



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 01:38 PM UTC

PDB ID : 7NVL / pdb_00007nvl
EMDB ID : EMD-12605
Title : Human TRiC complex in closed state with nanobody bound (Consensus Map)
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 : 2.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

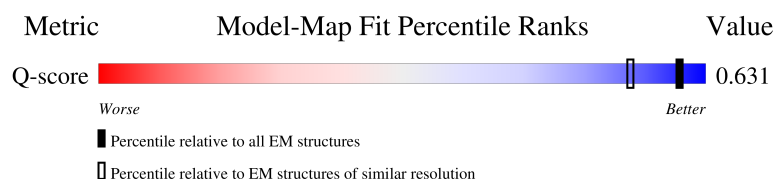
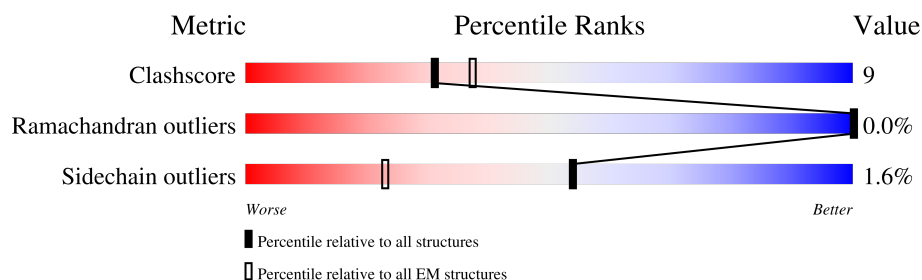
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	 75% 21% .
1	a	556	 73% 23% .
2	B	535	 80% 17% ..
2	b	535	 79% 18% ..

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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	

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
12	AF3	E	603	-	-	X	-
12	AF3	H	603	-	-	X	-
12	AF3	h	603	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 66477 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	534	Total	C	N	O	S	0	0
			4054	2540	709	782	23		
1	a	534	Total	C	N	O	S	0	0
			4054	2540	709	782	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	526	Total	C	N	O	S	0	0
			3952	2473	696	764	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	518	Total	C	N	O	S	0	0
			3908	2445	678	762	23		
3	d	518	Total	C	N	O	S	0	0
			3908	2445	678	762	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	534	Total	C	N	O	S	1	0
			4124	2586	717	790	31		
4	e	534	Total	C	N	O	S	1	0
			4124	2586	717	790	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	523	Total	C	N	O	S	0	0
			4064	2534	718	782	30		
5	g	523	Total	C	N	O	S	0	0
			4064	2534	718	782	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	520	Total	C	N	O	S	0	0
			3996	2526	691	756	23		
6	h	520	Total	C	N	O	S	0	0
			3996	2526	691	756	23		

- Molecule 7 is a protein called Nanobody Nb18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	104	Total	C	N	O	S	0	0
			820	510	151	155	4		
7	n	104	Total	C	N	O	S	0	0
			820	510	151	155	4		

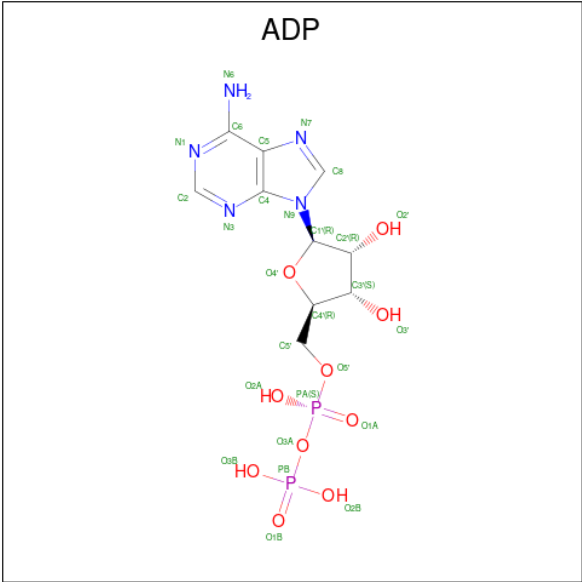
- Molecule 8 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	529	Total	C	N	O	S	0	0
			4029	2543	685	774	27		
8	q	529	Total	C	N	O	S	0	0
			4029	2543	685	774	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	525	Total	C	N	O	S	0	0
			4022	2528	704	769	21		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

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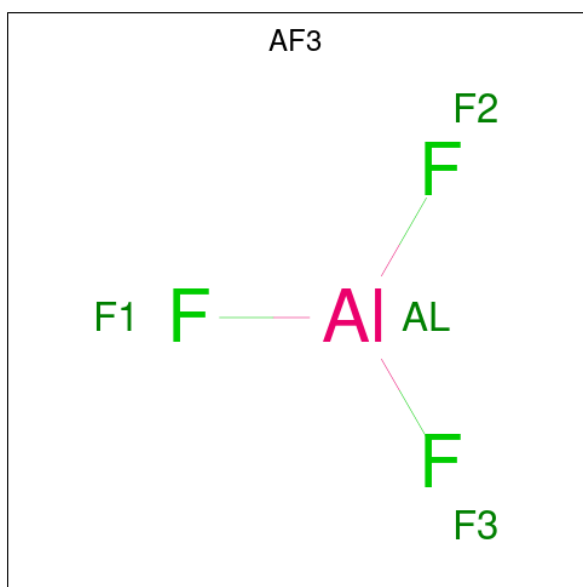
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Mol	Chain	Residues	Atoms					AltConf
10	q	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	z	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 12 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF₃).



Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	Al	F	0
			4	1	3	
12	B	1	Total	Al	F	0
			4	1	3	
12	D	1	Total	Al	F	0
			4	1	3	
12	E	1	Total	Al	F	0
			4	1	3	
12	G	1	Total	Al	F	0
			4	1	3	
12	H	1	Total	Al	F	0
			4	1	3	
12	Q	1	Total	Al	F	0
			4	1	3	
12	Z	1	Total	Al	F	0
			4	1	3	
12	a	1	Total	Al	F	0
			4	1	3	
12	b	1	Total	Al	F	0
			4	1	3	
12	d	1	Total	Al	F	0
			4	1	3	
12	e	1	Total	Al	F	0
			4	1	3	
12	g	1	Total	Al	F	0
			4	1	3	
12	h	1	Total	Al	F	0
			4	1	3	

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Mol	Chain	Residues	Atoms			AltConf
12	q	1	Total 4	Al 1	F 3	0
12	z	1	Total 4	Al 1	F 3	0

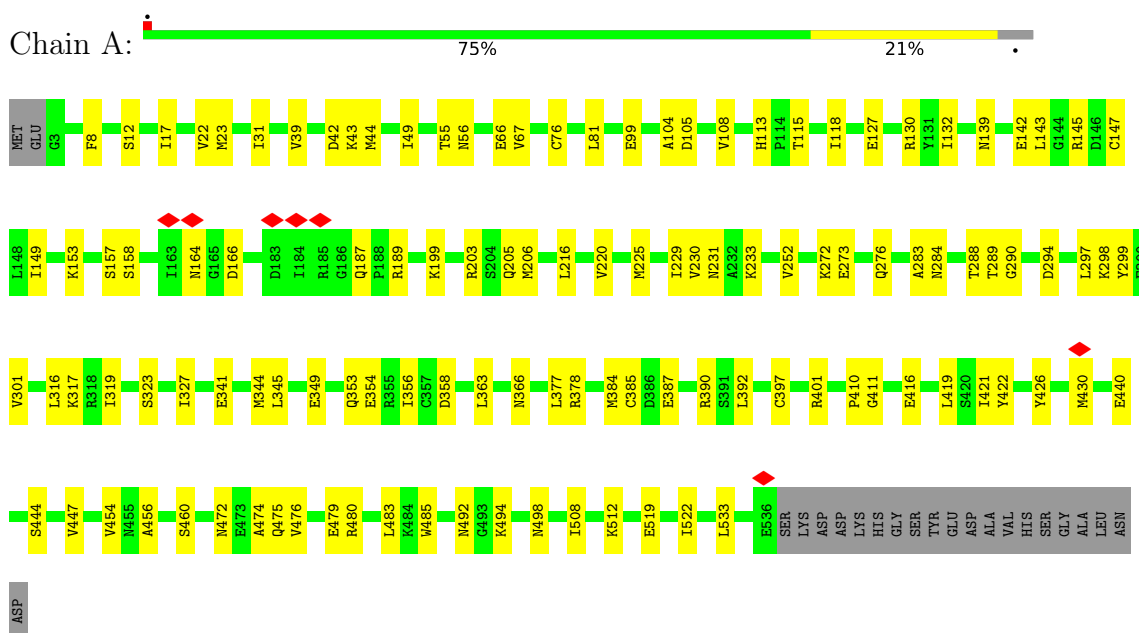
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	2	Total 2	O 2	0
13	B	3	Total 3	O 3	0
13	D	2	Total 2	O 2	0
13	E	1	Total 1	O 1	0
13	G	1	Total 1	O 1	0
13	H	2	Total 2	O 2	0
13	Q	1	Total 1	O 1	0
13	Z	1	Total 1	O 1	0
13	a	3	Total 3	O 3	0
13	b	2	Total 2	O 2	0
13	d	2	Total 2	O 2	0
13	e	2	Total 2	O 2	0
13	g	1	Total 1	O 1	0
13	h	2	Total 2	O 2	0
13	q	1	Total 1	O 1	0
13	z	1	Total 1	O 1	0

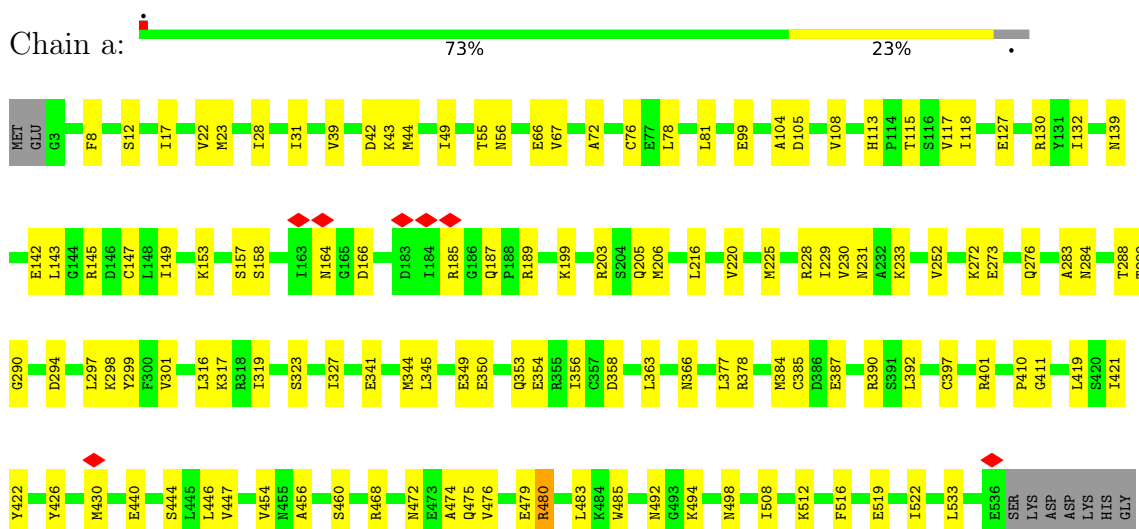
3 Residue-property plots [i](#)

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



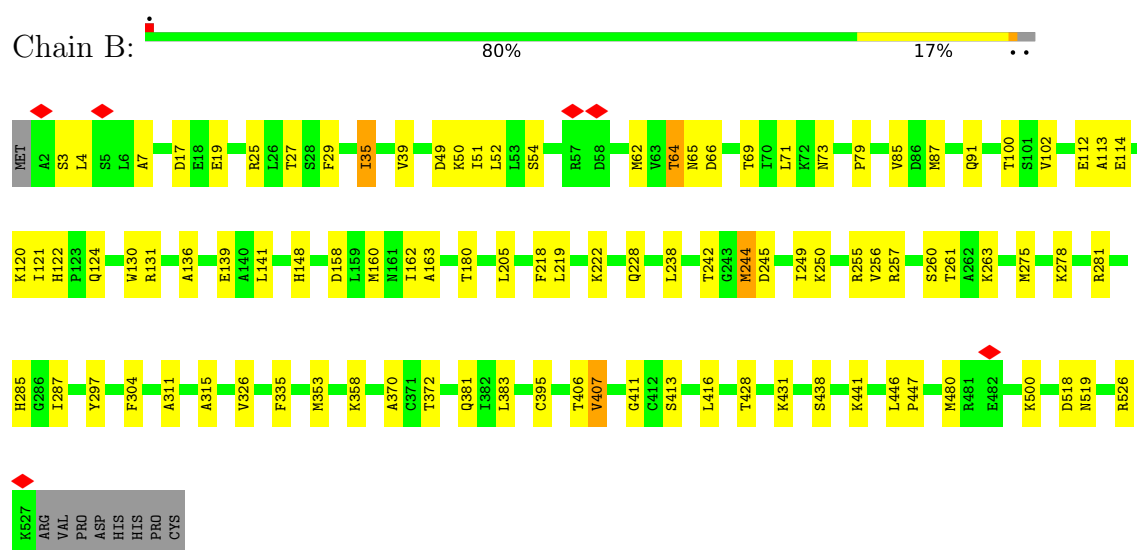
- Molecule 1: T-complex protein 1 subunit alpha



SER
TYR
GLU
ASP
ALA
VAL
HIS
SER
GLY
ALA
LEU
ASN
ASP

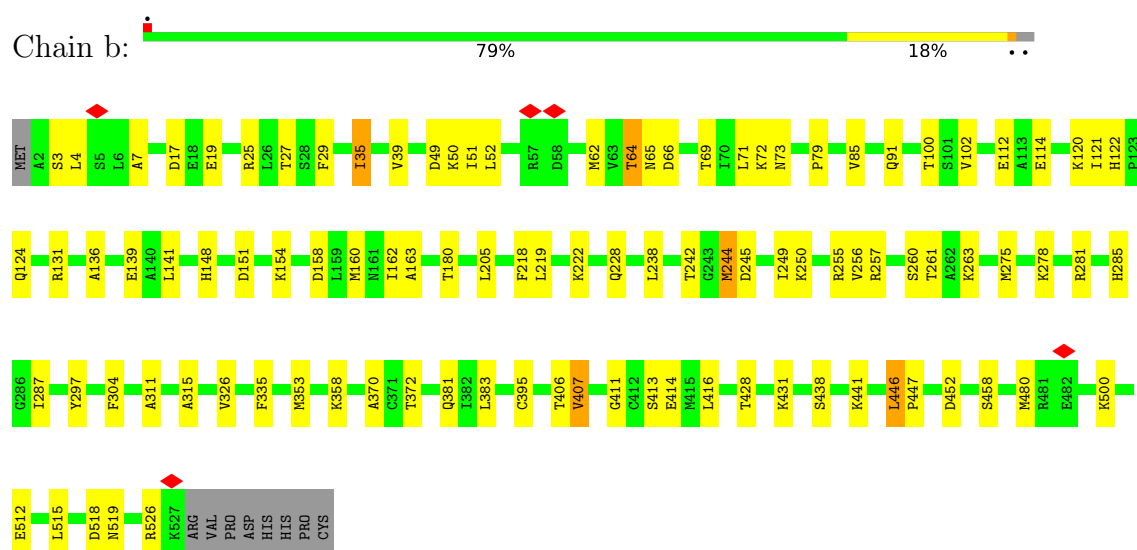
• Molecule 2: T-complex protein 1 subunit beta

Chain B:



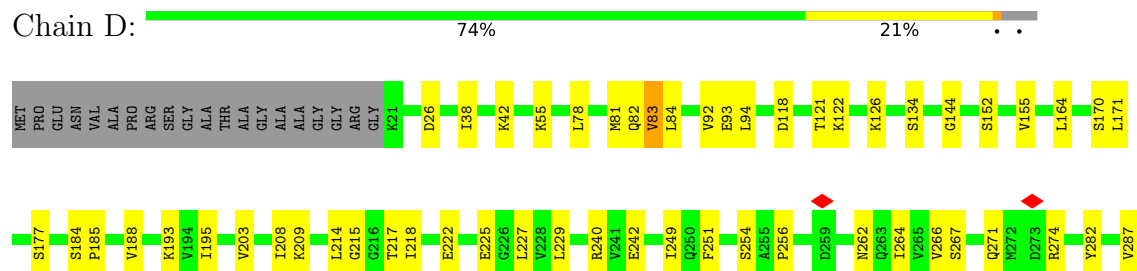
• Molecule 2: T-complex protein 1 subunit beta

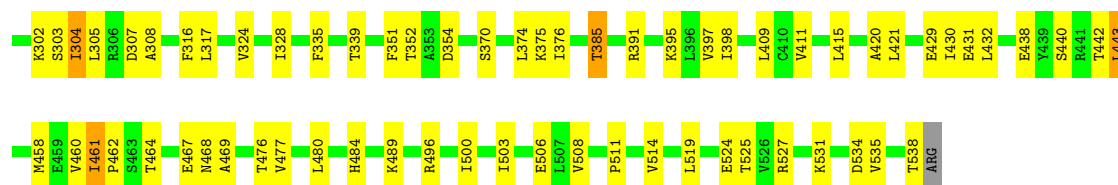
Chain b:



• Molecule 3: T-complex protein 1 subunit delta

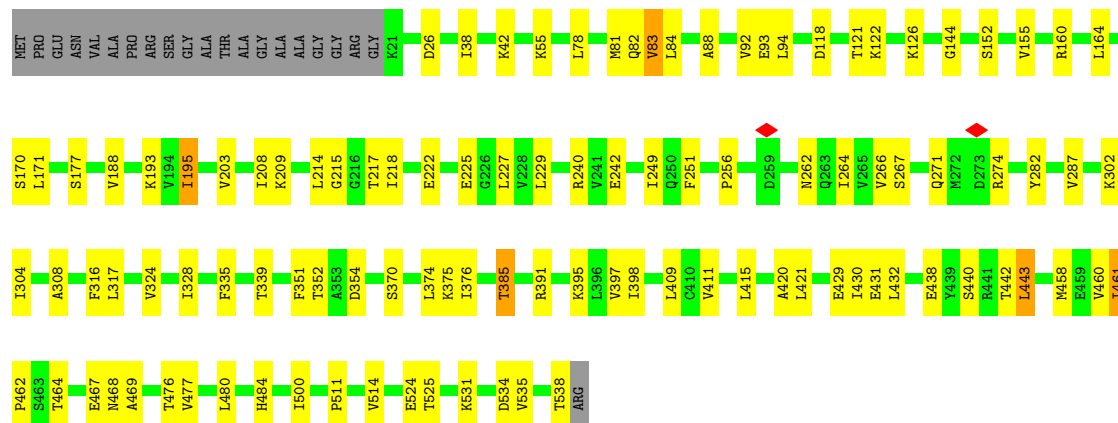
Chain D:





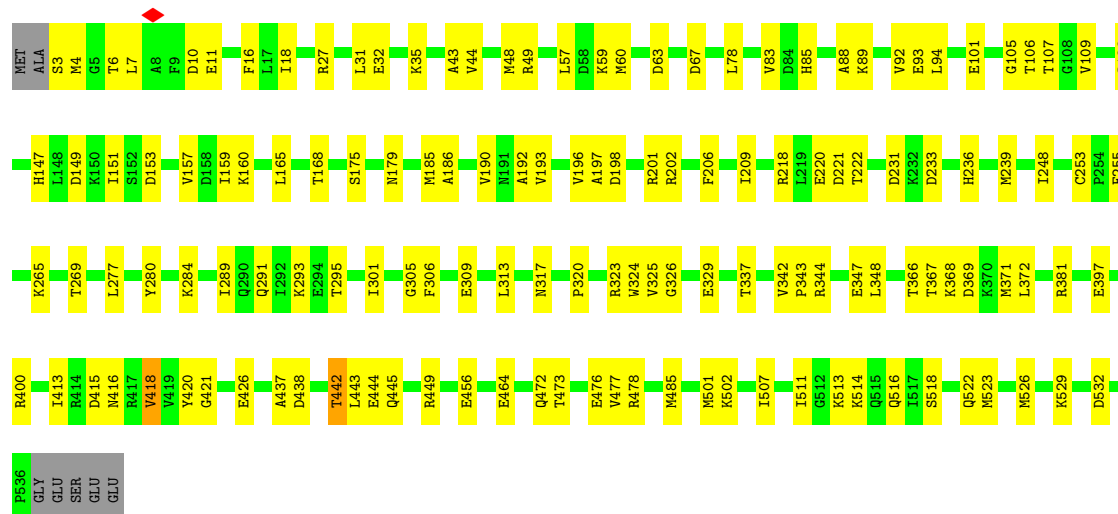
• Molecule 3: T-complex protein 1 subunit delta

Chain d: 76% 19% ..



• Molecule 4: T-complex protein 1 subunit epsilon

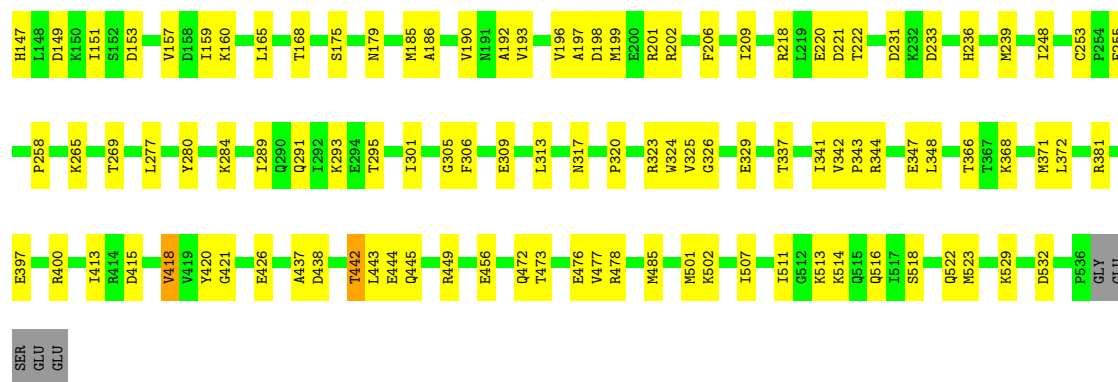
Chain E: 73% 26% .



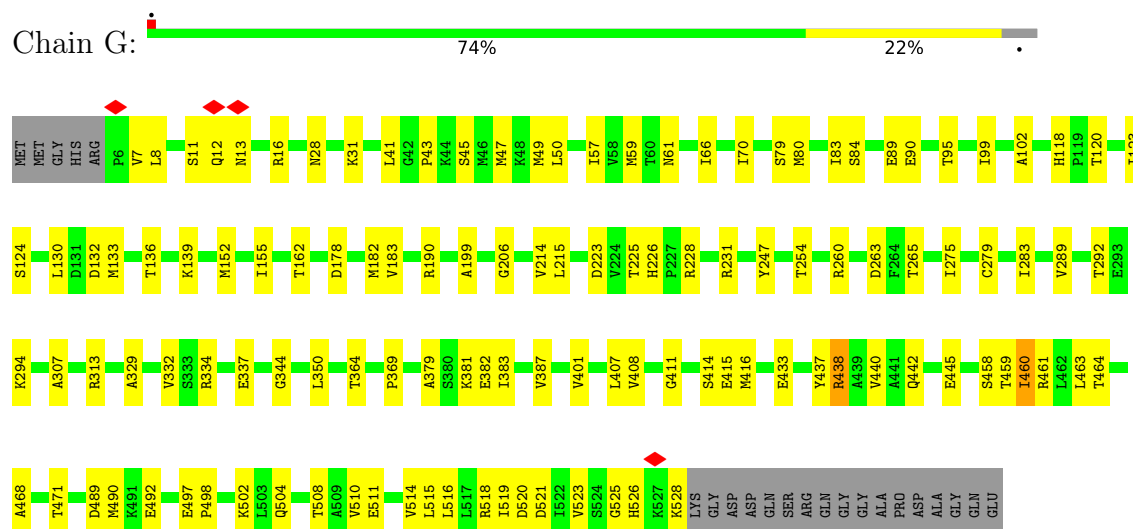
• Molecule 4: T-complex protein 1 subunit epsilon

Chain e: 74% 25% ..

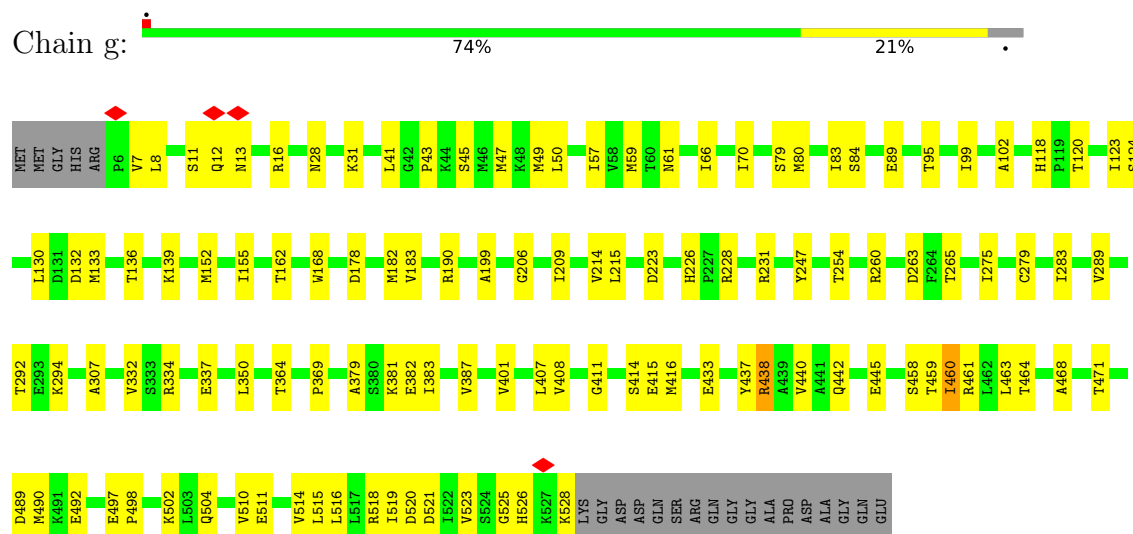




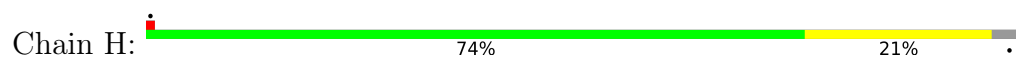
• Molecule 5: T-complex protein 1 subunit gamma

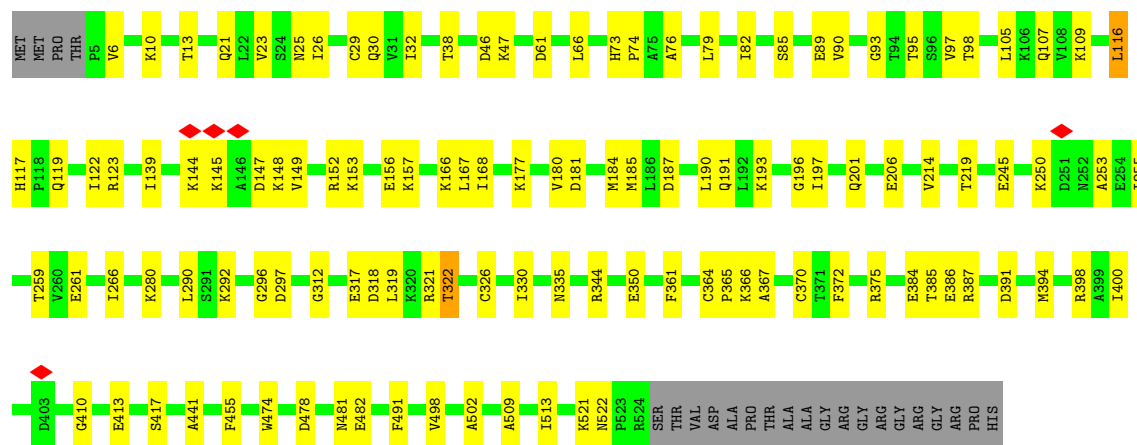


• Molecule 5: T-complex protein 1 subunit gamma

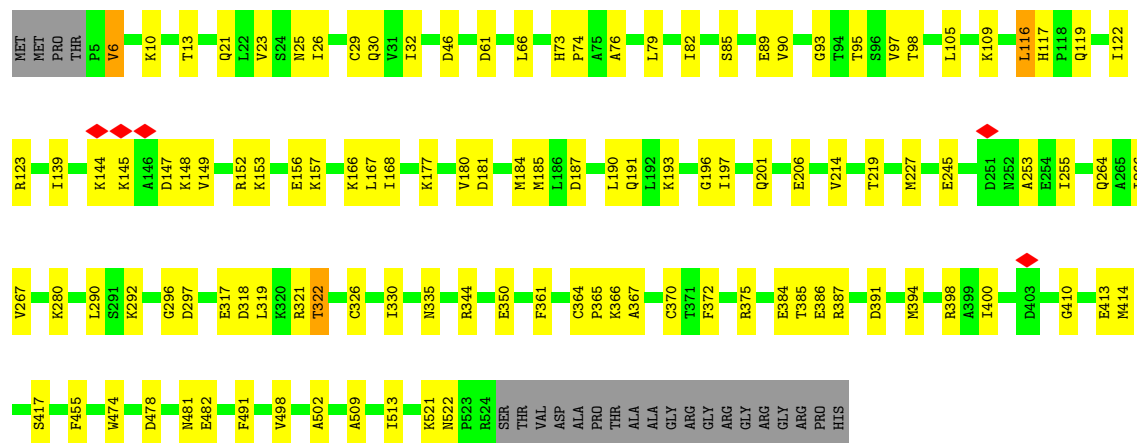
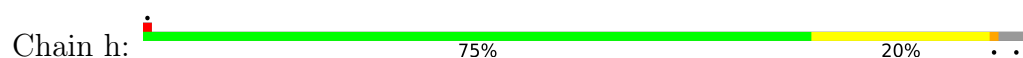


