GLY:HA3	1.84	0.42
9:Z:14:ALA:O	9:Z:520:GLU:HA	2.19	0.42
4:e:102:ILE:O	4:e:407:CYS:HB3	2.19	0.42
1:A:31:ILE:HG21	1:A:65:LEU:HD11	2.02	0.42
1:A:102:LYS:NZ	1:A:102:LYS:HB3	2.34	0.42
2:B:208:SER:HB3	3:D:520:THR:CG2	2.50	0.42
3:D:511:PRO:HG2	3:D:514:VAL:HG23	2.01	0.42
4:E:28:LEU:O	4:E:532:ASP:HA	2.20	0.42
5:G:411:GLY:HA3	5:G:490:MET:HE3	2.01	0.42
7:N:64:LYS:H	7:N:66:ARG:HH22	1.68	0.42
9:Z:221:MET:HE1	9:Z:312:ALA:HB3	2.01	0.42
6:h:344:ARG:CZ	6:h:344:ARG:HB2	2.50	0.42
8:q:118:LEU:O	8:q:121:ILE:HG12	2.19	0.42
11:P:67:ASP:O	11:P:71:ILE:HG13	2.20	0.42
3:D:149:THR:O	3:D:152:SER:OG	2.37	0.42
8:Q:148:CYS:SG	8:Q:149:CYS:N	2.93	0.42
8:Q:199:VAL:HG13	8:Q:400:LYS:HD3	2.02	0.42
2:b:151:ASP:OD1	2:b:153:VAL:HG12	2.19	0.42
3:d:476:THR:HG23	3:d:500:ILE:HD11	2.02	0.42
5:g:220:ILE:HG12	5:g:361:THR:HB	2.02	0.42
5:g:435:TRP:HB2	5:g:436:PRO:HD3	2.00	0.42
7:n:90:THR:HG23	7:n:115:VAL:HG23	2.02	0.42
11:P:47:THR:HG22	11:P:48:TYR:N	2.35	0.42
1:A:239:PHE:O	1:A:288:THR:OG1	2.36	0.42
2:B:86:ASP:CG	4:E:392:LYS:HG2	2.45	0.42
2:B:187:VAL:HG21	2:B:397:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:LYS:HE3	2:B:315:ALA:HA	2.02	0.42
5:G:445:GLU:O	5:G:449:ARG:HG3	2.20	0.42
6:H:242:VAL:O	6:H:291:SER:OG	2.34	0.42
6:H:290:LEU:HD11	6:H:361:PHE:CZ	2.55	0.42
6:H:527:VAL:HG23	6:H:528:ASP:N	2.33	0.42
7:N:7:SER:OG	7:N:21:SER:HB3	2.20	0.42
3:d:472:ASN:HD22	3:d:474:ILE:HG22	1.85	0.42
4:e:289:ILE:HG13	4:e:313:LEU:HB3	2.01	0.42
6:h:85:SER:OG	8:q:209:GLY:HA2	2.20	0.42
9:z:207:ILE:HD13	9:z:375:LEU:HB2	2.01	0.42
10:K:262:PHE:HZ	10:K:309:ILE:HG13	1.85	0.42
1:A:104:ALA:O	1:A:108:VAL:HG23	2.19	0.42
2:B:244:MET:HA	2:B:275:MET:HE1	2.02	0.42
5:G:220:ILE:HG12	5:G:361:THR:HB	2.01	0.42
6:H:499:ARG:HD3	6:H:499:ARG:HA	1.79	0.42
1:a:163:ILE:HB	5:g:127:ARG:HH21	1.84	0.42
1:a:204:SER:OG	5:g:511:GLU:OE2	2.31	0.42
1:a:277:LYS:HZ3	1:a:338:GLU:HG2	1.85	0.42
2:b:51:ILE:HB	3:d:535:VAL:HG22	2.02	0.42
2:b:54:SER:HA	3:d:538:THR:OG1	2.20	0.42
8:q:33:ILE:HG21	8:q:116:GLU:HB2	2.02	0.42
10:K:368:SER:HA	10:K:371:HIS:ND1	2.35	0.42
1:A:185:ARG:HB2	1:A:187:GLN:HG3	2.02	0.42
2:B:440:ALA:O	2:B:444:ARG:HG3	2.19	0.42
5:G:466:LEU:HD13	5:G:487:LEU:HD22	2.01	0.42
8:Q:291:VAL:HB	8:Q:312:LEU:HD12	2.00	0.42
9:Z:196:MET:HE2	9:Z:355:LEU:HD12	2.00	0.42
2:b:205:LEU:O	2:b:376:ARG:NH2	2.53	0.42
5:g:225:THR:HG22	5:g:313:ARG:HG2	2.01	0.42
6:h:48:LEU:HG	6:h:58:ILE:HG12	2.01	0.42
9:z:430:LYS:O	9:z:430:LYS:HG3	2.20	0.42
1:A:158:SER:OG	12:A:601:ADP:O2A	2.38	0.41
1:A:452:LEU:HB3	1:A:490:LEU:HD11	2.02	0.41
2:B:291:ILE:HD13	2:B:323:LEU:HD13	2.02	0.41
3:D:161:GLU:HA	3:D:161:GLU:OE1	2.19	0.41
4:E:226:LYS:HA	4:E:383:VAL:HG23	2.02	0.41
5:G:256:ILE:HG22	5:G:257:GLU:N	2.34	0.41
9:Z:135:GLU:HA	9:Z:138:LYS:HD3	2.02	0.41
9:Z:526:MET:SD	9:Z:526:MET:N	2.88	0.41
1:a:347:GLN:HB2	1:a:368:LYS:HD3	2.02	0.41
2:b:244:MET:HA	2:b:275:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:168:THR:HG23	3:d:180:SER:OG	2.20	0.41
4:e:416:ASN:OD1	4:e:416:ASN:N	2.52	0.41
5:g:383:ILE:O	5:g:387:VAL:HG23	2.20	0.41
8:q:54:LYS:O	8:q:65:VAL:HA	2.20	0.41
8:q:212:ILE:HG13	8:q:213:SER:N	2.34	0.41
10:K:94:LEU:HB3	10:K:96:VAL:HG22	2.02	0.41
10:K:346:LEU:O	10:K:352:PHE:HB2	2.20	0.41
1:A:163:ILE:HB	5:G:127:ARG:HH21	1.85	0.41
2:B:25:ARG:NH2	3:d:26:ASP:O	2.52	0.41
4:E:248:ILE:HD12	4:E:337:THR:HG21	2.02	0.41
5:G:95:THR:OG1	14:G:603:AF3:F3	2.20	0.41
6:H:82:ILE:HD12	6:H:97:VAL:HG12	2.01	0.41
9:Z:404:ASP:OD2	9:Z:499:CYS:HB3	2.20	0.41
2:b:246:THR:OG1	3:d:259:ASP:OD1	2.35	0.41
3:d:375:LYS:HG2	3:d:377:THR:HG22	2.01	0.41
6:h:346:GLN:HB2	6:h:363:GLY:HA3	2.02	0.41
8:q:228:GLU:HB2	8:q:312:LEU:HB3	2.01	0.41
11:P:97:ILE:HD12	11:P:102:TYR:HA	2.02	0.41
11:P:115:VAL:HB	11:P:169:TYR:HB2	2.02	0.41
2:B:242:THR:HG21	2:B:335:PHE:CZ	2.55	0.41
3:D:65:LYS:HE3	3:D:65:LYS:HB2	1.66	0.41
3:D:185:PRO:O	3:D:189:ASN:ND2	2.53	0.41
3:D:242:GLU:OE1	3:D:242:GLU:N	2.53	0.41
3:D:274:ARG:O	3:D:278:GLU:HG3	2.21	0.41
4:E:78:LEU:HD11	4:E:110:VAL:HG21	2.02	0.41
5:G:80:MET:HE1	5:G:102:ALA:HB3	2.01	0.41
6:H:215:ALA:HA	6:H:359:ASN:O	2.20	0.41
7:N:66:ARG:HB3	7:N:83:ASN:ND2	2.35	0.41
8:Q:81:PRO:HB2	9:Z:46:MET:SD	2.60	0.41
8:Q:253:THR:HA	9:Z:241:LYS:HE2	2.01	0.41
1:a:5:LEU:HD23	1:a:5:LEU:HA	1.84	0.41
1:a:487:GLY:O	1:a:495:PRO:HA	2.20	0.41
3:d:519:LEU:HD12	3:d:519:LEU:HA	1.74	0.41
4:e:6:THR:HG21	6:h:31:VAL:HG11	2.01	0.41
4:e:226:LYS:HA	4:e:383:VAL:HG23	2.01	0.41
4:e:456:GLU:OE2	4:e:478:ARG:NH2	2.43	0.41
5:g:83:ILE:HG21	5:g:83:ILE:HD13	1.84	0.41
5:g:234:LYS:HB3	5:g:234:LYS:HE3	1.74	0.41
10:K:113:LYS:HB3	10:K:116:ARG:HH21	1.85	0.41
10:K:309:ILE:O	10:K:309:ILE:HG12	2.12	0.41
11:P:5:ASN:HA	11:P:11:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:LEU:O	2:B:376:ARG:NH2	2.53	0.41
2:B:410:GLY:HA2	12:B:601:ADP:N3	2.36	0.41
3:D:428:PRO:O	3:D:432:LEU:HB2	2.20	0.41
4:E:109:VAL:HG13	4:E:516:GLN:HG2	2.01	0.41
4:E:159:ILE:HD11	4:E:199:MET:SD	2.61	0.41
4:E:293:LYS:NZ	4:E:317:ASN:O	2.45	0.41
8:Q:118:LEU:O	8:Q:121:ILE:HG12	2.20	0.41
3:d:292:LYS:HE3	3:d:292:LYS:HB3	1.81	0.41
4:e:159:ILE:HD11	4:e:199:MET:SD	2.61	0.41
5:g:183:VAL:HG12	5:g:193:ILE:O	2.20	0.41
5:g:302:HIS:CE1	9:z:335:SER:HG	2.38	0.41
6:h:26:ILE:O	6:h:30:GLN:HG2	2.19	0.41
9:z:225:VAL:CG1	9:z:288:GLY:HA3	2.50	0.41
1:A:118:ILE:HG23	1:A:522:ILE:HG12	2.02	0.41
1:A:209:MET:HE3	1:A:376:ILE:HD12	2.03	0.41
3:D:438:GLU:O	3:D:442:THR:HG23	2.20	0.41
6:H:325:ALA:HB2	6:H:369:THR:OG1	2.20	0.41
1:a:36:LEU:HD13	1:a:95:ILE:HD12	2.02	0.41
2:b:237:ILE:HD11	2:b:346:CYS:SG	2.60	0.41
6:h:48:LEU:HD21	6:h:56:ALA:HB1	2.03	0.41
8:q:127:GLU:OE1	8:q:433:LEU:HD12	2.21	0.41
9:z:407:VAL:HG13	9:z:495:TRP:CE3	2.54	0.41
11:P:144:VAL:HB	11:P:146:PHE:HE1	1.86	0.41
3:D:214:LEU:HA	3:D:398:ILE:HD11	2.03	0.41
3:D:347:HIS:CD2	3:D:349:ASP:HB2	2.56	0.41
3:D:458:MET:HE3	3:D:458:MET:HB3	1.84	0.41
5:G:182:MET:HE2	5:G:372:CYS:HB3	2.02	0.41
5:G:183:VAL:HG21	5:G:199:ALA:HB2	2.01	0.41
5:G:418:VAL:HG13	5:G:444:LEU:HD12	2.02	0.41
6:H:447:ARG:HB2	6:H:461:LEU:HD11	2.02	0.41
5:g:162:THR:HG21	12:g:601:ADP:H5'1	2.01	0.41
6:h:165:SER:O	6:h:165:SER:OG	2.38	0.41
8:q:70:ALA:HB2	8:q:101:THR:HG21	2.02	0.41
4:E:150:LYS:HB2	4:E:150:LYS:HE3	1.80	0.41
4:E:178:VAL:HG11	4:E:398:ALA:HA	2.03	0.41
9:Z:157:ARG:HH11	9:Z:166:ASP:CG	2.27	0.41
2:b:35:ILE:HD12	2:b:71:LEU:HD22	2.03	0.41
2:b:326:VAL:O	2:b:365:VAL:HB	2.19	0.41
3:d:88:ALA:O	3:d:92:VAL:HG23	2.21	0.41
5:g:133:MET:HG2	5:g:418:VAL:HG11	2.03	0.41
5:g:314:ARG:NH1	11:P:57:GLU:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:269:ALA:HB2	8:q:262:ALA:HB1	2.01	0.41
6:h:468:HIS:NE2	6:h:475:TYR:O	2.28	0.41
7:n:47:LEU:O	7:n:60:ALA:HB2	2.20	0.41
7:n:66:ARG:HD2	7:n:84:SER:OG	2.21	0.41
10:K:183:ARG:HD3	10:K:183:ARG:HA	1.81	0.41
3:D:144:GLY:HA3	3:D:432:LEU:HD21	2.01	0.41
6:H:26:ILE:HG23	6:H:105:LEU:HB3	2.02	0.41
9:Z:257:GLU:O	9:Z:261:LYS:HD3	2.21	0.41
2:b:162:ILE:HG13	2:b:494:THR:HG23	2.01	0.41
4:e:201:ARG:HA	4:e:201:ARG:NE	2.36	0.41
5:g:49:MET:HE2	9:z:76:LEU:HD11	2.03	0.41
10:K:124:PHE:HZ	10:K:357:ILE:O	2.04	0.41
2:B:52:LEU:HD12	3:D:538:THR:OG1	2.20	0.41
2:B:271:GLU:HG2	4:E:274:TYR:OH	2.21	0.41
2:B:326:VAL:HG13	2:B:327:THR:HG23	2.02	0.41
2:B:465:LEU:HD23	2:B:465:LEU:HA	1.87	0.41
3:D:227:LEU:HD23	3:D:376:ILE:HD12	2.02	0.41
4:E:185:MET:O	4:E:188:ILE:HG12	2.20	0.41
6:H:255:ILE:HD13	6:H:266:ILE:HG21	2.02	0.41
6:H:384:GLU:OE1	6:H:387:ARG:NH1	2.40	0.41
9:Z:71:HIS:CE1	8:q:6:PRO:HG3	2.55	0.41
9:Z:84:GLN:O	9:Z:88:THR:OG1	2.37	0.41
1:a:38:PRO:HG3	12:a:601:ADP:C5	2.56	0.41
4:e:335:ILE:HD11	6:h:226:GLU:HB2	2.03	0.41
5:g:95:THR:OG1	14:g:603:AF3:F2	2.19	0.41
5:g:444:LEU:HD23	5:g:444:LEU:HA	1.91	0.41
6:h:215:ALA:HA	6:h:359:ASN:O	2.20	0.41
8:q:66:THR:HB	8:q:390:ARG:NH1	2.36	0.41
9:z:157:ARG:NH1	9:z:166:ASP:OD1	2.46	0.41
9:z:177:LEU:HD23	9:z:177:LEU:HA	1.93	0.41
9:z:211:VAL:HG23	9:z:373:THR:HG21	2.03	0.41
9:z:425:HIS:O	9:z:428:SER:OG	2.34	0.41
11:P:130:ILE:HD11	11:P:184:PHE:CD2	2.56	0.41
3:D:496:ARG:NE	3:D:506:GLU:OE2	2.30	0.41
4:E:342:VAL:HG21	4:E:348:LEU:HD13	2.03	0.41
5:G:57:ILE:HG21	9:Z:76:LEU:HD21	2.03	0.41
6:H:61:ASP:OD2	15:H:701:HOH:O	2.22	0.41
9:Z:358:GLU:HG3	9:Z:360:PHE:CE1	2.55	0.41
8:q:11:PHE:CD1	9:z:69:ILE:HD11	2.56	0.41
10:K:94:LEU:O	10:K:96:VAL:HG13	2.21	0.41
10:K:275:HIS:H	10:K:275:HIS:HD2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:351:THR:O	10:K:354:GLN:HB2	2.21	0.41
11:P:189:LEU:HA	11:P:193:GLU:OE1	2.21	0.41
2:B:212:SER:OG	2:B:375:LEU:HA	2.21	0.40
1:a:244:THR:N	1:a:267:GLU:O	2.48	0.40
2:b:390:LEU:HA	2:b:390:LEU:HD23	1.87	0.40
3:d:71:THR:HA	3:d:400:GLU:CD	2.46	0.40
4:e:37:HIS:NE2	4:e:533:ILE:HD11	2.35	0.40
5:g:192:GLU:HG2	5:g:193:ILE:N	2.37	0.40
6:h:6:VAL:HB	8:q:80:HIS:CD2	2.56	0.40
7:n:104:GLU:CD	7:n:104:GLU:H	2.29	0.40
8:q:470:VAL:HG12	8:q:475:ASN:HB2	2.03	0.40
11:P:88:LYS:HA	11:P:88:LYS:HD2	1.84	0.40
11:P:94:VAL:HG23	11:P:138:ALA:HB2	2.03	0.40
11:P:139:ARG:HB3	11:P:139:ARG:NH1	2.35	0.40
1:A:301:VAL:HG12	5:G:330:ARG:HH11	1.86	0.40
2:B:42:THR:HG22	2:B:48:MET:O	2.22	0.40
2:B:245:ASP:HB2	2:B:297:TYR:CE1	2.56	0.40
2:B:445:MET:O	2:B:449:ILE:HG12	2.20	0.40
3:D:220:ASP:O	3:D:222:GLU:HG2	2.21	0.40
4:E:132:ARG:NH1	4:E:443:LEU:HD23	2.36	0.40
4:E:289:ILE:HG13	4:E:313:LEU:HB3	2.02	0.40
4:E:418:VAL:HG22	4:E:508:GLU:O	2.22	0.40
5:G:83:ILE:HG13	5:G:84:SER:N	2.36	0.40
5:G:223:ASP:CG	5:G:231:ARG:HH12	2.27	0.40
8:Q:221:MET:HE3	8:Q:223:PHE:CZ	2.56	0.40
8:Q:239:ILE:HD13	8:Q:328:VAL:HG11	2.02	0.40
9:Z:229:TYR:CE2	9:Z:287:LYS:HD3	2.56	0.40
3:d:149:THR:O	3:d:152:SER:OG	2.39	0.40
6:h:183:VAL:HG12	6:h:400:ILE:HD12	2.03	0.40
6:h:323:MET:HE1	8:q:230:ASP:OD2	2.21	0.40
9:z:272:LYS:O	9:z:276:GLU:HG2	2.21	0.40
9:z:430:LYS:HE2	9:z:430:LYS:HB2	1.88	0.40
10:K:75:ILE:HD12	10:K:75:ILE:HA	1.88	0.40
10:K:113:LYS:H	10:K:113:LYS:HG3	1.54	0.40
2:B:122:HIS:HD2	2:B:124:GLN:HB2	1.86	0.40
2:B:224:ILE:HG23	2:B:310:MET:HG3	2.04	0.40
3:D:88:ALA:O	3:D:92:VAL:HG23	2.21	0.40
1:a:127:GLU:OE1	1:a:130:ARG:NH2	2.33	0.40
1:a:145:ARG:NH2	1:a:149:ILE:HD11	2.36	0.40
1:a:357:CYS:HB2	1:a:378:ARG:HH22	1.87	0.40
2:b:325:LEU:HB3	2:b:369:GLU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:170:LYS:O	4:e:182:HIS:NE2	2.54	0.40
6:h:185:MET:CE	6:h:370:CYS:HB3	2.51	0.40
8:q:242:TYR:CE1	8:q:333:LEU:HD12	2.56	0.40
10:K:305:MET:O	10:K:308:GLY:N	2.52	0.40
11:P:13:ILE:O	11:P:17:LYS:HG2	2.21	0.40
1:A:386:ASP:OD2	10:K:53:TYR:OH	2.39	0.40
4:E:234:PHE:HE1	4:E:299:LEU:HD11	1.86	0.40
4:E:289:ILE:HG13	4:E:313:LEU:CB	2.51	0.40
9:Z:170:GLU:OE1	9:Z:170:GLU:N	2.54	0.40
9:Z:229:TYR:HE2	9:Z:287:LYS:HD3	1.86	0.40
3:d:459:GLU:OE1	3:d:481:ARG:HD3	2.21	0.40
4:e:102:ILE:HD11	4:e:515:GLN:HG3	2.04	0.40
4:e:185:MET:O	4:e:188:ILE:HG12	2.21	0.40
5:g:37:ILE:H	5:g:37:ILE:HG13	1.82	0.40
6:h:219:THR:OG1	6:h:312:GLY:O	2.22	0.40
9:z:235:VAL:HG22	9:z:334:ASN:C	2.46	0.40
11:P:88:LYS:HB3	11:P:143:ASP:OD1	2.21	0.40
11:P:209:GLU:N	11:P:209:GLU:OE1	2.54	0.40
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.81	0.40
3:D:218:ILE:HD11	3:D:397:VAL:HG22	2.02	0.40
3:D:472:ASN:HB3	3:D:475:SER:HG	1.87	0.40
4:E:196:VAL:HG21	4:E:209:ILE:CG1	2.52	0.40
9:Z:514:ASN:O	9:Z:518:VAL:HG23	2.21	0.40
1:a:104:ALA:HB1	1:a:117:VAL:HG11	2.04	0.40
3:d:148:LEU:HD11	3:d:432:LEU:HD11	2.04	0.40
4:e:169:ALA:HB2	4:e:409:ILE:HD11	2.03	0.40
10:K:140:LEU:O	10:K:342:GLY:HA3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	534/556 (96%)	508 (95%)	26 (5%)	0	100	100
1	a	530/556 (95%)	502 (95%)	28 (5%)	0	100	100
2	B	524/535 (98%)	502 (96%)	21 (4%)	1 (0%)	43	73
2	b	523/535 (98%)	503 (96%)	19 (4%)	1 (0%)	43	73
3	D	518/539 (96%)	507 (98%)	11 (2%)	0	100	100
3	d	518/539 (96%)	487 (94%)	31 (6%)	0	100	100
4	E	534/541 (99%)	511 (96%)	20 (4%)	3 (1%)	21	52
4	e	539/541 (100%)	516 (96%)	22 (4%)	1 (0%)	43	73
5	G	524/545 (96%)	502 (96%)	22 (4%)	0	100	100
5	g	536/545 (98%)	519 (97%)	17 (3%)	0	100	100
6	H	526/543 (97%)	506 (96%)	20 (4%)	0	100	100
6	h	523/543 (96%)	505 (97%)	18 (3%)	0	100	100
7	N	117/129 (91%)	110 (94%)	7 (6%)	0	100	100
7	n	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
8	Q	536/548 (98%)	516 (96%)	18 (3%)	2 (0%)	30	61
8	q	531/548 (97%)	512 (96%)	18 (3%)	1 (0%)	43	73
9	Z	523/531 (98%)	504 (96%)	18 (3%)	1 (0%)	43	73
9	z	525/531 (99%)	505 (96%)	19 (4%)	1 (0%)	43	73
10	K	309/375 (82%)	275 (89%)	32 (10%)	2 (1%)	21	52
11	P	186/239 (78%)	169 (91%)	17 (9%)	0	100	100
All	All	9173/9548 (96%)	8770 (96%)	390 (4%)	13 (0%)	49	78