• Molecule 6: T-complex protein 1 subunit eta

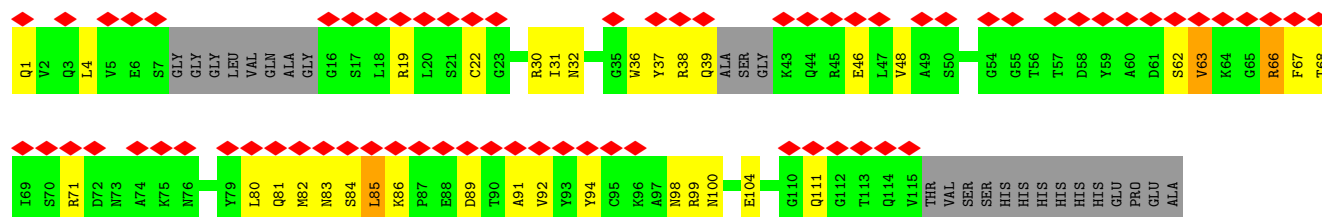




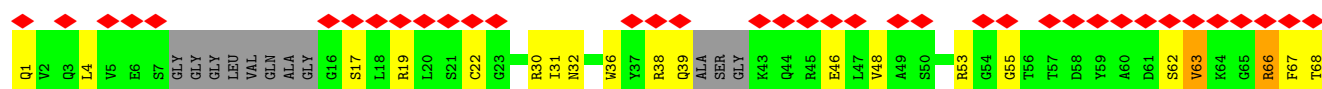
• Molecule 6: T-complex protein 1 subunit eta



• Molecule 7: Nanobody Nb18

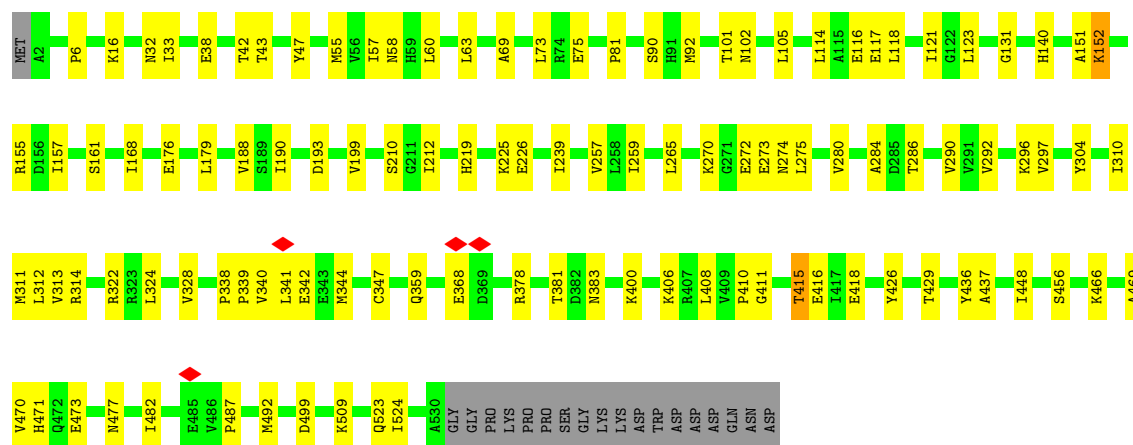
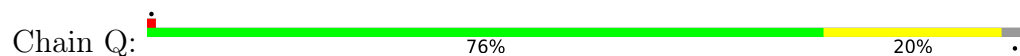


• Molecule 7: Nanobody Nb18

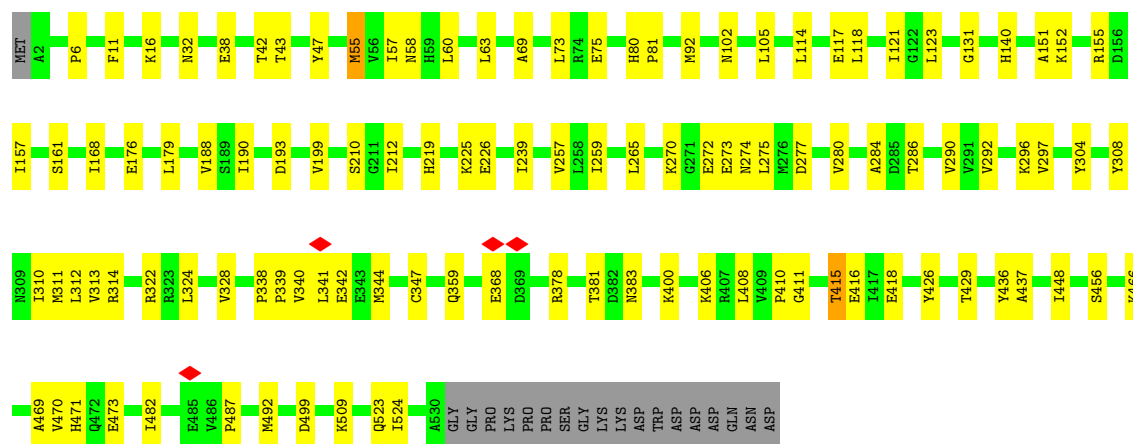
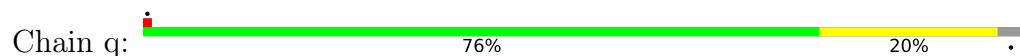




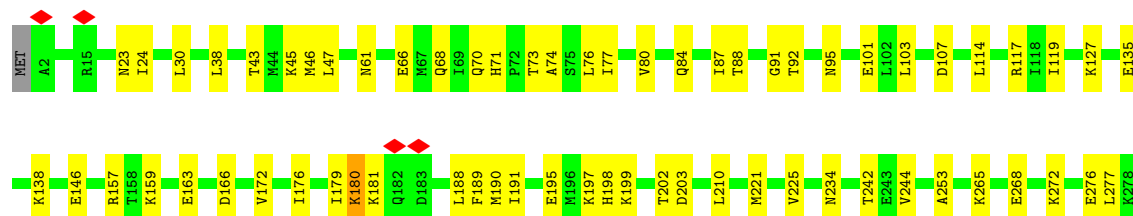
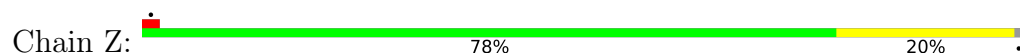
• Molecule 8: T-complex protein 1 subunit theta

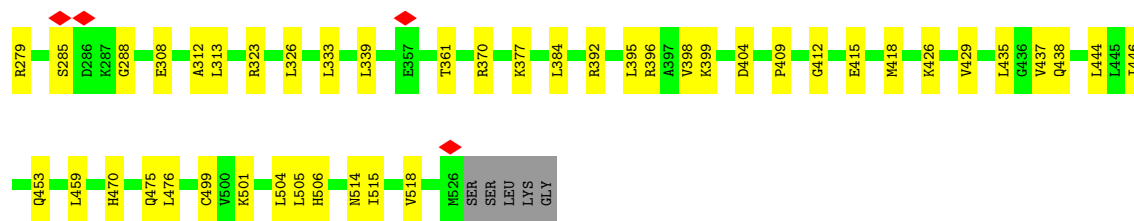


• Molecule 8: T-complex protein 1 subunit theta

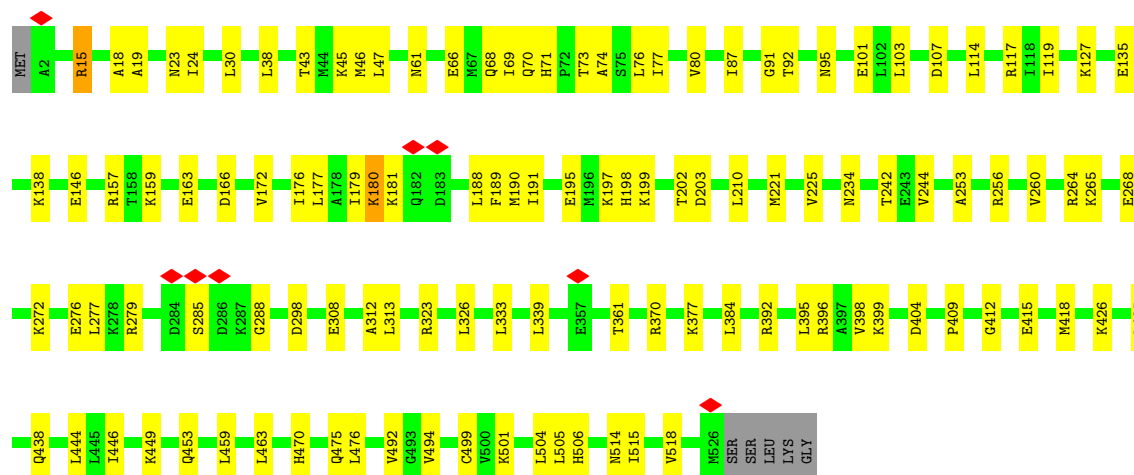
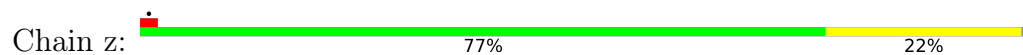


• Molecule 9: T-complex protein 1 subunit zeta





• Molecule 9: T-complex protein 1 subunit zeta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	316195	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	0.314	Depositor
Minimum map value	-0.123	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	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	0.22	0/4094	0.41	0/5528
1	a	0.22	0/4094	0.41	0/5528
2	B	0.21	0/3995	0.42	0/5386
2	b	0.21	0/3995	0.42	0/5386
3	D	0.22	0/3940	0.41	0/5319
3	d	0.21	0/3940	0.41	0/5319
4	E	0.22	0/4178	0.45	0/5628
4	e	0.22	0/4178	0.45	0/5628
5	G	0.20	0/4110	0.41	0/5544
5	g	0.20	0/4110	0.41	0/5544
6	H	0.21	0/4052	0.40	0/5468
6	h	0.21	0/4052	0.40	0/5468
7	N	0.26	0/835	0.67	0/1127
7	n	0.26	0/835	0.67	0/1127
8	Q	0.20	0/4087	0.42	0/5525
8	q	0.19	0/4087	0.42	0/5525
9	Z	0.23	0/4069	0.43	0/5486
9	z	0.22	0/4069	0.42	0/5486
All	All	0.22	0/66720	0.43	0/90022