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	10	ASP
9	Z	16	ALA
4	e	10	ASP
8	q	530	ALA
9	z	16	ALA
2	B	21	ALA
2	b	21	ALA
8	Q	534	LYS
4	E	9[B]	PHE
4	E	9[C]	PHE
10	K	333	PRO

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Mol	Chain	Res	Type
10	K	31	PHE
8	Q	533	PRO

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	447/463 (96%)	443 (99%)	4 (1%)	70	80
1	a	444/463 (96%)	441 (99%)	3 (1%)	76	82
2	B	418/427 (98%)	413 (99%)	5 (1%)	63	78
2	b	417/427 (98%)	411 (99%)	6 (1%)	59	76
3	D	442/452 (98%)	436 (99%)	6 (1%)	59	76
3	d	441/452 (98%)	436 (99%)	5 (1%)	65	78
4	E	452/456 (99%)	445 (98%)	7 (2%)	57	75
4	e	456/456 (100%)	449 (98%)	7 (2%)	57	75
5	G	456/469 (97%)	453 (99%)	3 (1%)	76	82
5	g	463/469 (99%)	456 (98%)	7 (2%)	57	75
6	H	435/443 (98%)	423 (97%)	12 (3%)	38	66
6	h	432/443 (98%)	422 (98%)	10 (2%)	44	70
7	N	96/105 (91%)	96 (100%)	0	100	100
7	n	96/105 (91%)	96 (100%)	0	100	100
8	Q	442/452 (98%)	437 (99%)	5 (1%)	65	78
8	q	438/452 (97%)	433 (99%)	5 (1%)	65	78
9	Z	437/442 (99%)	435 (100%)	2 (0%)	81	85
9	z	438/442 (99%)	436 (100%)	2 (0%)	81	85
10	K	264/318 (83%)	242 (92%)	22 (8%)	10	35
11	P	155/215 (72%)	150 (97%)	5 (3%)	34	64
All	All	7669/7951 (96%)	7553 (98%)	116 (2%)	55	75

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	352	VAL
1	A	526	ARG
1	A	537	SER
2	B	35	ILE
2	B	39	VAL
2	B	52	LEU
2	B	55	SER
2	B	513	VAL
3	D	83	VAL
3	D	385	THR
3	D	432	LEU
3	D	460	VAL
3	D	461	ILE
3	D	488	GLU
4	E	65	ASP
4	E	163	GLU
4	E	316	GLN
4	E	372	LEU
4	E	408	VAL
4	E	418	VAL
4	E	442	THR
5	G	50	LEU
5	G	442	GLN
5	G	460	ILE
6	H	6	VAL
6	H	9	LEU
6	H	22	LEU
6	H	85	SER
6	H	191	GLN
6	H	226	GLU
6	H	322	THR
6	H	338	SER
6	H	362	THR
6	H	400	ILE
6	H	405	VAL
6	H	460	ILE
8	Q	105	LEU
8	Q	212	ILE
8	Q	253	THR
8	Q	312	LEU
8	Q	534	LYS

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Mol	Chain	Res	Type
9	Z	246	SER
9	Z	281	VAL
1	a	352	VAL
1	a	387	GLU
1	a	526	ARG
2	b	35	ILE
2	b	39	VAL
2	b	52	LEU
2	b	55	SER
2	b	105	LEU
2	b	513	VAL
3	d	145	ILE
3	d	222	GLU
3	d	374	LEU
3	d	385	THR
3	d	404	SER
4	e	65	ASP
4	e	316	GLN
4	e	372	LEU
4	e	408	VAL
4	e	442	THR
4	e	535	LYS
4	e	540	GLU
5	g	8	LEU
5	g	163	LYS
5	g	192	GLU
5	g	365	ASP
5	g	460	ILE
5	g	528	LYS
5	g	529	LYS
6	h	9	LEU
6	h	22	LEU
6	h	85	SER
6	h	191	GLN
6	h	226	GLU
6	h	322	THR
6	h	338	SER
6	h	362	THR
6	h	400	ILE
6	h	460	ILE
8	q	105	LEU
8	q	212	ILE

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Mol	Chain	Res	Type
8	q	253	THR
8	q	312	LEU
8	q	534	LYS
9	z	15	ARG
9	z	526	MET
10	K	31	PHE
10	K	82	MET
10	K	85	ILE
10	K	88	HIS
10	K	91	TYR
10	K	100	GLU
10	K	113	LYS
10	K	183	ARG
10	K	213	LYS
10	K	221	LEU
10	K	261	LEU
10	K	275	HIS
10	K	303	THR
10	K	309	ILE
10	K	325	MET
10	K	328	LYS
10	K	336	LYS
10	K	359	LYS
10	K	364	GLU
10	K	370	VAL
10	K	371	HIS
10	K	375	PHE
11	P	15	ARG
11	P	91	PHE
11	P	139	ARG
11	P	154	CYS
11	P	165	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	103	ASN
1	A	150	ASN
1	A	164	ASN
1	A	170	ASN
1	A	217	ASN

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Mol	Chain	Res	Type
1	A	223	GLN
1	A	347	GLN
1	A	458	GLN
1	A	472	ASN
1	A	475	GLN
1	A	500	GLN
2	B	65	ASN
2	B	228	GLN
2	B	285	HIS
2	B	294	GLN
2	B	381	GLN
2	B	419	HIS
2	B	502	GLN
3	D	72	ASN
3	D	82	GLN
3	D	138	GLN
3	D	235	ASN
3	D	271	GLN
3	D	347	HIS
3	D	350	GLN
3	D	406	HIS
4	E	22	GLN
4	E	86	GLN
4	E	139	GLN
4	E	184	GLN
4	E	278	GLN
4	E	316	GLN
4	E	403	HIS
4	E	435	GLN
4	E	445	GLN
4	E	465	ASN
4	E	486	ASN
4	E	495	HIS
4	E	503	GLN
5	G	71	GLN
5	G	115	GLN
5	G	116	GLN
5	G	226	HIS
5	G	235	ASN
5	G	269	GLN
5	G	277	GLN
5	G	308	ASN

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Mol	Chain	Res	Type
5	G	390	ASN
5	G	392	GLN
5	G	400	ASN
5	G	420	HIS
5	G	472	GLN
5	G	504	GLN
6	H	228	GLN
6	H	252	ASN
6	H	272	ASN
6	H	331	GLN
6	H	448	GLN
6	H	459	ASN
6	H	470	GLN
6	H	522	ASN
7	N	13	GLN
7	N	81	GLN
8	Q	34	GLN
8	Q	102	ASN
8	Q	172	GLN
8	Q	175	ASN
8	Q	359	GLN
8	Q	472	GLN
9	Z	17	GLN
9	Z	68	GLN
9	Z	71	HIS
9	Z	95	ASN
9	Z	161	HIS
9	Z	198	HIS
9	Z	334	ASN
9	Z	425	HIS
9	Z	438	GLN
9	Z	475	GLN
9	Z	497	ASN
1	a	20	GLN
1	a	113	HIS
1	a	150	ASN
1	a	164	ASN
1	a	170	ASN
1	a	347	GLN
1	a	458	GLN
1	a	472	ASN
1	a	475	GLN

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Mol	Chain	Res	Type
2	b	122	HIS
2	b	174	HIS
2	b	228	GLN
2	b	294	GLN
2	b	298	ASN
2	b	381	GLN
2	b	423	GLN
2	b	502	GLN
3	d	80	GLN
3	d	178	GLN
3	d	301	GLN
3	d	406	HIS
3	d	472	ASN
3	d	486	GLN
4	e	22	GLN
4	e	86	GLN
4	e	139	GLN
4	e	167	GLN
4	e	184	GLN
4	e	278	GLN
4	e	316	GLN
4	e	391	ASN
4	e	403	HIS
4	e	445	GLN
4	e	465	ASN
4	e	486	ASN
4	e	495	HIS
5	g	28	ASN
5	g	64	ASN
5	g	111	HIS
5	g	116	GLN
5	g	226	HIS
5	g	235	ASN
5	g	253	GLN
5	g	276	GLN
5	g	284	GLN
5	g	301	GLN
5	g	453	GLN
5	g	504	GLN
5	g	544	GLN
6	h	264	GLN
6	h	272	ASN

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Mol	Chain	Res	Type
6	h	331	GLN
6	h	359	ASN
6	h	459	ASN
6	h	470	GLN
6	h	522	ASN
7	n	81	GLN
8	q	34	GLN
8	q	80	HIS
8	q	95	GLN
8	q	172	GLN
8	q	175	ASN
8	q	303	HIS
8	q	359	GLN
8	q	383	ASN
8	q	472	GLN
9	z	8	ASN
9	z	17	GLN
9	z	71	HIS
9	z	95	ASN
9	z	161	HIS
9	z	198	HIS
9	z	425	HIS
9	z	438	GLN
10	K	59	GLN
10	K	88	HIS
10	K	111	ASN
10	K	115	ASN
10	K	263	GLN
10	K	360	GLN
11	P	5	ASN
11	P	11	ASN
11	P	89	ASN
11	P	157	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 16 are monoatomic - leaving 32 for Mogul analysis.

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	$\# Z > 2$
12	ADP	H	601	13	28,29,29	1.38	5 (17%)	43,45,45	1.79	7 (16%)
12	ADP	A	601	13	28,29,29	1.39	5 (17%)	43,45,45	1.86	10 (23%)
12	ADP	d	601	13	28,29,29	1.37	5 (17%)	43,45,45	1.88	11 (25%)
14	AF3	e	603	-	0,3,3	-	-	-	-	-
12	ADP	z	601	13	28,29,29	1.39	5 (17%)	43,45,45	1.80	8 (18%)
14	AF3	q	603	-	0,3,3	-	-	-	-	-
12	ADP	E	601	13	28,29,29	1.41	4 (14%)	43,45,45	1.89	10 (23%)
12	ADP	a	601	13	28,29,29	1.40	5 (17%)	43,45,45	1.86	12 (27%)
12	ADP	e	601	13	28,29,29	1.40	4 (14%)	43,45,45	1.85	9 (20%)
12	ADP	G	601	13	28,29,29	1.40	5 (17%)	43,45,45	1.67	9 (20%)
14	AF3	b	603	-	0,3,3	-	-	-	-	-
14	AF3	D	603	-	0,3,3	-	-	-	-	-
12	ADP	D	601	13	28,29,29	1.38	5 (17%)	43,45,45	1.86	10 (23%)
14	AF3	H	603	-	0,3,3	-	-	-	-	-
14	AF3	z	603	-	0,3,3	-	-	-	-	-
14	AF3	G	603	-	0,3,3	-	-	-	-	-
14	AF3	a	603	-	0,3,3	-	-	-	-	-
12	ADP	b	601	13	28,29,29	1.39	5 (17%)	43,45,45	1.82	10 (23%)
14	AF3	d	603	-	0,3,3	-	-	-	-	-
12	ADP	B	601	13	28,29,29	1.39	5 (17%)	43,45,45	1.81	10 (23%)
14	AF3	E	603	-	0,3,3	-	-	-	-	-
14	AF3	Q	603	-	0,3,3	-	-	-	-	-
12	ADP	Q	601	13	28,29,29	1.35	5 (17%)	43,45,45	1.83	9 (20%)
14	AF3	Z	603	-	0,3,3	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	ADP	Z	601	13	28,29,29	1.37	5 (17%)	43,45,45	1.82	10 (23%)
12	ADP	g	601	13	28,29,29	1.38	5 (17%)	43,45,45	1.77	8 (18%)
12	ADP	h	601	13	28,29,29	1.35	5 (17%)	43,45,45	1.83	9 (20%)
14	AF3	h	603	-	0,3,3	-	-	-		
14	AF3	B	603	-	0,3,3	-	-	-		
12	ADP	q	601	13	28,29,29	1.37	5 (17%)	43,45,45	1.82	10 (23%)
14	AF3	A	603	-	0,3,3	-	-	-		
14	AF3	g	603	-	0,3,3	-	-	-		

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
12	ADP	H	601	13	-	6/16/32/32	0/3/3/3
12	ADP	a	601	13	-	1/16/32/32	0/3/3/3
12	ADP	g	601	13	-	8/16/32/32	0/3/3/3
12	ADP	e	601	13	-	1/16/32/32	0/3/3/3
12	ADP	A	601	13	-	1/16/32/32	0/3/3/3
12	ADP	b	601	13	-	2/16/32/32	0/3/3/3
12	ADP	B	601	13	-	1/16/32/32	0/3/3/3
12	ADP	d	601	13	-	0/16/32/32	0/3/3/3
12	ADP	G	601	13	-	7/16/32/32	0/3/3/3
12	ADP	h	601	13	-	6/16/32/32	0/3/3/3
12	ADP	z	601	13	-	0/16/32/32	0/3/3/3
12	ADP	q	601	13	-	4/16/32/32	0/3/3/3
12	ADP	D	601	13	-	1/16/32/32	0/3/3/3
12	ADP	Q	601	13	-	3/16/32/32	0/3/3/3
12	ADP	E	601	13	-	1/16/32/32	0/3/3/3
12	ADP	Z	601	13	-	0/16/32/32	0/3/3/3