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4054	0	4213	82	0
1	a	4054	0	4213	85	0
2	B	3952	0	4070	69	0
2	b	3952	0	4070	71	0
3	D	3908	0	4115	82	0
3	d	3908	0	4115	73	0
4	E	4124	0	4242	97	0
4	e	4124	0	4242	98	0
5	G	4064	0	4202	79	0
5	g	4064	0	4202	77	0
6	H	3996	0	4101	81	0
6	h	3996	0	4101	82	0
7	N	820	0	768	22	0
7	n	820	0	768	22	0
8	Q	4029	0	4099	73	0
8	q	4029	0	4099	72	0
9	Z	4022	0	4161	73	0
9	z	4022	0	4161	78	0
10	A	27	0	12	1	0
10	B	27	0	12	1	0
10	D	27	0	12	1	0
10	E	27	0	12	3	0
10	G	27	0	12	0	0
10	H	27	0	12	3	0
10	Q	27	0	12	0	0
10	Z	27	0	12	2	0
10	a	27	0	12	1	0
10	b	27	0	12	1	0
10	d	27	0	12	1	0
10	e	27	0	12	3	0
10	g	27	0	12	0	0
10	h	27	0	12	3	0
10	q	27	0	12	0	0
10	z	27	0	12	2	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	G	1	0	0	0	0
11	H	1	0	0	0	0
11	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Z	1	0	0	0	0
11	a	1	0	0	0	0
11	b	1	0	0	0	0
11	d	1	0	0	0	0
11	e	1	0	0	0	0
11	g	1	0	0	0	0
11	h	1	0	0	0	0
11	q	1	0	0	0	0
11	z	1	0	0	0	0
12	A	4	0	0	0	0
12	B	4	0	0	0	0
12	D	4	0	0	1	0
12	E	4	0	0	2	0
12	G	4	0	0	1	0
12	H	4	0	0	2	0
12	Q	4	0	0	0	0
12	Z	4	0	0	1	0
12	a	4	0	0	0	0
12	b	4	0	0	0	0
12	d	4	0	0	1	0
12	e	4	0	0	1	0
12	g	4	0	0	1	0
12	h	4	0	0	2	0
12	q	4	0	0	0	0
12	z	4	0	0	1	0
13	A	2	0	0	1	0
13	B	3	0	0	0	0
13	D	2	0	0	0	0
13	E	1	0	0	0	0
13	G	1	0	0	0	0
13	H	2	0	0	2	0
13	Q	1	0	0	0	0
13	Z	1	0	0	0	0
13	a	3	0	0	1	0
13	b	2	0	0	0	0
13	d	2	0	0	0	0
13	e	2	0	0	0	0
13	g	1	0	0	0	0
13	h	2	0	0	2	0
13	q	1	0	0	0	0
13	z	1	0	0	0	0
All	All	66477	0	68134	1183	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 (1183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:432:LEU:HD23	3:d:458:MET:CE	1.85	1.06
3:D:432:LEU:HD23	3:D:458:MET:CE	1.84	1.05
3:d:432:LEU:HD23	3:d:458:MET:HE1	1.03	1.02
3:D:432:LEU:HD23	3:D:458:MET:HE1	1.03	1.01
3:d:432:LEU:CD2	3:d:458:MET:HE1	1.94	0.98
3:D:432:LEU:CD2	3:D:458:MET:HE1	1.94	0.97
5:G:206:GLY:HA3	9:Z:87:ILE:HG13	1.59	0.84
5:g:206:GLY:HA3	9:z:87:ILE:HG13	1.59	0.84
8:Q:280:VAL:HG21	8:Q:304:TYR:HB3	1.61	0.82
8:q:280:VAL:HG21	8:q:304:TYR:HB3	1.61	0.82
6:h:335:ASN:ND2	8:q:273:GLU:OE2	2.12	0.82
6:H:335:ASN:ND2	8:Q:273:GLU:OE2	2.13	0.81
1:a:474:ALA:HB2	1:a:483:LEU:HB2	1.63	0.80
1:A:474:ALA:HB2	1:A:483:LEU:HB2	1.63	0.79
7:n:19:ARG:HB2	7:n:81:GLN:HE21	1.45	0.79
7:N:19:ARG:HB2	7:N:81:GLN:HE21	1.45	0.78
1:A:44:MET:HE3	5:G:519:ILE:HD13	1.65	0.77
1:a:44:MET:HE3	5:g:519:ILE:HD13	1.65	0.77
2:B:64:THR:HG22	2:B:66:ASP:H	1.50	0.76
2:b:64:THR:HG22	2:b:66:ASP:H	1.50	0.75
7:n:19:ARG:HB2	7:n:81:GLN:NE2	2.01	0.75
5:g:45:SER:O	9:z:117:ARG:NH2	2.19	0.74
3:D:195:ILE:HG21	3:D:203:VAL:HG22	1.70	0.73
7:N:19:ARG:HB2	7:N:81:GLN:NE2	2.01	0.73
7:n:68:THR:HB	7:n:81:GLN:HB2	1.70	0.73
5:G:45:SER:O	9:Z:117:ARG:NH2	2.21	0.73
3:d:195:ILE:HG21	3:d:203:VAL:HG22	1.70	0.73
4:e:295:THR:HG21	4:e:348:LEU:HG	1.71	0.72
6:h:366:LYS:H	6:h:366:LYS:HD3	1.55	0.72
7:N:68:THR:HB	7:N:81:GLN:HB2	1.70	0.72
2:B:91:GLN:HG3	2:B:102:VAL:HG11	1.72	0.72
9:z:15:ARG:O	9:z:19:ALA:N	2.17	0.71
4:E:78:LEU:HB3	4:E:92:VAL:HG22	1.72	0.71
4:E:305:GLY:HA2	4:E:323:ARG:HB2	1.71	0.71
2:b:91:GLN:HG3	2:b:102:VAL:HG11	1.72	0.70
3:D:287:VAL:HG21	3:D:316:PHE:HB3	1.73	0.70
4:E:295:THR:HG21	4:E:348:LEU:HG	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:415:ASP:HB3	4:e:511:ILE:HD11	1.72	0.70
4:E:426:GLU:OE2	4:E:513:LYS:NZ	2.25	0.70
6:H:366:LYS:HD3	6:H:366:LYS:H	1.55	0.70
4:e:305:GLY:HA2	4:e:323:ARG:HB2	1.71	0.70
4:e:78:LEU:HB3	4:e:92:VAL:HG22	1.72	0.70
4:E:438:ASP:OD1	4:E:449:ARG:NH2	2.26	0.69
3:d:287:VAL:HG21	3:d:316:PHE:HB3	1.73	0.69
4:e:472:GLN:O	4:e:476:GLU:HG3	1.92	0.69
4:E:415:ASP:HB3	4:E:511:ILE:HD11	1.72	0.69
5:G:223:ASP:OD1	5:G:231:ARG:NH1	2.25	0.69
8:q:466:LYS:NZ	8:q:487:PRO:O	2.26	0.69
5:g:223:ASP:OD1	5:g:231:ARG:NH1	2.25	0.69
4:E:472:GLN:O	4:E:476:GLU:HG3	1.92	0.68
2:b:326:VAL:HG23	2:b:370:ALA:HB3	1.75	0.68
5:G:279:CYS:O	5:G:283:ILE:HG13	1.94	0.68
8:Q:55:MET:CG	8:Q:63:LEU:HD11	2.23	0.68
5:G:292:THR:HG22	5:G:294:LYS:H	1.58	0.68
5:g:292:THR:HG22	5:g:294:LYS:H	1.58	0.68
4:e:438:ASP:OD1	4:e:449:ARG:NH2	2.26	0.68
2:b:438:SER:HA	2:b:441:LYS:HE2	1.76	0.68
5:g:155:ILE:HG21	5:g:401:VAL:HG21	1.76	0.68
5:g:279:CYS:O	5:g:283:ILE:HG13	1.94	0.68
6:h:197:ILE:HG21	6:h:386:GLU:HG3	1.76	0.67
8:Q:466:LYS:NZ	8:Q:487:PRO:O	2.26	0.67
5:G:438:ARG:O	5:G:442:GLN:HG2	1.95	0.67
6:H:82:ILE:HG21	6:H:509:ALA:HB2	1.77	0.67
2:B:438:SER:HA	2:B:441:LYS:HE2	1.76	0.67
4:e:94:LEU:HD13	4:e:523:MET:HG3	1.75	0.67
2:B:326:VAL:HG23	2:B:370:ALA:HB3	1.75	0.66
6:H:197:ILE:HG21	6:H:386:GLU:HG3	1.76	0.66
4:E:201:ARG:NH2	6:H:350:GLU:O	2.28	0.66
5:G:155:ILE:HG21	5:G:401:VAL:HG21	1.76	0.66
6:H:166:LYS:NZ	12:H:603:AF3:F1	2.19	0.66
3:d:214:LEU:O	3:d:391:ARG:NH1	2.29	0.66
5:g:438:ARG:O	5:g:442:GLN:HG2	1.95	0.66
4:E:94:LEU:HD13	4:E:523:MET:HG3	1.75	0.66
6:h:521:LYS:HG2	8:q:57:ILE:HD12	1.77	0.66
1:A:56:ASN:ND2	13:A:702:HOH:O	2.29	0.66
3:D:214:LEU:O	3:D:391:ARG:NH1	2.29	0.66
3:d:464:THR:HA	3:d:467:GLU:HG2	1.77	0.66
1:a:56:ASN:ND2	13:a:703:HOH:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:353:GLN:O	5:g:190:ARG:NH2	2.28	0.65
6:h:166:LYS:NZ	12:h:603:AF3:F1	2.19	0.65
8:q:523:GLN:HB2	9:z:45:LYS:HD2	1.78	0.65
1:A:353:GLN:O	5:G:190:ARG:NH2	2.30	0.65
6:h:82:ILE:HG21	6:h:509:ALA:HB2	1.77	0.65
2:b:228:GLN:NE2	2:b:311:ALA:H	1.95	0.65
3:D:464:THR:HA	3:D:467:GLU:HG2	1.77	0.65
1:A:252:VAL:HB	5:G:254:THR:HA	1.79	0.65
8:Q:225:LYS:NZ	8:Q:314:ARG:O	2.29	0.65
4:E:236:HIS:HB3	4:E:239:MET:HG3	1.79	0.64
6:H:156:GLU:HG2	6:H:180:VAL:HG21	1.79	0.64
4:e:201:ARG:NH2	6:h:350:GLU:O	2.30	0.64
8:q:225:LYS:NZ	8:q:314:ARG:O	2.29	0.64
1:a:288:THR:HG22	1:a:290:GLY:H	1.62	0.64
1:A:411:GLY:O	1:A:498:ASN:ND2	2.27	0.64
2:B:228:GLN:NE2	2:B:311:ALA:H	1.95	0.64
8:Q:219:HIS:NE2	8:Q:368:GLU:OE1	2.31	0.64
2:b:50:LYS:HD2	3:d:534:ASP:HB3	1.80	0.64
3:d:240:ARG:NH1	3:d:242:GLU:OE2	2.31	0.64
3:d:214:LEU:HD12	3:d:398:ILE:HD12	1.80	0.64
8:q:219:HIS:NE2	8:q:368:GLU:OE1	2.31	0.64
1:A:288:THR:HG22	1:A:290:GLY:H	1.62	0.63
8:Q:55:MET:HG3	8:Q:63:LEU:HD11	1.79	0.63
9:Z:279:ARG:NH1	9:Z:308:GLU:OE2	2.29	0.63
4:e:236:HIS:HB3	4:e:239:MET:HG3	1.79	0.63
8:q:270:LYS:O	8:q:274:ASN:ND2	2.25	0.63
8:Q:157:ILE:O	8:Q:161:SER:OG	2.17	0.63
3:D:214:LEU:HD12	3:D:398:ILE:HD12	1.80	0.63
6:h:280:LYS:NZ	6:h:335:ASN:OD1	2.31	0.63
3:D:240:ARG:NH1	3:D:242:GLU:OE2	2.31	0.63
6:h:156:GLU:HG2	6:h:180:VAL:HG21	1.79	0.63
3:D:78:LEU:HB3	3:D:92:VAL:HG22	1.79	0.62
1:a:252:VAL:HB	5:g:254:THR:HA	1.82	0.62
3:d:78:LEU:HB3	3:d:92:VAL:HG22	1.79	0.62
9:z:279:ARG:NH1	9:z:308:GLU:OE2	2.29	0.62
6:h:478:ASP:OD2	6:h:481:ASN:ND2	2.33	0.62
6:H:167:LEU:H	6:H:167:LEU:HD23	1.65	0.61
6:H:521:LYS:HG2	8:Q:57:ILE:HD12	1.81	0.61
8:Q:523:GLN:HB2	9:Z:45:LYS:HD2	1.83	0.61
4:E:193:VAL:O	4:E:197:ALA:HB2	2.01	0.61
4:e:193:VAL:O	4:e:197:ALA:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:163:ALA:HB3	2:b:180:THR:HG23	1.83	0.61
2:B:163:ALA:HB3	2:B:180:THR:HG23	1.83	0.61
6:H:478:ASP:OD2	6:H:481:ASN:ND2	2.33	0.61
1:a:199:LYS:HB3	1:a:385:CYS:HB3	1.83	0.61
6:h:167:LEU:H	6:h:167:LEU:HD23	1.65	0.61
2:b:242:THR:HG21	2:b:335:PHE:CE2	2.36	0.61
1:a:411:GLY:O	1:a:498:ASN:ND2	2.27	0.61
9:Z:103:LEU:HD21	9:Z:515:ILE:HG21	1.83	0.60
9:z:103:LEU:HD21	9:z:515:ILE:HG21	1.83	0.60
2:B:50:LYS:HD2	3:D:534:ASP:HB3	1.82	0.60
3:D:430:ILE:HG13	3:D:480:LEU:HD13	1.83	0.60
1:A:199:LYS:HB3	1:A:385:CYS:HB3	1.83	0.60
2:B:242:THR:HG21	2:B:335:PHE:CE2	2.36	0.60
4:E:201:ARG:HG3	4:E:201:ARG:HH11	1.67	0.60
6:H:38:THR:HG1	6:H:47:LYS:HZ1	1.49	0.60
1:a:203:ARG:HA	5:g:504:GLN:HE22	1.66	0.60
4:e:201:ARG:HG3	4:e:201:ARG:HH11	1.67	0.60
8:Q:38:GLU:O	8:Q:42:THR:HG23	2.02	0.59
3:d:430:ILE:HG13	3:d:480:LEU:HD13	1.82	0.59
8:Q:280:VAL:HG21	8:Q:304:TYR:CB	2.32	0.59
3:D:430:ILE:HG12	3:D:462:PRO:HG2	1.85	0.59
7:N:63:VAL:HB	7:N:67:PHE:HZ	1.68	0.59
8:q:157:ILE:O	8:q:161:SER:OG	2.17	0.59
3:D:352:THR:OG1	3:D:354:ASP:OD1	2.20	0.59
4:E:206:PHE:HD1	4:E:209:ILE:HD12	1.68	0.59
2:b:52:LEU:HD12	2:b:62:MET:HE2	1.84	0.59
1:A:203:ARG:HA	5:G:504:GLN:HE22	1.68	0.59
3:d:430:ILE:HG12	3:d:462:PRO:HG2	1.85	0.59
1:A:289:THR:HG23	1:A:316:LEU:HD22	1.84	0.59
4:e:293:LYS:HD2	4:e:317:ASN:HB3	1.85	0.59
1:a:132:ILE:HD11	1:a:419:LEU:HD11	1.85	0.58
1:A:8:PHE:HB2	3:D:84:LEU:HD11	1.86	0.58
4:E:529:LYS:NZ	6:H:46:ASP:OD1	2.37	0.58
4:E:293:LYS:HD2	4:E:317:ASN:HB3	1.85	0.58
1:a:387:GLU:OE1	1:a:390:ARG:NH1	2.37	0.58
2:b:244:MET:HE1	2:b:304:PHE:HE2	1.68	0.58
4:E:485:MET:O	7:N:30:ARG:HD3	2.03	0.58
8:q:38:GLU:O	8:q:42:THR:HG23	2.02	0.58
6:H:280:LYS:NZ	6:H:335:ASN:OD1	2.31	0.58
8:Q:226:GLU:OE2	8:Q:359:GLN:NE2	2.37	0.58
9:Z:189:PHE:O	9:Z:323:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:437:ALA:O	4:e:445:GLN:NE2	2.37	0.58
4:E:18:ILE:HA	6:H:73:HIS:HB2	1.86	0.58
2:b:260:SER:OG	3:d:274:ARG:NH1	2.37	0.58
9:z:114:LEU:HD23	9:z:119:ILE:HD11	1.86	0.58
9:z:189:PHE:O	9:z:323:ARG:NH2	2.36	0.58
1:A:127:GLU:HG3	1:A:426:TYR:CZ	2.39	0.58
1:A:387:GLU:OE1	1:A:390:ARG:NH1	2.37	0.58
2:B:52:LEU:HD12	2:B:62:MET:HE2	1.84	0.58
2:b:79:PRO:HB2	4:e:60:MET:SD	2.44	0.58
3:d:480:LEU:HG	3:d:500:ILE:HD12	1.85	0.58
8:q:226:GLU:OE2	8:q:359:GLN:NE2	2.37	0.58
2:B:353:MET:SD	2:B:358:LYS:HG3	2.44	0.58
1:a:289:THR:HG23	1:a:316:LEU:HD22	1.84	0.58
2:b:285:HIS:HE1	2:b:335:PHE:HB3	1.69	0.58
7:n:63:VAL:HB	7:n:67:PHE:HZ	1.68	0.58
3:D:164:LEU:HD22	3:D:188:VAL:HG21	1.86	0.57
4:E:7:LEU:HD23	5:g:7:VAL:HG21	1.85	0.57
4:e:206:PHE:HD1	4:e:209:ILE:HD12	1.68	0.57
3:d:164:LEU:HD22	3:d:188:VAL:HG21	1.87	0.57
6:h:32:ILE:HG13	6:h:76:ALA:HB1	1.86	0.57
2:B:79:PRO:HB2	4:E:60:MET:SD	2.44	0.57
2:B:244:MET:HE1	2:B:304:PHE:HE2	1.68	0.57
3:D:480:LEU:HG	3:D:500:ILE:HD12	1.85	0.57
3:D:55:LYS:HG3	3:D:469:ALA:HA	1.86	0.57
3:D:26:ASP:O	2:b:25:ARG:NH2	2.38	0.57
5:G:8:LEU:CD1	5:G:12:GLN:HG3	2.35	0.57
9:Z:114:LEU:HD23	9:Z:119:ILE:HD11	1.86	0.57
9:z:195:GLU:HB2	9:z:384:LEU:HD13	1.87	0.57
3:d:55:LYS:HG3	3:d:469:ALA:HA	1.86	0.57
1:A:377:LEU:HD21	1:A:392:LEU:HD22	1.86	0.57
4:E:437:ALA:O	4:E:445:GLN:NE2	2.37	0.57
1:a:127:GLU:HG3	1:a:426:TYR:CZ	2.39	0.57
1:a:377:LEU:HD21	1:a:392:LEU:HD22	1.86	0.57
5:g:283:ILE:HD13	5:g:307:ALA:HB2	1.87	0.57
1:A:229:ILE:HD13	1:A:284:ASN:HB2	1.87	0.56
2:b:353:MET:SD	2:b:358:LYS:HG3	2.44	0.56
5:g:8:LEU:CD1	5:g:12:GLN:HG3	2.35	0.56
5:G:7:VAL:HG21	4:e:7:LEU:HD23	1.86	0.56
8:q:55:MET:HG3	8:q:63:LEU:HD11	1.87	0.56
1:A:132:ILE:HD11	1:A:419:LEU:HD11	1.85	0.56
6:H:32:ILE:HG13	6:H:76:ALA:HB1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:97:VAL:HG22	6:H:502:ALA:HA	1.87	0.56
8:Q:411:GLY:O	8:Q:492:MET:HG3	2.05	0.56
9:Z:24:ILE:HD13	9:Z:107:ASP:HB2	1.88	0.56
4:e:426:GLU:OE2	4:e:513:LYS:NZ	2.25	0.56
6:h:97:VAL:HG22	6:h:502:ALA:HA	1.86	0.56
8:q:280:VAL:HG21	8:q:304:TYR:CB	2.32	0.56
8:q:284:ALA:HB2	8:q:310:ILE:HD11	1.87	0.56
2:B:120:LYS:NZ	3:d:26:ASP:OD1	2.26	0.56
2:B:285:HIS:HE1	2:B:335:PHE:HB3	1.69	0.56
3:D:38:ILE:HG21	3:D:121:THR:OG1	2.05	0.56
8:Q:270:LYS:O	8:Q:274:ASN:ND2	2.25	0.56
1:a:317:LYS:HA	1:a:327:ILE:HD11	1.88	0.56
3:d:38:ILE:HG21	3:d:121:THR:OG1	2.05	0.56
5:g:520:ASP:OD1	5:g:521:ASP:N	2.35	0.56
7:N:31:ILE:O	7:N:71:ARG:NH2	2.38	0.56
8:Q:296:LYS:HG2	8:Q:297:VAL:H	1.71	0.56
1:a:42:ASP:OD1	5:g:518:ARG:NH2	2.31	0.56
3:d:214:LEU:HD22	3:d:395:LYS:HZ3	1.71	0.56
6:h:365:PRO:HD2	6:h:366:LYS:HD3	1.88	0.56
5:G:95:THR:OG1	12:G:603:AF3:F1	2.13	0.56
1:a:229:ILE:HD13	1:a:284:ASN:HB2	1.87	0.56
4:e:109:VAL:HG13	4:e:516:GLN:HG2	1.88	0.56
2:b:519:ASN:HB3	4:e:59:LYS:HD3	1.86	0.56
4:e:63:ASP:OD1	4:e:67:ASP:N	2.38	0.56
6:h:144:LYS:CD	6:h:144:LYS:H	2.18	0.56
7:n:31:ILE:O	7:n:71:ARG:NH2	2.38	0.56
2:B:260:SER:OG	3:D:274:ARG:NH1	2.39	0.56
9:Z:234:ASN:N	9:Z:333:LEU:O	2.37	0.56
5:g:132:ASP:OD2	5:g:437:TYR:OH	2.23	0.56
5:G:283:ILE:HD13	5:G:307:ALA:HB2	1.87	0.56
8:q:411:GLY:O	8:q:492:MET:HG3	2.05	0.56
4:E:63:ASP:OD1	4:E:67:ASP:N	2.38	0.56
5:G:489:ASP:HB3	5:G:492:GLU:HG2	1.88	0.56
3:D:429:GLU:HG2	3:D:461:ILE:HB	1.89	0.55
4:E:109:VAL:HG13	4:E:516:GLN:HG2	1.88	0.55
6:H:144:LYS:H	6:H:144:LYS:CD	2.18	0.55
8:Q:284:ALA:HB2	8:Q:310:ILE:HD11	1.87	0.55
5:g:497:GLU:HG3	5:g:498:PRO:HD2	1.88	0.55
4:E:153:ASP:O	4:E:418:VAL:N	2.32	0.55
2:B:25:ARG:NH2	3:d:26:ASP:O	2.38	0.55
9:Z:195:GLU:HB2	9:Z:384:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:8:PHE:HB2	3:d:84:LEU:HD11	1.88	0.55
5:g:95:THR:OG1	12:g:603:AF3:F1	2.13	0.55
1:A:354:GLU:HG3	1:A:363:LEU:HD12	1.88	0.55
5:G:497:GLU:HG3	5:G:498:PRO:HD2	1.88	0.55
6:H:365:PRO:HD2	6:H:366:LYS:HD3	1.88	0.55
3:D:171:LEU:O	3:D:177:SER:OG	2.24	0.55
8:Q:55:MET:HG2	8:Q:63:LEU:HD11	1.88	0.55
1:a:354:GLU:HG3	1:a:363:LEU:HD12	1.89	0.55
3:d:208:ILE:HD13	3:d:409:LEU:HD22	1.89	0.55
4:e:175:SER:OG	10:e:601:ADP:O1A	2.20	0.55
6:h:522:ASN:HD22	8:q:58:ASN:HA	1.71	0.55
9:z:24:ILE:HD13	9:z:107:ASP:HB2	1.88	0.55
2:B:49:ASP:OD1	3:D:531:LYS:NZ	2.37	0.55
6:H:292:LYS:HB2	6:H:319:LEU:HD12	1.90	0.55
8:Q:292:VAL:HG22	8:Q:313:VAL:HB	1.89	0.55
8:q:16:LYS:HE3	9:z:70:GLN:HG2	1.89	0.55
9:Z:459:LEU:HD12	9:Z:459:LEU:H	1.73	0.54
2:b:244:MET:HA	2:b:275:MET:HE1	1.88	0.54
4:e:18:ILE:HA	6:h:73:HIS:HB2	1.89	0.54
1:A:317:LYS:HA	1:A:327:ILE:HD11	1.88	0.54
2:B:519:ASN:HB3	4:E:59:LYS:HD3	1.89	0.54
8:q:55:MET:CG	8:q:63:LEU:HD11	2.37	0.54
3:D:208:ILE:HD13	3:D:409:LEU:HD22	1.89	0.54
9:Z:47:LEU:HD13	9:Z:66:GLU:HB2	1.89	0.54
3:d:429:GLU:HG2	3:d:461:ILE:HB	1.89	0.54
5:G:66:ILE:O	5:G:70:ILE:HG23	2.08	0.54
1:A:164:ASN:CG	1:A:206:MET:SD	2.91	0.54
6:H:522:ASN:HD22	8:Q:58:ASN:HA	1.72	0.54
4:e:344:ARG:NE	4:e:347:GLU:OE2	2.38	0.54
5:g:489:ASP:HB3	5:g:492:GLU:HG2	1.88	0.54
6:h:292:LYS:HB2	6:h:319:LEU:HD12	1.90	0.54
9:z:47:LEU:HD13	9:z:66:GLU:HB2	1.89	0.54
2:B:244:MET:HA	2:B:275:MET:HE1	1.88	0.54
2:B:255:ARG:HD3	4:E:265:LYS:HD2	1.89	0.54
5:G:520:ASP:OD1	5:G:521:ASP:N	2.35	0.54
2:b:407:VAL:HG13	2:b:413:SER:OG	2.08	0.54
3:d:352:THR:OG1	3:d:354:ASP:OD1	2.20	0.54
1:A:397:CYS:O	1:A:401:ARG:HG2	2.08	0.54
2:b:49:ASP:OD1	3:d:531:LYS:NZ	2.39	0.54
2:b:242:THR:HG21	2:b:335:PHE:HE2	1.73	0.54
3:d:122:LYS:HE3	3:d:126:LYS:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:229:LEU:HD12	3:d:374:LEU:HD12	1.89	0.54
9:z:459:LEU:H	9:z:459:LEU:HD12	1.73	0.54
4:E:175:SER:OG	10:E:601:ADP:O1A	2.20	0.54
2:B:218:PHE:HB2	2:B:326:VAL:HG11	1.90	0.53
7:N:36:TRP:O	7:N:48:VAL:N	2.41	0.53
3:d:171:LEU:O	3:d:177:SER:OG	2.24	0.53
5:g:66:ILE:O	5:g:70:ILE:HG23	2.08	0.53
2:B:219:LEU:HB2	2:B:372:THR:HG21	1.91	0.53
3:D:229:LEU:HD12	3:D:374:LEU:HD12	1.89	0.53
4:E:85:HIS:O	4:E:89:LYS:HG3	2.08	0.53
2:b:218:PHE:HB2	2:b:326:VAL:HG11	1.90	0.53
5:G:16:ARG:HG3	5:G:523:VAL:HG22	1.90	0.53
5:G:382:GLU:N	5:G:382:GLU:OE1	2.41	0.53
8:Q:16:LYS:HE3	9:Z:70:GLN:HG2	1.90	0.53
4:e:255:PHE:HB2	4:e:306:PHE:CB	2.38	0.53
5:g:382:GLU:N	5:g:382:GLU:OE1	2.41	0.53
8:q:296:LYS:HG2	8:q:297:VAL:H	1.71	0.53
1:a:397:CYS:O	1:a:401:ARG:HG2	2.08	0.53
6:h:21:GLN:OE1	6:h:25:ASN:ND2	2.37	0.53
3:D:26:ASP:OD1	3:D:26:ASP:N	2.41	0.53
3:D:122:LYS:HE3	3:D:126:LYS:HE3	1.90	0.53
4:E:255:PHE:HB2	4:E:306:PHE:CB	2.38	0.53
2:b:219:LEU:HB2	2:b:372:THR:HG21	1.91	0.53
8:q:292:VAL:HG22	8:q:313:VAL:HB	1.89	0.53
3:D:26:ASP:OD1	2:b:120:LYS:NZ	2.27	0.53
1:A:42:ASP:OD1	5:G:518:ARG:NH2	2.31	0.53
8:Q:151:ALA:HB3	8:Q:406:LYS:HE2	1.91	0.53
8:Q:157:ILE:HG13	8:Q:188:VAL:HG21	1.91	0.53
8:Q:286:THR:HG21	8:Q:338:PRO:HB2	1.89	0.53
2:b:250:LYS:NZ	4:e:309:GLU:OE1	2.42	0.53
6:h:73:HIS:HB3	6:h:76:ALA:HB3	1.91	0.53
6:h:157:LYS:HD3	6:h:491:PHE:HB3	1.91	0.53
4:E:426:GLU:N	4:E:426:GLU:OE1	2.42	0.53
1:a:118:ILE:HG12	1:a:522:ILE:HG13	1.91	0.53
2:b:39:VAL:HG22	2:b:100:THR:HG23	1.91	0.53
9:Z:268:GLU:O	9:Z:272:LYS:HD3	2.09	0.53
3:d:26:ASP:OD1	3:d:26:ASP:N	2.41	0.53
4:e:153:ASP:O	4:e:418:VAL:N	2.32	0.53
4:e:426:GLU:N	4:e:426:GLU:OE1	2.42	0.53
6:h:391:ASP:OD1	13:h:701:HOH:O	2.18	0.53
7:n:36:TRP:O	7:n:48:VAL:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:344:ARG:NE	4:E:347:GLU:OE2	2.38	0.53
5:G:289:VAL:HG21	5:G:350:LEU:HD13	1.91	0.53
9:Z:38:LEU:HG	10:Z:601:ADP:H5'1	1.91	0.53
2:b:278:LYS:NZ	2:b:281:ARG:HE	2.07	0.53
4:e:85:HIS:O	4:e:89:LYS:HG3	2.09	0.53
5:g:16:ARG:HG3	5:g:523:VAL:HG22	1.90	0.53
1:A:349:GLU:HB2	1:A:366:ASN:HB2	1.91	0.52
2:B:242:THR:HG21	2:B:335:PHE:HE2	1.73	0.52
2:B:407:VAL:HG13	2:B:413:SER:OG	2.08	0.52
6:H:185:MET:SD	6:H:370:CYS:HB3	2.49	0.52
1:a:349:GLU:HB2	1:a:366:ASN:HB2	1.91	0.52
8:q:286:THR:HG21	8:q:338:PRO:HB2	1.89	0.52
6:H:73:HIS:HB3	6:H:76:ALA:HB3	1.91	0.52
8:q:157:ILE:HG13	8:q:188:VAL:HG21	1.91	0.52
1:A:56:ASN:ND2	1:A:56:ASN:O	2.42	0.52
2:B:39:VAL:HG22	2:B:100:THR:HG23	1.91	0.52
6:H:93:GLY:O	6:H:97:VAL:HG23	2.09	0.52
9:z:268:GLU:O	9:z:272:LYS:HD3	2.09	0.52
1:A:118:ILE:HG12	1:A:522:ILE:HG13	1.91	0.52
9:Z:43:THR:O	9:Z:45:LYS:NZ	2.42	0.52
5:g:289:VAL:HG21	5:g:350:LEU:HD13	1.91	0.52
8:q:426:TYR:O	8:q:429:THR:HG22	2.09	0.52
1:a:56:ASN:ND2	1:a:56:ASN:O	2.42	0.52
6:h:185:MET:SD	6:h:370:CYS:HB3	2.49	0.52
9:z:418:MET:HE1	9:z:505:LEU:HD21	1.92	0.52
1:a:143:LEU:HB3	1:a:147:CYS:HB2	1.91	0.52
8:q:151:ALA:HB3	8:q:406:LYS:HE2	1.91	0.52
8:Q:131:GLY:HA3	8:Q:437:ALA:HB3	1.91	0.52
8:Q:426:TYR:O	8:Q:429:THR:HG22	2.09	0.52
9:Z:179:ILE:HD13	9:Z:191:ILE:HG13	1.92	0.52
9:Z:242:THR:OG1	9:Z:244:VAL:O	2.27	0.52
4:e:442:THR:HG22	4:e:444:GLU:H	1.75	0.52
9:z:43:THR:O	9:z:45:LYS:NZ	2.42	0.52
5:G:124:SER:OG	5:G:433:GLU:OE2	2.27	0.52
10:Z:601:ADP:O1B	12:Z:603:AF3:F1	2.17	0.52
9:z:38:LEU:HG	10:z:601:ADP:H5'1	1.91	0.52
1:A:143:LEU:HB3	1:A:147:CYS:HB2	1.91	0.52
9:Z:404:ASP:OD2	9:Z:499:CYS:HB3	2.10	0.52
9:Z:418:MET:HE3	9:Z:444:LEU:HD13	1.92	0.52
1:a:164:ASN:CG	1:a:206:MET:SD	2.93	0.52
6:h:93:GLY:O	6:h:97:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:q:381:THR:HG22	8:q:383:ASN:H	1.75	0.52
8:Q:117:GLU:O	8:Q:121:ILE:HG23	2.10	0.52
8:Q:328:VAL:HG12	8:Q:347:CYS:SG	2.50	0.52
4:e:529:LYS:NZ	6:h:46:ASP:OD1	2.39	0.52
8:q:117:GLU:O	8:q:121:ILE:HG23	2.10	0.52
4:e:185:MET:HE1	4:e:222:THR:HB	1.91	0.51
7:n:66:ARG:HB2	7:n:83:ASN:OD1	2.10	0.51
8:q:131:GLY:HA3	8:q:437:ALA:HB3	1.90	0.51
8:q:259:ILE:HG21	8:q:265:LEU:HB2	1.93	0.51
9:z:179:ILE:HD13	9:z:191:ILE:HG13	1.92	0.51
1:A:187:GLN:O	1:A:189:ARG:NH2	2.43	0.51
3:D:214:LEU:HD22	3:D:395:LYS:HZ3	1.74	0.51
4:E:442:THR:HG22	4:E:444:GLU:H	1.75	0.51
5:G:28:ASN:HA	5:G:31:LYS:HG2	1.91	0.51
6:H:455:PHE:CE1	6:H:482:GLU:HG2	2.45	0.51
7:N:66:ARG:HB2	7:N:83:ASN:OD1	2.10	0.51
8:q:328:VAL:HG12	8:q:347:CYS:SG	2.51	0.51
9:z:418:MET:HE3	9:z:444:LEU:HD13	1.92	0.51
5:G:460:ILE:O	5:G:464:THR:OG1	2.20	0.51
2:b:131:ARG:NH2	4:e:179:ASN:OD1	2.42	0.51
3:d:152:SER:OG	3:d:420:ALA:HB1	2.11	0.51
5:g:28:ASN:HA	5:g:31:LYS:HG2	1.91	0.51
1:A:23:MET:HG2	4:e:11:GLU:HG2	1.90	0.51
3:D:222:GLU:OE2	3:D:375:LYS:NZ	2.42	0.51
4:E:198:ASP:HB3	4:E:201:ARG:HB2	1.93	0.51
8:Q:415:THR:HG23	8:Q:416:GLU:OE1	2.10	0.51
10:z:601:ADP:O1B	12:z:603:AF3:F1	2.17	0.51
4:E:93:GLU:OE1	6:H:201:GLN:NE2	2.44	0.51
6:H:93:GLY:HA2	10:H:601:ADP:O2B	2.11	0.51
6:H:157:LYS:HD3	6:H:491:PHE:HB3	1.91	0.51
4:e:196:VAL:O	4:e:196:VAL:HG23	2.10	0.51
5:g:468:ALA:O	5:g:471:THR:OG1	2.27	0.51
2:B:278:LYS:NZ	2:B:281:ARG:HE	2.07	0.51
8:Q:259:ILE:HG21	8:Q:265:LEU:HB2	1.93	0.51
3:d:144:GLY:CA	3:d:432:LEU:HD11	2.41	0.51
5:g:260:ARG:NH2	5:g:263:ASP:OD2	2.44	0.51
6:h:93:GLY:HA2	10:h:601:ADP:O2B	2.11	0.51
6:h:455:PHE:CE1	6:h:482:GLU:HG2	2.46	0.51
5:G:468:ALA:O	5:G:471:THR:OG1	2.27	0.51
6:H:152:ARG:NH2	6:H:184:MET:SD	2.84	0.51
4:e:192:ALA:O	4:e:196:VAL:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:247:TYR:HB2	5:g:275:ILE:HD11	1.92	0.51
3:D:144:GLY:CA	3:D:432:LEU:HD11	2.41	0.51
4:E:11:GLU:HG2	1:a:23:MET:HG2	1.91	0.51
4:E:192:ALA:O	4:E:196:VAL:HG22	2.11	0.51
5:G:260:ARG:NH2	5:G:263:ASP:OD2	2.44	0.51
6:H:318:ASP:OD1	6:H:321:ARG:NH1	2.44	0.51
8:q:415:THR:HG23	8:q:416:GLU:OE1	2.10	0.51
9:z:404:ASP:OD2	9:z:499:CYS:HB3	2.10	0.51
1:A:220:VAL:HB	1:A:225:MET:HE3	1.93	0.51
4:E:456:GLU:OE2	4:E:478:ARG:NH2	2.40	0.51
1:a:479:GLU:HG3	1:a:480:ARG:HG2	1.93	0.51
4:e:198:ASP:HB3	4:e:201:ARG:HB2	1.93	0.51
2:B:52:LEU:O	3:D:538:THR:HG23	2.11	0.51
1:a:187:GLN:O	1:a:189:ARG:NH2	2.43	0.51
4:E:185:MET:HE1	4:E:222:THR:HB	1.91	0.50
7:N:39:GLN:N	7:N:92:VAL:O	2.39	0.50
4:e:485:MET:O	7:n:30:ARG:HD3	2.11	0.50
5:g:415:GLU:OE1	5:g:415:GLU:N	2.44	0.50
5:g:460:ILE:O	5:g:464:THR:OG1	2.20	0.50
5:G:155:ILE:HG12	5:G:407:LEU:HD11	1.93	0.50
4:E:280:TYR:O	4:E:284:LYS:HG2	2.11	0.50
8:Q:381:THR:HG22	8:Q:383:ASN:H	1.75	0.50
1:a:283:ALA:HB2	1:a:345:LEU:HD21	1.93	0.50
2:b:71:LEU:HB3	2:b:85:VAL:HG22	1.92	0.50
6:h:318:ASP:OD1	6:h:321:ARG:NH1	2.44	0.50
8:q:410:PRO:O	8:q:415:THR:HG22	2.11	0.50
2:B:71:LEU:HB3	2:B:85:VAL:HG22	1.92	0.50
5:G:247:TYR:HB2	5:G:275:ILE:HD11	1.93	0.50
8:Q:469:ALA:O	8:Q:473:GLU:HG3	2.11	0.50
9:Z:418:MET:HE1	9:Z:505:LEU:HD21	1.92	0.50
4:E:4:MET:HB2	4:E:7:LEU:HD11	1.93	0.50
4:E:196:VAL:O	4:E:196:VAL:HG23	2.10	0.50
7:n:4:LEU:HD22	7:n:22:CYS:SG	2.51	0.50
4:E:44:VAL:O	4:E:48:MET:HG2	2.12	0.50
5:G:133:MET:HE1	5:G:440:VAL:HG22	1.93	0.50
6:H:391:ASP:OD1	13:H:701:HOH:O	2.19	0.50
7:N:4:LEU:HD22	7:N:22:CYS:SG	2.51	0.50
4:e:93:GLU:OE1	6:h:201:GLN:NE2	2.44	0.50
5:g:155:ILE:HG12	5:g:407:LEU:HD11	1.93	0.50
9:z:114:LEU:HD22	9:z:435:LEU:HD12	1.94	0.50
9:z:242:THR:OG1	9:z:244:VAL:O	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ALA:HB2	1:A:345:LEU:HD21	1.93	0.50
3:D:152:SER:OG	3:D:420:ALA:HB1	2.11	0.50
9:Z:114:LEU:HD22	9:Z:435:LEU:HD12	1.94	0.50
5:g:133:MET:HE1	5:g:440:VAL:HG22	1.94	0.50
6:h:522:ASN:ND2	8:q:75:GLU:O	2.45	0.50
10:H:601:ADP:O1B	12:H:603:AF3:F2	2.20	0.50
4:e:255:PHE:HB2	4:e:306:PHE:HB3	1.94	0.50
5:g:332:VAL:HG12	5:g:334:ARG:H	1.76	0.50
6:h:95:THR:HB	10:h:601:ADP:O3B	2.11	0.50
1:A:533:LEU:HD13	3:D:82:GLN:HG2	1.94	0.50
2:B:250:LYS:NZ	4:E:309:GLU:OE1	2.45	0.50
3:d:317:LEU:HD13	3:d:324:VAL:HG21	1.94	0.50
9:z:277:LEU:HD22	9:z:339:LEU:HG	1.93	0.50
4:E:397:GLU:OE1	4:E:400:ARG:HD2	2.12	0.49
1:a:220:VAL:HB	1:a:225:MET:HE3	1.93	0.49
4:e:397:GLU:OE1	4:e:400:ARG:HD2	2.12	0.49
1:A:479:GLU:HG3	1:A:480:ARG:HG2	1.93	0.49
5:G:130:LEU:HB2	5:G:510:VAL:HG11	1.94	0.49
6:H:95:THR:HB	10:H:601:ADP:O3B	2.11	0.49
9:Z:277:LEU:HD22	9:Z:339:LEU:HG	1.93	0.49
4:e:44:VAL:O	4:e:48:MET:HG2	2.12	0.49
5:g:411:GLY:HA3	5:g:490:MET:HE3	1.94	0.49
6:h:152:ARG:NH2	6:h:184:MET:SD	2.84	0.49
10:h:601:ADP:O1B	12:h:603:AF3:F2	2.20	0.49
9:z:234:ASN:N	9:z:333:LEU:O	2.37	0.49
2:b:29:PHE:CD2	2:b:114:GLU:HB2	2.47	0.49
2:b:238:LEU:HB2	2:b:287:ILE:HG21	1.94	0.49
5:g:124:SER:OG	5:g:433:GLU:OE2	2.27	0.49
1:A:216:LEU:HD13	1:A:319:ILE:HD11	1.93	0.49
3:D:227:LEU:HD23	3:D:376:ILE:HD12	1.94	0.49
5:G:84:SER:HB2	5:G:99:ILE:HD11	1.94	0.49
8:Q:114:LEU:O	8:Q:117:GLU:HG2	2.13	0.49
8:Q:410:PRO:O	8:Q:415:THR:HG22	2.11	0.49
3:d:430:ILE:HD11	3:d:477:VAL:HG13	1.95	0.49
3:d:438:GLU:O	3:d:442:THR:HG23	2.13	0.49
4:e:4:MET:HB2	4:e:7:LEU:HD11	1.93	0.49
6:h:144:LYS:H	6:h:144:LYS:HD3	1.77	0.49
9:z:23:ASN:OD1	9:z:73:THR:OG1	2.30	0.49
4:E:220:GLU:CD	4:E:220:GLU:H	2.21	0.49
4:E:255:PHE:HB2	4:E:306:PHE:HB3	1.94	0.49
9:Z:172:VAL:HG13	9:Z:395:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:130:ARG:NH2	1:a:422:TYR:OH	2.44	0.49
1:a:216:LEU:HD13	1:a:319:ILE:HD11	1.94	0.49
2:b:52:LEU:O	3:d:538:THR:HG23	2.11	0.49
8:q:469:ALA:O	8:q:473:GLU:HG3	2.11	0.49
9:z:188:LEU:HD11	9:z:399:LYS:HD2	1.95	0.49
3:D:144:GLY:HA2	3:D:432:LEU:HD11	1.95	0.49
5:G:332:VAL:HG12	5:G:334:ARG:H	1.76	0.49
6:H:145:LYS:HD3	6:H:147:ASP:HB2	1.95	0.49
6:h:145:LYS:HD3	6:h:147:ASP:HB2	1.95	0.49
5:G:459:THR:O	5:G:463:LEU:HB2	2.13	0.49
5:g:136:THR:O	5:g:139:LYS:HG2	2.12	0.49
3:D:317:LEU:HD13	3:D:324:VAL:HG21	1.94	0.49
3:D:438:GLU:O	3:D:442:THR:HG23	2.12	0.49
5:G:411:GLY:HA3	5:G:490:MET:HE3	1.94	0.49
6:H:144:LYS:H	6:H:144:LYS:HD3	1.77	0.49
1:a:230:VAL:HG23	1:a:231:ASN:H	1.78	0.49
8:q:272:GLU:HG2	9:z:253:ALA:HB2	1.95	0.49
1:A:384:MET:HG3	5:G:515:LEU:HD13	1.95	0.49
2:B:29:PHE:CD2	2:B:114:GLU:HB2	2.47	0.49
9:Z:23:ASN:OD1	9:Z:73:THR:OG1	2.30	0.49
6:h:153:LYS:O	6:h:157:LYS:HG3	2.13	0.49
9:z:15:ARG:H	9:z:18:ALA:HB3	1.78	0.49
2:B:52:LEU:HD13	2:B:73:ASN:HB2	1.95	0.49
2:b:222:LYS:HE3	2:b:315:ALA:HA	1.95	0.49
5:g:84:SER:HB2	5:g:99:ILE:HD11	1.95	0.49
8:q:114:LEU:O	8:q:117:GLU:HG2	2.12	0.49
2:B:64:THR:HG21	2:B:69:THR:HB	1.95	0.48
3:D:170:SER:HB3	3:D:411:VAL:HG21	1.95	0.48
5:g:130:LEU:HB2	5:g:510:VAL:HG11	1.94	0.48
9:z:181:LYS:HE2	9:z:370:ARG:HD3	1.94	0.48
1:A:49:ILE:HD11	5:G:528:LYS:HE3	1.94	0.48
5:G:136:THR:O	5:G:139:LYS:HG2	2.12	0.48
9:Z:188:LEU:HD11	9:Z:399:LYS:HD2	1.95	0.48
9:Z:453:GLN:OE1	9:Z:459:LEU:HD11	2.13	0.48
1:a:49:ILE:HD11	5:g:528:LYS:HE3	1.94	0.48
3:d:227:LEU:HD23	3:d:376:ILE:HD12	1.94	0.48
4:e:220:GLU:CD	4:e:220:GLU:H	2.21	0.48
4:e:280:TYR:O	4:e:284:LYS:HG2	2.11	0.48
2:B:222:LYS:HE3	2:B:315:ALA:HA	1.95	0.48
1:a:12:SER:HB3	1:a:17:ILE:HB	1.95	0.48
3:d:431:GLU:OE2	3:d:484:HIS:ND1	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:459:THR:O	5:g:463:LEU:HB2	2.13	0.48
8:q:339:PRO:HG2	8:q:344:MET:HE3	1.95	0.48
2:B:131:ARG:NH2	4:E:179:ASN:OD1	2.45	0.48
4:E:518:SER:O	4:E:522:GLN:HG2	2.14	0.48
6:H:219:THR:O	6:H:219:THR:OG1	2.31	0.48
8:Q:6:PRO:HG3	9:z:71:HIS:CE1	2.48	0.48
2:b:64:THR:HG21	2:b:69:THR:HB	1.95	0.48
9:z:172:VAL:HG13	9:z:395:LEU:HD23	1.94	0.48
1:A:12:SER:HB3	1:A:17:ILE:HB	1.95	0.48
6:H:21:GLN:OE1	6:H:25:ASN:ND2	2.37	0.48
6:H:61:ASP:OD2	13:H:701:HOH:O	2.20	0.48
2:B:238:LEU:HB2	2:B:287:ILE:HG21	1.94	0.48
9:Z:71:HIS:CE1	8:q:6:PRO:HG3	2.48	0.48
1:a:297:LEU:O	1:a:301:VAL:HG23	2.14	0.48
4:e:168:THR:HG23	4:e:507:ILE:HG22	1.96	0.48
8:q:239:ILE:HD13	8:q:328:VAL:HG11	1.96	0.48
1:a:492:ASN:HB2	1:a:494:LYS:HG2	1.94	0.48
2:b:52:LEU:HD13	2:b:73:ASN:HB2	1.95	0.48
6:h:219:THR:O	6:h:219:THR:OG1	2.31	0.48
1:A:230:VAL:HG23	1:A:231:ASN:H	1.78	0.48
8:q:16:LYS:HZ2	9:z:68:GLN:HA	1.78	0.48
3:D:430:ILE:HD11	3:D:477:VAL:HG13	1.95	0.48
8:Q:16:LYS:HZ2	9:Z:68:GLN:HA	1.79	0.48
8:Q:168:ILE:HD13	8:Q:179:LEU:HB2	1.96	0.48
4:e:518:SER:O	4:e:522:GLN:HG2	2.14	0.48
1:A:153:LYS:HE2	1:A:166:ASP:HA	1.95	0.48
1:A:297:LEU:O	1:A:301:VAL:HG23	2.14	0.48
1:A:492:ASN:HB2	1:A:494:LYS:HG2	1.94	0.48
2:B:35:ILE:HD12	2:B:71:LEU:HD22	1.96	0.48
7:N:63:VAL:HB	7:N:67:PHE:CZ	2.48	0.48
1:a:384:MET:HG3	5:g:515:LEU:HD13	1.96	0.48
5:g:226:HIS:HD2	5:g:228:ARG:H	1.61	0.48
8:q:168:ILE:HD13	8:q:179:LEU:HB2	1.96	0.48
9:z:15:ARG:N	9:z:18:ALA:HB3	2.29	0.48
9:z:453:GLN:OE1	9:z:459:LEU:HD11	2.13	0.48
3:D:94:LEU:HD13	3:D:525:THR:OG1	2.13	0.47
6:H:153:LYS:O	6:H:157:LYS:HG3	2.13	0.47
8:Q:239:ILE:HD13	8:Q:328:VAL:HG11	1.96	0.47
9:Z:181:LYS:HE2	9:Z:370:ARG:HD3	1.94	0.47
1:a:153:LYS:HE2	1:a:166:ASP:HA	1.96	0.47
3:d:302:LYS:N	3:d:328:ILE:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:61:ASP:OD2	13:h:701:HOH:O	2.20	0.47
8:Q:339:PRO:HG2	8:Q:344:MET:HE3	1.95	0.47
1:a:288:THR:HG22	1:a:290:GLY:N	2.27	0.47
3:d:170:SER:HB3	3:d:411:VAL:HG21	1.95	0.47
4:e:196:VAL:HG12	4:e:381:ARG:O	2.15	0.47
5:g:59:MET:HE3	9:z:514:ASN:HB3	1.97	0.47
4:e:196:VAL:HG21	4:e:209:ILE:HG13	1.96	0.47
5:g:182:MET:HE3	5:g:369:PRO:HG2	1.97	0.47
7:n:63:VAL:HB	7:n:67:PHE:CZ	2.48	0.47
1:A:66:GLU:OE2	5:G:11:SER:OG	2.31	0.47
6:h:116:LEU:HD12	6:h:117:HIS:H	1.80	0.47
6:H:32:ILE:CG1	6:H:76:ALA:HB1	2.44	0.47
6:H:394:MET:O	6:H:398:ARG:HG2	2.15	0.47
3:d:144:GLY:HA2	3:d:432:LEU:HD11	1.95	0.47
5:g:57:ILE:HG21	9:z:76:LEU:HD21	1.96	0.47
8:q:81:PRO:HB2	9:z:46:MET:SD	2.54	0.47
1:A:288:THR:HG22	1:A:290:GLY:N	2.27	0.47
1:A:319:ILE:O	1:A:323:SER:OG	2.29	0.47
8:Q:118:LEU:O	8:Q:121:ILE:HG12	2.15	0.47
1:a:158:SER:OG	10:a:601:ADP:O2A	2.21	0.47
1:a:533:LEU:HD13	3:d:82:GLN:HG2	1.96	0.47
2:b:35:ILE:HD12	2:b:71:LEU:HD22	1.96	0.47
3:d:94:LEU:HD13	3:d:525:THR:OG1	2.13	0.47
1:A:273:GLU:HA	1:A:276:GLN:HE21	1.80	0.47
3:D:467:GLU:HG3	3:D:468:ASN:N	2.30	0.47
4:E:168:THR:HG23	4:E:507:ILE:HG22	1.96	0.47
5:G:415:GLU:OE1	5:G:415:GLU:N	2.44	0.47
8:Q:123:LEU:HD11	8:Q:436:TYR:HB2	1.97	0.47
3:d:303:SER:HB3	3:d:308:ALA:HB2	1.96	0.47
4:e:109:VAL:HG12	4:e:516:GLN:HA	1.97	0.47
8:q:123:LEU:HD11	8:q:436:TYR:HB2	1.96	0.47
8:q:416:GLU:OE1	8:q:416:GLU:N	2.44	0.47
5:G:226:HIS:HD2	5:G:228:ARG:H	1.61	0.47
4:E:367:THR:OG1	4:E:369:ASP:OD1	2.24	0.47
1:a:273:GLU:HA	1:a:276:GLN:HE21	1.80	0.47
2:b:4:LEU:HA	4:e:43:ALA:HB1	1.96	0.47
3:d:266:VAL:HG13	3:d:271:GLN:HB2	1.97	0.47
8:q:32:ASN:HD21	8:q:524:ILE:HD11	1.79	0.47
9:z:426:LYS:NZ	9:z:438:GLN:HE21	2.13	0.47
1:A:81:LEU:HD11	3:D:215:GLY:HA2	1.96	0.47
4:E:109:VAL:HG12	4:E:516:GLN:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:80:MET:HE1	5:G:102:ALA:HB3	1.97	0.47
5:G:414:SER:HB2	5:G:502:LYS:NZ	2.30	0.47
6:H:196:GLY:O	6:H:372:PHE:N	2.35	0.47
8:Q:32:ASN:HD21	8:Q:524:ILE:HD11	1.79	0.47
8:Q:140:HIS:NE2	8:Q:509:LYS:HE3	2.30	0.47
8:Q:340:VAL:CG2	8:Q:342:GLU:HG3	2.45	0.47
9:Z:176:ILE:HD13	9:Z:398:VAL:HB	1.97	0.47
3:d:256:PRO:HD3	3:d:282:TYR:CD2	2.50	0.47
7:n:85:LEU:HD12	7:n:86:LYS:H	1.80	0.47
8:q:340:VAL:CG2	8:q:342:GLU:HG3	2.45	0.47
9:z:190:MET:SD	9:z:326:LEU:HD12	2.55	0.47
3:D:256:PRO:HD3	3:D:282:TYR:CD2	2.50	0.46
5:G:183:VAL:HG21	5:G:199:ALA:HB2	1.98	0.46
9:Z:415:GLU:OE2	9:Z:501:LYS:NZ	2.41	0.46
3:d:467:GLU:HG3	3:d:468:ASN:N	2.30	0.46
8:q:118:LEU:O	8:q:121:ILE:HG12	2.15	0.46
3:D:302:LYS:N	3:D:328:ILE:O	2.46	0.46
3:D:303:SER:HB3	3:D:308:ALA:HB2	1.96	0.46
4:E:159:ILE:HG13	4:E:159:ILE:O	2.16	0.46
6:H:191:GLN:OE1	6:H:193:LYS:HE3	2.16	0.46
6:H:522:ASN:ND2	8:Q:75:GLU:O	2.47	0.46
2:b:255:ARG:HD3	4:e:265:LYS:HD2	1.96	0.46
8:q:140:HIS:NE2	8:q:509:LYS:HE3	2.30	0.46
6:H:116:LEU:HD12	6:H:117:HIS:H	1.80	0.46
6:H:181:ASP:O	6:H:185:MET:HG2	2.16	0.46
6:H:319:LEU:HD23	6:H:319:LEU:HA	1.78	0.46
5:g:414:SER:HB2	5:g:502:LYS:NZ	2.30	0.46
5:g:516:LEU:HA	5:g:519:ILE:HD12	1.98	0.46
2:B:4:LEU:HA	4:E:43:ALA:HB1	1.97	0.46
3:D:266:VAL:HG13	3:D:271:GLN:HB2	1.97	0.46
5:G:13:ASN:O	5:G:525:GLY:HA3	2.16	0.46
7:N:85:LEU:HD12	7:N:86:LYS:H	1.80	0.46
5:g:13:ASN:O	5:g:525:GLY:HA3	2.16	0.46
2:B:52:LEU:HA	2:B:52:LEU:HD23	1.63	0.46
5:G:123:ILE:HG23	5:G:514:VAL:HG22	1.97	0.46
5:G:182:MET:HE3	5:G:369:PRO:HG2	1.97	0.46
1:a:294:ASP:O	1:a:298:LYS:HG2	2.16	0.46
2:b:249:ILE:HG21	4:e:277:LEU:HG	1.98	0.46
6:h:32:ILE:CG1	6:h:76:ALA:HB1	2.44	0.46
7:n:38:ARG:HD3	7:n:91:ALA:HB3	1.97	0.46
7:n:111:GLN:O	7:n:111:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:31:LEU:HG	4:E:35:LYS:HE2	1.98	0.46
4:E:196:VAL:HG21	4:E:209:ILE:HG13	1.96	0.46
4:E:368:LYS:O	4:E:368:LYS:HG2	2.16	0.46
7:N:111:GLN:O	7:N:111:GLN:HG2	2.16	0.46
9:Z:190:MET:SD	9:Z:326:LEU:HD12	2.55	0.46
4:e:368:LYS:O	4:e:368:LYS:HG2	2.16	0.46
9:z:412:GLY:HA2	9:z:415:GLU:OE1	2.16	0.46
1:A:130:ARG:NH2	1:A:422:TYR:OH	2.44	0.46
1:A:341:GLU:HB2	1:A:344:MET:SD	2.56	0.46
4:E:101:GLU:OE1	6:H:375:ARG:NH2	2.46	0.46
1:A:358:ASP:HB2	5:G:89:GLU:HB3	1.98	0.46
4:E:253:CYS:HB3	4:E:343:PRO:O	2.16	0.46
6:H:26:ILE:O	6:H:30:GLN:HG2	2.16	0.46
9:Z:66:GLU:O	9:Z:68:GLN:NE2	2.49	0.46
9:Z:146:GLU:CD	9:Z:146:GLU:H	2.24	0.46
6:h:191:GLN:OE1	6:h:193:LYS:HE3	2.16	0.46
9:z:146:GLU:H	9:z:146:GLU:CD	2.24	0.46
2:B:249:ILE:HG21	4:E:277:LEU:HG	1.97	0.46
2:B:285:HIS:CE1	2:B:335:PHE:HB3	2.50	0.46
3:D:415:LEU:HD12	3:D:415:LEU:HA	1.78	0.46
5:G:118:HIS:ND1	5:G:120:THR:HG23	2.31	0.46
9:Z:30:LEU:HD11	9:Z:74:ALA:HA	1.98	0.46
9:Z:426:LYS:NZ	9:Z:438:GLN:HE21	2.13	0.46
1:a:341:GLU:HB2	1:a:344:MET:SD	2.56	0.46
3:d:222:GLU:OE2	3:d:375:LYS:NZ	2.42	0.46
3:d:267:SER:H	3:d:271:GLN:NE2	2.14	0.46
4:e:31:LEU:HG	4:e:35:LYS:HE2	1.98	0.46
5:g:123:ILE:HG23	5:g:514:VAL:HG22	1.97	0.46
6:h:26:ILE:O	6:h:30:GLN:HG2	2.16	0.46
6:h:384:GLU:OE1	6:h:387:ARG:NH1	2.41	0.46
6:h:394:MET:O	6:h:398:ARG:HG2	2.15	0.46
5:G:79:SER:O	5:G:83:ILE:HG23	2.16	0.46
1:a:421:ILE:HG23	1:a:472:ASN:HD22	1.81	0.46
5:g:79:SER:O	5:g:83:ILE:HG23	2.16	0.46
5:g:183:VAL:HG21	5:g:199:ALA:HB2	1.97	0.46
1:A:294:ASP:O	1:A:298:LYS:HG2	2.16	0.45
3:D:254:SER:OG	3:D:307:ASP:O	2.34	0.45
8:Q:456:SER:OG	8:Q:482:ILE:HG22	2.17	0.45
4:e:157:VAL:HA	4:e:165:LEU:HD11	1.98	0.45
5:g:80:MET:HE1	5:g:102:ALA:HB3	1.98	0.45
6:h:196:GLY:O	6:h:372:PHE:N	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:THR:HG22	3:D:264:ILE:HD13	1.98	0.45
4:E:196:VAL:HG12	4:E:381:ARG:O	2.14	0.45
5:G:57:ILE:HG21	9:Z:76:LEU:HD21	1.99	0.45
5:G:59:MET:HE3	9:Z:514:ASN:HB3	1.98	0.45
5:G:516:LEU:HA	5:G:519:ILE:HD12	1.97	0.45
1:a:81:LEU:HD11	3:d:215:GLY:HA2	1.98	0.45
1:a:358:ASP:HB2	5:g:89:GLU:HB3	1.98	0.45
3:d:511:PRO:HG2	3:d:514:VAL:HG23	1.99	0.45
4:e:253:CYS:HB3	4:e:343:PRO:O	2.16	0.45
7:n:66:ARG:NE	7:n:84:SER:HB3	2.31	0.45
3:D:511:PRO:HG2	3:D:514:VAL:HG23	1.99	0.45
4:E:88:ALA:O	4:E:92:VAL:HG23	2.16	0.45
2:b:151:ASP:OD2	2:b:154:LYS:NZ	2.38	0.45
4:e:280:TYR:OH	6:h:264:GLN:OE1	2.22	0.45
2:b:141:LEU:HD21	2:b:500:LYS:HB3	1.99	0.45
4:e:231:ASP:HA	4:e:371:MET:HG2	1.98	0.45
9:z:30:LEU:HD11	9:z:74:ALA:HA	1.98	0.45
1:A:157:SER:O	1:A:158:SER:OG	2.35	0.45
3:D:267:SER:H	3:D:271:GLN:NE2	2.14	0.45
6:H:156:GLU:OE2	6:H:177:LYS:HA	2.16	0.45
8:Q:416:GLU:OE1	8:Q:416:GLU:N	2.44	0.45
9:Z:221:MET:HE1	9:Z:312:ALA:HB3	1.99	0.45
4:e:456:GLU:OE2	4:e:478:ARG:NH2	2.41	0.45
6:h:10:LYS:O	6:h:13:THR:OG1	2.31	0.45
9:z:180:LYS:HG2	9:z:181:LYS:N	2.28	0.45
6:H:29:CYS:SG	6:H:513:ILE:HD13	2.57	0.45
6:h:29:CYS:SG	6:h:513:ILE:HD13	2.57	0.45
8:q:456:SER:OG	8:q:482:ILE:HG22	2.17	0.45
2:B:148:HIS:HD2	2:B:158:ASP:OD2	2.00	0.45
4:E:305:GLY:HA3	4:E:324:TRP:CE2	2.52	0.45
5:G:43:PRO:HA	5:G:162:THR:HA	1.99	0.45
8:Q:272:GLU:HG2	9:Z:253:ALA:HB2	1.98	0.45
4:e:107:THR:HB	10:e:601:ADP:O2B	2.17	0.45
5:g:43:PRO:HA	5:g:162:THR:HA	1.99	0.45
6:h:90:VAL:HG11	6:h:498:VAL:HG22	1.99	0.45
9:z:176:ILE:HD13	9:z:398:VAL:HB	1.97	0.45
1:A:39:VAL:HG21	1:A:456:ALA:HB2	1.99	0.45
1:A:421:ILE:HG23	1:A:472:ASN:HD22	1.81	0.45
2:B:162:ILE:HD11	2:B:406:THR:HG22	1.99	0.45
4:e:159:ILE:HG13	4:e:159:ILE:O	2.16	0.45
9:z:127:LYS:HE2	9:z:506:HIS:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:TYR:HA	1:A:475:GLN:HE22	1.82	0.45
4:E:231:ASP:HA	4:E:371:MET:HG2	1.98	0.45
5:G:265:THR:HG21	9:Z:265:LYS:HB3	1.99	0.45
6:H:317:GLU:H	6:H:317:GLU:CD	2.25	0.45
7:N:32:ASN:N	7:N:98:ASN:O	2.50	0.45
7:N:38:ARG:HD3	7:N:91:ALA:HB3	1.97	0.45
7:N:66:ARG:NE	7:N:84:SER:HB3	2.31	0.45
1:a:39:VAL:HG21	1:a:456:ALA:HB2	1.99	0.45
3:d:209:LYS:HB2	3:d:335:PHE:CZ	2.52	0.45
6:h:74:PRO:HB2	8:q:55:MET:HG2	1.98	0.45
7:n:104:GLU:H	7:n:104:GLU:HG3	1.62	0.45
9:z:66:GLU:O	9:z:68:GLN:NE2	2.49	0.45
1:A:519:GLU:HG3	3:D:217:THR:HG22	1.99	0.45
3:D:432:LEU:HD12	3:D:432:LEU:HA	1.79	0.45
9:Z:412:GLY:HA2	9:Z:415:GLU:OE1	2.16	0.45
2:b:381:GLN:HE22	3:d:93:GLU:HG3	1.82	0.45
6:h:156:GLU:OE2	6:h:177:LYS:HA	2.16	0.45
6:h:181:ASP:O	6:h:185:MET:HG2	2.16	0.45
6:h:326:CYS:HB3	6:h:344:ARG:H	1.81	0.45
1:A:508:ILE:HD11	1:A:512:LYS:NZ	2.32	0.44
4:E:342:VAL:HG21	4:E:348:LEU:HD13	1.99	0.44
6:H:364:CYS:HB2	6:H:367:ALA:HB2	1.99	0.44
1:a:508:ILE:HD11	1:a:512:LYS:NZ	2.32	0.44
2:b:148:HIS:HD2	2:b:158:ASP:OD2	1.99	0.44
10:d:601:ADP:O3B	12:d:603:AF3:F1	2.25	0.44
4:e:368:LYS:HE2	4:e:368:LYS:HB3	1.69	0.44
5:g:118:HIS:ND1	5:g:120:THR:HG23	2.31	0.44
5:g:416:MET:SD	5:g:445:GLU:HG2	2.57	0.44
9:z:221:MET:HE1	9:z:312:ALA:HB3	1.99	0.44
5:G:132:ASP:OD2	5:G:437:TYR:OH	2.23	0.44
6:H:23:VAL:HG13	6:H:109:LYS:HE3	1.99	0.44
6:H:255:ILE:HD13	6:H:266:ILE:HG21	1.99	0.44
9:Z:392:ARG:O	9:Z:396:ARG:HG2	2.18	0.44
1:a:157:SER:O	1:a:158:SER:OG	2.35	0.44
4:e:88:ALA:O	4:e:92:VAL:HG23	2.17	0.44
6:h:148:LYS:HE2	6:h:148:LYS:HA	1.99	0.44
9:z:514:ASN:O	9:z:518:VAL:HG23	2.18	0.44
3:D:218:ILE:HD11	3:D:397:VAL:HG22	2.00	0.44
6:H:89:GLU:OE1	8:Q:378:ARG:NH2	2.47	0.44
8:Q:81:PRO:HB2	9:Z:46:MET:SD	2.57	0.44
4:e:305:GLY:HA3	4:e:324:TRP:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:342:VAL:HG21	4:e:348:LEU:HD13	1.99	0.44
9:z:47:LEU:HD13	9:z:66:GLU:CB	2.48	0.44
2:B:121:ILE:HG12	2:B:431:LYS:HD3	1.99	0.44
4:E:107:THR:HB	10:E:601:ADP:O2B	2.17	0.44
4:E:473:THR:O	4:E:477:VAL:HG13	2.18	0.44
7:N:67:PHE:CD2	7:N:82:MET:HE1	2.53	0.44
5:G:379:ALA:HB1	9:Z:80:VAL:HG23	2.00	0.44
8:Q:275:LEU:HD22	9:Z:253:ALA:HB1	1.99	0.44
2:b:65:ASN:O	2:b:65:ASN:ND2	2.51	0.44
9:z:225:VAL:CG1	9:z:288:GLY:HA3	2.47	0.44
2:B:141:LEU:HD21	2:B:500:LYS:HB3	1.98	0.44
3:D:209:LYS:HB2	3:D:335:PHE:CZ	2.52	0.44
3:D:489:LYS:HB3	3:D:489:LYS:HE3	1.75	0.44
10:D:601:ADP:O3B	12:D:603:AF3:F1	2.25	0.44
4:E:301:ILE:HG23	4:E:325:VAL:HG21	2.00	0.44
6:H:90:VAL:HG11	6:H:498:VAL:HG22	1.99	0.44
6:H:318:ASP:O	6:H:322:THR:OG1	2.34	0.44
6:H:326:CYS:HB3	6:H:344:ARG:H	1.81	0.44
7:N:89:ASP:N	7:N:89:ASP:OD1	2.51	0.44
8:Q:324:LEU:O	8:Q:328:VAL:HG22	2.17	0.44
1:a:422:TYR:HA	1:a:475:GLN:HE22	1.82	0.44
2:b:244:MET:HB3	2:b:244:MET:HE3	1.72	0.44
4:e:233:ASP:OD1	4:e:233:ASP:N	2.51	0.44
7:n:39:GLN:N	7:n:92:VAL:O	2.38	0.44
7:n:67:PHE:CD2	7:n:82:MET:HE1	2.53	0.44
8:q:324:LEU:O	8:q:328:VAL:HG22	2.17	0.44
9:z:77:ILE:O	9:z:80:VAL:HG12	2.18	0.44
9:z:392:ARG:O	9:z:396:ARG:HG2	2.18	0.44
4:E:157:VAL:HA	4:E:165:LEU:HD11	1.99	0.44
4:E:233:ASP:N	4:E:233:ASP:OD1	2.51	0.44
6:H:297:ASP:OD1	6:H:297:ASP:N	2.51	0.44
1:a:205:GLN:HE21	1:a:384:MET:HE3	1.83	0.44
2:b:480:MET:HG3	10:b:601:ADP:C2	2.53	0.44
6:h:187:ASP:O	6:h:190:LEU:HD23	2.18	0.44
2:B:205:LEU:HA	2:B:383:LEU:HD11	1.99	0.44
4:E:202:ARG:NH2	4:E:413:ILE:O	2.51	0.44
8:Q:322:ARG:CZ	8:Q:322:ARG:HB3	2.48	0.44
9:Z:91:GLY:O	9:Z:95:ASN:HB2	2.17	0.44
9:Z:127:LYS:HE2	9:Z:506:HIS:HA	1.99	0.44
9:Z:225:VAL:CG1	9:Z:288:GLY:HA3	2.47	0.44
4:e:202:ARG:NH2	4:e:413:ILE:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:247:TYR:HB2	5:g:275:ILE:CD1	2.48	0.44
6:h:23:VAL:HG13	6:h:109:LYS:HE3	1.99	0.44
6:h:255:ILE:HD13	6:h:266:ILE:HG21	1.99	0.44
6:h:290:LEU:HD11	6:h:361:PHE:CZ	2.53	0.44
9:z:15:ARG:O	9:z:19:ALA:CB	2.65	0.44
9:z:135:GLU:HA	9:z:138:LYS:HD3	2.00	0.44
1:A:104:ALA:O	1:A:108:VAL:HG23	2.17	0.44
2:B:3:SER:O	2:B:7:ALA:HB2	2.18	0.44
9:Z:77:ILE:O	9:Z:80:VAL:HG12	2.18	0.44
9:Z:135:GLU:HA	9:Z:138:LYS:HD3	2.00	0.44
2:b:162:ILE:HD11	2:b:406:THR:HG22	1.99	0.44
6:h:297:ASP:OD1	6:h:297:ASP:N	2.51	0.44
6:h:319:LEU:HD23	6:h:319:LEU:HA	1.78	0.44
7:n:89:ASP:N	7:n:89:ASP:OD1	2.51	0.44
1:A:158:SER:OG	10:A:601:ADP:O2A	2.21	0.43
1:A:205:GLN:HE21	1:A:384:MET:HE3	1.83	0.43
4:E:186:ALA:O	4:E:190:VAL:HG23	2.18	0.43
2:b:205:LEU:HA	2:b:383:LEU:HD11	1.99	0.43
3:d:218:ILE:HD11	3:d:397:VAL:HG22	1.99	0.43
2:B:65:ASN:O	2:B:65:ASN:ND2	2.51	0.43
5:G:152:MET:HA	5:G:155:ILE:HD12	2.00	0.43
5:G:416:MET:SD	5:G:445:GLU:HG2	2.57	0.43
7:N:32:ASN:ND2	7:N:100:ASN:O	2.42	0.43
1:a:55:THR:HA	1:a:387:GLU:OE1	2.18	0.43
4:e:186:ALA:O	4:e:190:VAL:HG23	2.18	0.43
8:q:92:MET:HE1	9:z:197:LYS:O	2.17	0.43
9:z:91:GLY:O	9:z:95:ASN:HB2	2.17	0.43
9:z:313:LEU:HD11	9:z:361:THR:HG21	2.00	0.43
2:B:245:ASP:HB2	2:B:297:TYR:CE1	2.54	0.43
4:E:368:LYS:HB3	4:E:368:LYS:HE2	1.68	0.43
4:E:416:ASN:OD1	4:E:416:ASN:N	2.51	0.43
5:G:247:TYR:HB2	5:G:275:ILE:CD1	2.48	0.43
8:Q:152:LYS:HB2	8:Q:152:LYS:HE2	1.51	0.43
9:Z:514:ASN:O	9:Z:518:VAL:HG23	2.18	0.43
2:b:452:ASP:OD1	2:b:458:SER:OG	2.29	0.43
2:b:518:ASP:OD2	4:e:57:LEU:HB2	2.19	0.43
6:h:364:CYS:HB2	6:h:367:ALA:HB2	1.99	0.43
8:q:275:LEU:HD22	9:z:253:ALA:HB1	2.00	0.43
8:q:418:GLU:OE1	8:q:471:HIS:ND1	2.41	0.43
2:B:411:GLY:HA3	2:B:447:PRO:HB3	2.01	0.43
4:E:6:THR:HG21	4:E:18:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:155:ARG:HH11	8:Q:193:ASP:HA	1.84	0.43
1:a:104:ALA:O	1:a:108:VAL:HG23	2.17	0.43
6:h:168:ILE:HG21	6:h:385:THR:HG23	2.00	0.43
6:h:317:GLU:H	6:h:317:GLU:CD	2.25	0.43
1:A:43:LYS:HA	5:G:520:ASP:O	2.17	0.43
1:A:55:THR:HA	1:A:387:GLU:OE1	2.18	0.43
2:B:260:SER:HB2	2:B:263:LYS:HG3	2.01	0.43
4:E:147:HIS:O	4:E:151:ILE:HG12	2.19	0.43
6:H:66:LEU:HD11	6:H:98:THR:HG21	1.99	0.43
6:H:74:PRO:HB2	8:Q:55:MET:HG2	2.01	0.43
6:H:253:ALA:HA	8:Q:257:VAL:HB	2.00	0.43
9:Z:47:LEU:HD13	9:Z:66:GLU:CB	2.48	0.43
9:Z:77:ILE:HA	9:Z:80:VAL:HG12	2.01	0.43
2:b:285:HIS:CE1	2:b:335:PHE:HB3	2.50	0.43
4:e:83:VAL:HG11	4:e:88:ALA:HB3	2.01	0.43
5:g:49:MET:HE2	9:z:76:LEU:HD11	1.99	0.43
9:z:177:LEU:HD23	9:z:177:LEU:HA	1.87	0.43
6:H:410:GLY:HA2	6:H:413:GLU:OE1	2.19	0.43
9:Z:180:LYS:HG2	9:Z:181:LYS:N	2.28	0.43
1:a:66:GLU:OE2	5:g:11:SER:OG	2.32	0.43
2:b:3:SER:O	2:b:7:ALA:HB2	2.18	0.43
2:b:136:ALA:O	2:b:139:GLU:HG3	2.19	0.43
8:q:277:ASP:OD1	8:q:308:TYR:OH	2.21	0.43
2:B:136:ALA:O	2:B:139:GLU:HG3	2.19	0.43
6:H:290:LEU:HD11	6:H:361:PHE:CZ	2.53	0.43
9:Z:501:LYS:HA	9:Z:504:LEU:HD12	2.01	0.43
1:a:43:LYS:HA	5:g:520:ASP:O	2.18	0.43
1:a:66:GLU:CD	5:g:526:HIS:HA	2.44	0.43
1:a:426:TYR:OH	1:a:430:MET:SD	2.70	0.43
2:b:245:ASP:HB2	2:b:297:TYR:CE1	2.54	0.43
2:b:411:GLY:HA3	2:b:447:PRO:HB3	2.01	0.43
6:h:253:ALA:HA	8:q:257:VAL:HB	1.99	0.43
9:z:157:ARG:NH1	9:z:166:ASP:OD1	2.45	0.43
5:G:504:GLN:O	5:G:508:THR:OG1	2.35	0.43
6:H:26:ILE:HG23	6:H:105:LEU:HB3	2.01	0.43
6:H:187:ASP:O	6:H:190:LEU:HD23	2.18	0.43
8:Q:466:LYS:O	8:Q:470:VAL:HG23	2.19	0.43
9:Z:61:ASN:HB2	9:Z:92:THR:HG21	2.01	0.43
1:a:228:ARG:NE	1:a:350:GLU:OE2	2.49	0.43
2:b:121:ILE:HG12	2:b:431:LYS:HD3	1.99	0.43
4:e:147:HIS:O	4:e:151:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:q:155:ARG:HH11	8:q:193:ASP:HA	1.84	0.43
1:A:66:GLU:CD	5:G:526:HIS:HA	2.43	0.43
1:A:472:ASN:O	1:A:476:VAL:HG22	2.18	0.43
6:H:148:LYS:HE2	6:H:148:LYS:HA	1.99	0.43
2:b:526:ARG:HG3	2:b:526:ARG:HH11	1.84	0.43
4:e:248:ILE:HD12	4:e:337:THR:HG21	2.01	0.43
4:e:473:THR:O	4:e:477:VAL:HG13	2.18	0.43
6:h:66:LEU:HD11	6:h:98:THR:HG21	1.99	0.43
8:q:322:ARG:CZ	8:q:322:ARG:HB3	2.48	0.43
1:A:203:ARG:HG3	1:A:378:ARG:NH1	2.34	0.43
2:B:381:GLN:HE22	3:D:93:GLU:HG3	1.84	0.43
2:B:480:MET:HG3	10:B:601:ADP:C2	2.53	0.43
6:H:206:GLU:H	6:H:206:GLU:CD	2.27	0.43
8:Q:418:GLU:OE1	8:Q:471:HIS:ND1	2.41	0.43
1:a:67:VAL:HG21	1:a:76:CYS:SG	2.59	0.43
1:a:203:ARG:HG3	1:a:378:ARG:NH1	2.34	0.43
1:a:472:ASN:O	1:a:476:VAL:HG22	2.18	0.43
3:d:242:GLU:OE1	3:d:242:GLU:N	2.52	0.43
10:e:601:ADP:O3B	12:e:603:AF3:F3	2.26	0.43
5:g:152:MET:HA	5:g:155:ILE:HD12	2.00	0.43
6:h:6:VAL:HB	8:q:80:HIS:CD2	2.54	0.43
2:B:257:ARG:O	4:E:269:THR:HG22	2.19	0.42
6:H:219:THR:OG1	6:H:312:GLY:O	2.26	0.42
1:a:185:ARG:HE	1:a:185:ARG:HB3	1.40	0.42
1:a:519:GLU:HG3	3:d:217:THR:HG22	2.01	0.42
2:b:131:ARG:NH2	2:b:512:GLU:OE2	2.44	0.42
1:A:440:GLU:O	1:A:444:SER:OG	2.37	0.42
2:B:160:MET:SD	2:B:180:THR:HG22	2.60	0.42
2:B:395:CYS:HB3	4:E:366:THR:HG21	2.01	0.42
4:E:49:ARG:NH1	4:E:464:GLU:OE1	2.52	0.42
4:E:248:ILE:HD12	4:E:337:THR:HG21	2.01	0.42
5:g:265:THR:HG21	9:z:265:LYS:HB3	2.00	0.42
6:h:79:LEU:HA	6:h:82:ILE:HG12	2.02	0.42
9:z:501:LYS:HA	9:z:504:LEU:HD12	2.01	0.42
1:A:233:LYS:HB3	1:A:345:LEU:HD13	2.01	0.42
2:B:112:GLU:HB3	2:B:438:SER:HB3	2.01	0.42
4:E:420:TYR:CZ	4:E:502:LYS:HD2	2.55	0.42
10:E:601:ADP:O3B	12:E:603:AF3:F3	2.26	0.42
9:Z:313:LEU:HD11	9:Z:361:THR:HG21	2.00	0.42
9:Z:409:PRO:HG2	9:Z:476:LEU:HD13	2.02	0.42
3:d:193:LYS:NZ	3:d:225:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:16:PHE:CE2	4:e:18:ILE:HD11	2.55	0.42
4:e:149:ASP:OD1	4:e:514:LYS:HD3	2.19	0.42
6:h:206:GLU:H	6:h:206:GLU:CD	2.27	0.42
8:q:340:VAL:HG23	8:q:342:GLU:HG3	2.01	0.42
1:A:67:VAL:HG21	1:A:76:CYS:SG	2.59	0.42
2:B:518:ASP:OD2	4:E:57:LEU:HB2	2.19	0.42
3:D:480:LEU:HD23	3:D:480:LEU:HA	1.89	0.42
4:E:16:PHE:CE2	4:E:18:ILE:HD11	2.55	0.42
4:E:291:GLN:O	4:E:295:THR:HG23	2.19	0.42
6:H:10:LYS:O	6:H:13:THR:OG1	2.30	0.42
1:a:440:GLU:O	1:a:444:SER:OG	2.37	0.42
2:b:72:LYS:HB2	2:b:72:LYS:HE2	1.91	0.42
2:b:112:GLU:HB3	2:b:438:SER:HB3	2.01	0.42
2:b:260:SER:HB2	2:b:263:LYS:HG3	2.01	0.42
3:d:249:ILE:HD11	3:d:351:PHE:CE2	2.55	0.42
4:e:301:ILE:HG23	4:e:325:VAL:HG21	2.00	0.42
1:A:139:ASN:HB2	1:A:142:GLU:OE2	2.20	0.42
2:B:51:ILE:HB	3:D:535:VAL:HG22	2.02	0.42
4:E:532:ASP:HB3	6:H:47:LYS:HD2	2.02	0.42
5:G:49:MET:HE2	9:Z:76:LEU:HD11	2.02	0.42
9:Z:285:SER:O	9:Z:285:SER:OG	2.30	0.42
1:a:99:GLU:HG2	1:a:447:VAL:HB	2.02	0.42
2:b:160:MET:SD	2:b:180:THR:HG22	2.60	0.42
3:d:81:MET:O	3:d:83:VAL:N	2.52	0.42
3:d:415:LEU:HD12	3:d:415:LEU:HA	1.78	0.42
9:z:61:ASN:HB2	9:z:92:THR:HG21	2.01	0.42
1:A:127:GLU:HG3	1:A:426:TYR:CE2	2.54	0.42
1:A:272:LYS:O	1:A:276:GLN:HG3	2.19	0.42
2:B:244:MET:HE3	2:B:244:MET:HB3	1.72	0.42
4:E:83:VAL:HG11	4:E:88:ALA:HB3	2.01	0.42
4:E:105:GLY:O	4:E:109:VAL:HG22	2.19	0.42
6:H:168:ILE:HG21	6:H:385:THR:HG23	2.00	0.42
8:Q:199:VAL:HG13	8:Q:400:LYS:HD3	2.02	0.42
1:a:384:MET:HE1	5:g:511:GLU:HG2	2.02	0.42
2:b:395:CYS:HB3	4:e:366:THR:HG21	2.02	0.42
3:d:339:THR:OG1	3:d:385:THR:HG21	2.19	0.42
5:G:47:MET:SD	5:G:61:ASN:ND2	2.93	0.42
6:H:245:GLU:HB3	6:H:296:GLY:HA3	2.01	0.42
1:a:272:LYS:O	1:a:276:GLN:HG3	2.19	0.42
4:e:105:GLY:O	4:e:109:VAL:HG22	2.19	0.42
5:g:47:MET:SD	5:g:61:ASN:ND2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:q:466:LYS:O	8:q:470:VAL:HG23	2.19	0.42
9:z:77:ILE:HA	9:z:80:VAL:HG12	2.01	0.42
9:z:285:SER:O	9:z:285:SER:OG	2.30	0.42
1:A:22:VAL:HG21	1:A:105:ASP:CB	2.50	0.42
2:B:278:LYS:HZ1	2:B:281:ARG:HE	1.67	0.42
3:D:42:LYS:HD2	3:D:118:ASP:OD1	2.19	0.42
4:E:149:ASP:OD1	4:E:514:LYS:HD3	2.19	0.42
5:G:497:GLU:HG3	5:G:498:PRO:CD	2.50	0.42
9:Z:114:LEU:HD12	9:Z:114:LEU:HA	1.89	0.42
2:b:261:THR:HG22	3:d:264:ILE:HD13	2.02	0.42
4:e:6:THR:HG21	4:e:18:ILE:HD12	2.00	0.42
4:e:196:VAL:HG21	4:e:209:ILE:CG1	2.50	0.42
6:h:139:ILE:HD12	6:h:474:TRP:CH2	2.55	0.42
6:h:245:GLU:HB3	6:h:296:GLY:HA3	2.01	0.42
2:B:54:SER:HA	3:D:538:THR:OG1	2.20	0.42
3:D:249:ILE:HD11	3:D:351:PHE:CE2	2.55	0.42
8:Q:92:MET:HE1	9:Z:197:LYS:O	2.20	0.42
9:Z:84:GLN:HE21	9:Z:91:GLY:HA3	1.85	0.42
9:Z:101:GLU:HG2	9:Z:446:ILE:HB	2.02	0.42
1:a:113:HIS:HD2	1:a:115:THR:H	1.67	0.42
3:d:458:MET:HE2	3:d:458:MET:HB3	1.81	0.42
4:e:291:GLN:O	4:e:295:THR:HG23	2.19	0.42
5:g:178:ASP:HB2	5:g:214:VAL:HG11	2.01	0.42
6:h:384:GLU:OE1	6:h:387:ARG:HD2	2.20	0.42
8:q:290:VAL:HG22	8:q:311:MET:HB3	2.02	0.42
1:A:384:MET:HE1	5:G:511:GLU:HG2	2.02	0.42
2:B:19:GLU:OE1	2:B:27:THR:HG21	2.20	0.42
2:B:256:VAL:O	3:D:262:ASN:HA	2.19	0.42
3:D:242:GLU:N	3:D:242:GLU:OE1	2.52	0.42
4:E:218:ARG:HB2	4:E:221:ASP:OD1	2.20	0.42
6:H:139:ILE:HD12	6:H:474:TRP:CH2	2.55	0.42
7:N:37:TYR:O	7:N:94:TYR:N	2.52	0.42
9:Z:199:LYS:HB3	9:Z:203:ASP:OD2	2.20	0.42
1:a:233:LYS:HB3	1:a:345:LEU:HD13	2.01	0.42
2:b:19:GLU:OE1	2:b:27:THR:HG21	2.20	0.42
5:g:215:LEU:HB3	5:g:364:THR:HG22	2.02	0.42
1:A:23:MET:HG2	4:e:11:GLU:CG	2.50	0.41
1:A:164:ASN:OD1	1:A:206:MET:SD	2.77	0.41
1:A:410:PRO:HG3	1:A:485:TRP:HE3	1.85	0.41
5:G:408:VAL:HG21	5:G:502:LYS:HD2	2.02	0.41
2:b:35:ILE:HD13	2:b:35:ILE:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:239:MET:HE2	4:e:320:PRO:HA	2.02	0.41
1:A:416:GLU:OE1	1:A:416:GLU:N	2.51	0.41
2:B:526:ARG:HG3	2:B:526:ARG:HH11	1.84	0.41
3:D:193:LYS:NZ	3:D:225:GLU:OE1	2.52	0.41
3:D:339:THR:OG1	3:D:385:THR:HG21	2.19	0.41
4:E:196:VAL:HG21	4:E:209:ILE:CG1	2.50	0.41
5:G:133:MET:HE1	5:G:440:VAL:CG2	2.50	0.41
5:G:334:ARG:HB2	5:G:337:GLU:HG3	2.02	0.41
6:H:214:VAL:HG11	6:H:322:THR:HG23	2.02	0.41
8:Q:477:ASN:O	8:Q:492:MET:N	2.45	0.41
9:Z:198:HIS:CE1	9:Z:377:LYS:HE2	2.55	0.41
3:d:155:VAL:CG2	3:d:421:LEU:HB2	2.50	0.41
6:h:26:ILE:HG23	6:h:105:LEU:HB3	2.01	0.41
6:h:318:ASP:O	6:h:322:THR:OG1	2.34	0.41
9:z:409:PRO:HG2	9:z:476:LEU:HD13	2.02	0.41
1:A:99:GLU:HG2	1:A:447:VAL:HB	2.01	0.41
1:A:426:TYR:OH	1:A:430:MET:SD	2.70	0.41
3:D:431:GLU:OE2	3:D:484:HIS:ND1	2.40	0.41
6:H:79:LEU:HA	6:H:82:ILE:HG12	2.01	0.41
8:Q:341:LEU:HD23	8:Q:342:GLU:N	2.36	0.41
1:a:139:ASN:HB2	1:a:142:GLU:OE2	2.20	0.41
1:a:145:ARG:NH2	1:a:149:ILE:HD11	2.35	0.41
2:b:256:VAL:O	3:d:262:ASN:HA	2.19	0.41
3:d:249:ILE:HD12	3:d:251:PHE:CE2	2.55	0.41
5:g:16:ARG:HE	5:g:521:ASP:CG	2.28	0.41
7:n:32:ASN:N	7:n:98:ASN:O	2.50	0.41
9:z:198:HIS:CE1	9:z:377:LYS:HE2	2.55	0.41
9:z:272:LYS:O	9:z:276:GLU:HG2	2.20	0.41
9:z:470:HIS:HD2	9:z:475:GLN:O	2.03	0.41
1:A:145:ARG:NH2	1:A:149:ILE:HD11	2.35	0.41
3:D:440:SER:HA	3:D:443:LEU:HG	2.03	0.41
4:E:239:MET:HE2	4:E:320:PRO:HA	2.02	0.41
5:G:178:ASP:HB2	5:G:214:VAL:HG11	2.01	0.41
8:Q:416:GLU:OE2	8:Q:448:ILE:HG21	2.21	0.41
9:Z:84:GLN:O	9:Z:88:THR:OG1	2.36	0.41
1:a:22:VAL:HG21	1:a:105:ASP:CB	2.50	0.41
3:d:440:SER:HA	3:d:443:LEU:HG	2.03	0.41
4:e:289:ILE:HG13	4:e:313:LEU:HB3	2.02	0.41
5:g:334:ARG:HB2	5:g:337:GLU:HG3	2.02	0.41
9:Z:272:LYS:O	9:Z:276:GLU:HG2	2.20	0.41
3:d:160:ARG:HG2	3:d:164:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:420:TYR:CZ	4:e:502:LYS:HD2	2.55	0.41
5:g:8:LEU:HD12	5:g:12:GLN:HG3	2.01	0.41
5:g:379:ALA:HB1	9:z:80:VAL:HG23	2.03	0.41
6:h:410:GLY:HA2	6:h:413:GLU:OE1	2.19	0.41
8:q:43:THR:OG1	8:q:105:LEU:HD23	2.21	0.41
8:q:416:GLU:OE2	8:q:448:ILE:HG21	2.21	0.41
9:z:492:VAL:HG23	9:z:494:VAL:HG23	2.03	0.41
2:B:122:HIS:C	2:B:124:GLN:H	2.28	0.41
6:H:107:GLN:HG3	6:H:441:ALA:HB2	2.03	0.41
8:Q:290:VAL:HG22	8:Q:311:MET:HB3	2.02	0.41
8:Q:408:LEU:HD23	8:Q:499:ASP:O	2.21	0.41
1:a:78:LEU:HD11	1:a:516:PHE:HB3	2.02	0.41
1:a:410:PRO:HG3	1:a:485:TRP:HE3	1.85	0.41
4:e:3:SER:HA	4:e:27:ARG:O	2.21	0.41
6:h:89:GLU:OE1	8:q:378:ARG:NH2	2.48	0.41
6:h:344:ARG:CZ	6:h:344:ARG:HB2	2.51	0.41
8:q:341:LEU:HD23	8:q:342:GLU:N	2.36	0.41
9:z:264:ARG:NH2	9:z:298:ASP:OD2	2.52	0.41
3:D:155:VAL:CG2	3:D:421:LEU:HB2	2.50	0.41
3:D:496:ARG:NE	3:D:506:GLU:OE2	2.39	0.41
6:H:384:GLU:OE1	6:H:387:ARG:HD2	2.20	0.41
2:b:122:HIS:C	2:b:124:GLN:H	2.28	0.41
4:e:199:MET:HE3	4:e:202:ARG:NH1	2.36	0.41
4:e:218:ARG:HB2	4:e:221:ASP:OD1	2.20	0.41
4:e:258:PRO:HB3	6:h:267:VAL:HG11	2.02	0.41
4:e:341:ILE:HD12	6:h:227:MET:HE2	2.03	0.41
5:g:497:GLU:HG3	5:g:498:PRO:CD	2.50	0.41
9:z:101:GLU:HG2	9:z:446:ILE:HB	2.02	0.41
9:z:199:LYS:HB3	9:z:203:ASP:OD2	2.20	0.41
9:z:256:ARG:O	9:z:260:VAL:HG23	2.21	0.41
1:A:31:ILE:O	1:A:43:LYS:HE3	2.21	0.41
1:A:203:ARG:NH2	5:G:90:GLU:OE2	2.54	0.41
4:E:3:SER:HA	4:E:27:ARG:O	2.21	0.41
4:E:289:ILE:HG13	4:E:313:LEU:HB3	2.02	0.41
8:Q:340:VAL:HG23	8:Q:342:GLU:HG3	2.01	0.41
1:a:31:ILE:O	1:a:43:LYS:HE3	2.21	0.41
3:d:42:LYS:HD2	3:d:118:ASP:OD1	2.19	0.41
1:A:454:VAL:HG23	1:A:460:SER:OG	2.21	0.41
3:D:81:MET:O	3:D:83:VAL:N	2.52	0.41
3:D:155:VAL:HG21	3:D:421:LEU:HB2	2.02	0.41
3:D:249:ILE:HD12	3:D:251:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:106:THR:OG1	12:E:603:AF3:F3	2.23	0.41
4:E:442:THR:CG2	4:E:443:LEU:N	2.84	0.41
5:G:383:ILE:O	5:G:387:VAL:HG23	2.21	0.41
7:N:36:TRP:CD1	7:N:80:LEU:HB2	2.56	0.41
9:Z:157:ARG:NH1	9:Z:166:ASP:OD1	2.45	0.41
9:Z:470:HIS:HD2	9:Z:475:GLN:O	2.03	0.41
1:a:454:VAL:HG23	1:a:460:SER:OG	2.21	0.41
2:b:51:ILE:HB	3:d:535:VAL:HG22	2.01	0.41
4:e:101:GLU:OE1	6:h:375:ARG:NH2	2.47	0.41
5:g:133:MET:HE1	5:g:440:VAL:CG2	2.50	0.41
6:h:122:ILE:HG13	6:h:123:ARG:N	2.36	0.41
3:D:503:ILE:HG13	3:D:508:VAL:HB	2.03	0.41
4:E:32:GLU:OE1	4:E:32:GLU:HA	2.21	0.41
5:G:329:ALA:HB2	5:G:344:GLY:HA3	2.03	0.41
6:H:250:LYS:HB3	6:H:253:ALA:HB2	2.03	0.41
8:Q:43:THR:OG1	8:Q:105:LEU:HD23	2.21	0.41
1:a:127:GLU:HG3	1:a:426:TYR:CE2	2.55	0.41
3:d:88:ALA:O	3:d:92:VAL:HG23	2.21	0.41
6:h:410:GLY:O	6:h:414:MET:HG2	2.21	0.41
8:q:140:HIS:HE2	8:q:509:LYS:HE3	1.86	0.41
8:q:408:LEU:HD23	8:q:499:ASP:O	2.21	0.41
9:z:449:LYS:HE3	9:z:463:LEU:HD22	2.03	0.41
3:D:519:LEU:HD12	3:D:519:LEU:HA	1.73	0.40
4:E:326:GLY:O	4:E:329:GLU:HG2	2.22	0.40
5:G:458:SER:OG	5:G:461:ARG:HG3	2.21	0.40
8:Q:33:ILE:HD13	8:Q:116:GLU:HB2	2.03	0.40
8:Q:69:ALA:O	8:Q:73:LEU:HG	2.22	0.40
8:Q:90:SER:OG	8:Q:101:THR:HB	2.21	0.40
4:e:28:LEU:O	4:e:532:ASP:HA	2.21	0.40
5:g:383:ILE:O	5:g:387:VAL:HG23	2.21	0.40
6:h:119:GLN:HA	6:h:122:ILE:HG12	2.03	0.40
1:A:113:HIS:HD2	1:A:115:THR:H	1.68	0.40
2:B:87:MET:HE2	2:B:87:MET:HB3	2.00	0.40
3:D:458:MET:HE2	3:D:458:MET:HB3	1.81	0.40
3:D:476:THR:HG22	3:D:500:ILE:HD11	2.04	0.40
5:G:215:LEU:HB3	5:G:364:THR:HG22	2.02	0.40
6:H:259:THR:HG22	6:H:261:GLU:H	1.86	0.40
1:a:104:ALA:HB1	1:a:117:VAL:HG11	2.04	0.40
1:a:272:LYS:HG3	1:a:299:TYR:CZ	2.57	0.40
1:a:319:ILE:O	1:a:323:SER:OG	2.29	0.40
4:e:326:GLY:O	4:e:329:GLU:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:442:THR:CG2	4:e:443:LEU:N	2.84	0.40
4:e:442:THR:HG23	4:e:443:LEU:N	2.36	0.40
5:g:408:VAL:HG21	5:g:502:LYS:HD2	2.02	0.40
6:h:214:VAL:HG11	6:h:322:THR:HG23	2.02	0.40
8:q:11:PHE:CE1	9:z:69:ILE:HD11	2.56	0.40
8:q:199:VAL:HG13	8:q:400:LYS:HD3	2.01	0.40
3:D:134:SER:HB3	3:D:527:ARG:HE	1.87	0.40
5:G:225:THR:HG22	5:G:313:ARG:HB2	2.03	0.40
6:H:119:GLN:HA	6:H:122:ILE:HG12	2.03	0.40
7:N:67:PHE:CE2	7:N:82:MET:HE1	2.56	0.40
8:Q:47:TYR:HD1	8:Q:102:ASN:HB3	1.85	0.40
8:Q:168:ILE:HD11	8:Q:176:GLU:O	2.22	0.40
9:Z:429:VAL:HG21	9:Z:437:VAL:HG21	2.04	0.40
1:a:28:ILE:HG13	1:a:72:ALA:HB1	2.03	0.40
5:g:168:TRP:CE2	5:g:209:ILE:HG21	2.57	0.40
8:q:47:TYR:HD1	8:q:102:ASN:HB3	1.85	0.40
2:B:113:ALA:HB2	2:B:130:TRP:CH2	2.56	0.40
3:D:184:SER:N	3:D:185:PRO:HD2	2.37	0.40
3:D:304:ILE:HD12	3:D:305:LEU:HG	2.04	0.40
5:G:8:LEU:HD12	5:G:12:GLN:HG3	2.01	0.40
1:a:164:ASN:OD1	1:a:206:MET:SD	2.80	0.40
2:b:515:LEU:HD12	2:b:515:LEU:HA	1.91	0.40
3:d:155:VAL:HG21	3:d:421:LEU:HB2	2.02	0.40
4:e:421:GLY:O	4:e:501:MET:HG3	2.22	0.40
5:g:458:SER:OG	5:g:461:ARG:HG3	2.21	0.40
7:n:17:SER:HA	7:n:82:MET:O	2.22	0.40
7:n:36:TRP:CD1	7:n:80:LEU:HB2	2.56	0.40
8:q:69:ALA:O	8:q:73:LEU:HG	2.21	0.40
8:q:176:GLU:OE1	8:q:176:GLU:N	2.54	0.40
1:A:272:LYS:HG3	1:A:299:TYR:CZ	2.57	0.40
4:E:421:GLY:O	4:E:501:MET:HG3	2.22	0.40
4:E:526:MET:HE3	4:E:526:MET:HB2	2.01	0.40
6:H:122:ILE:HG13	6:H:123:ARG:N	2.36	0.40
1:a:446:LEU:HD11	1:a:468:ARG:HD3	2.03	0.40
2:b:257:ARG:O	4:e:269:THR:HG22	2.21	0.40
2:b:414:GLU:HG2	2:b:446:LEU:HD23	2.04	0.40
3:d:476:THR:HG22	3:d:500:ILE:HD11	2.04	0.40
7:n:53:ARG:C	7:n:55:GLY:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	532/556 (96%)	511 (96%)	21 (4%)	0	100	100
1	a	532/556 (96%)	510 (96%)	22 (4%)	0	100	100
2	B	524/535 (98%)	503 (96%)	21 (4%)	0	100	100
2	b	524/535 (98%)	502 (96%)	22 (4%)	0	100	100
3	D	516/539 (96%)	502 (97%)	14 (3%)	0	100	100
3	d	516/539 (96%)	501 (97%)	15 (3%)	0	100	100
4	E	533/541 (98%)	513 (96%)	19 (4%)	1 (0%)	43	63
4	e	533/541 (98%)	514 (96%)	18 (3%)	1 (0%)	43	63
5	G	521/545 (96%)	501 (96%)	20 (4%)	0	100	100
5	g	521/545 (96%)	501 (96%)	20 (4%)	0	100	100
6	H	518/543 (95%)	506 (98%)	12 (2%)	0	100	100
6	h	518/543 (95%)	506 (98%)	12 (2%)	0	100	100
7	N	98/129 (76%)	95 (97%)	3 (3%)	0	100	100
7	n	98/129 (76%)	95 (97%)	3 (3%)	0	100	100
8	Q	527/548 (96%)	512 (97%)	14 (3%)	1 (0%)	43	63
8	q	527/548 (96%)	512 (97%)	14 (3%)	1 (0%)	43	63
9	Z	523/531 (98%)	508 (97%)	15 (3%)	0	100	100
9	z	523/531 (98%)	508 (97%)	15 (3%)	0	100	100
All	All	8584/8934 (96%)	8300 (97%)	280 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	10	ASP
8	Q	210	SER
4	e	10	ASP
8	q	210	SER

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	445/463 (96%)	444 (100%)	1 (0%)	87	95
1	a	445/463 (96%)	443 (100%)	2 (0%)	84	93
2	B	418/427 (98%)	410 (98%)	8 (2%)	50	76
2	b	418/427 (98%)	410 (98%)	8 (2%)	50	76
3	D	441/452 (98%)	433 (98%)	8 (2%)	51	77
3	d	441/452 (98%)	432 (98%)	9 (2%)	48	75
4	E	452/456 (99%)	447 (99%)	5 (1%)	65	84
4	e	452/456 (99%)	447 (99%)	5 (1%)	65	84
5	G	454/469 (97%)	449 (99%)	5 (1%)	65	84
5	g	454/469 (97%)	449 (99%)	5 (1%)	65	84
6	H	427/443 (96%)	419 (98%)	8 (2%)	50	76
6	h	427/443 (96%)	419 (98%)	8 (2%)	50	76
7	N	83/105 (79%)	75 (90%)	8 (10%)	8	17
7	n	83/105 (79%)	75 (90%)	8 (10%)	8	17
8	Q	436/452 (96%)	430 (99%)	6 (1%)	59	81
8	q	436/452 (96%)	429 (98%)	7 (2%)	55	79
9	Z	437/442 (99%)	432 (99%)	5 (1%)	65	84
9	z	437/442 (99%)	431 (99%)	6 (1%)	59	81
All	All	7186/7418 (97%)	7074 (98%)	112 (2%)	54	79