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	z	601	ADP	C5-C4	4.59	1.47	1.39
12	E	601	ADP	C5-C4	4.47	1.47	1.39
12	a	601	ADP	C5-C4	4.46	1.47	1.39
12	g	601	ADP	C5-C4	4.44	1.47	1.39
12	G	601	ADP	C5-C4	4.42	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	601	ADP	C5-C4	4.42	1.47	1.39
12	D	601	ADP	C5-C4	4.41	1.47	1.39
12	Z	601	ADP	C5-C4	4.41	1.47	1.39
12	A	601	ADP	C5-C4	4.38	1.46	1.39
12	e	601	ADP	C5-C4	4.38	1.46	1.39
12	b	601	ADP	C5-C4	4.36	1.46	1.39
12	B	601	ADP	C5-C4	4.33	1.46	1.39
12	d	601	ADP	C5-C4	4.29	1.46	1.39
12	h	601	ADP	C5-C4	4.26	1.46	1.39
12	q	601	ADP	C5-C4	4.19	1.46	1.39
12	Q	601	ADP	C5-C4	4.18	1.46	1.39
12	E	601	ADP	C5-C6	2.67	1.48	1.41
12	q	601	ADP	C5-C6	2.63	1.48	1.41
12	G	601	ADP	C5-C6	2.63	1.48	1.41
12	D	601	ADP	C5-C6	2.62	1.48	1.41
12	Z	601	ADP	C5-C6	2.58	1.48	1.41
12	a	601	ADP	C5-C6	2.58	1.48	1.41
12	z	601	ADP	C5-N7	-2.57	1.34	1.39
12	g	601	ADP	C5-C6	2.56	1.48	1.41
12	z	601	ADP	C5-C6	2.56	1.48	1.41
12	Q	601	ADP	C5-C6	2.56	1.48	1.41
12	d	601	ADP	C5-C6	2.54	1.48	1.41
12	e	601	ADP	C5-C6	2.53	1.48	1.41
12	A	601	ADP	C5-C6	2.53	1.48	1.41
12	B	601	ADP	C5-C6	2.52	1.48	1.41
12	e	601	ADP	C5-N7	-2.52	1.34	1.39
12	B	601	ADP	C5-N7	-2.49	1.34	1.39
12	H	601	ADP	C5-C6	2.48	1.47	1.41
12	b	601	ADP	C5-C6	2.48	1.47	1.41
12	d	601	ADP	C5-N7	-2.48	1.34	1.39
12	h	601	ADP	C5-N7	-2.47	1.34	1.39
12	q	601	ADP	C5-N7	-2.46	1.34	1.39
12	a	601	ADP	C5-N7	-2.46	1.34	1.39
12	H	601	ADP	C5-N7	-2.45	1.34	1.39
12	b	601	ADP	C5-N7	-2.45	1.34	1.39
12	Z	601	ADP	C5-N7	-2.45	1.34	1.39
12	A	601	ADP	C5-N7	-2.44	1.34	1.39
12	g	601	ADP	C5-N7	-2.43	1.34	1.39
12	b	601	ADP	C4-N9	-2.43	1.32	1.37
12	G	601	ADP	C5-N7	-2.42	1.34	1.39
12	B	601	ADP	C4-N9	-2.42	1.32	1.37
12	E	601	ADP	C5-N7	-2.39	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	q	601	ADP	C8-N7	2.39	1.36	1.31
12	h	601	ADP	C5-C6	2.38	1.47	1.41
12	D	601	ADP	C5-N7	-2.37	1.34	1.39
12	Q	601	ADP	C5-N7	-2.36	1.34	1.39
12	Q	601	ADP	C8-N7	2.32	1.36	1.31
12	B	601	ADP	C8-N7	2.31	1.36	1.31
12	d	601	ADP	C8-N7	2.31	1.36	1.31
12	A	601	ADP	C8-N7	2.30	1.36	1.31
12	G	601	ADP	C4-N9	-2.27	1.33	1.37
12	z	601	ADP	C8-N7	2.26	1.36	1.31
12	g	601	ADP	C8-N7	2.26	1.36	1.31
12	q	601	ADP	C4-N9	-2.26	1.33	1.37
12	D	601	ADP	C8-N7	2.24	1.36	1.31
12	Z	601	ADP	C8-N7	2.24	1.36	1.31
12	G	601	ADP	C8-N7	2.23	1.36	1.31
12	E	601	ADP	C8-N7	2.23	1.36	1.31
12	b	601	ADP	C8-N7	2.21	1.35	1.31
12	D	601	ADP	C4-N9	-2.20	1.33	1.37
12	a	601	ADP	C8-N7	2.20	1.35	1.31
12	e	601	ADP	C8-N7	2.17	1.35	1.31
12	Z	601	ADP	C4-N9	-2.15	1.33	1.37
12	Q	601	ADP	C4-N9	-2.13	1.33	1.37
12	h	601	ADP	C4-N9	-2.13	1.33	1.37
12	h	601	ADP	C8-N7	2.12	1.35	1.31
12	H	601	ADP	C8-N7	2.11	1.35	1.31
12	z	601	ADP	C4-N9	-2.10	1.33	1.37
12	a	601	ADP	C4-N9	-2.09	1.33	1.37
12	d	601	ADP	C4-N9	-2.04	1.33	1.37
12	H	601	ADP	C4-N9	-2.03	1.33	1.37
12	A	601	ADP	C4-N9	-2.02	1.33	1.37
12	g	601	ADP	C4-N9	-2.00	1.33	1.37

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	601	ADP	C5-C4-N3	-6.12	118.29	126.72
12	e	601	ADP	C5-C4-N3	-5.96	118.51	126.72
12	z	601	ADP	C5-C4-N3	-5.92	118.57	126.72
12	g	601	ADP	C5-C4-N3	-5.92	118.57	126.72
12	Z	601	ADP	C5-C4-N3	-5.77	118.77	126.72
12	d	601	ADP	C5-C4-N3	-5.74	118.81	126.72
12	H	601	ADP	C5-C4-N3	-5.72	118.84	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	601	ADP	C5-C4-N3	-5.70	118.87	126.72
12	q	601	ADP	C5-C4-N3	-5.66	118.93	126.72
12	a	601	ADP	C5-C4-N3	-5.63	118.97	126.72
12	Q	601	ADP	C5-C4-N3	-5.58	119.04	126.72
12	h	601	ADP	C5-C4-N3	-5.57	119.05	126.72
12	D	601	ADP	C5-C4-N3	-5.44	119.23	126.72
12	G	601	ADP	C5-C4-N3	-5.39	119.30	126.72
12	B	601	ADP	C5-C4-N3	-5.20	119.56	126.72
12	b	601	ADP	C5-C4-N3	-5.07	119.73	126.72
12	e	601	ADP	N3-C4-N9	4.74	135.22	127.17
12	h	601	ADP	N3-C4-N9	4.64	135.07	127.17
12	E	601	ADP	N3-C4-N9	4.62	135.03	127.17
12	H	601	ADP	N3-C4-N9	4.61	135.01	127.17
12	z	601	ADP	N3-C4-N9	4.55	134.91	127.17
12	Z	601	ADP	N3-C4-N9	4.53	134.87	127.17
12	a	601	ADP	N3-C4-N9	4.52	134.85	127.17
12	g	601	ADP	N3-C4-N9	4.50	134.82	127.17
12	A	601	ADP	N3-C4-N9	4.48	134.79	127.17
12	d	601	ADP	N3-C4-N9	4.41	134.66	127.17
12	D	601	ADP	N3-C4-N9	4.32	134.52	127.17
12	Q	601	ADP	N3-C4-N9	4.28	134.45	127.17
12	b	601	ADP	N3-C4-N9	4.12	134.17	127.17
12	q	601	ADP	N3-C4-N9	4.09	134.13	127.17
12	G	601	ADP	N3-C4-N9	4.06	134.08	127.17
12	B	601	ADP	N3-C4-N9	4.02	134.01	127.17
12	E	601	ADP	C2-N3-C4	3.88	121.32	111.83
12	q	601	ADP	C2-N3-C4	3.86	121.26	111.83
12	Q	601	ADP	C2-N3-C4	3.81	121.13	111.83
12	e	601	ADP	C2-N3-C4	3.80	121.11	111.83
12	q	601	ADP	C4-C5-N7	-3.79	106.25	110.58
12	d	601	ADP	C2-N3-C4	3.71	120.89	111.83
12	g	601	ADP	C2-N3-C4	3.70	120.87	111.83
12	A	601	ADP	C2-N3-C4	3.70	120.87	111.83
12	g	601	ADP	C4-C5-N7	-3.67	106.39	110.58
12	a	601	ADP	C2-N3-C4	3.67	120.79	111.83
12	G	601	ADP	C4-C5-N7	-3.65	106.40	110.58
12	E	601	ADP	C4-C5-N7	-3.62	106.45	110.58
12	Q	601	ADP	C4-C5-N7	-3.61	106.45	110.58
12	d	601	ADP	C4-C5-N7	-3.61	106.46	110.58
12	h	601	ADP	C2-N3-C4	3.60	120.63	111.83
12	H	601	ADP	C2-N3-C4	3.59	120.60	111.83
12	Q	601	ADP	N3-C2-N1	-3.58	123.17	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	601	ADP	C2-N3-C4	3.57	120.56	111.83
12	z	601	ADP	C2-N3-C4	3.57	120.54	111.83
12	D	601	ADP	C2-N3-C4	3.52	120.42	111.83
12	q	601	ADP	N3-C2-N1	-3.51	123.27	128.58
12	A	601	ADP	C4-C5-N7	-3.51	106.57	110.58
12	Z	601	ADP	C4-C5-N7	-3.50	106.58	110.58
12	z	601	ADP	C4-C5-N7	-3.50	106.58	110.58
12	D	601	ADP	C4-C5-N7	-3.50	106.58	110.58
12	B	601	ADP	C4-C5-N7	-3.46	106.63	110.58
12	B	601	ADP	C2-N3-C4	3.43	120.20	111.83
12	G	601	ADP	C2-N3-C4	3.42	120.18	111.83
12	a	601	ADP	C4-C5-N7	-3.42	106.68	110.58
12	e	601	ADP	N3-C2-N1	-3.38	123.47	128.58
12	b	601	ADP	C2-N3-C4	3.38	120.08	111.83
12	A	601	ADP	N3-C2-N1	-3.36	123.49	128.58
12	e	601	ADP	C4-C5-N7	-3.33	106.78	110.58
12	b	601	ADP	C4-C5-N7	-3.33	106.78	110.58
12	E	601	ADP	N3-C2-N1	-3.32	123.55	128.58
12	d	601	ADP	N3-C2-N1	-3.32	123.56	128.58
12	a	601	ADP	N3-C2-N1	-3.31	123.58	128.58
12	h	601	ADP	N3-C2-N1	-3.30	123.59	128.58
12	H	601	ADP	C4-C5-N7	-3.26	106.85	110.58
12	h	601	ADP	C4-C5-N7	-3.21	106.91	110.58
12	g	601	ADP	N3-C2-N1	-3.18	123.76	128.58
12	b	601	ADP	C4-N9-C8	3.18	109.08	105.74
12	h	601	ADP	C4-N9-C8	3.18	109.07	105.74
12	b	601	ADP	N3-C2-N1	-3.13	123.85	128.58
12	H	601	ADP	N3-C2-N1	-3.12	123.86	128.58
12	D	601	ADP	N3-C2-N1	-3.09	123.91	128.58
12	B	601	ADP	N3-C2-N1	-3.04	123.99	128.58
12	D	601	ADP	C4-N9-C8	3.00	108.89	105.74
12	Z	601	ADP	N3-C2-N1	-3.00	124.05	128.58
12	z	601	ADP	N3-C2-N1	-2.95	124.11	128.58
12	Q	601	ADP	C4-N9-C8	2.90	108.78	105.74
12	B	601	ADP	C4-N9-C8	2.90	108.78	105.74
12	a	601	ADP	C4-N9-C8	2.89	108.78	105.74
12	G	601	ADP	N3-C2-N1	-2.87	124.24	128.58
12	A	601	ADP	C4-N9-C8	2.80	108.68	105.74
12	Z	601	ADP	C4-N9-C8	2.78	108.66	105.74
12	d	601	ADP	C4-N9-C8	2.69	108.56	105.74
12	H	601	ADP	C4-N9-C8	2.66	108.54	105.74
12	Q	601	ADP	C5-N7-C8	2.65	107.62	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	601	ADP	C4-N9-C8	2.65	108.52	105.74
12	G	601	ADP	C4-N9-C8	2.64	108.51	105.74
12	d	601	ADP	C5-N7-C8	2.63	107.58	103.45
12	A	601	ADP	C5-N7-C8	2.60	107.53	103.45
12	q	601	ADP	C5-N7-C8	2.58	107.51	103.45
12	g	601	ADP	C5-N7-C8	2.58	107.51	103.45
12	q	601	ADP	C6-C5-N7	2.56	137.03	132.09
12	E	601	ADP	C5-N7-C8	2.54	107.45	103.45
12	D	601	ADP	C5-N7-C8	2.52	107.42	103.45
12	a	601	ADP	C5-N7-C8	2.52	107.42	103.45
12	D	601	ADP	C3'-C2'-C1'	2.52	106.23	101.46
12	q	601	ADP	C4-N9-C8	2.51	108.37	105.74
12	b	601	ADP	O3B-PB-O2B	2.50	117.19	107.80
12	G	601	ADP	C5-N7-C8	2.50	107.39	103.45
12	g	601	ADP	C4-N9-C8	2.49	108.35	105.74
12	Z	601	ADP	C5-N7-C8	2.49	107.36	103.45
12	Q	601	ADP	C6-C5-N7	2.46	136.84	132.09
12	e	601	ADP	C5-N7-C8	2.46	107.32	103.45
12	h	601	ADP	C5-N7-C8	2.45	107.30	103.45
12	z	601	ADP	C5-N7-C8	2.41	107.24	103.45
12	B	601	ADP	C5-N7-C8	2.40	107.23	103.45
12	d	601	ADP	C3'-C2'-C1'	2.40	106.00	101.46
12	B	601	ADP	O3B-PB-O2B	2.40	116.80	107.80
12	b	601	ADP	C5-N7-C8	2.39	107.21	103.45
12	E	601	ADP	C4-N9-C8	2.38	108.24	105.74
12	A	601	ADP	C2'-C3'-C4'	2.38	107.20	102.61
12	z	601	ADP	C4-N9-C8	2.37	108.22	105.74
12	H	601	ADP	C5-N7-C8	2.35	107.14	103.45
12	E	601	ADP	C2'-C3'-C4'	2.33	107.11	102.61
12	Q	601	ADP	N9-C8-N7	-2.33	110.63	113.94
12	G	601	ADP	C6-C5-N7	2.32	136.56	132.09
12	a	601	ADP	C2'-C3'-C4'	2.30	107.06	102.61
12	D	601	ADP	C6-C5-N7	2.26	136.45	132.09
12	B	601	ADP	C6-C5-N7	2.25	136.43	132.09
12	d	601	ADP	C6-C5-N7	2.24	136.41	132.09
12	q	601	ADP	O4'-C1'-N9	2.23	112.37	108.09
12	A	601	ADP	C6-C5-N7	2.20	136.34	132.09
12	b	601	ADP	N9-C8-N7	-2.20	110.82	113.94
12	b	601	ADP	C6-C5-N7	2.19	136.31	132.09
12	a	601	ADP	C6-C5-N7	2.19	136.30	132.09
12	h	601	ADP	N9-C8-N7	-2.18	110.84	113.94
12	E	601	ADP	C6-C5-N7	2.18	136.29	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	601	ADP	N9-C8-N7	-2.17	110.86	113.94
12	E	601	ADP	O3B-PB-O2B	2.16	115.92	107.80
12	d	601	ADP	N9-C8-N7	-2.16	110.87	113.94
12	A	601	ADP	N9-C8-N7	-2.16	110.87	113.94
12	e	601	ADP	C2'-C3'-C4'	2.16	106.78	102.61
12	a	601	ADP	O4'-C1'-N9	2.15	112.22	108.09
12	g	601	ADP	C6-C5-N7	2.15	136.23	132.09
12	d	601	ADP	O5'-C5'-C4'	2.14	116.27	108.99
12	h	601	ADP	O2A-PA-O1A	2.12	122.31	112.44
12	a	601	ADP	C2'-C1'-N9	-2.12	108.03	113.30
12	B	601	ADP	N9-C8-N7	-2.12	110.93	113.94
12	q	601	ADP	N9-C8-N7	-2.12	110.93	113.94
12	Z	601	ADP	O2A-PA-O1A	2.11	122.24	112.44
12	a	601	ADP	N9-C8-N7	-2.10	110.95	113.94
12	z	601	ADP	O2A-PA-O1A	2.10	122.22	112.44
12	Z	601	ADP	N9-C8-N7	-2.04	111.05	113.94
12	e	601	ADP	O3B-PB-O2B	2.02	115.38	107.80
12	G	601	ADP	N9-C8-N7	-2.01	111.09	113.94
12	Z	601	ADP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	601	ADP	PA-O3A-PB-O3B
12	G	601	ADP	C5'-O5'-PA-O2A
12	G	601	ADP	C5'-O5'-PA-O3A
12	H	601	ADP	PA-O3A-PB-O2B
12	H	601	ADP	PB-O3A-PA-O5'
12	Q	601	ADP	C5'-O5'-PA-O3A
12	g	601	ADP	PA-O3A-PB-O3B
12	g	601	ADP	C5'-O5'-PA-O2A
12	g	601	ADP	C5'-O5'-PA-O3A
12	q	601	ADP	C5'-O5'-PA-O3A
12	H	601	ADP	C3'-C4'-C5'-O5'
12	h	601	ADP	O4'-C4'-C5'-O5'
12	H	601	ADP	O4'-C4'-C5'-O5'
12	h	601	ADP	C3'-C4'-C5'-O5'
12	E	601	ADP	PB-O3A-PA-O5'
12	g	601	ADP	PB-O3A-PA-O5'
12	h	601	ADP	PA-O3A-PB-O2B
12	g	601	ADP	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
12	Q	601	ADP	PB-O3A-PA-O2A
12	q	601	ADP	PB-O3A-PA-O2A
12	D	601	ADP	C5'-O5'-PA-O1A
12	G	601	ADP	C5'-O5'-PA-O1A
12	q	601	ADP	C5'-O5'-PA-O1A
12	B	601	ADP	O4'-C4'-C5'-O5'
12	b	601	ADP	O4'-C4'-C5'-O5'
12	h	601	ADP	PB-O3A-PA-O2A
12	e	601	ADP	PB-O3A-PA-O5'
12	g	601	ADP	O4'-C1'-N9-C8
12	G	601	ADP	PA-O3A-PB-O1B
12	G	601	ADP	PA-O3A-PB-O2B
12	H	601	ADP	PA-O3A-PB-O3B
12	g	601	ADP	PA-O3A-PB-O2B
12	h	601	ADP	PA-O3A-PB-O3B
12	a	601	ADP	PB-O3A-PA-O2A
12	h	601	ADP	PB-O3A-PA-O1A
12	g	601	ADP	C2'-C1'-N9-C4
12	H	601	ADP	PA-O3A-PB-O1B
12	A	601	ADP	PB-O3A-PA-O2A
12	Q	601	ADP	PB-O3A-PA-O1A
12	q	601	ADP	PB-O3A-PA-O1A
12	G	601	ADP	C3'-C4'-C5'-O5'
12	b	601	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