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356	ILE
2	B	17	ASP
2	B	35	ILE
2	B	64	THR
2	B	244	MET
2	B	407	VAL

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Mol	Chain	Res	Type
2	B	416	LEU
2	B	428	THR
2	B	446	LEU
3	D	83	VAL
3	D	304	ILE
3	D	370	SER
3	D	385	THR
3	D	443	LEU
3	D	460	VAL
3	D	461	ILE
3	D	524	GLU
4	E	122	GLN
4	E	160	LYS
4	E	372	LEU
4	E	418	VAL
4	E	442	THR
5	G	41	LEU
5	G	50	LEU
5	G	381	LYS
5	G	438	ARG
5	G	460	ILE
6	H	6	VAL
6	H	85	SER
6	H	116	LEU
6	H	149	VAL
6	H	322	THR
6	H	330	ILE
6	H	400	ILE
6	H	417	SER
7	N	1	GLN
7	N	46	GLU
7	N	62	SER
7	N	63	VAL
7	N	66	ARG
7	N	85	LEU
7	N	99	ARG
7	N	104	GLU
8	Q	60	LEU
8	Q	152	LYS
8	Q	190	ILE
8	Q	212	ILE
8	Q	312	LEU

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Mol	Chain	Res	Type
8	Q	415	THR
9	Z	159	LYS
9	Z	163	GLU
9	Z	180	LYS
9	Z	202	THR
9	Z	210	LEU
1	a	356	ILE
1	a	480	ARG
2	b	17	ASP
2	b	35	ILE
2	b	64	THR
2	b	244	MET
2	b	407	VAL
2	b	416	LEU
2	b	428	THR
2	b	446	LEU
3	d	83	VAL
3	d	195	ILE
3	d	304	ILE
3	d	370	SER
3	d	385	THR
3	d	443	LEU
3	d	460	VAL
3	d	461	ILE
3	d	524	GLU
4	e	122	GLN
4	e	160	LYS
4	e	372	LEU
4	e	418	VAL
4	e	442	THR
5	g	41	LEU
5	g	50	LEU
5	g	381	LYS
5	g	438	ARG
5	g	460	ILE
6	h	6	VAL
6	h	85	SER
6	h	116	LEU
6	h	149	VAL
6	h	322	THR
6	h	330	ILE
6	h	400	ILE

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Mol	Chain	Res	Type
6	h	417	SER
7	n	1	GLN
7	n	46	GLU
7	n	62	SER
7	n	63	VAL
7	n	66	ARG
7	n	85	LEU
7	n	99	ARG
7	n	104	GLU
8	q	55	MET
8	q	60	LEU
8	q	152	LYS
8	q	190	ILE
8	q	212	ILE
8	q	312	LEU
8	q	415	THR
9	z	15	ARG
9	z	159	LYS
9	z	163	GLU
9	z	180	LYS
9	z	202	THR
9	z	210	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (158) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	56	ASN
1	A	110	GLN
1	A	113	HIS
1	A	135	ASN
1	A	251	GLN
1	A	276	GLN
1	A	472	ASN
1	A	475	GLN
2	B	65	ASN
2	B	148	HIS
2	B	174	HIS
2	B	228	GLN
2	B	285	HIS
2	B	294	GLN
2	B	381	GLN

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Mol	Chain	Res	Type
2	B	423	GLN
2	B	502	GLN
3	D	72	ASN
3	D	82	GLN
3	D	138	GLN
3	D	271	GLN
3	D	315	HIS
3	D	347	HIS
3	D	406	HIS
4	E	86	GLN
4	E	139	GLN
4	E	184	GLN
4	E	278	GLN
4	E	379	ASN
4	E	403	HIS
4	E	465	ASN
4	E	486	ASN
4	E	495	HIS
4	E	503	GLN
4	E	504	GLN
4	E	505	HIS
5	G	13	ASN
5	G	64	ASN
5	G	71	GLN
5	G	115	GLN
5	G	226	HIS
5	G	235	ASN
5	G	277	GLN
5	G	284	GLN
5	G	390	ASN
5	G	392	GLN
5	G	396	GLN
5	G	420	HIS
5	G	472	GLN
5	G	504	GLN
6	H	252	ASN
6	H	272	ASN
6	H	331	GLN
6	H	470	GLN
6	H	522	ASN
7	N	81	GLN
8	Q	32	ASN