29 monomers are involved in 45 short contacts:

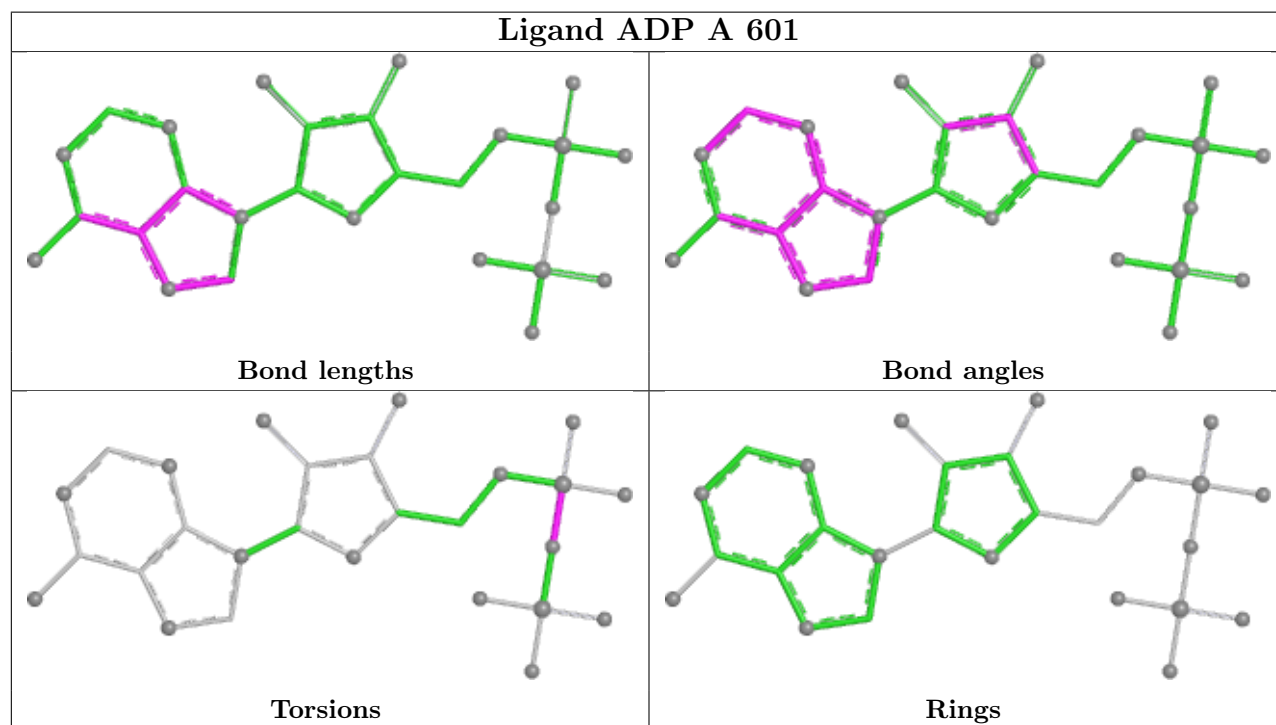
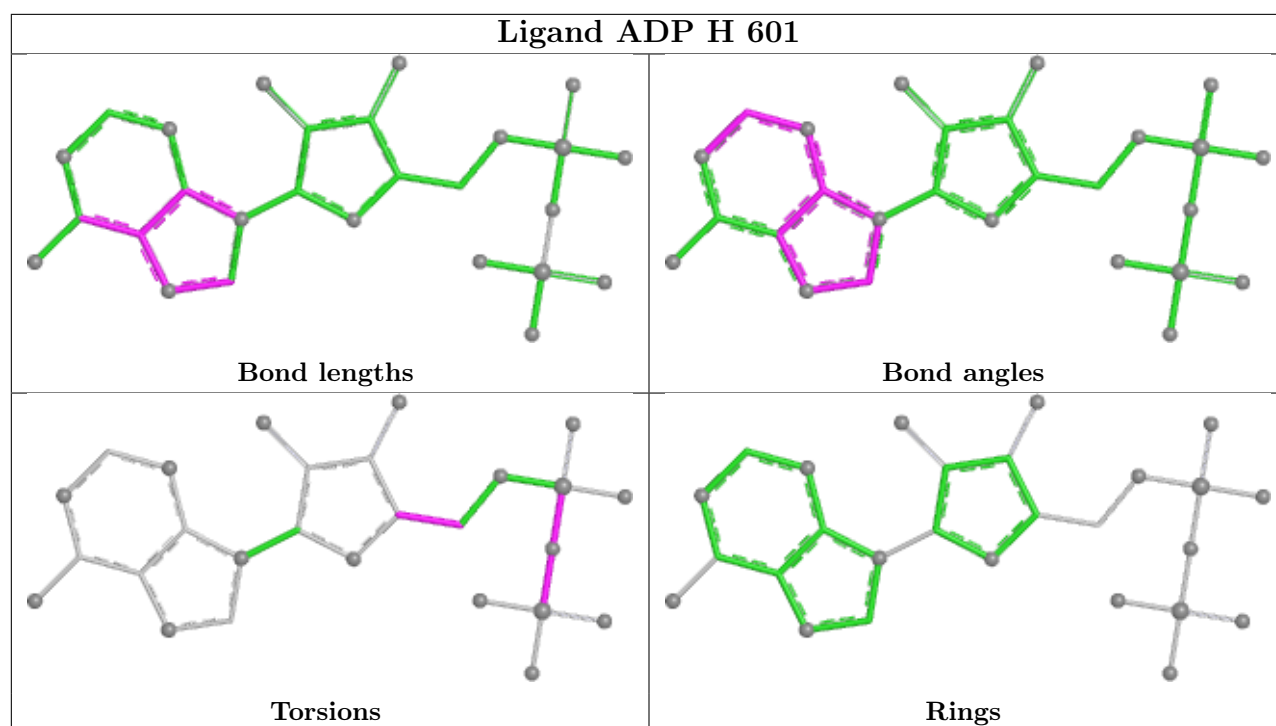
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	601	ADP	1	0
12	A	601	ADP	1	0
12	d	601	ADP	2	0
14	e	603	AF3	2	0
12	z	601	ADP	2	0
14	q	603	AF3	2	0
12	E	601	ADP	4	0
12	a	601	ADP	1	0
12	e	601	ADP	2	0
12	G	601	ADP	1	0
14	b	603	AF3	1	0
12	D	601	ADP	2	0
14	H	603	AF3	2	0

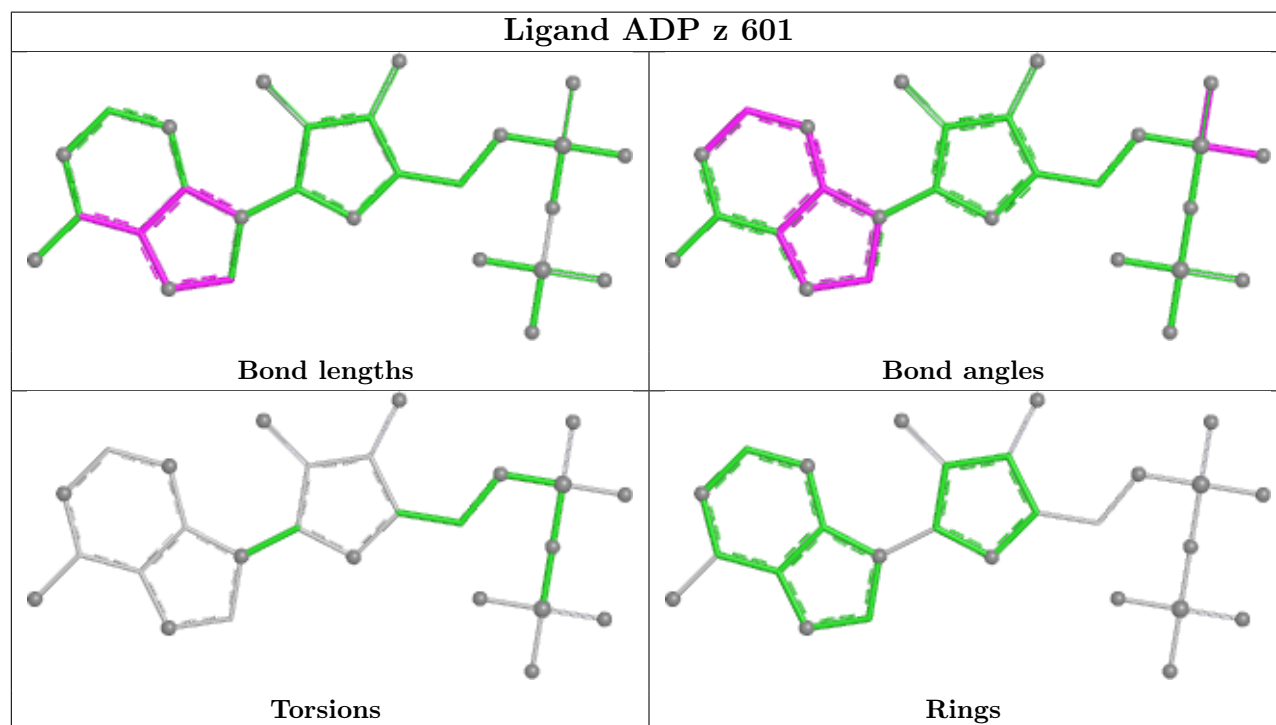
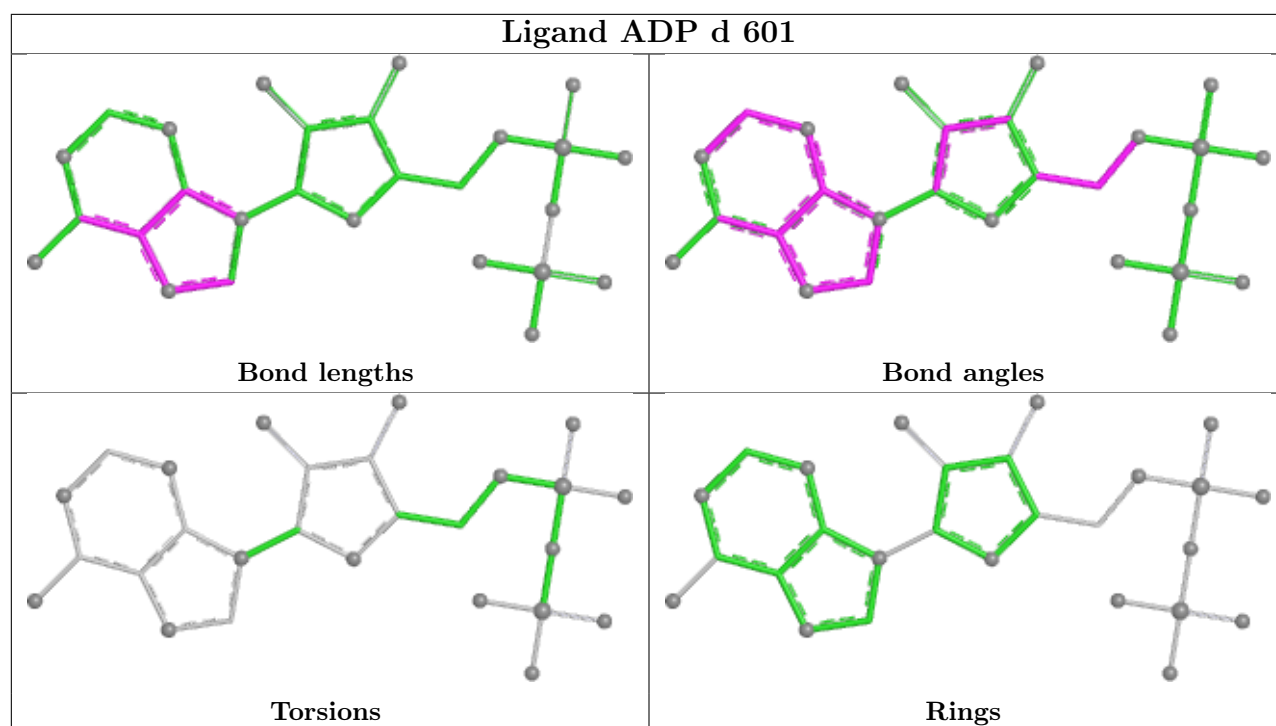
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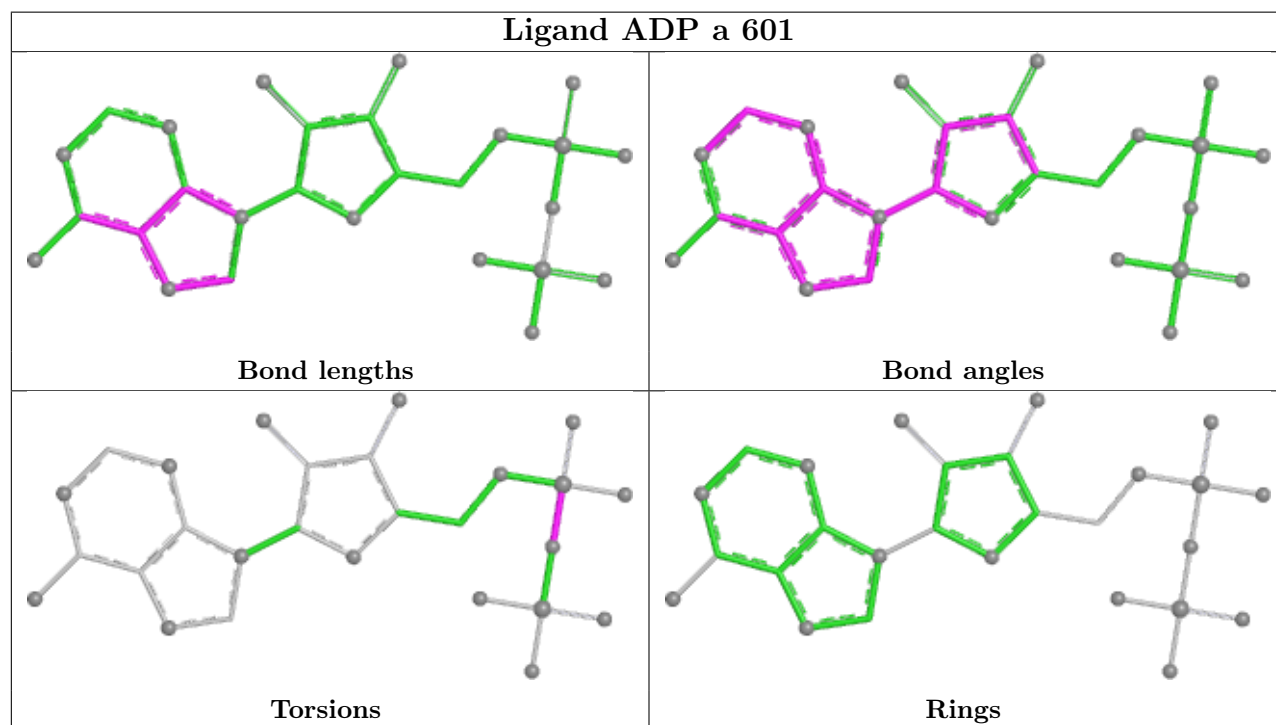
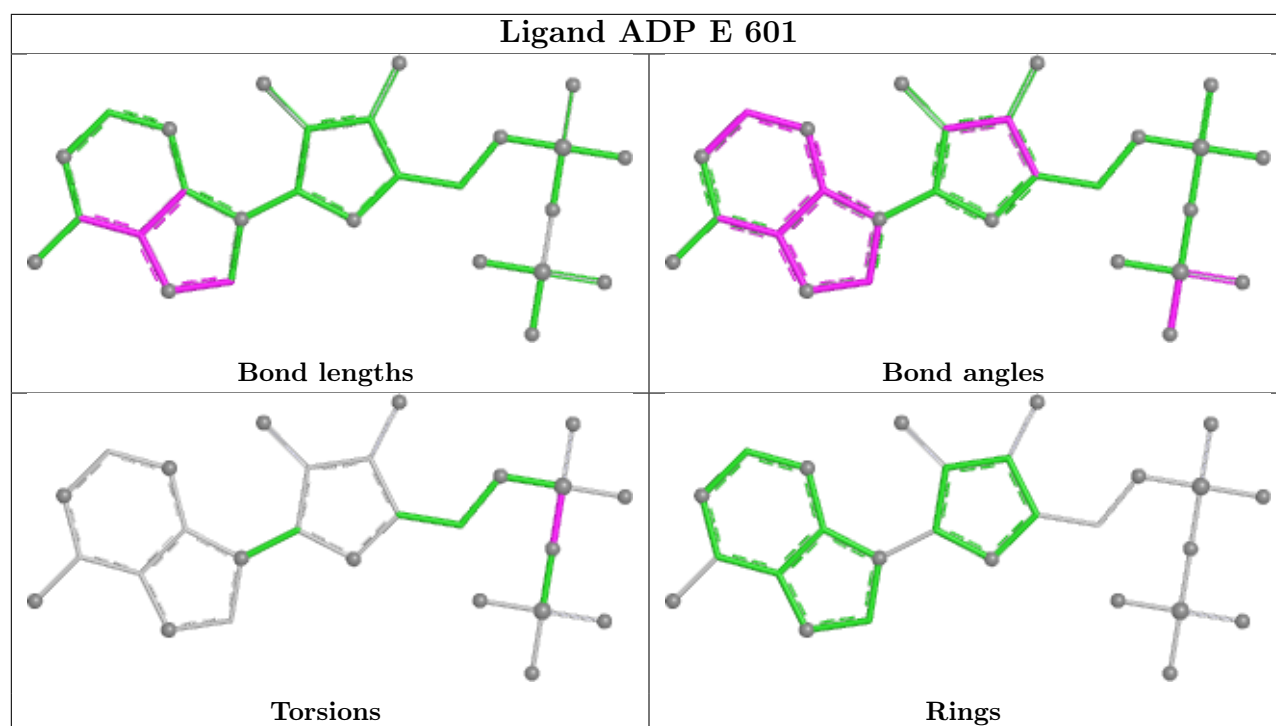
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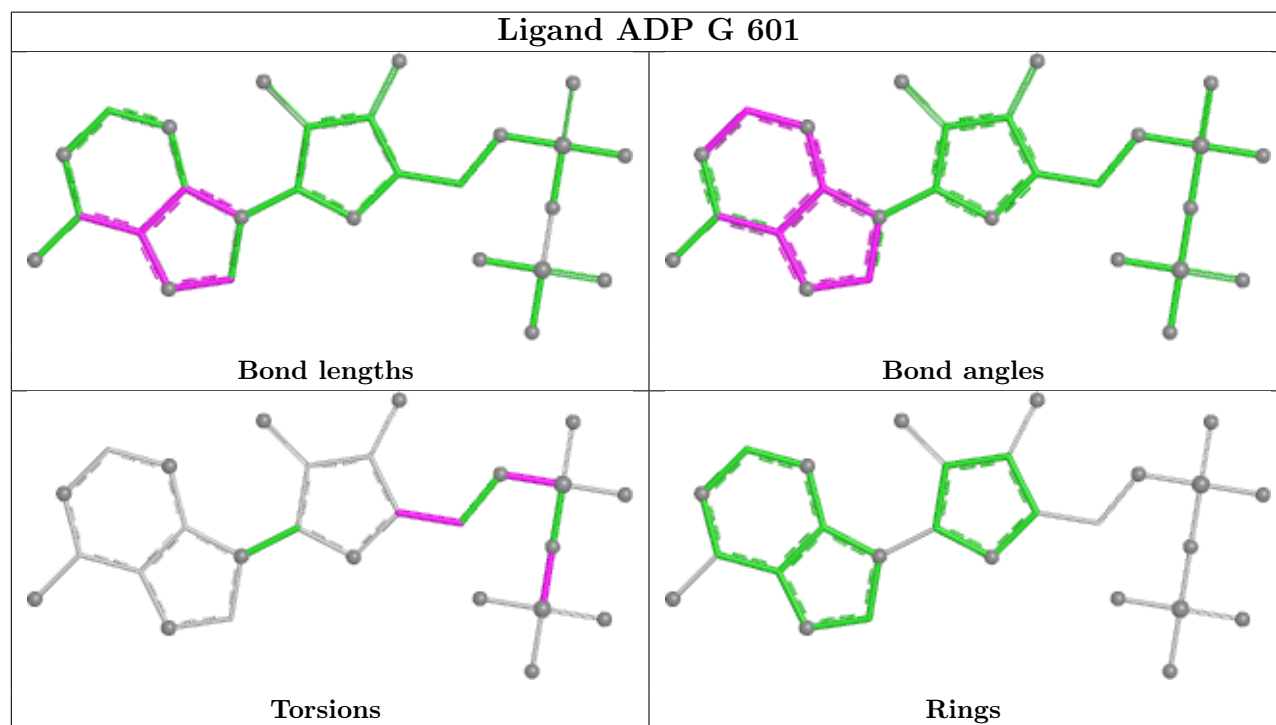
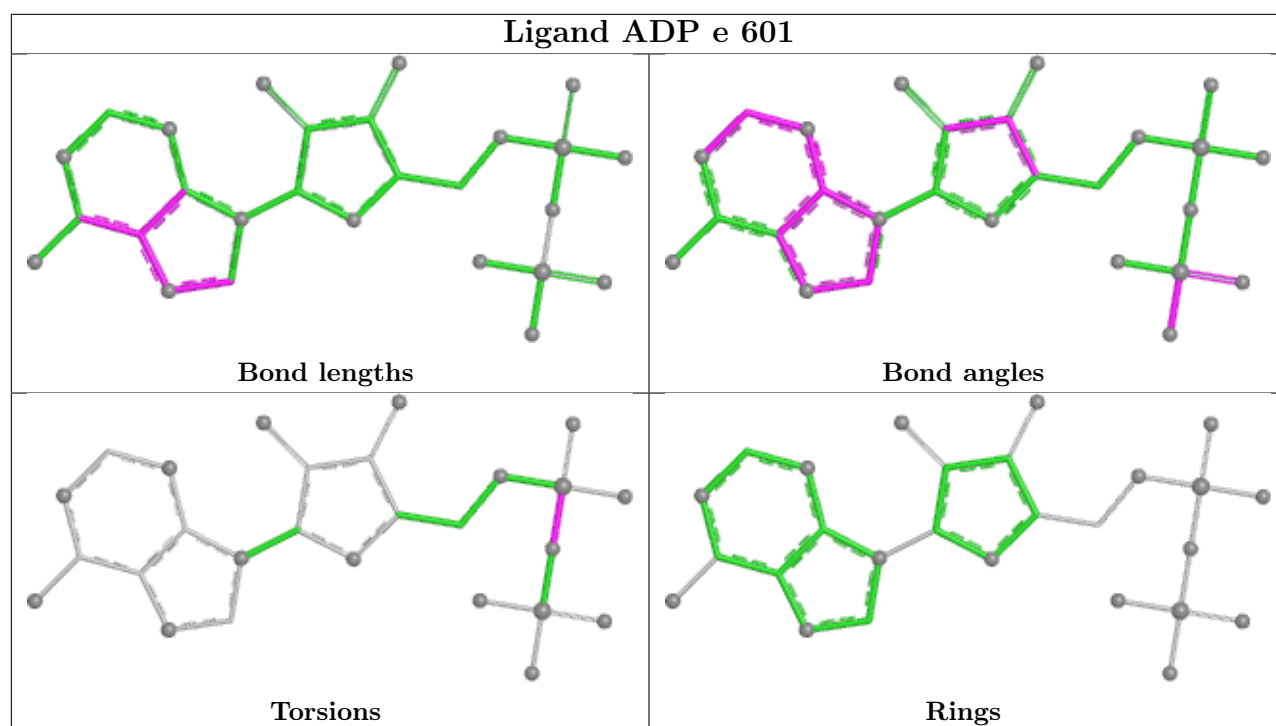
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	z	603	AF3	2	0
14	G	603	AF3	2	0
12	b	601	ADP	3	0
14	d	603	AF3	3	0
12	B	601	ADP	4	0
14	E	603	AF3	3	0
14	Q	603	AF3	2	0
12	Q	601	ADP	1	0
14	Z	603	AF3	2	0
12	Z	601	ADP	2	0
12	g	601	ADP	3	0
12	h	601	ADP	2	0
14	h	603	AF3	2	0
14	B	603	AF3	1	0
12	q	601	ADP	2	0
14	g	603	AF3	2	0