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Mol	Chain	Res	Type
8	Q	34	GLN
8	Q	80	HIS
8	Q	95	GLN
8	Q	303	HIS
8	Q	359	GLN
8	Q	365	HIS
8	Q	383	ASN
8	Q	461	ASN
9	Z	61	ASN
9	Z	65	HIS
9	Z	68	GLN
9	Z	71	HIS
9	Z	95	ASN
9	Z	161	HIS
9	Z	198	HIS
9	Z	234	ASN
9	Z	368	ASN
9	Z	438	GLN
9	Z	460	GLN
9	Z	470	HIS
1	a	20	GLN
1	a	56	ASN
1	a	110	GLN
1	a	113	HIS
1	a	135	ASN
1	a	251	GLN
1	a	276	GLN
1	a	472	ASN
1	a	475	GLN
2	b	65	ASN
2	b	122	HIS
2	b	148	HIS
2	b	174	HIS
2	b	228	GLN
2	b	285	HIS
2	b	294	GLN
2	b	381	GLN
2	b	423	GLN
2	b	502	GLN
3	d	72	ASN
3	d	82	GLN
3	d	138	GLN

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Mol	Chain	Res	Type
3	d	271	GLN
3	d	318	ASN
3	d	347	HIS
3	d	406	HIS
4	e	86	GLN
4	e	139	GLN
4	e	184	GLN
4	e	278	GLN
4	e	379	ASN
4	e	403	HIS
4	e	465	ASN
4	e	486	ASN
4	e	495	HIS
4	e	503	GLN
4	e	505	HIS
5	g	13	ASN
5	g	64	ASN
5	g	71	GLN
5	g	115	GLN
5	g	116	GLN
5	g	226	HIS
5	g	235	ASN
5	g	277	GLN
5	g	390	ASN
5	g	392	GLN
5	g	396	GLN
5	g	420	HIS
5	g	504	GLN
6	h	234	ASN
6	h	252	ASN
6	h	272	ASN
6	h	331	GLN
6	h	470	GLN
6	h	522	ASN
7	n	81	GLN
8	q	32	ASN
8	q	34	GLN
8	q	80	HIS
8	q	95	GLN
8	q	172	GLN
8	q	175	ASN
8	q	303	HIS

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Mol	Chain	Res	Type
8	q	359	GLN
8	q	383	ASN
8	q	461	ASN
8	q	472	GLN
9	z	61	ASN
9	z	65	HIS
9	z	68	GLN
9	z	71	HIS
9	z	95	ASN
9	z	161	HIS
9	z	198	HIS
9	z	234	ASN
9	z	368	ASN
9	z	438	GLN
9	z	460	GLN
9	z	470	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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
10	ADP	q	601	11	28,29,29	1.37	5 (17%)	43,45,45	1.86	11 (25%)
10	ADP	Q	601	11	28,29,29	1.37	5 (17%)	43,45,45	1.86	11 (25%)
10	ADP	h	601	11	28,29,29	1.39	5 (17%)	43,45,45	1.91	11 (25%)
12	AF3	E	603	-	0,3,3	-	-	-	-	-
10	ADP	B	601	11	28,29,29	1.38	5 (17%)	43,45,45	1.80	8 (18%)
12	AF3	Q	603	-	0,3,3	-	-	-	-	-
12	AF3	e	603	-	0,3,3	-	-	-	-	-
12	AF3	B	603	-	0,3,3	-	-	-	-	-
10	ADP	Z	601	11	28,29,29	1.37	5 (17%)	43,45,45	1.88	11 (25%)
10	ADP	e	601	11	28,29,29	1.42	6 (21%)	43,45,45	1.89	10 (23%)
10	ADP	H	601	11	28,29,29	1.39	5 (17%)	43,45,45	1.92	11 (25%)
10	ADP	g	601	11	28,29,29	1.40	5 (17%)	43,45,45	1.74	8 (18%)
10	ADP	a	601	11	28,29,29	1.40	5 (17%)	43,45,45	1.86	11 (25%)
12	AF3	h	603	-	0,3,3	-	-	-	-	-
10	ADP	A	601	11	28,29,29	1.40	5 (17%)	43,45,45	1.85	11 (25%)
12	AF3	a	603	-	0,3,3	-	-	-	-	-
12	AF3	z	603	-	0,3,3	-	-	-	-	-
12	AF3	b	603	-	0,3,3	-	-	-	-	-
10	ADP	z	601	11	28,29,29	1.37	5 (17%)	43,45,45	1.88	11 (25%)
12	AF3	D	603	-	0,3,3	-	-	-	-	-
12	AF3	A	603	-	0,3,3	-	-	-	-	-
10	ADP	D	601	11	28,29,29	1.38	4 (14%)	43,45,45	1.77	9 (20%)
10	ADP	d	601	11	28,29,29	1.37	4 (14%)	43,45,45	1.77	9 (20%)
12	AF3	H	603	-	0,3,3	-	-	-	-	-
10	ADP	G	601	11	28,29,29	1.40	5 (17%)	43,45,45	1.74	8 (18%)
12	AF3	Z	603	-	0,3,3	-	-	-	-	-
12	AF3	d	603	-	0,3,3	-	-	-	-	-
12	AF3	g	603	-	0,3,3	-	-	-	-	-
12	AF3	G	603	-	0,3,3	-	-	-	-	-
10	ADP	b	601	11	28,29,29	1.39	4 (14%)	43,45,45	1.80	10 (23%)
10	ADP	E	601	11	28,29,29	1.43	6 (21%)	43,45,45	1.89	10 (23%)
12	AF3	q	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
10	ADP	q	601	11	-	2/16/32/32	0/3/3/3
10	ADP	Q	601	11	-	2/16/32/32	0/3/3/3
10	ADP	e	601	11	-	1/16/32/32	0/3/3/3
10	ADP	h	601	11	-	7/16/32/32	0/3/3/3
10	ADP	H	601	11	-	7/16/32/32	0/3/3/3
10	ADP	G	601	11	-	4/16/32/32	0/3/3/3
10	ADP	g	601	11	-	4/16/32/32	0/3/3/3
10	ADP	B	601	11	-	1/16/32/32	0/3/3/3
10	ADP	z	601	11	-	0/16/32/32	0/3/3/3
10	ADP	D	601	11	-	6/16/32/32	0/3/3/3
10	ADP	b	601	11	-	1/16/32/32	0/3/3/3
10	ADP	a	601	11	-	4/16/32/32	0/3/3/3
10	ADP	d	601	11	-	6/16/32/32	0/3/3/3
10	ADP	E	601	11	-	1/16/32/32	0/3/3/3
10	ADP	A	601	11	-	4/16/32/32	0/3/3/3
10	ADP	Z	601	11	-	0/16/32/32	0/3/3/3

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Z	601	ADP	C5-C4	4.47	1.47	1.39
10	z	601	ADP	C5-C4	4.47	1.47	1.39
10	A	601	ADP	C5-C4	4.47	1.47	1.39
10	a	601	ADP	C5-C4	4.47	1.47	1.39
10	G	601	ADP	C5-C4	4.47	1.47	1.39
10	D	601	ADP	C5-C4	4.45	1.47	1.39
10	B	601	ADP	C5-C4	4.43	1.47	1.39
10	b	601	ADP	C5-C4	4.43	1.47	1.39
10	g	601	ADP	C5-C4	4.42	1.47	1.39
10	d	601	ADP	C5-C4	4.40	1.46	1.39
10	e	601	ADP	C5-C4	4.40	1.46	1.39
10	E	601	ADP	C5-C4	4.39	1.46	1.39
10	H	601	ADP	C5-C4	4.38	1.46	1.39
10	h	601	ADP	C5-C4	4.38	1.46	1.39
10	q	601	ADP	C5-C4	4.36	1.46	1.39
10	Q	601	ADP	C5-C4	4.35	1.46	1.39
10	Q	601	ADP	C5-C6	2.74	1.48	1.41
10	q	601	ADP	C5-C6	2.74	1.48	1.41
10	E	601	ADP	C5-C6	2.71	1.48	1.41
10	e	601	ADP	C5-C6	2.68	1.48	1.41
10	d	601	ADP	C5-C6	2.68	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	601	ADP	C5-C6	2.65	1.48	1.41
10	H	601	ADP	C5-C6	2.62	1.48	1.41
10	B	601	ADP	C5-C6	2.62	1.48	1.41
10	A	601	ADP	C5-C6	2.60	1.48	1.41
10	Z	601	ADP	C5-C6	2.60	1.48	1.41
10	h	601	ADP	C5-C6	2.60	1.48	1.41
10	b	601	ADP	C5-C6	2.59	1.48	1.41
10	z	601	ADP	C5-C6	2.58	1.48	1.41
10	a	601	ADP	C5-C6	2.58	1.48	1.41
10	G	601	ADP	C5-C6	2.57	1.48	1.41
10	g	601	ADP	C5-C6	2.57	1.48	1.41
10	B	601	ADP	C5-N7	-2.43	1.34	1.39
10	b	601	ADP	C5-N7	-2.43	1.34	1.39
10	A	601	ADP	C5-N7	-2.41	1.34	1.39
10	a	601	ADP	C5-N7	-2.41	1.34	1.39
10	G	601	ADP	C5-N7	-2.40	1.34	1.39
10	g	601	ADP	C5-N7	-2.40	1.34	1.39
10	Z	601	ADP	C5-N7	-2.38	1.34	1.39
10	D	601	ADP	C5-N7	-2.38	1.34	1.39
10	d	601	ADP	C5-N7	-2.38	1.34	1.39
10	H	601	ADP	C5-N7	-2.36	1.34	1.39
10	E	601	ADP	C5-N7	-2.36	1.34	1.39
10	h	601	ADP	C5-N7	-2.35	1.34	1.39
10	z	601	ADP	C5-N7	-2.35	1.34	1.39
10	q	601	ADP	C8-N7	2.34	1.36	1.31
10	e	601	ADP	C5-N7	-2.34	1.34	1.39
10	Q	601	ADP	C8-N7	2.32	1.36	1.31
10	E	601	ADP	C8-N7	2.27	1.36	1.31
10	Q	601	ADP	C5-N7	-2.26	1.35	1.39
10	e	601	ADP	C8-N7	2.25	1.36	1.31
10	q	601	ADP	C5-N7	-2.22	1.35	1.39
10	G	601	ADP	C4-N9	-2.22	1.33	1.37
10	g	601	ADP	C4-N9	-2.20	1.33	1.37
10	D	601	ADP	C8-N7	2.20	1.35	1.31
10	b	601	ADP	C8-N7	2.20	1.35	1.31
10	G	601	ADP	C8-N7	2.20	1.35	1.31
10	g	601	ADP	C8-N7	2.19	1.35	1.31
10	H	601	ADP	C8-N7	2.19	1.35	1.31
10	B	601	ADP	C8-N7	2.19	1.35	1.31
10	h	601	ADP	C8-N7	2.16	1.35	1.31
10	d	601	ADP	C8-N7	2.15	1.35	1.31
10	A	601	ADP	C8-N7	2.15	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	601	ADP	C8-N7	2.15	1.35	1.31
10	z	601	ADP	C8-N7	2.14	1.35	1.31
10	Q	601	ADP	C4-N9	-2.12	1.33	1.37
10	q	601	ADP	C4-N9	-2.09	1.33	1.37
10	E	601	ADP	PA-O3A	2.09	1.61	1.59
10	Z	601	ADP	C8-N7	2.09	1.35	1.31
10	a	601	ADP	C4-N9	-2.06	1.33	1.37
10	A	601	ADP	C4-N9	-2.05	1.33	1.37
10	e	601	ADP	PA-O3A	2.05	1.61	1.59
10	H	601	ADP	C4-N9	-2.04	1.33	1.37
10	h	601	ADP	C4-N9	-2.04	1.33	1.37
10	e	601	ADP	C4-N9	-2.03	1.33	1.37
10	Z	601	ADP	C4-N9	-2.03	1.33	1.37
10	z	601	ADP	C4-N9	-2.03	1.33	1.37
10	E	601	ADP	C4-N9	-2.02	1.33	1.37
10	B	601	ADP	C4-N9	-2.01	1.33	1.37

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	601	ADP	C5-C4-N3	-5.86	118.65	126.72
10	b	601	ADP	C5-C4-N3	-5.82	118.71	126.72
10	D	601	ADP	C5-C4-N3	-5.77	118.78	126.72
10	d	601	ADP	C5-C4-N3	-5.76	118.78	126.72
10	e	601	ADP	C5-C4-N3	-5.74	118.81	126.72
10	E	601	ADP	C5-C4-N3	-5.73	118.83	126.72
10	H	601	ADP	C5-C4-N3	-5.72	118.84	126.72
10	h	601	ADP	C5-C4-N3	-5.72	118.84	126.72
10	Z	601	ADP	C5-C4-N3	-5.72	118.84	126.72
10	A	601	ADP	C5-C4-N3	-5.71	118.86	126.72
10	a	601	ADP	C5-C4-N3	-5.70	118.87	126.72
10	z	601	ADP	C5-C4-N3	-5.69	118.88	126.72
10	Q	601	ADP	C5-C4-N3	-5.61	118.99	126.72
10	q	601	ADP	C5-C4-N3	-5.60	119.00	126.72
10	G	601	ADP	C5-C4-N3	-5.51	119.13	126.72
10	g	601	ADP	C5-C4-N3	-5.48	119.17	126.72
10	Z	601	ADP	N3-C4-N9	4.59	134.98	127.17
10	H	601	ADP	N3-C4-N9	4.59	134.97	127.17
10	h	601	ADP	N3-C4-N9	4.58	134.95	127.17
10	a	601	ADP	N3-C4-N9	4.58	134.95	127.17
10	B	601	ADP	N3-C4-N9	4.58	134.95	127.17
10	A	601	ADP	N3-C4-N9	4.57	134.95	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	z	601	ADP	N3-C4-N9	4.57	134.94	127.17
10	b	601	ADP	N3-C4-N9	4.57	134.94	127.17
10	D	601	ADP	N3-C4-N9	4.54	134.89	127.17
10	d	601	ADP	N3-C4-N9	4.52	134.86	127.17
10	e	601	ADP	N3-C4-N9	4.40	134.65	127.17
10	E	601	ADP	N3-C4-N9	4.38	134.62	127.17
10	G	601	ADP	N3-C4-N9	4.27	134.43	127.17
10	g	601	ADP	N3-C4-N9	4.24	134.38	127.17
10	Q	601	ADP	N3-C4-N9	4.21	134.33	127.17
10	q	601	ADP	N3-C4-N9	4.21	134.32	127.17
10	Q	601	ADP	C2-N3-C4	3.83	121.19	111.83
10	q	601	ADP	C2-N3-C4	3.81	121.14	111.83
10	B	601	ADP	C2-N3-C4	3.78	121.07	111.83
10	q	601	ADP	C4-C5-N7	-3.78	106.26	110.58
10	H	601	ADP	C2-N3-C4	3.78	121.06	111.83
10	Q	601	ADP	C4-C5-N7	-3.78	106.26	110.58
10	h	601	ADP	C2-N3-C4	3.77	121.04	111.83
10	b	601	ADP	C2-N3-C4	3.76	121.03	111.83
10	D	601	ADP	C2-N3-C4	3.73	120.95	111.83
10	d	601	ADP	C2-N3-C4	3.73	120.95	111.83
10	e	601	ADP	C2-N3-C4	3.73	120.95	111.83
10	E	601	ADP	C2-N3-C4	3.73	120.94	111.83
10	a	601	ADP	C2-N3-C4	3.72	120.92	111.83
10	A	601	ADP	C2-N3-C4	3.70	120.87	111.83
10	e	601	ADP	C4-C5-N7	-3.68	106.37	110.58
10	E	601	ADP	C4-C5-N7	-3.67	106.39	110.58
10	Z	601	ADP	C2-N3-C4	3.60	120.62	111.83
10	z	601	ADP	C2-N3-C4	3.59	120.61	111.83
10	G	601	ADP	C4-C5-N7	-3.55	106.53	110.58
10	B	601	ADP	C4-C5-N7	-3.55	106.53	110.58
10	b	601	ADP	C4-C5-N7	-3.55	106.53	110.58
10	D	601	ADP	C4-C5-N7	-3.54	106.54	110.58
10	d	601	ADP	C4-C5-N7	-3.53	106.54	110.58
10	g	601	ADP	C4-C5-N7	-3.51	106.57	110.58
10	h	601	ADP	C4-C5-N7	-3.49	106.59	110.58
10	q	601	ADP	N3-C2-N1	-3.47	123.33	128.58
10	G	601	ADP	C2-N3-C4	3.47	120.30	111.83
10	Q	601	ADP	N3-C2-N1	-3.47	123.33	128.58
10	g	601	ADP	C2-N3-C4	3.46	120.29	111.83
10	Z	601	ADP	C4-C5-N7	-3.46	106.62	110.58
10	A	601	ADP	C4-C5-N7	-3.46	106.63	110.58
10	H	601	ADP	C4-C5-N7	-3.46	106.63	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	z	601	ADP	C4-C5-N7	-3.45	106.64	110.58
10	a	601	ADP	C4-C5-N7	-3.44	106.65	110.58
10	H	601	ADP	N3-C2-N1	-3.43	123.39	128.58
10	h	601	ADP	N3-C2-N1	-3.40	123.43	128.58
10	a	601	ADP	N3-C2-N1	-3.39	123.45	128.58
10	B	601	ADP	N3-C2-N1	-3.35	123.50	128.58
10	b	601	ADP	N3-C2-N1	-3.35	123.51	128.58
10	A	601	ADP	N3-C2-N1	-3.33	123.54	128.58
10	E	601	ADP	N3-C2-N1	-3.33	123.54	128.58
10	D	601	ADP	N3-C2-N1	-3.32	123.55	128.58
10	e	601	ADP	N3-C2-N1	-3.31	123.57	128.58
10	d	601	ADP	N3-C2-N1	-3.31	123.58	128.58
10	z	601	ADP	N3-C2-N1	-3.19	123.75	128.58
10	Z	601	ADP	N3-C2-N1	-3.14	123.82	128.58
10	g	601	ADP	N3-C2-N1	-2.97	124.08	128.58
10	H	601	ADP	C4-N9-C8	2.94	108.82	105.74
10	G	601	ADP	N3-C2-N1	-2.93	124.14	128.58
10	h	601	ADP	C4-N9-C8	2.91	108.80	105.74
10	a	601	ADP	C4-N9-C8	2.88	108.76	105.74
10	A	601	ADP	C4-N9-C8	2.86	108.74	105.74
10	z	601	ADP	C4-N9-C8	2.85	108.73	105.74
10	h	601	ADP	O2A-PA-O3A	2.83	114.93	107.27
10	e	601	ADP	O4'-C1'-N9	2.82	113.51	108.09
10	Z	601	ADP	C4-N9-C8	2.81	108.69	105.74
10	E	601	ADP	O4'-C1'-N9	2.81	113.48	108.09
10	H	601	ADP	O2A-PA-O3A	2.80	114.84	107.27
10	q	601	ADP	C4-N9-C8	2.77	108.65	105.74
10	Q	601	ADP	C4-N9-C8	2.75	108.62	105.74
10	e	601	ADP	C4-N9-C8	2.73	108.61	105.74
10	D	601	ADP	C4-N9-C8	2.71	108.59	105.74
10	E	601	ADP	C4-N9-C8	2.71	108.59	105.74
10	G	601	ADP	C4-N9-C8	2.69	108.57	105.74
10	d	601	ADP	C4-N9-C8	2.67	108.55	105.74
10	g	601	ADP	C4-N9-C8	2.67	108.55	105.74
10	b	601	ADP	C4-N9-C8	2.67	108.54	105.74
10	Q	601	ADP	C5-N7-C8	2.66	107.64	103.45
10	q	601	ADP	C5-N7-C8	2.66	107.64	103.45
10	E	601	ADP	C5-N7-C8	2.65	107.61	103.45
10	e	601	ADP	C5-N7-C8	2.64	107.60	103.45
10	B	601	ADP	C4-N9-C8	2.64	108.50	105.74
10	d	601	ADP	C5-N7-C8	2.59	107.53	103.45
10	D	601	ADP	C5-N7-C8	2.58	107.51	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	601	ADP	C6-C5-N7	2.58	137.07	132.09
10	q	601	ADP	C6-C5-N7	2.58	137.06	132.09
10	b	601	ADP	C5-N7-C8	2.58	107.50	103.45
10	H	601	ADP	C5-N7-C8	2.57	107.49	103.45
10	A	601	ADP	C5-N7-C8	2.57	107.48	103.45
10	h	601	ADP	C5-N7-C8	2.56	107.48	103.45
10	B	601	ADP	C5-N7-C8	2.56	107.47	103.45
10	a	601	ADP	C5-N7-C8	2.55	107.46	103.45
10	Z	601	ADP	C5-N7-C8	2.54	107.44	103.45
10	z	601	ADP	C5-N7-C8	2.51	107.39	103.45
10	G	601	ADP	C5-N7-C8	2.46	107.31	103.45
10	g	601	ADP	C5-N7-C8	2.44	107.28	103.45
10	e	601	ADP	C6-C5-N7	2.31	136.54	132.09
10	E	601	ADP	C6-C5-N7	2.30	136.53	132.09
10	A	601	ADP	O4'-C1'-C2'	-2.23	101.85	106.62
10	q	601	ADP	N9-C8-N7	-2.23	110.78	113.94
10	a	601	ADP	O4'-C1'-C2'	-2.22	101.86	106.62
10	Q	601	ADP	N9-C8-N7	-2.22	110.79	113.94
10	h	601	ADP	C6-C5-N7	2.22	136.36	132.09
10	b	601	ADP	C6-C5-N7	2.20	136.34	132.09
10	D	601	ADP	C6-C5-N7	2.20	136.33	132.09
10	d	601	ADP	C6-C5-N7	2.20	136.33	132.09
10	H	601	ADP	C6-C5-N7	2.19	136.32	132.09
10	B	601	ADP	C6-C5-N7	2.19	136.31	132.09
10	G	601	ADP	C6-C5-N7	2.17	136.28	132.09
10	A	601	ADP	C6-C5-N7	2.17	136.28	132.09
10	H	601	ADP	N9-C8-N7	-2.16	110.87	113.94
10	E	601	ADP	N9-C8-N7	-2.16	110.87	113.94
10	a	601	ADP	C6-C5-N7	2.15	136.24	132.09
10	e	601	ADP	N9-C8-N7	-2.14	110.90	113.94
10	g	601	ADP	C6-C5-N7	2.14	136.22	132.09
10	q	601	ADP	O4'-C1'-N9	2.13	112.18	108.09
10	h	601	ADP	N9-C8-N7	-2.12	110.92	113.94
10	Q	601	ADP	O4'-C1'-N9	2.12	112.16	108.09
10	Z	601	ADP	O4'-C1'-N9	2.11	112.13	108.09
10	A	601	ADP	N9-C8-N7	-2.10	110.96	113.94
10	a	601	ADP	N9-C8-N7	-2.10	110.96	113.94
10	z	601	ADP	O4'-C1'-N9	2.06	112.05	108.09
10	a	601	ADP	O3A-PB-O1B	-2.06	100.20	111.04
10	Z	601	ADP	C6-C5-N7	2.05	136.05	132.09
10	z	601	ADP	C6-C5-N7	2.05	136.05	132.09
10	d	601	ADP	N9-C8-N7	-2.05	111.03	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	601	ADP	N9-C8-N7	-2.05	111.03	113.94
10	A	601	ADP	O3A-PB-O1B	-2.04	100.28	111.04
10	h	601	ADP	O3A-PA-O1A	-2.04	104.58	110.70
10	H	601	ADP	O3A-PA-O1A	-2.02	104.62	110.70
10	Z	601	ADP	N9-C8-N7	-2.02	111.07	113.94
10	z	601	ADP	N9-C8-N7	-2.02	111.07	113.94
10	z	601	ADP	O3B-PB-O3A	-2.02	97.86	104.64
10	b	601	ADP	N9-C8-N7	-2.02	111.08	113.94
10	Z	601	ADP	O3B-PB-O3A	-2.01	97.90	104.64
10	b	601	ADP	O4'-C1'-N9	2.01	111.95	108.09
10	Q	601	ADP	O3B-PB-O2B	2.01	115.33	107.80
10	q	601	ADP	O3B-PB-O2B	2.01	115.33	107.80

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	601	ADP	PA-O3A-PB-O2B
10	A	601	ADP	O4'-C4'-C5'-O5'
10	D	601	ADP	C5'-O5'-PA-O1A
10	D	601	ADP	C5'-O5'-PA-O3A
10	G	601	ADP	PA-O3A-PB-O2B
10	H	601	ADP	PA-O3A-PB-O2B
10	H	601	ADP	PA-O3A-PB-O3B
10	a	601	ADP	PA-O3A-PB-O2B
10	a	601	ADP	O4'-C4'-C5'-O5'
10	d	601	ADP	C5'-O5'-PA-O1A
10	d	601	ADP	C5'-O5'-PA-O3A
10	g	601	ADP	PA-O3A-PB-O2B
10	h	601	ADP	PA-O3A-PB-O2B
10	h	601	ADP	PA-O3A-PB-O3B
10	A	601	ADP	C3'-C4'-C5'-O5'
10	a	601	ADP	C3'-C4'-C5'-O5'
10	G	601	ADP	PB-O3A-PA-O1A
10	g	601	ADP	PB-O3A-PA-O1A
10	E	601	ADP	PB-O3A-PA-O5'
10	e	601	ADP	PB-O3A-PA-O5'
10	D	601	ADP	C3'-C4'-C5'-O5'
10	d	601	ADP	C3'-C4'-C5'-O5'
10	H	601	ADP	PB-O3A-PA-O1A
10	H	601	ADP	PB-O3A-PA-O2A
10	Q	601	ADP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
10	h	601	ADP	PB-O3A-PA-O1A
10	h	601	ADP	PB-O3A-PA-O2A
10	q	601	ADP	PB-O3A-PA-O2A
10	D	601	ADP	O4'-C4'-C5'-O5'
10	d	601	ADP	O4'-C4'-C5'-O5'
10	D	601	ADP	C5'-O5'-PA-O2A
10	H	601	ADP	C5'-O5'-PA-O1A
10	H	601	ADP	C5'-O5'-PA-O2A
10	H	601	ADP	C5'-O5'-PA-O3A
10	d	601	ADP	C5'-O5'-PA-O2A
10	h	601	ADP	C5'-O5'-PA-O1A
10	h	601	ADP	C5'-O5'-PA-O2A
10	h	601	ADP	C5'-O5'-PA-O3A
10	G	601	ADP	PB-O3A-PA-O2A
10	g	601	ADP	PB-O3A-PA-O2A
10	A	601	ADP	PA-O3A-PB-O1B
10	a	601	ADP	PA-O3A-PB-O1B
10	G	601	ADP	PA-O3A-PB-O3B
10	g	601	ADP	PA-O3A-PB-O3B
10	Q	601	ADP	PB-O3A-PA-O1A
10	q	601	ADP	PB-O3A-PA-O1A
10	B	601	ADP	PB-O3A-PA-O2A
10	D	601	ADP	PB-O3A-PA-O2A
10	b	601	ADP	PB-O3A-PA-O2A
10	d	601	ADP	PB-O3A-PA-O2A

There are no ring outliers.