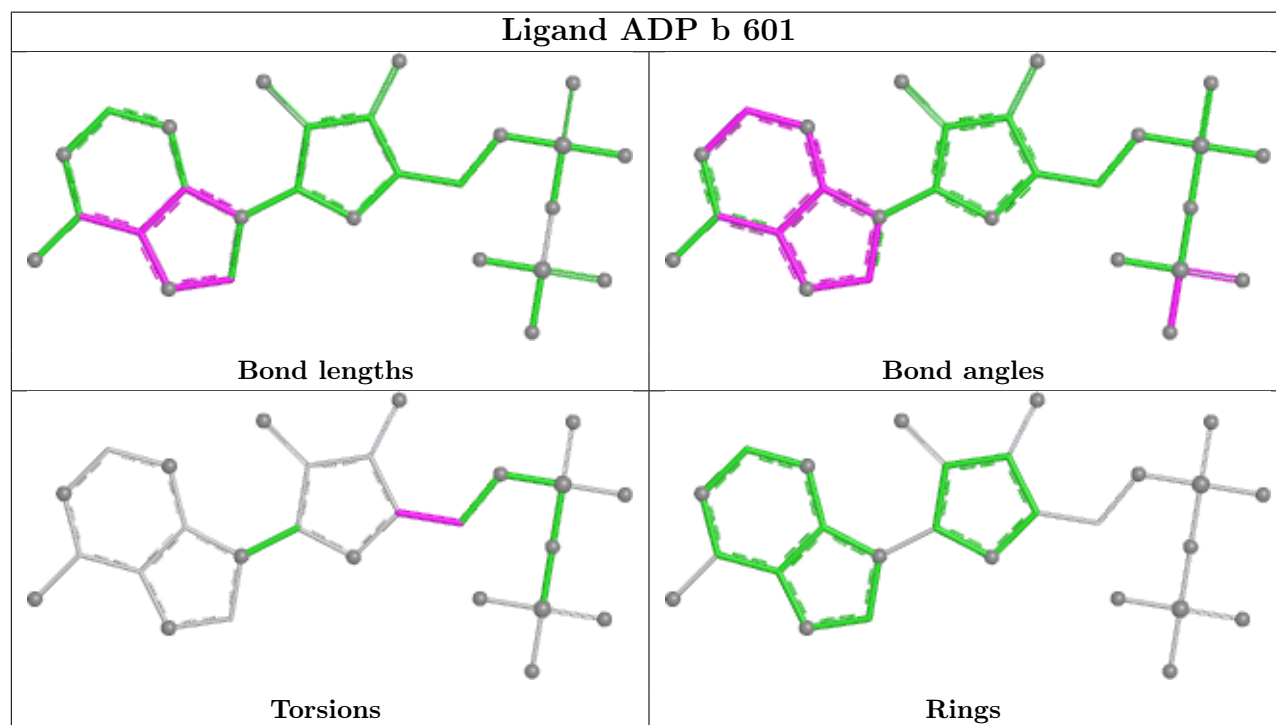
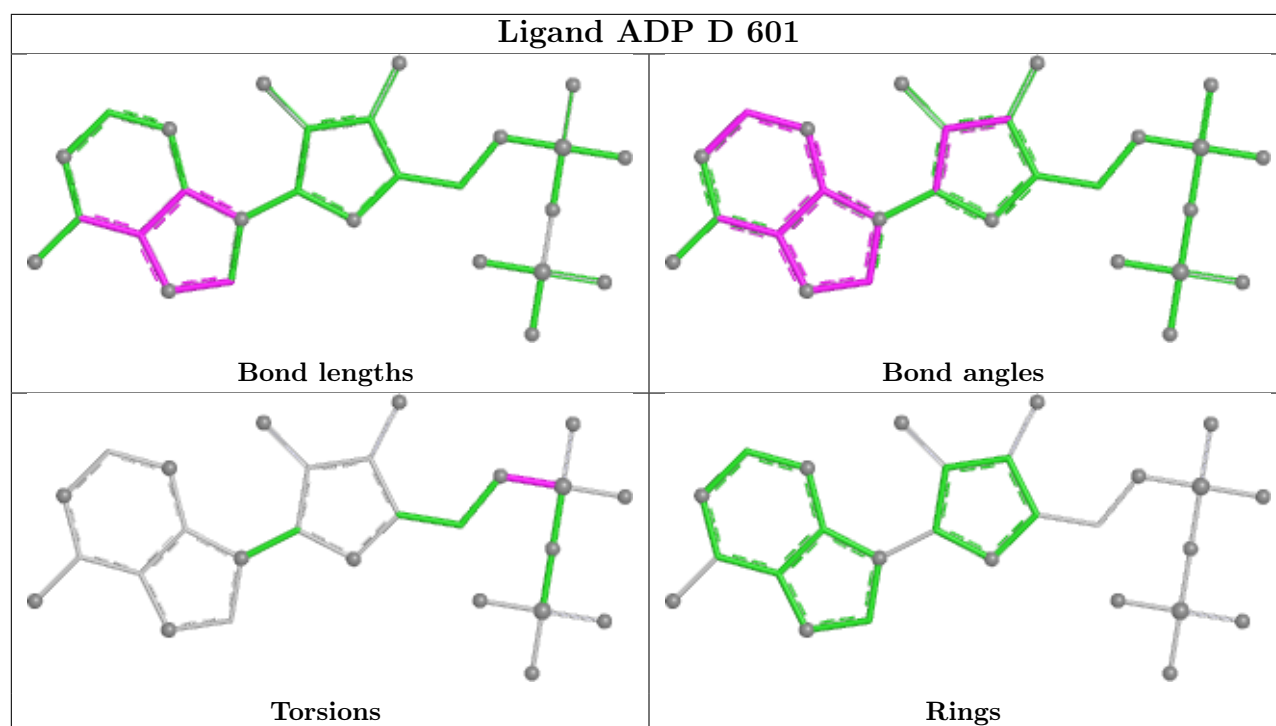
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

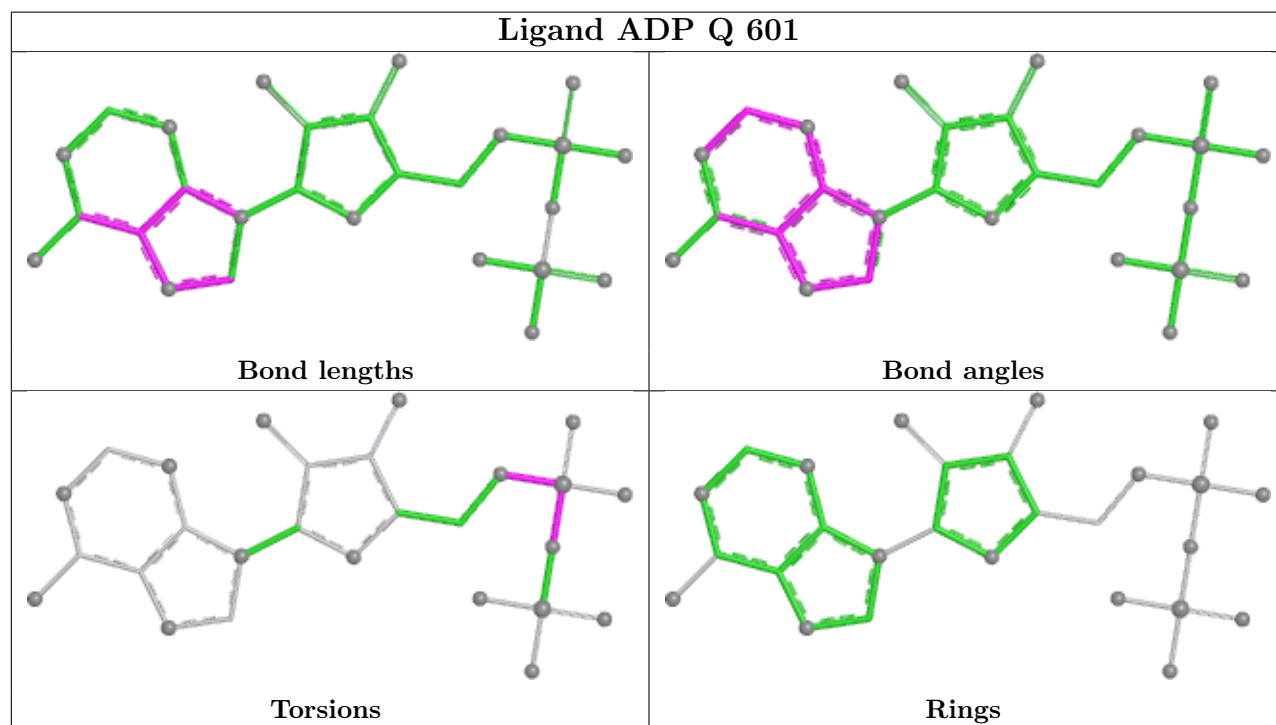
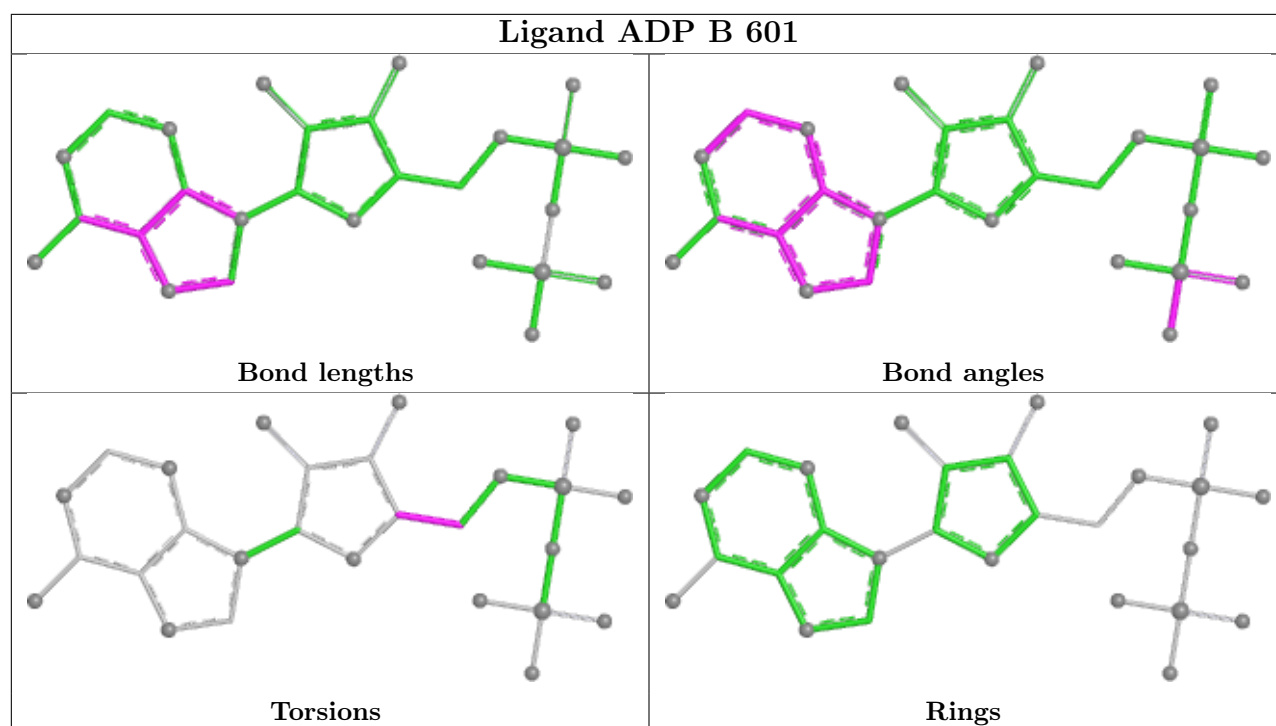


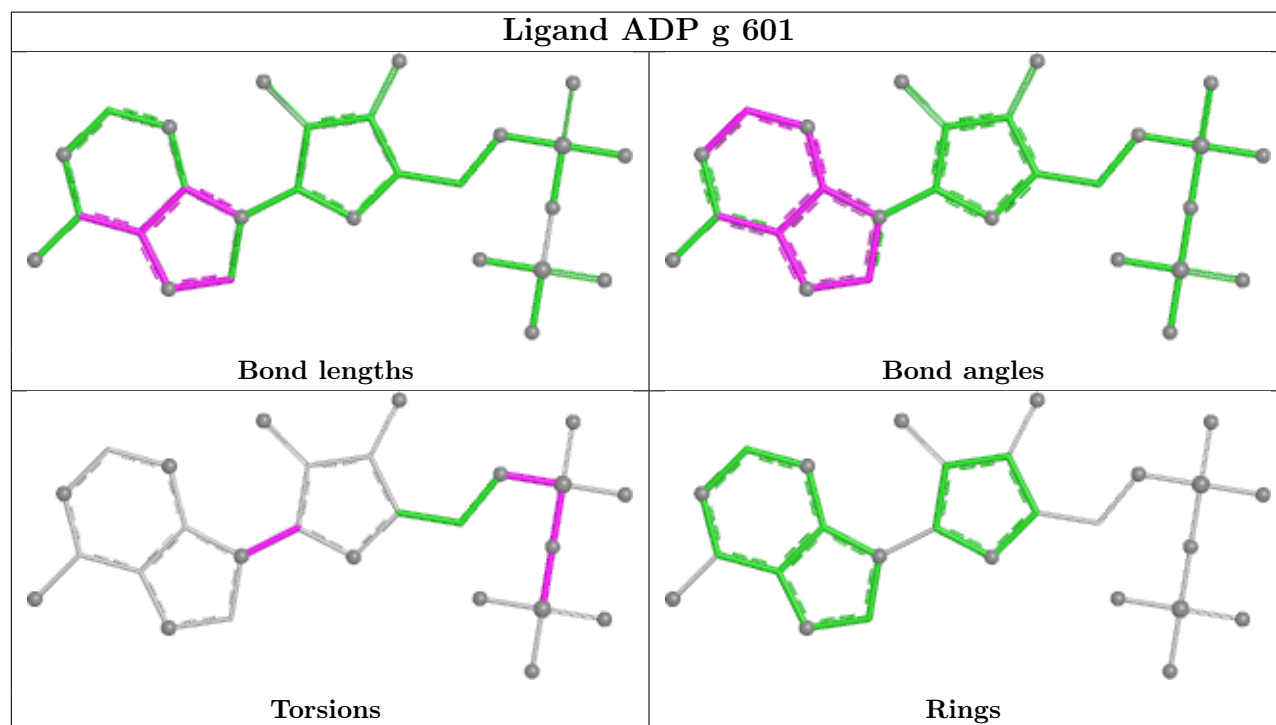
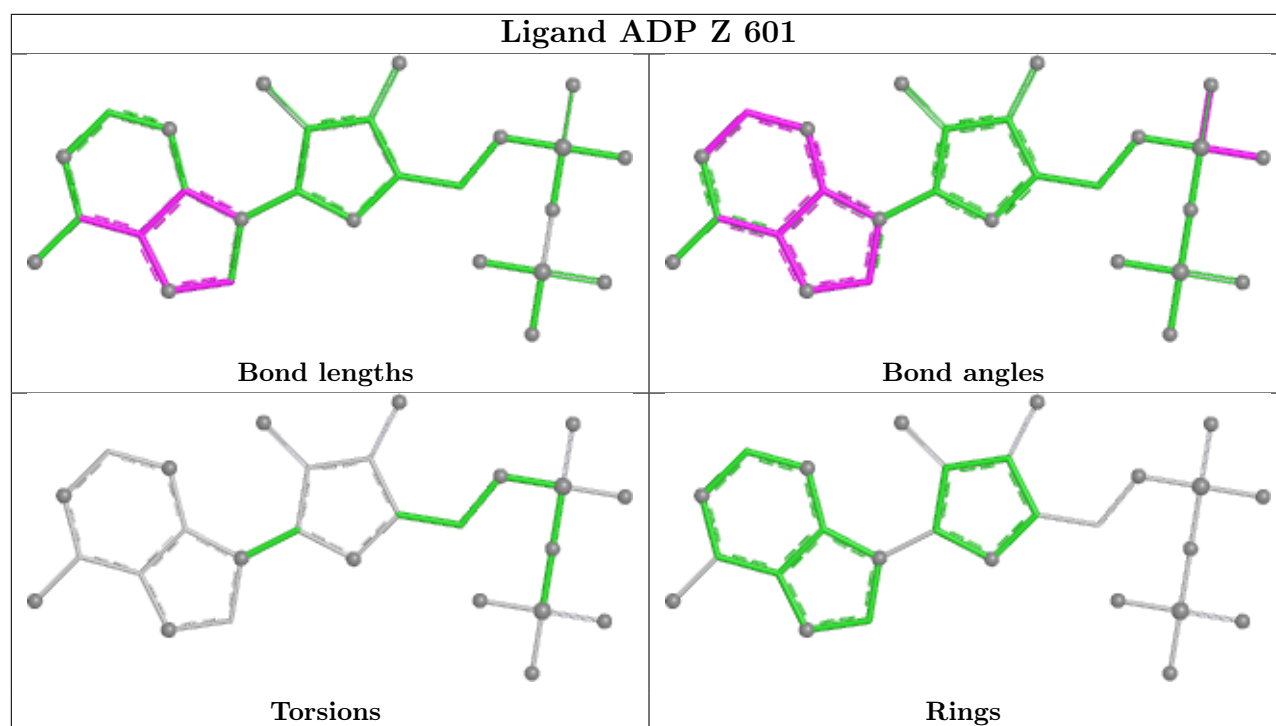


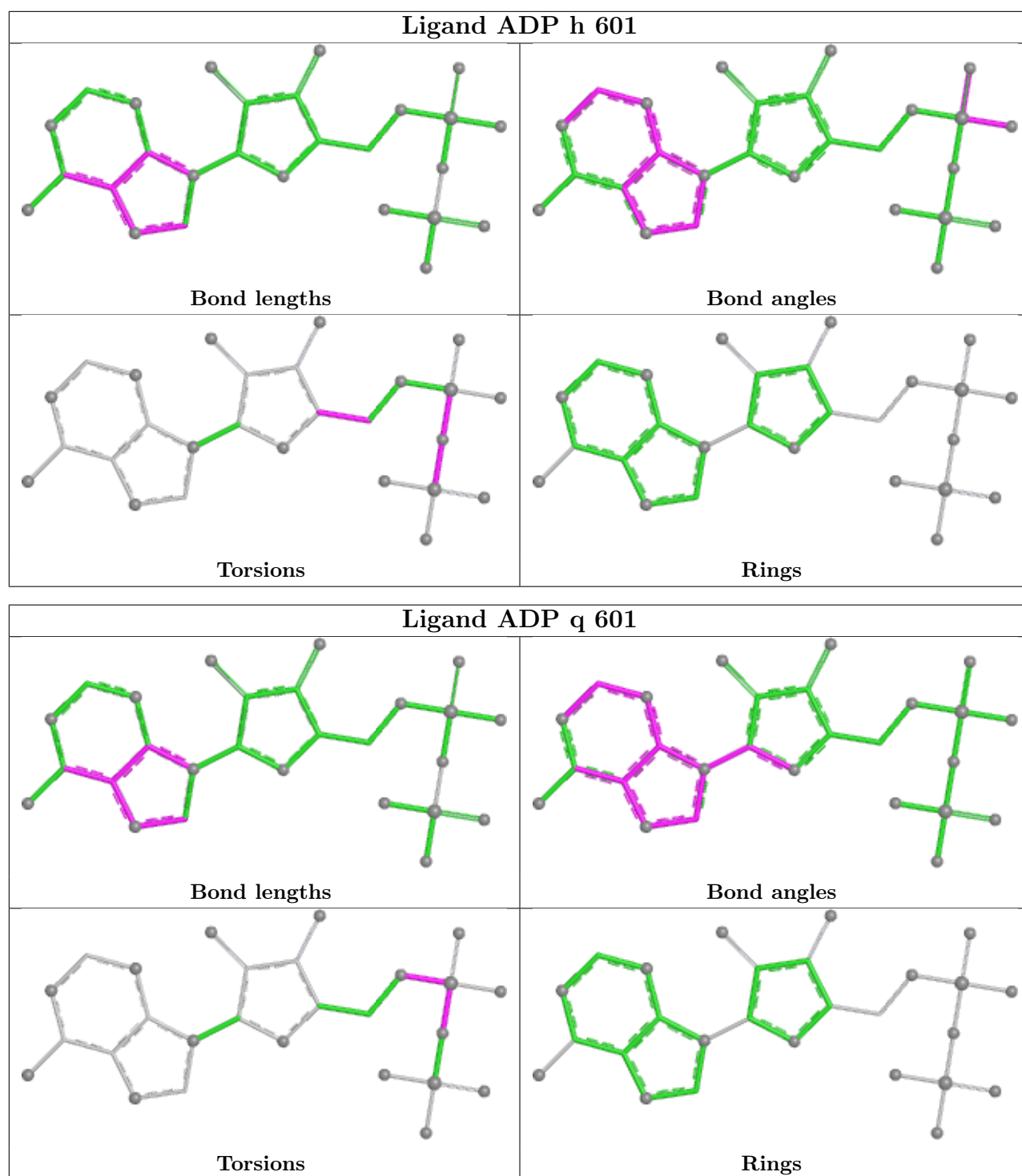












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

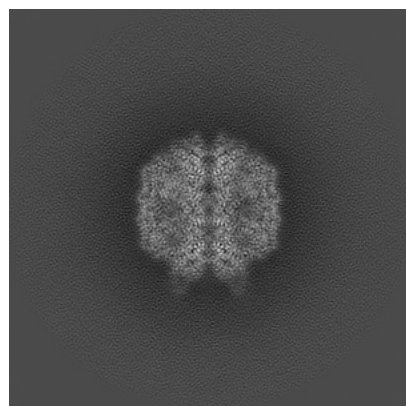
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12606. These allow visual inspection of the internal detail of the map and identification of artifacts.

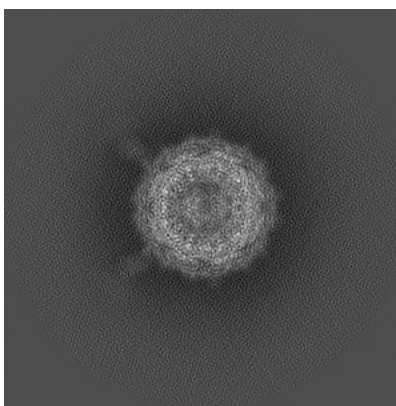
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

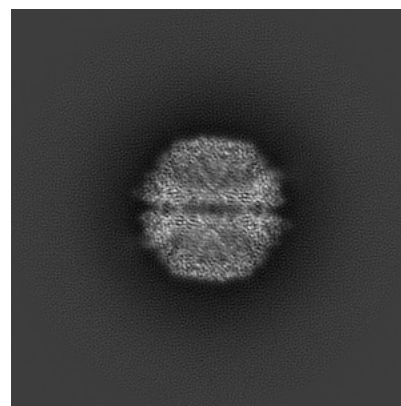
6.1.1 Primary map



X

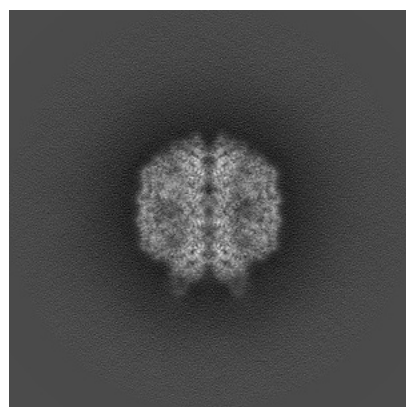


Y

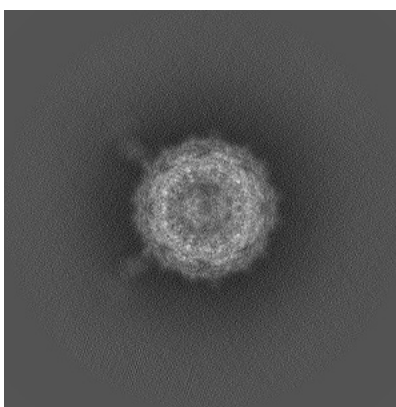


Z

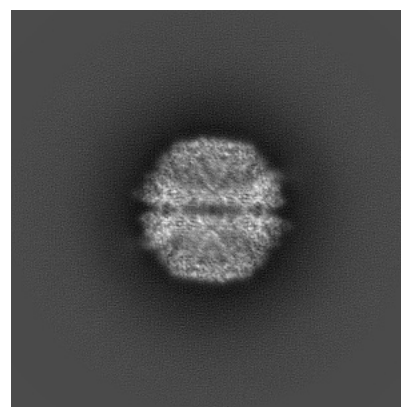
6.1.2 Raw map



X



Y

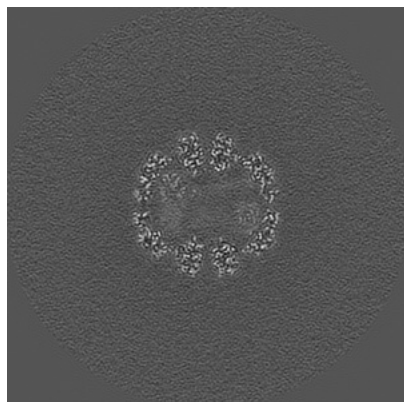


Z

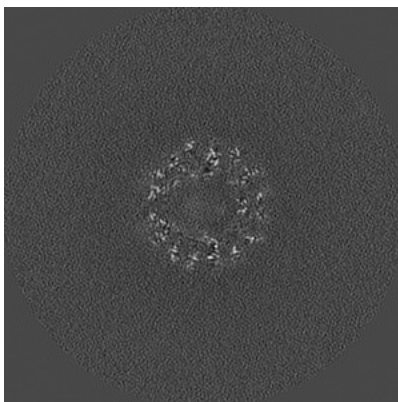
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

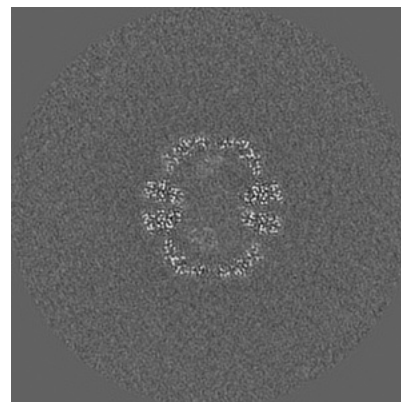
6.2.1 Primary map



X Index: 200

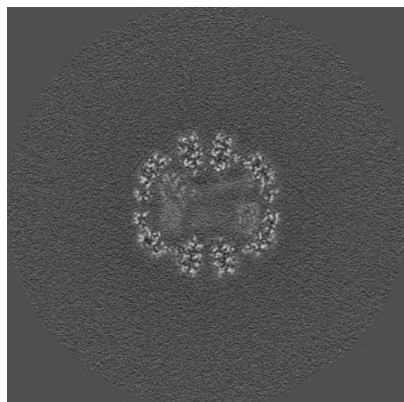


Y Index: 200

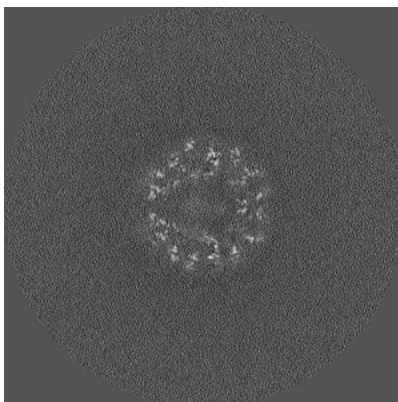


Z Index: 200

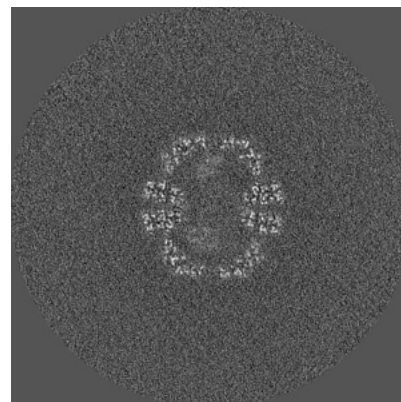
6.2.2 Raw map



X Index: 200



Y Index: 200

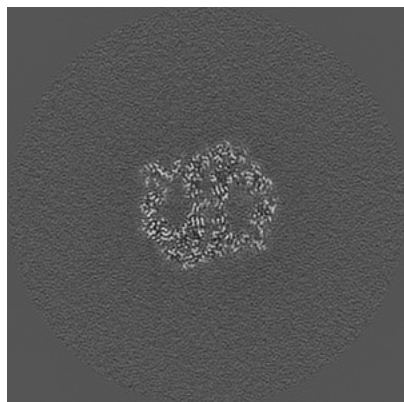


Z Index: 200

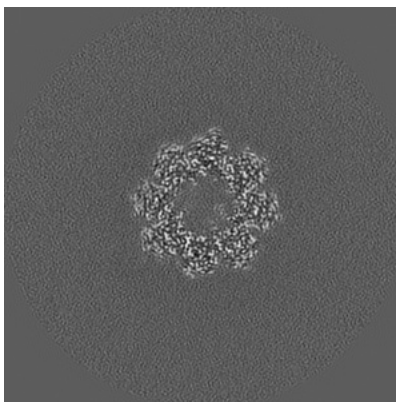
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