22 monomers are involved in 27 short contacts:

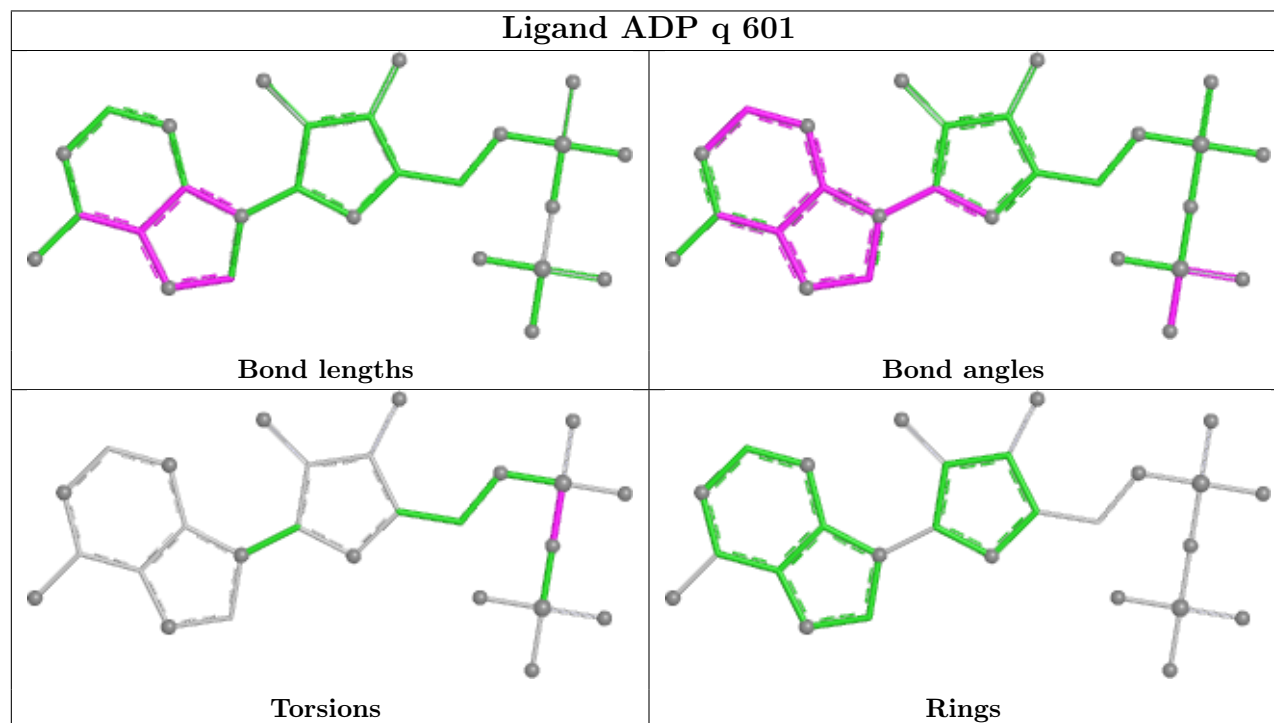
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	h	601	ADP	3	0
12	E	603	AF3	2	0
10	B	601	ADP	1	0
12	e	603	AF3	1	0
10	Z	601	ADP	2	0
10	e	601	ADP	3	0
10	H	601	ADP	3	0
10	a	601	ADP	1	0
12	h	603	AF3	2	0
10	A	601	ADP	1	0
12	z	603	AF3	1	0
10	z	601	ADP	2	0

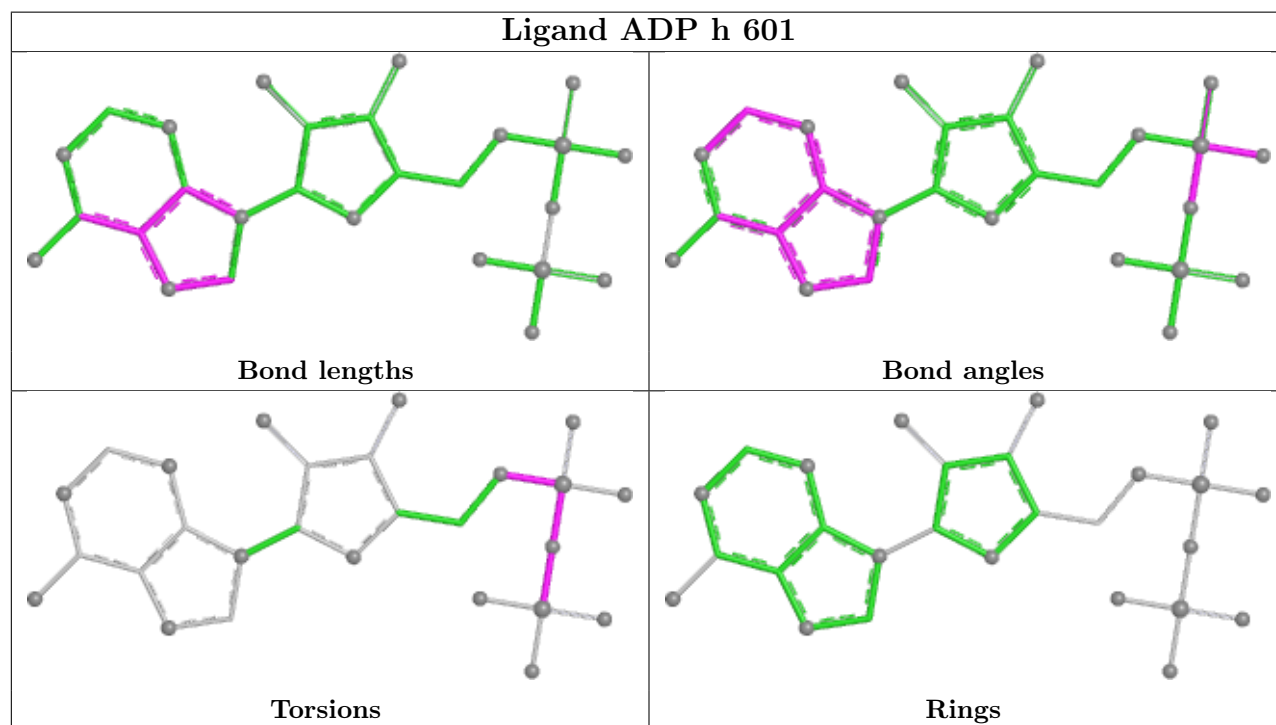
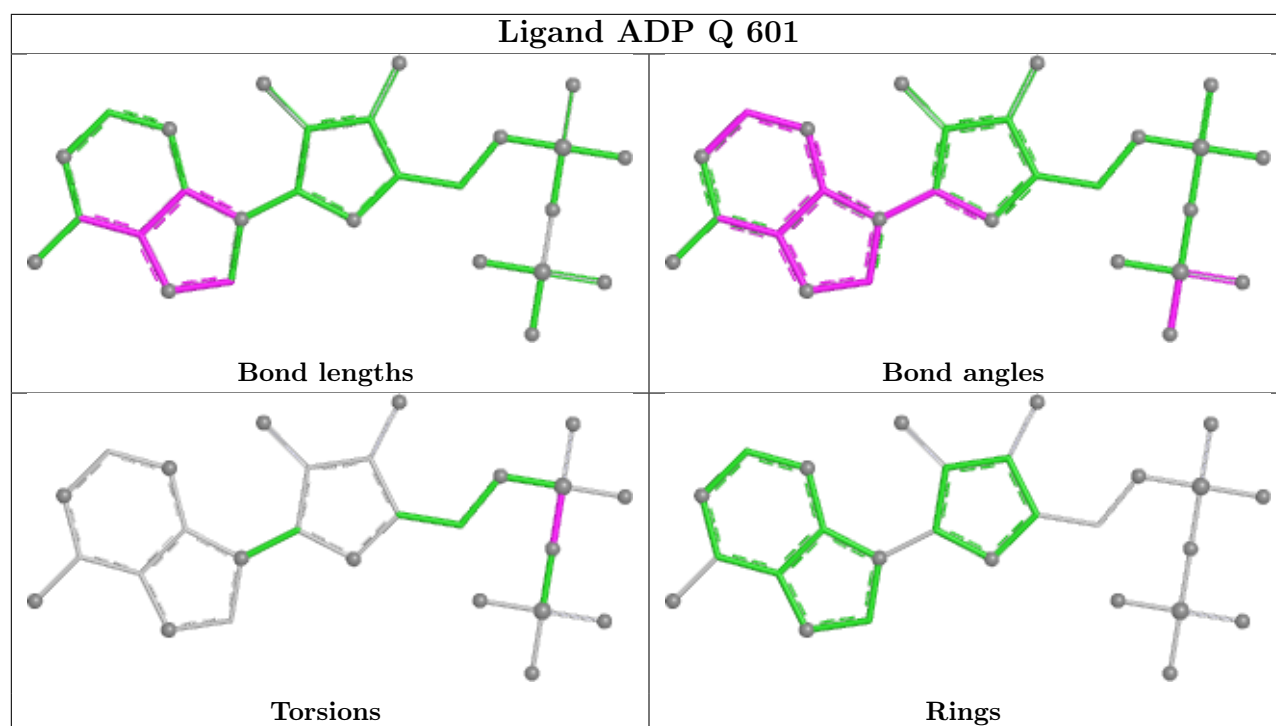
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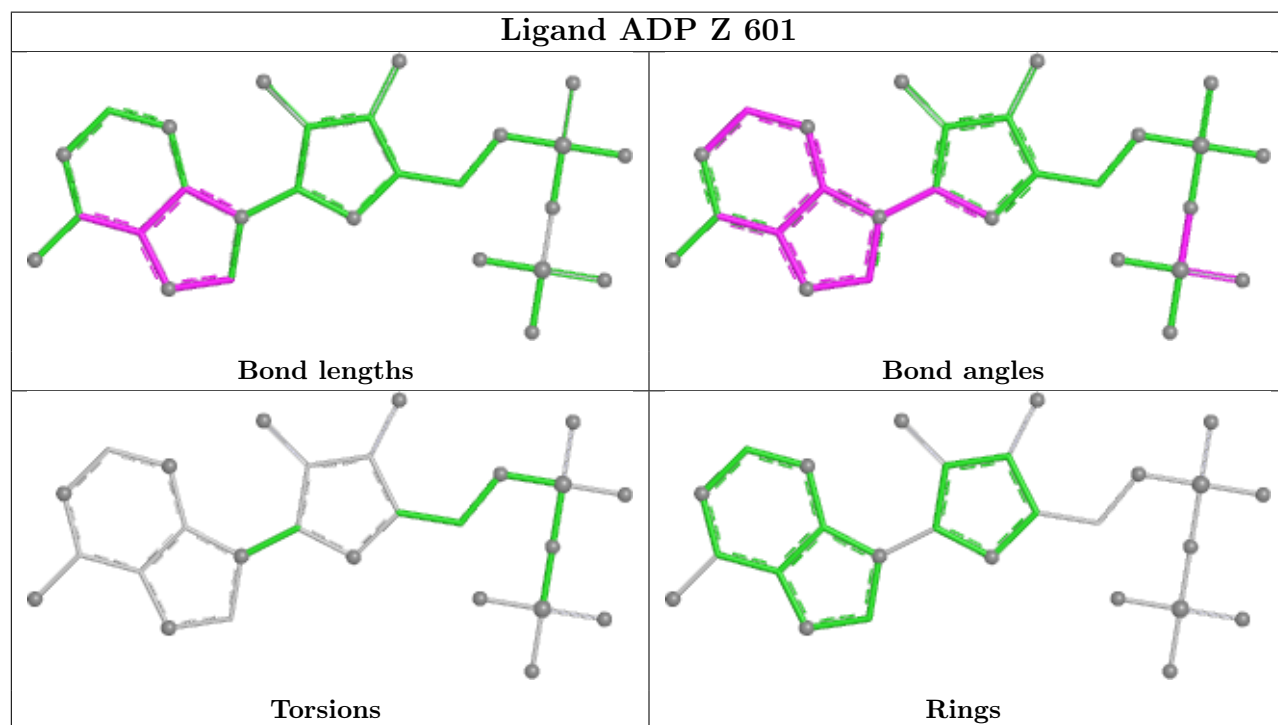
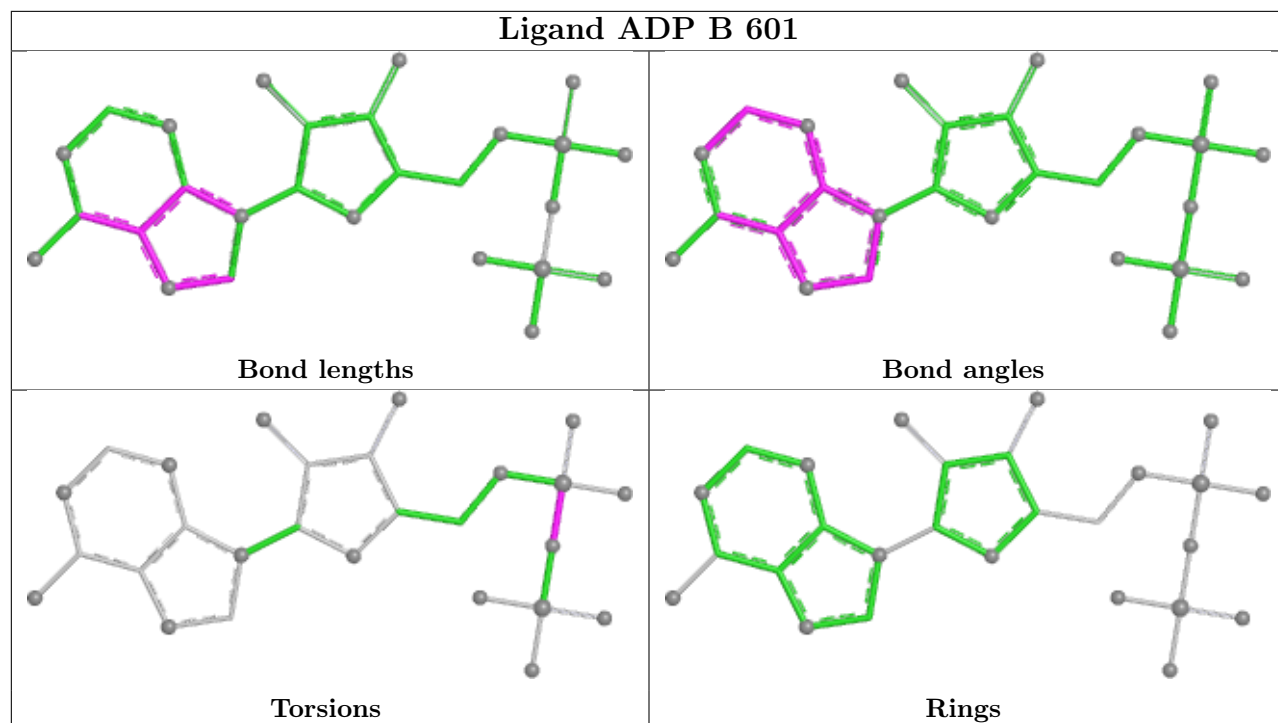
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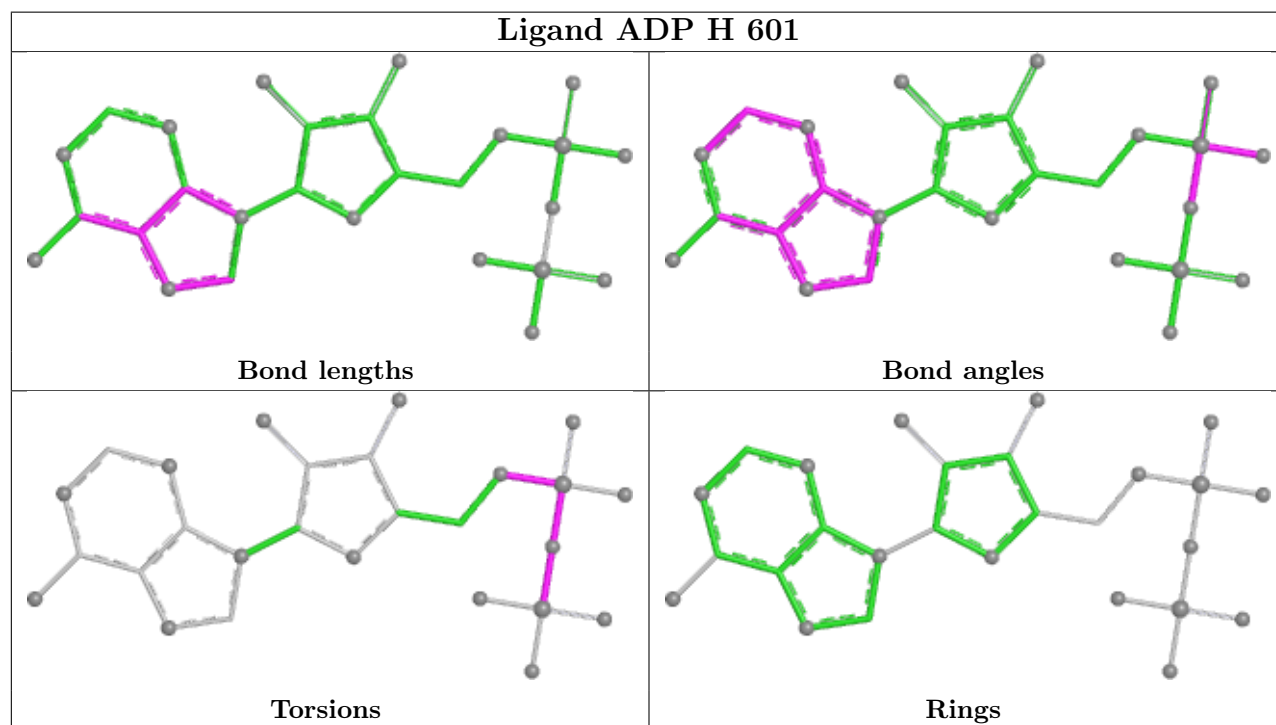
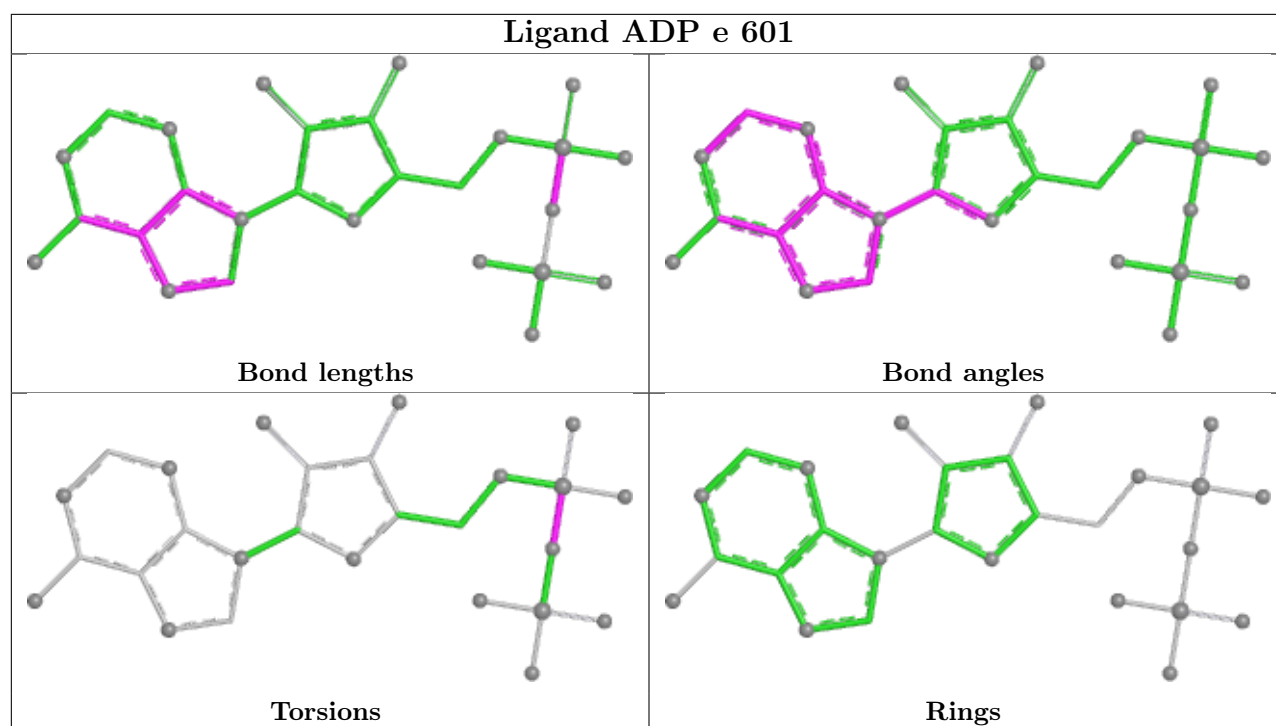
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	603	AF3	1	0
10	D	601	ADP	1	0
10	d	601	ADP	1	0
12	H	603	AF3	2	0
12	Z	603	AF3	1	0
12	d	603	AF3	1	0
12	g	603	AF3	1	0
12	G	603	AF3	1	0
10	b	601	ADP	1	0
10	E	601	ADP	3	0

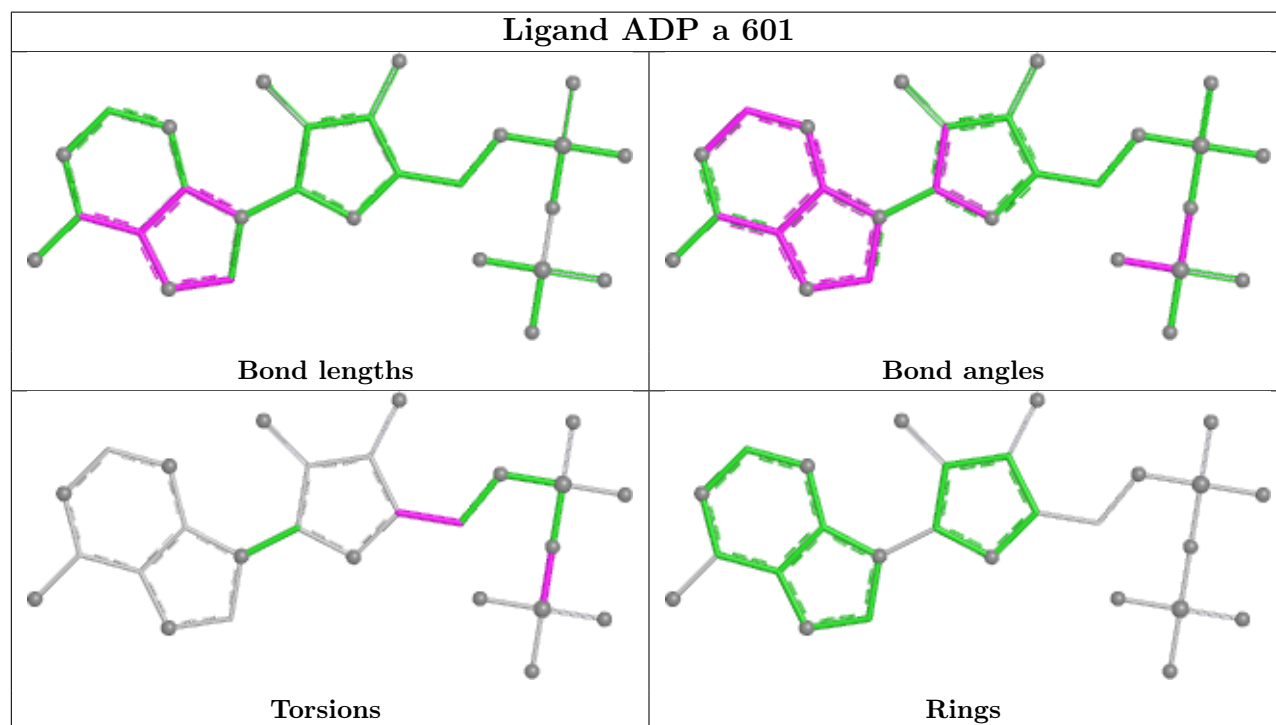
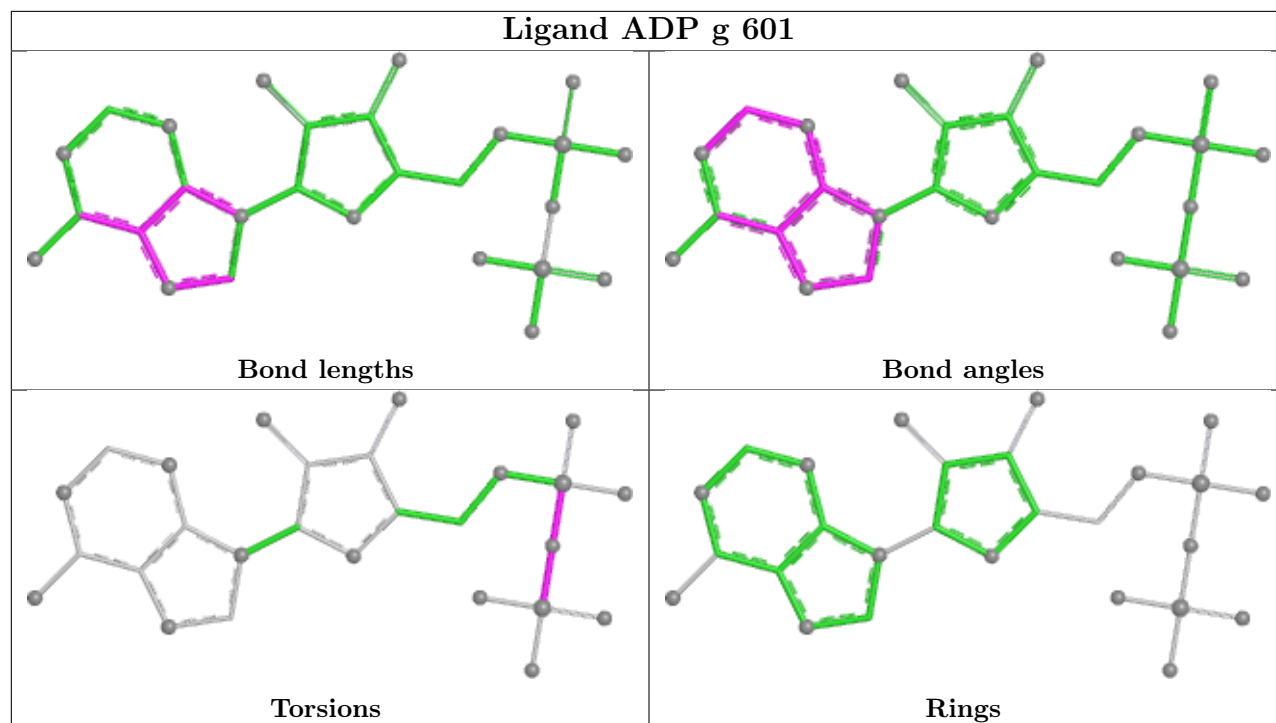
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

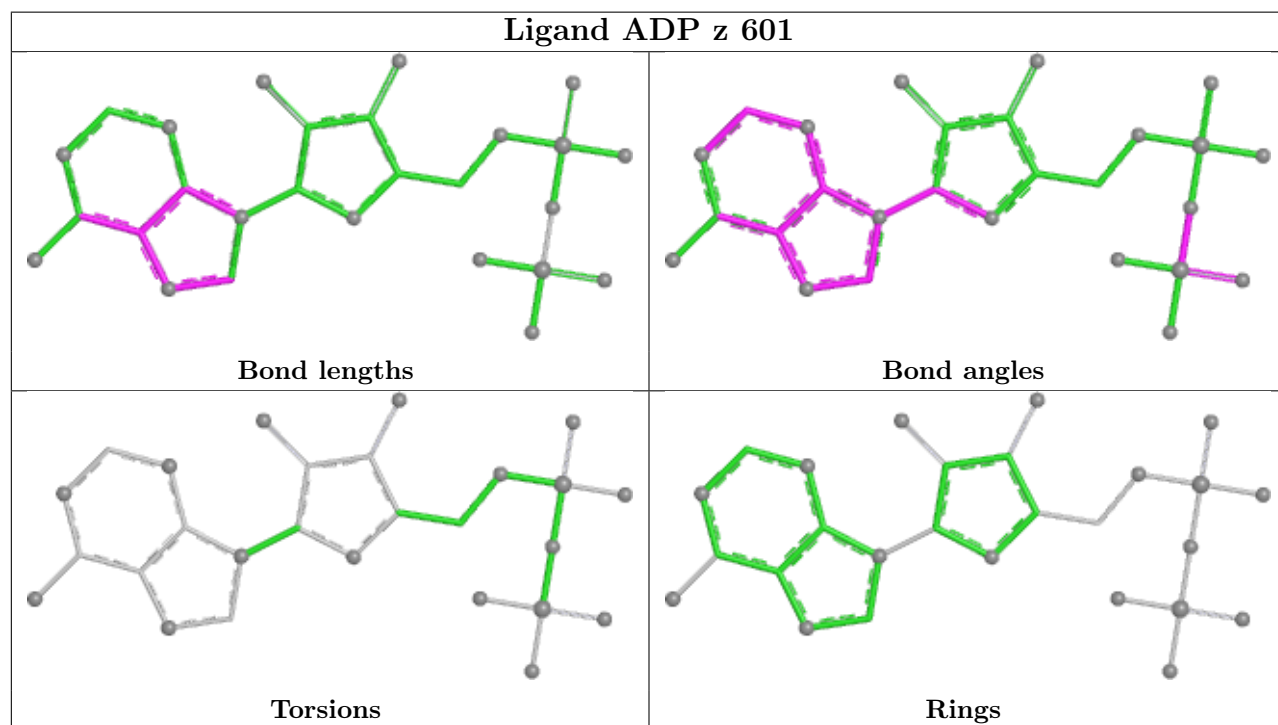
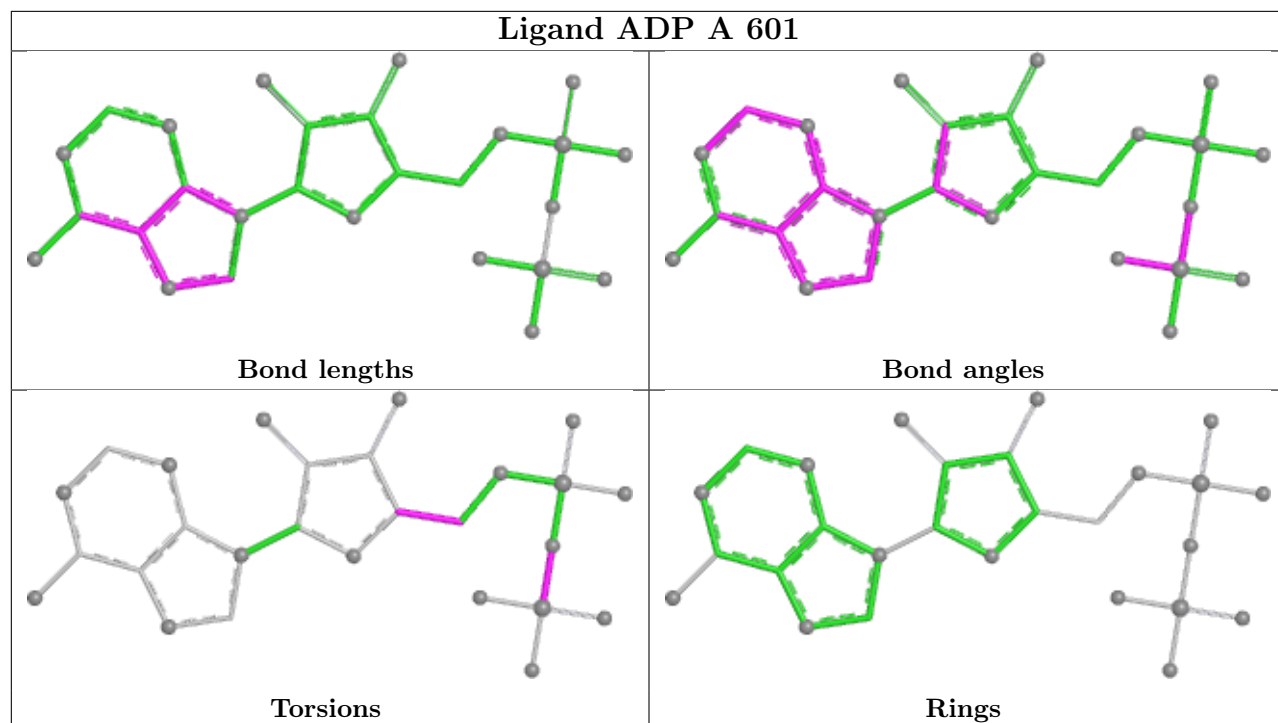