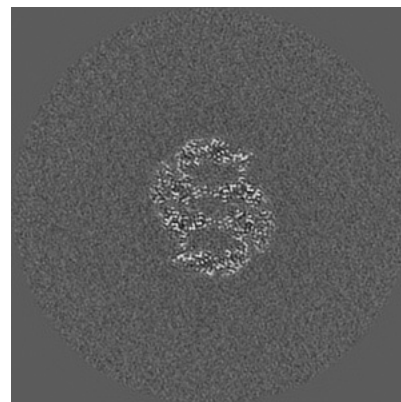
6.3.1 Primary map



X Index: 169

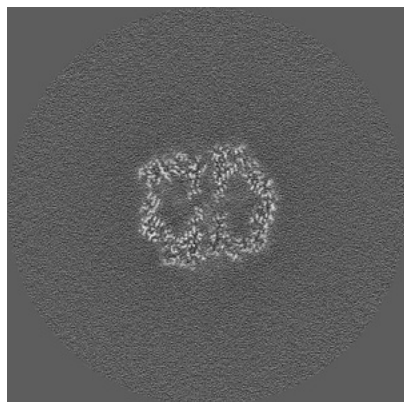


Y Index: 186

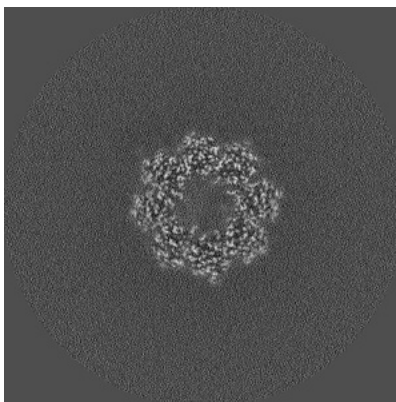


Z Index: 166

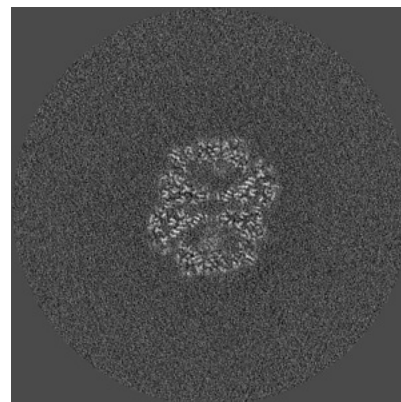
6.3.2 Raw map



X Index: 173



Y Index: 212

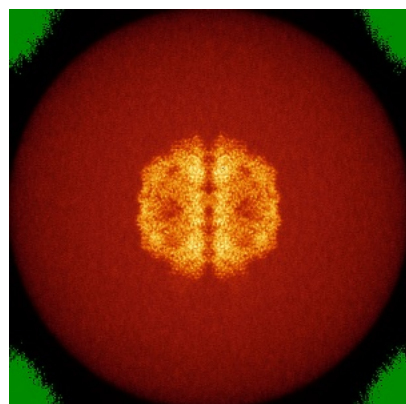


Z Index: 231

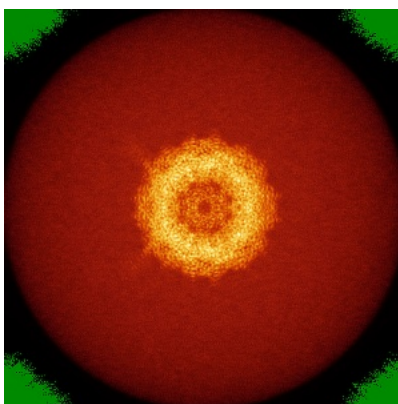
The images above show the largest variance slices of the map in three orthogonal directions.

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

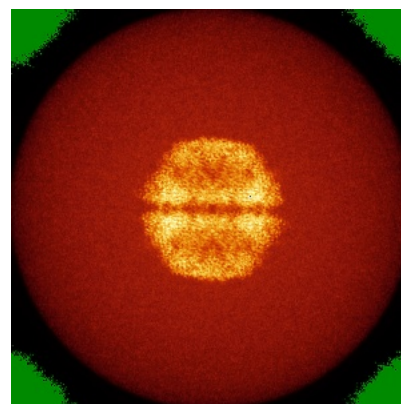
6.4.1 Primary map



X

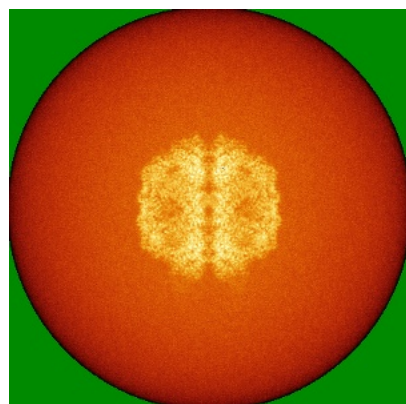


Y

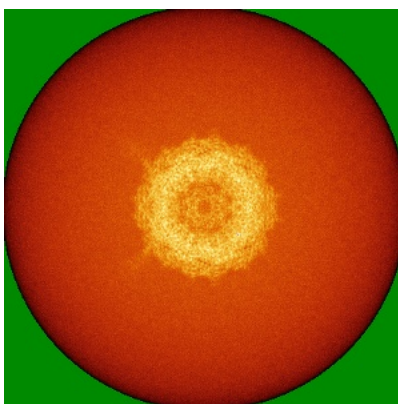


Z

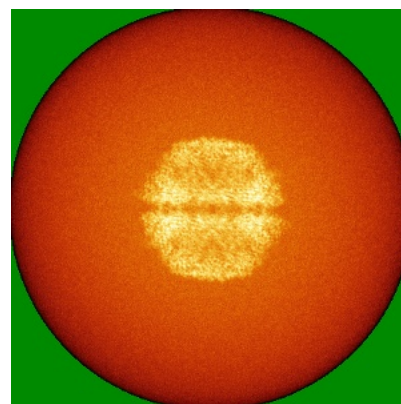
6.4.2 Raw map



X



Y

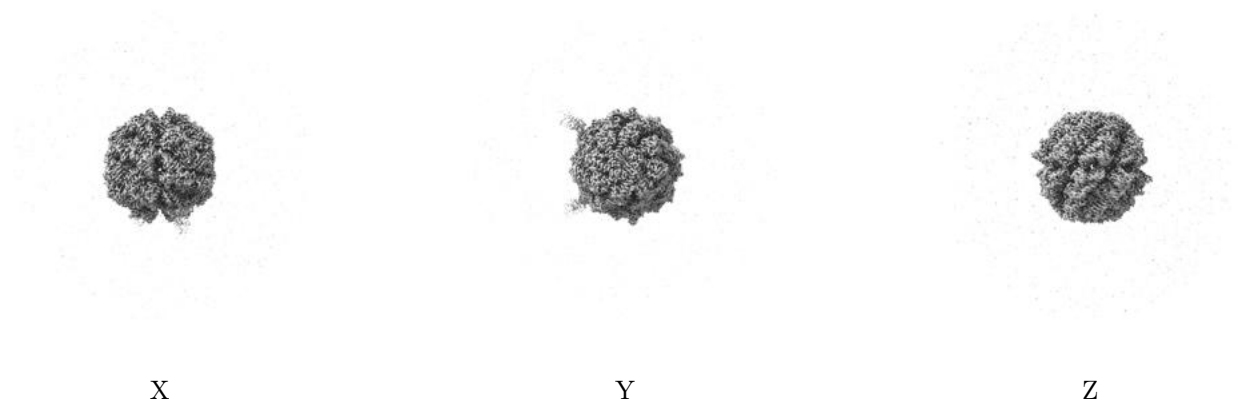


Z

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.

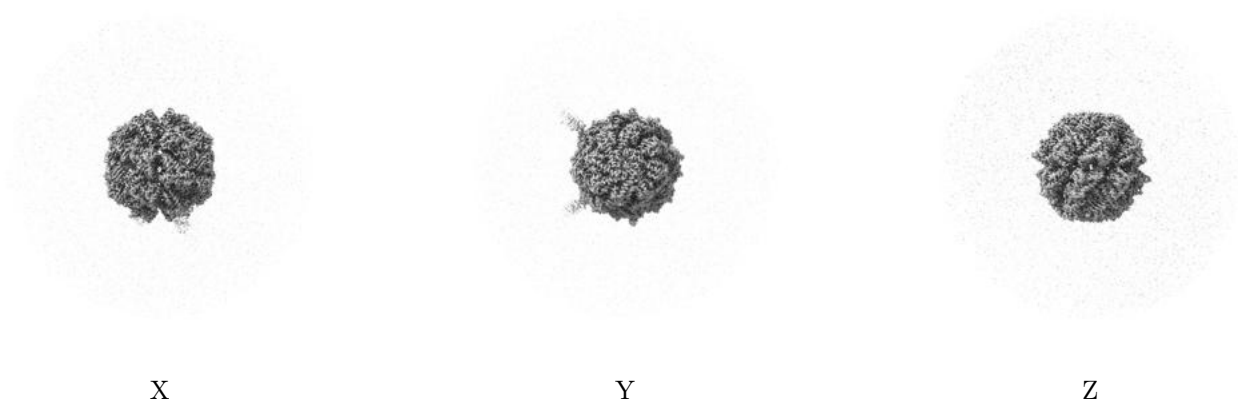
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

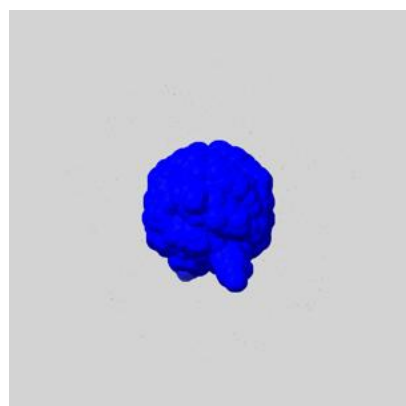
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

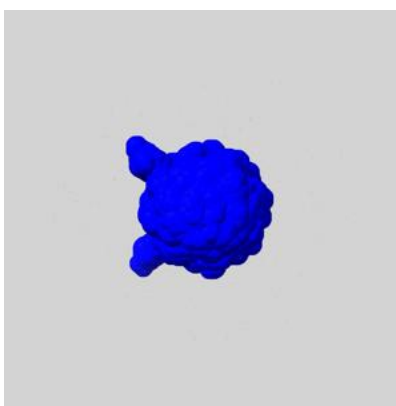
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

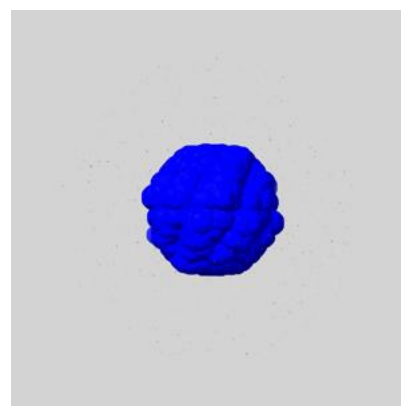
6.6.1 emd_12606_msk_1.map [i](#)



X



Y

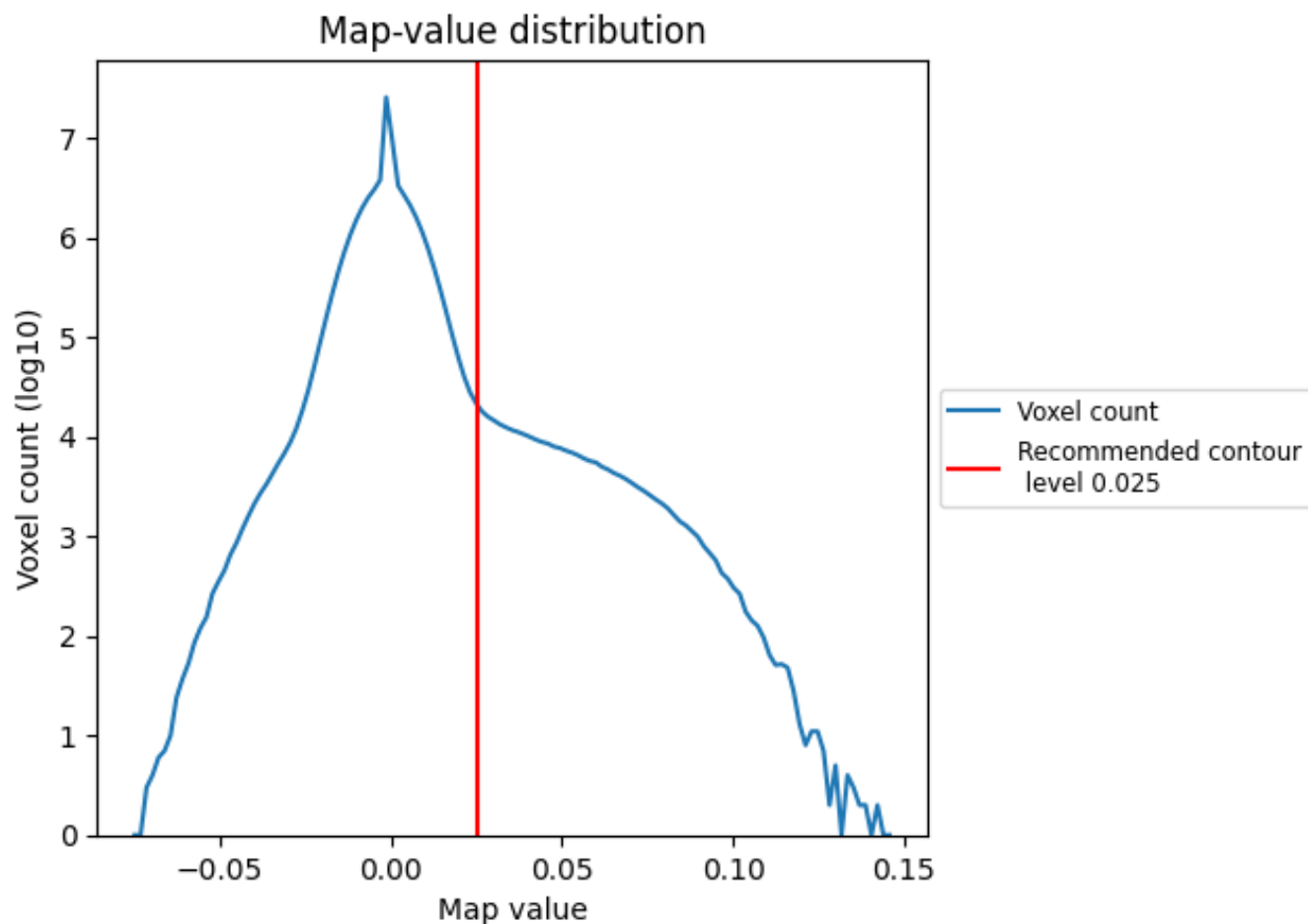


Z

7 Map analysis [i](#)

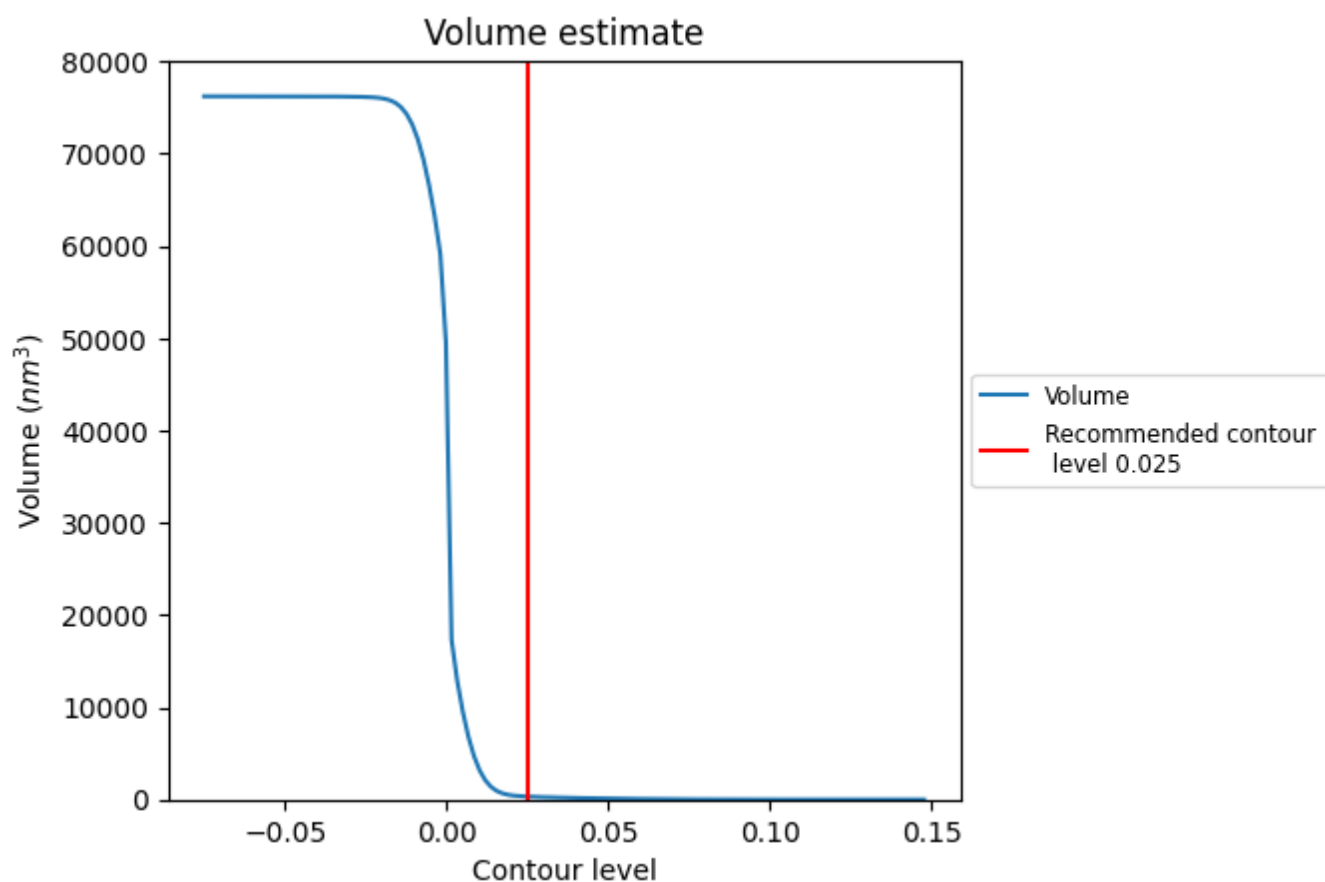
This section contains the results of statistical analysis of the map.

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.

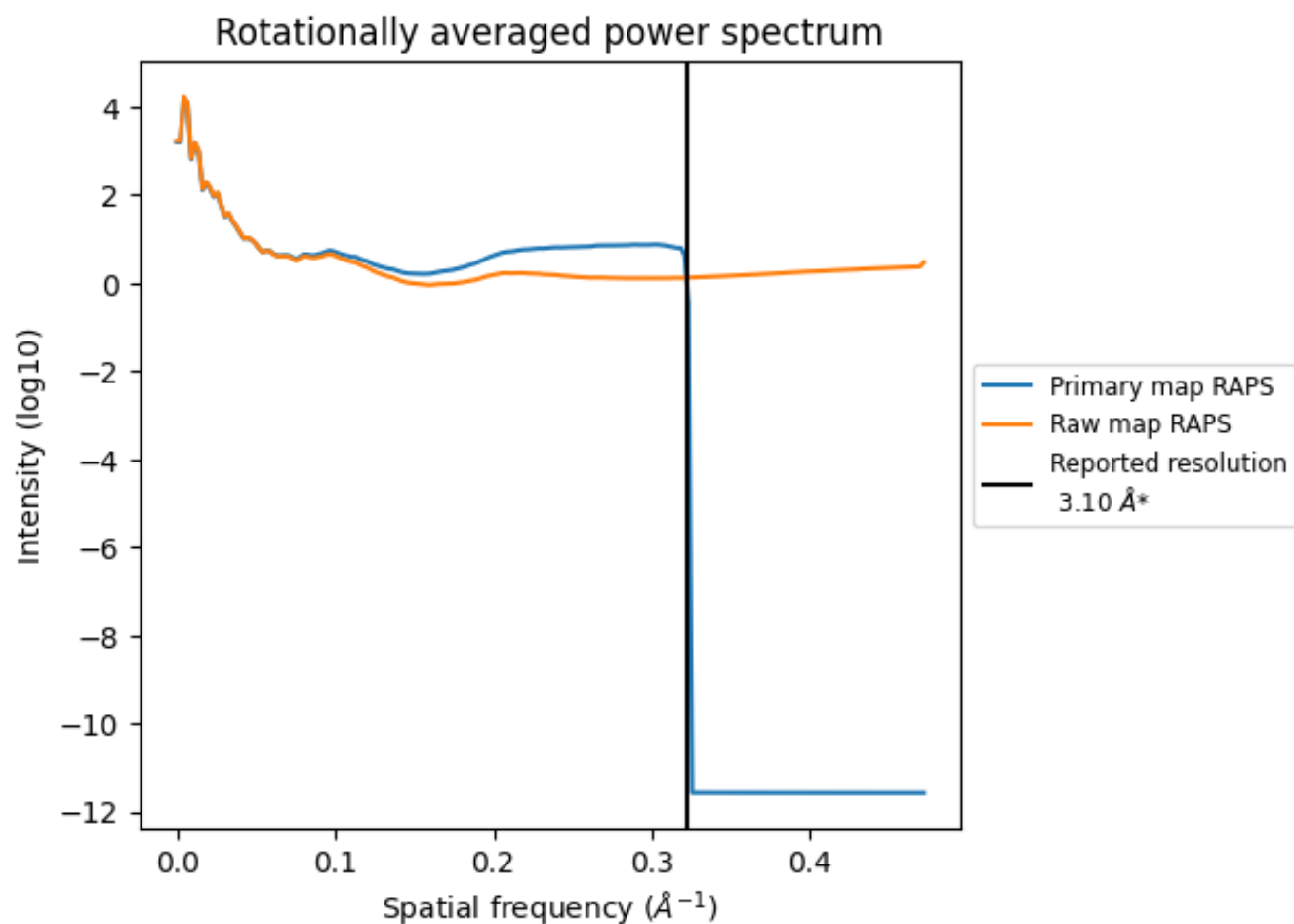
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 321 nm³; this corresponds to an approximate mass of 290 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 ⓘ

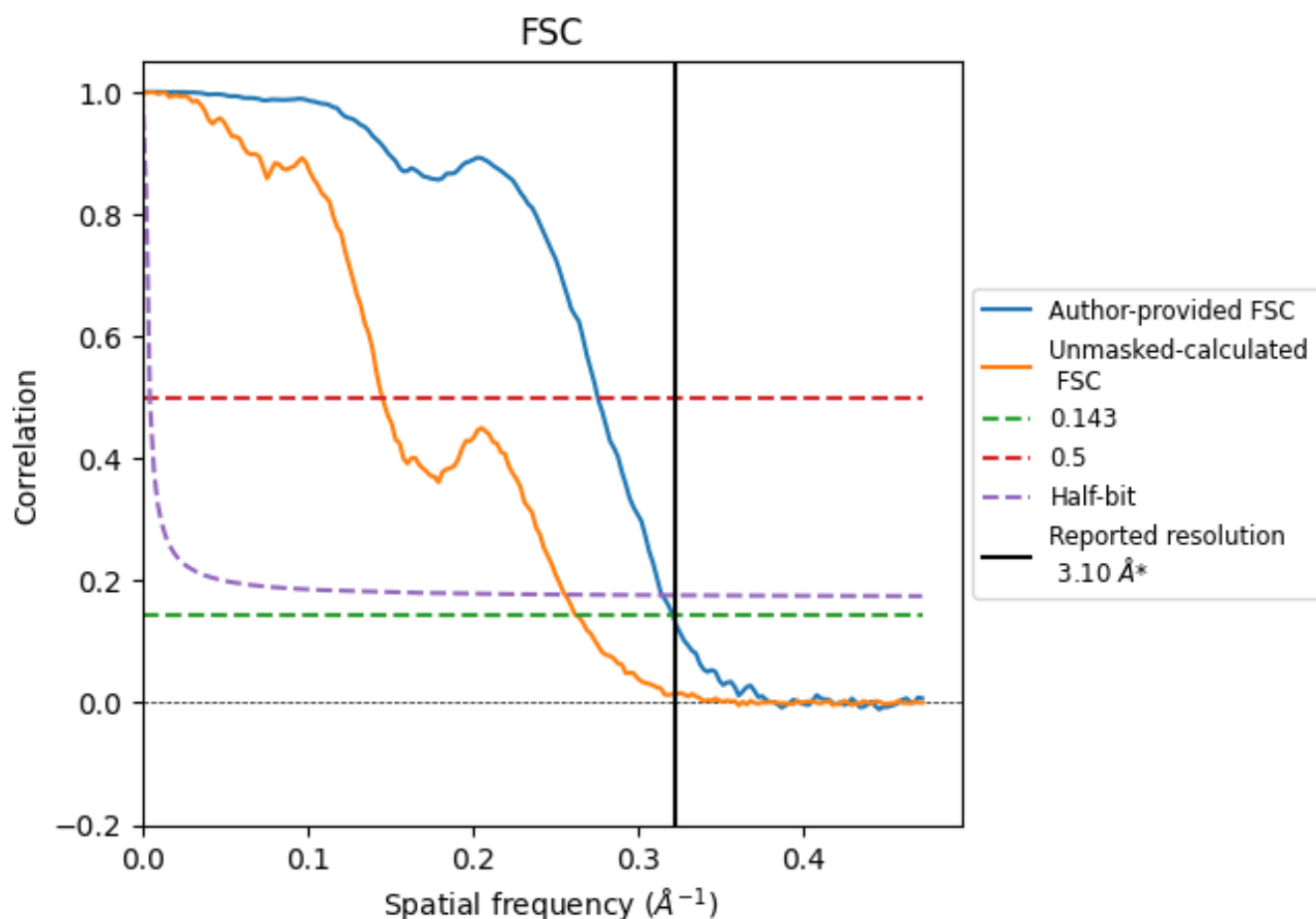


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

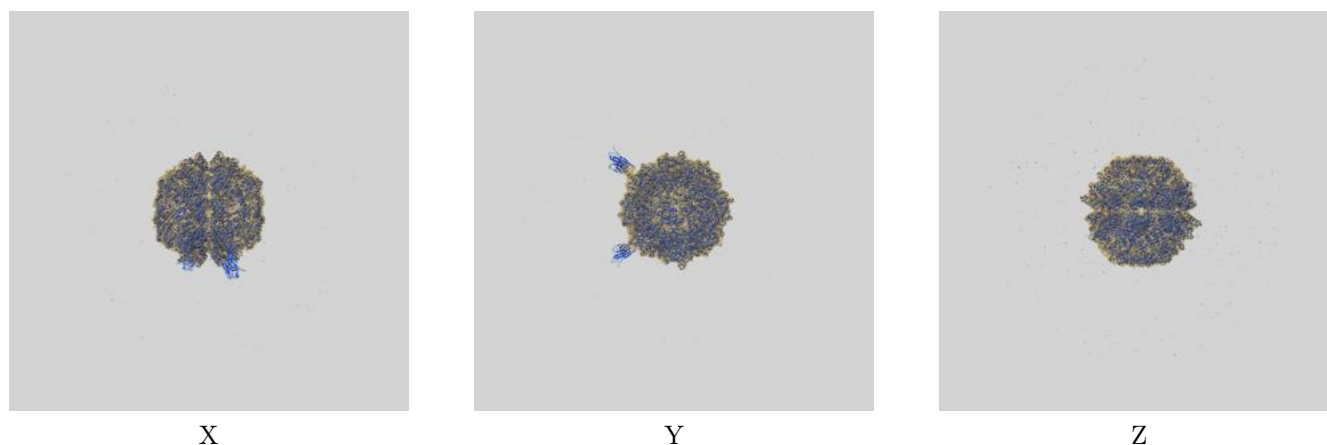
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.63	3.18
Unmasked-calculated*	3.81	6.89	3.91

*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 3.81 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

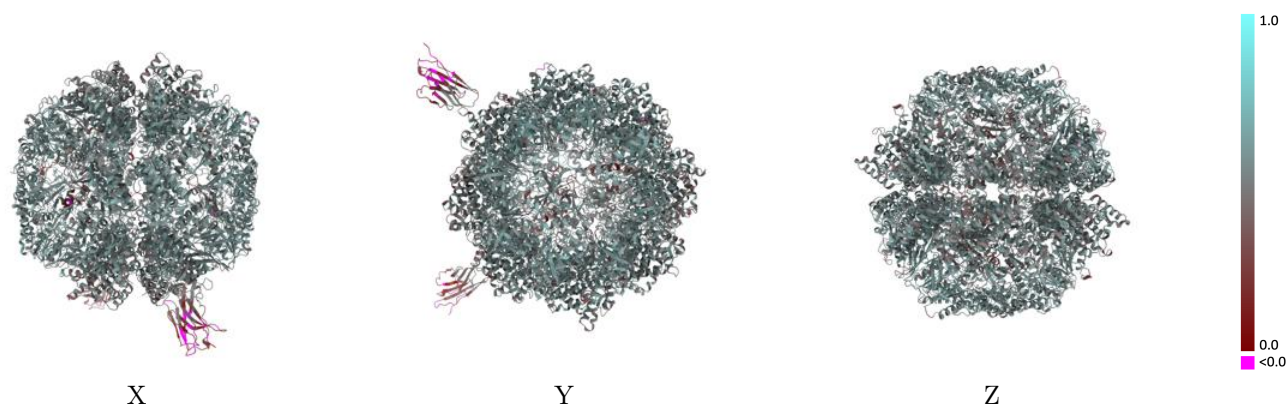
This section contains information regarding the fit between EMDB map EMD-12606 and PDB model 7NVM. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



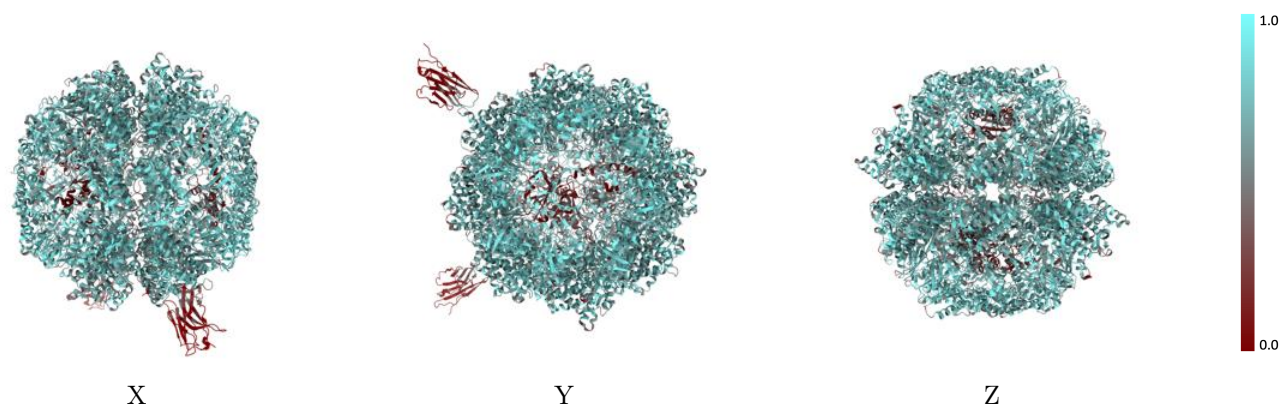
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



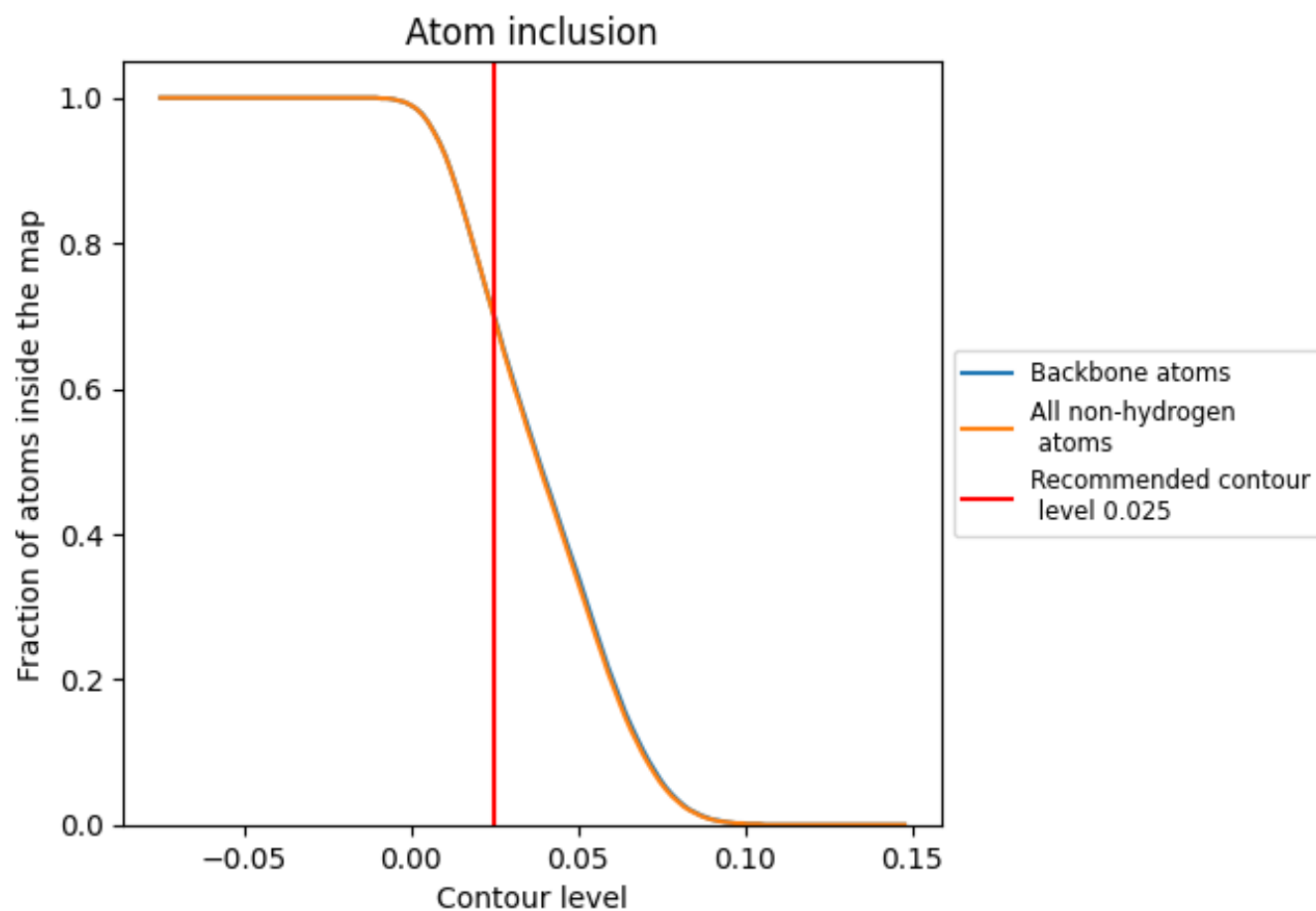
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6950	 0.5290
A	 0.7380	 0.5380
B	 0.7220	 0.5310
D	 0.7330	 0.5420
E	 0.7550	 0.5440
G	 0.7390	 0.5360
H	 0.7800	 0.5680
K	 0.2580	 0.4280
N	 0.1700	 0.2840
P	 0.1830	 0.4180
Q	 0.7490	 0.5530
Z	 0.7350	 0.5380
a	 0.7470	 0.5420
b	 0.7290	 0.5270
d	 0.7340	 0.5380
e	 0.7380	 0.5420
g	 0.7280	 0.5360
h	 0.7750	 0.5630
n	 0.1530	 0.2660
q	 0.7670	 0.5560
z	 0.7320	 0.5320