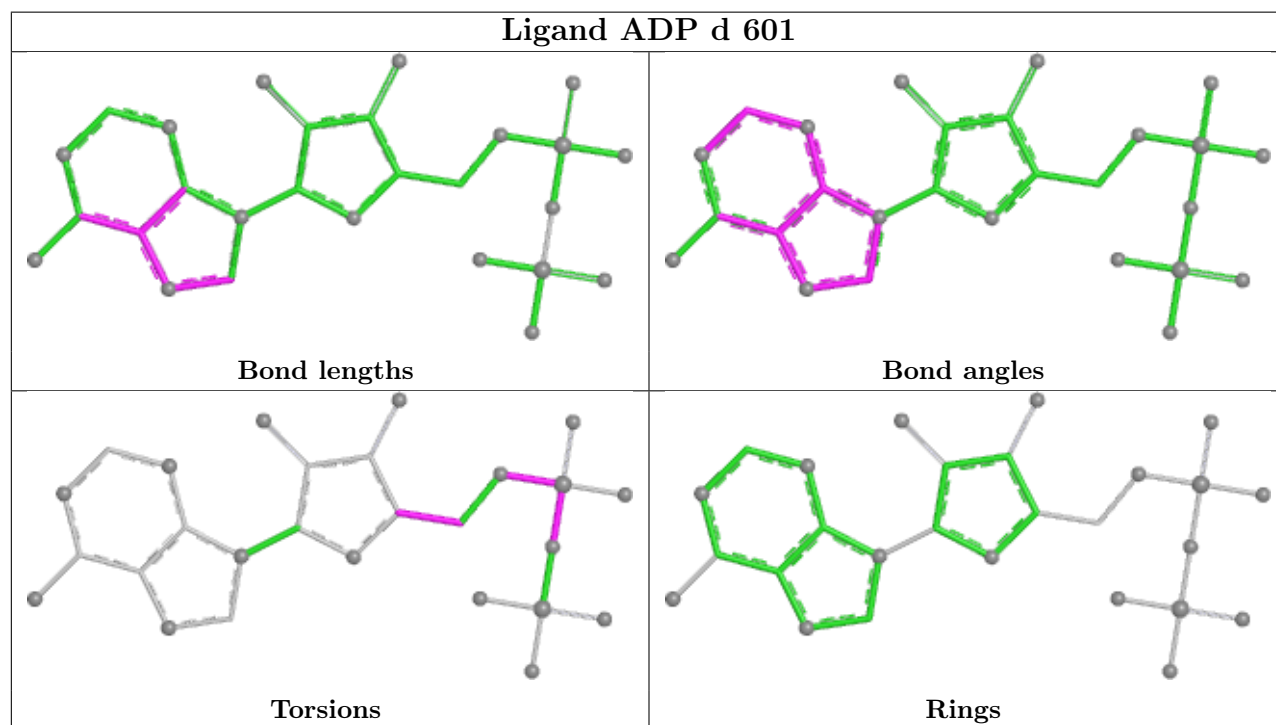
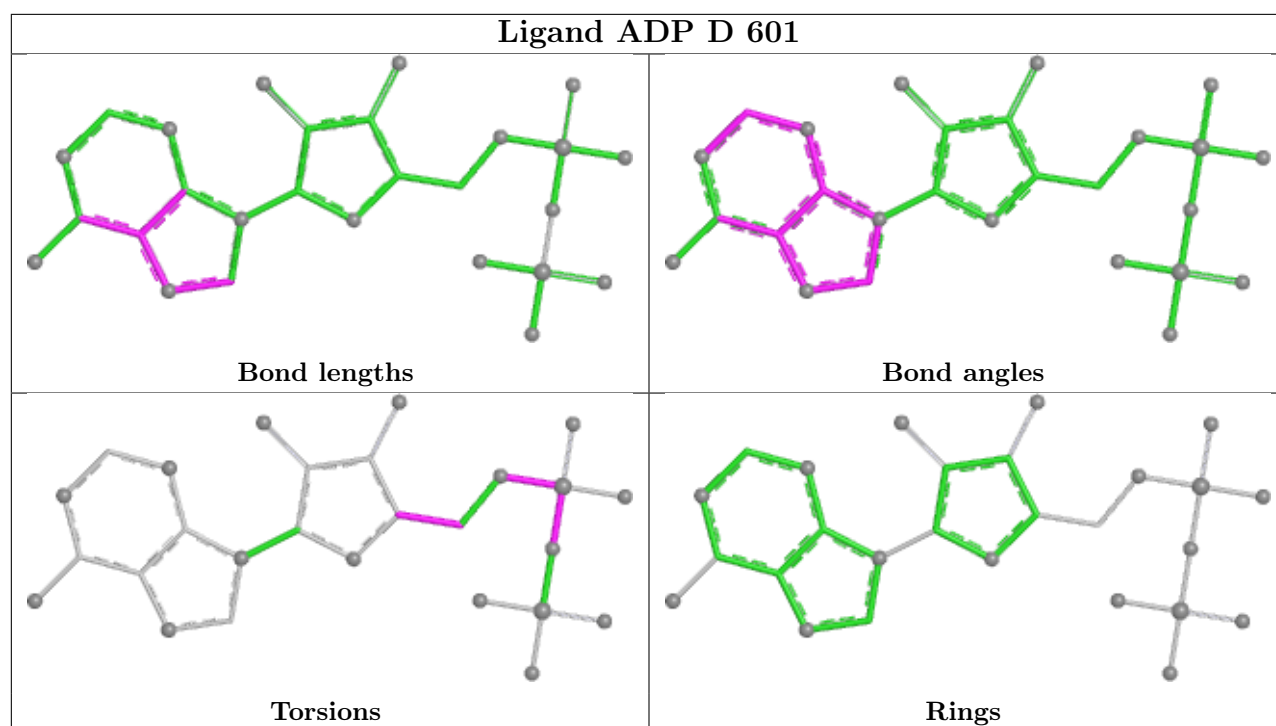


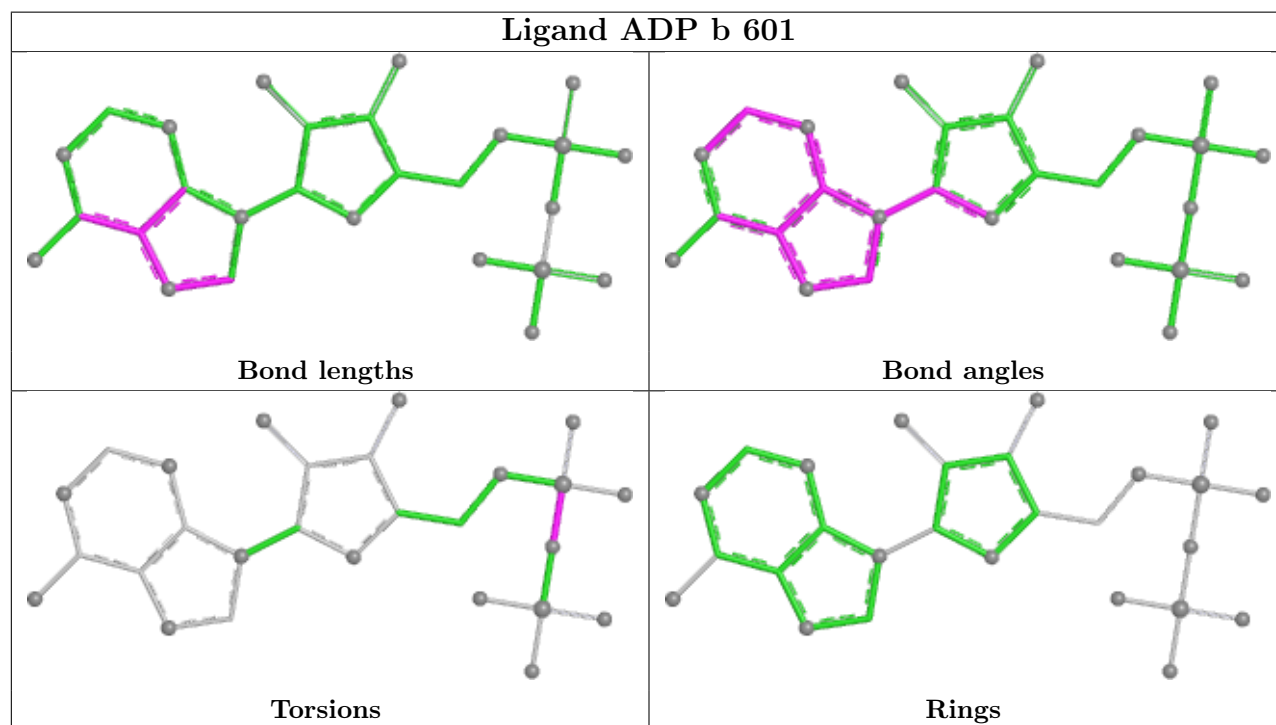
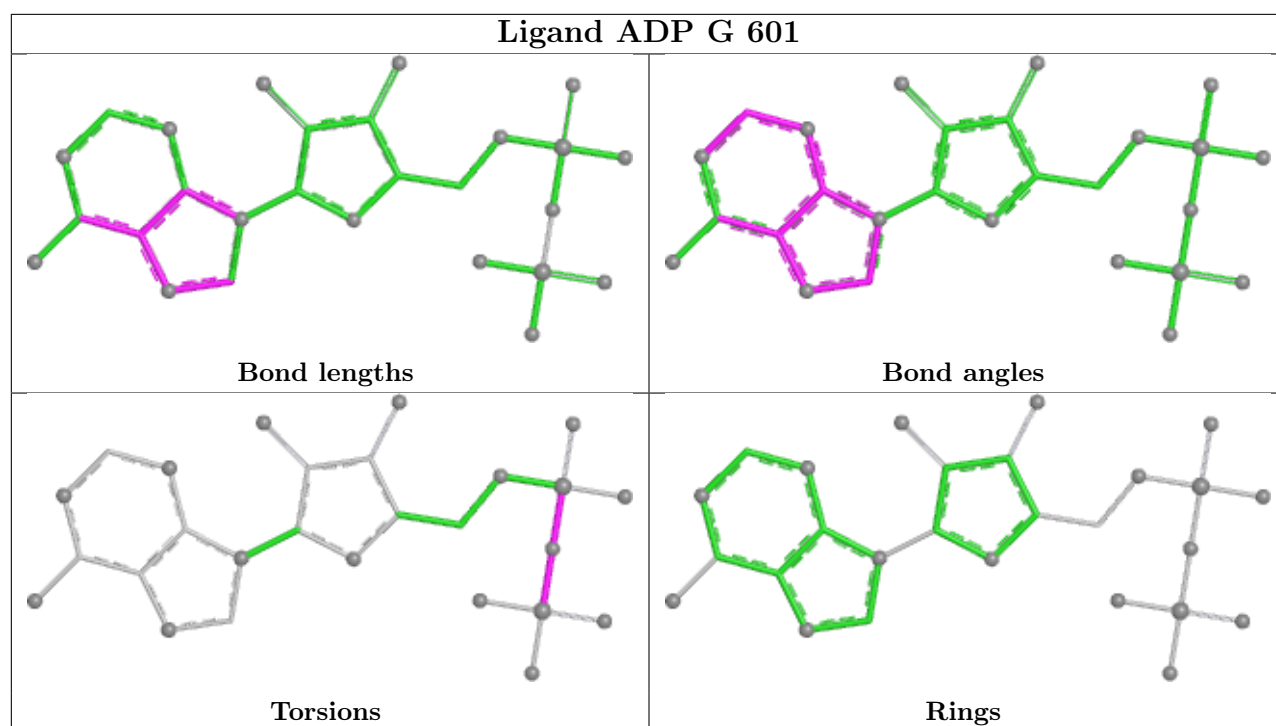


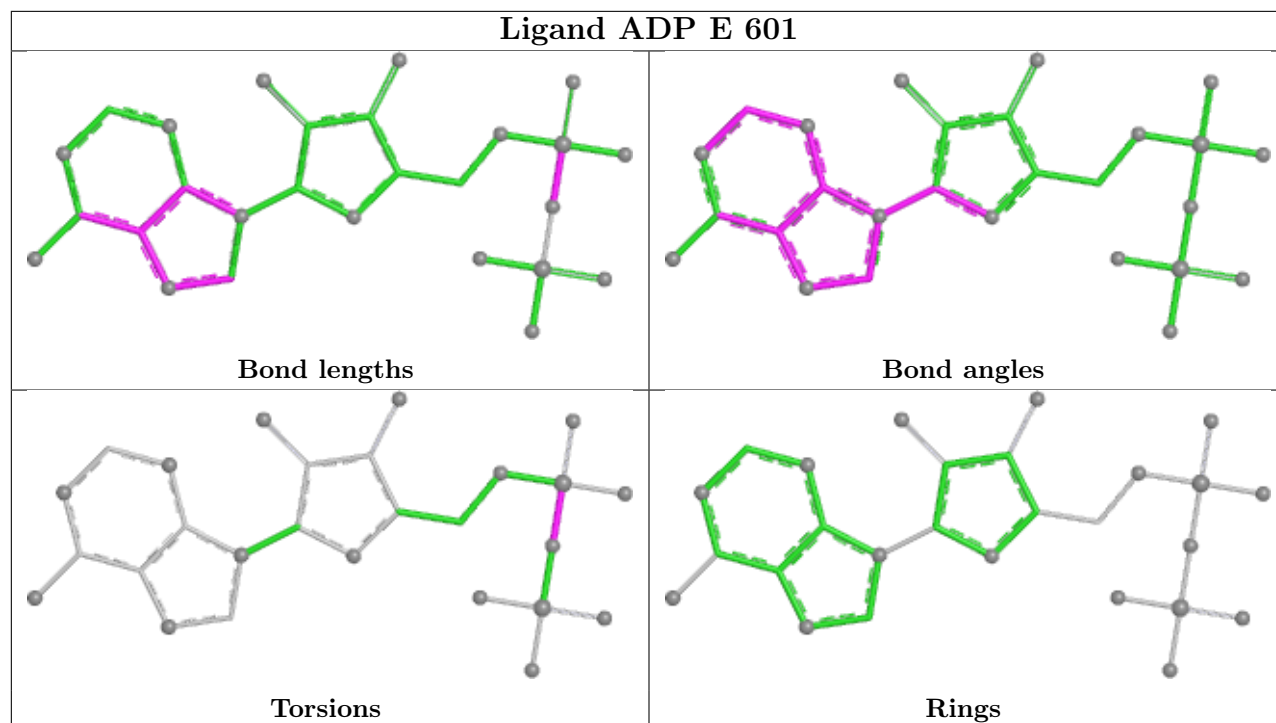












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

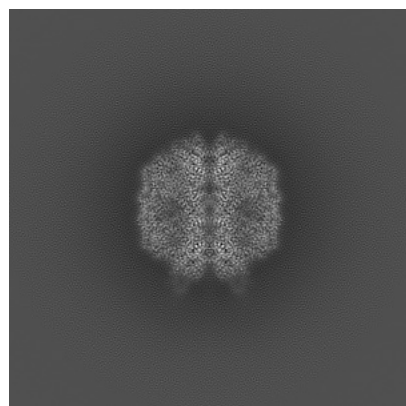
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12605. These allow visual inspection of the internal detail of the map and identification of artifacts.

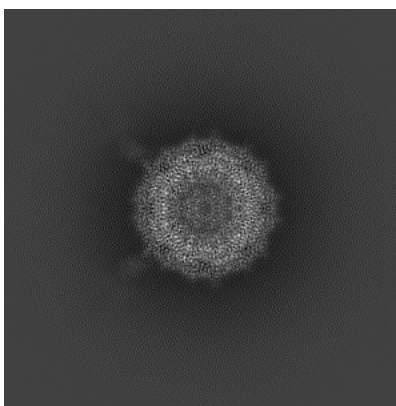
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

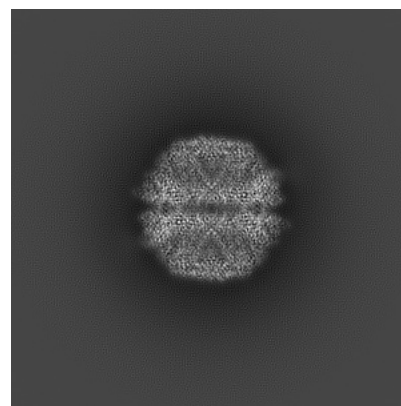
6.1.1 Primary map



X

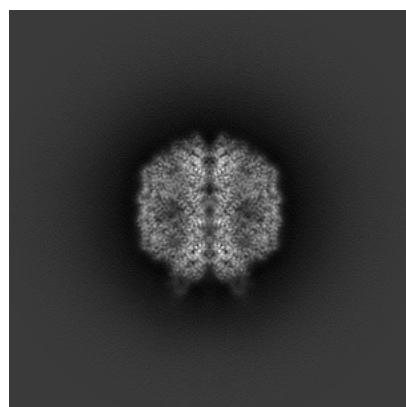


Y

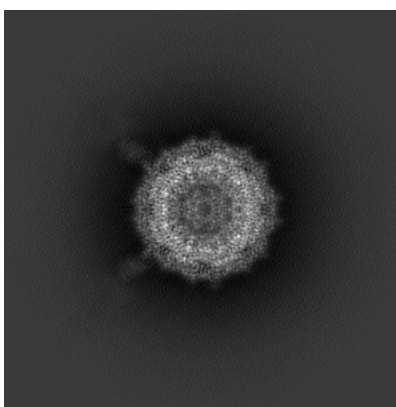


Z

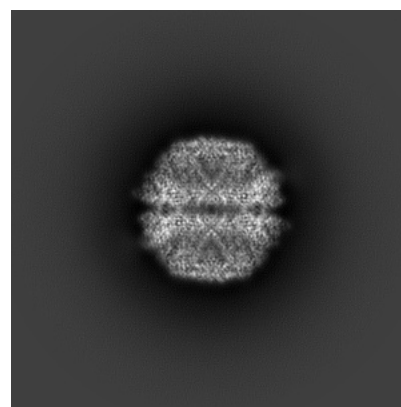
6.1.2 Raw map



X



Y

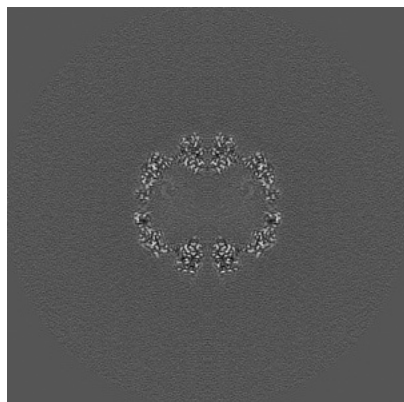


Z

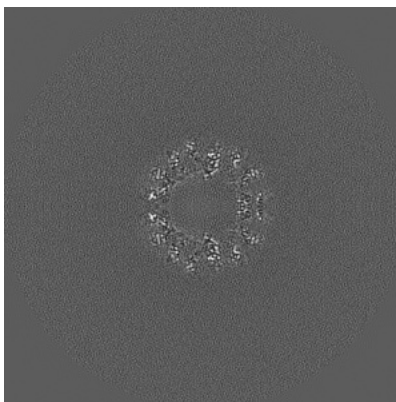
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

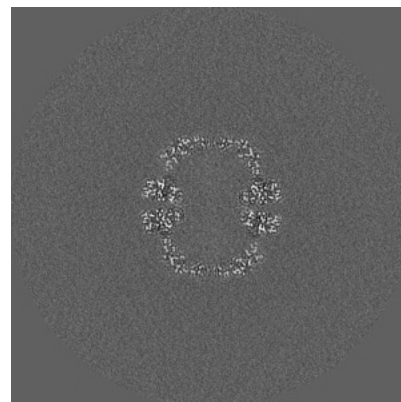
6.2.1 Primary map



X Index: 200

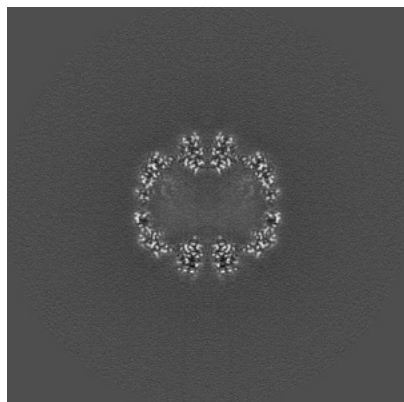


Y Index: 200

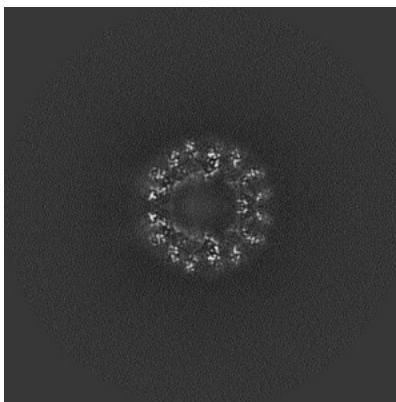


Z Index: 200

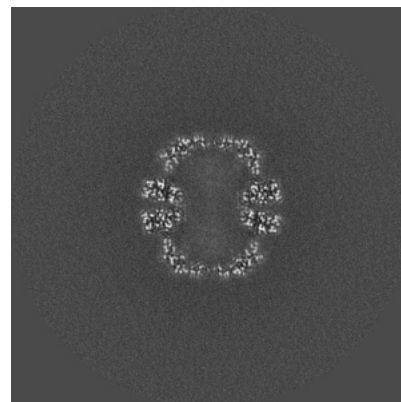
6.2.2 Raw map



X Index: 200



Y Index: 200

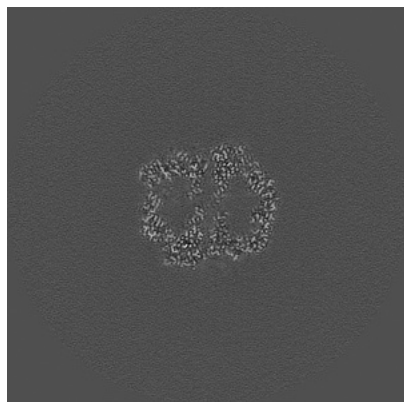


Z Index: 200

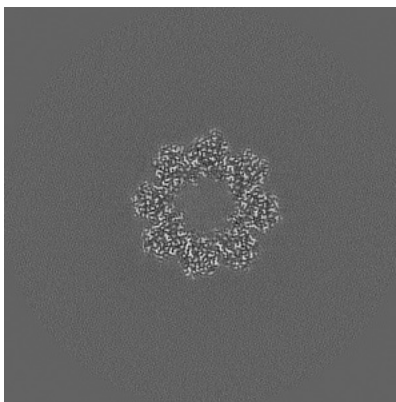
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

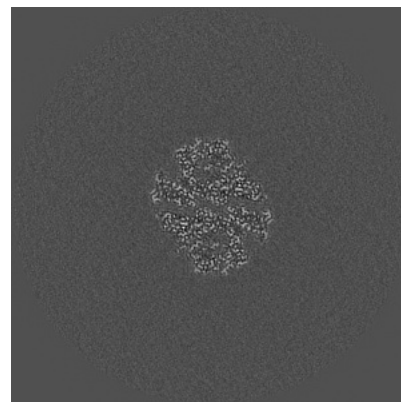
6.3.1 Primary map



X Index: 172

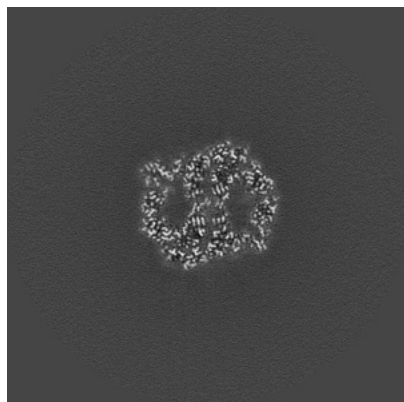


Y Index: 187

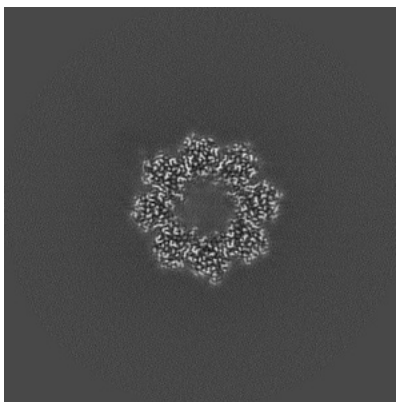


Z Index: 161

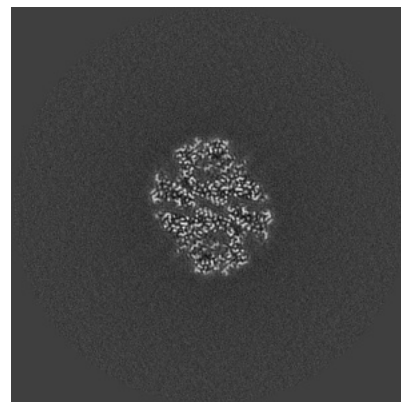
6.3.2 Raw map



X Index: 168



Y Index: 213

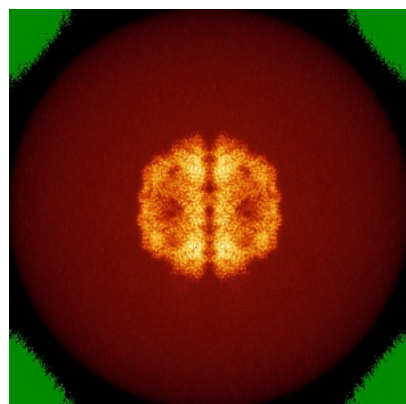


Z Index: 161

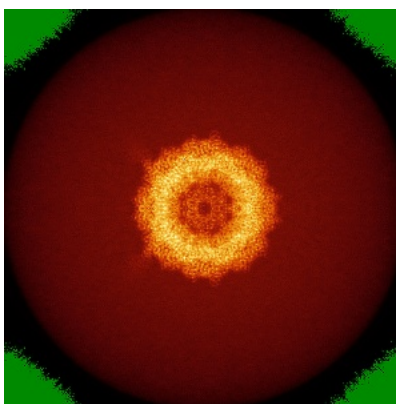
The images above show the largest variance slices of the map in three orthogonal directions.

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

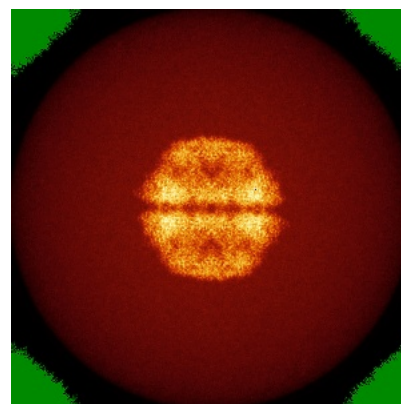
6.4.1 Primary map



X

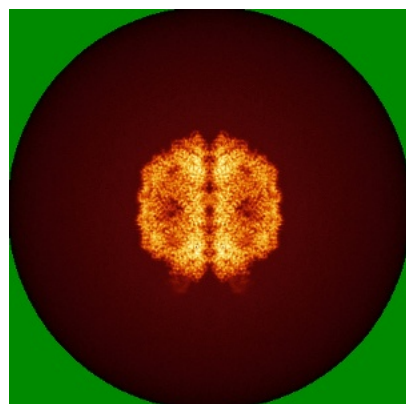


Y

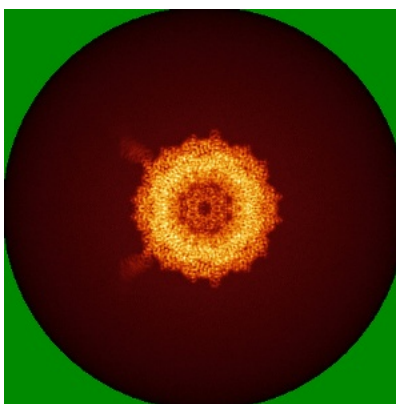


Z

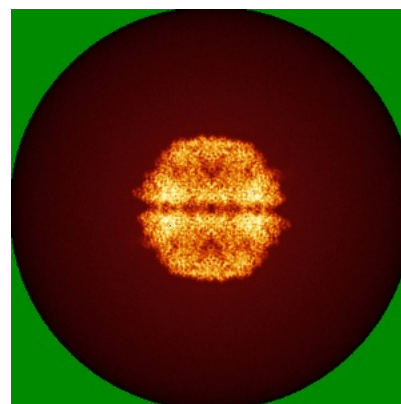
6.4.2 Raw map



X



Y

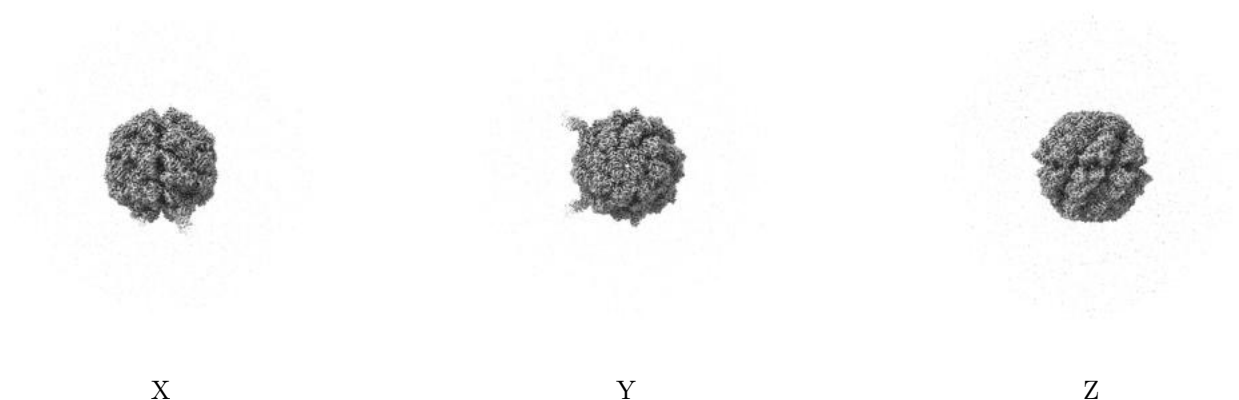


Z

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.

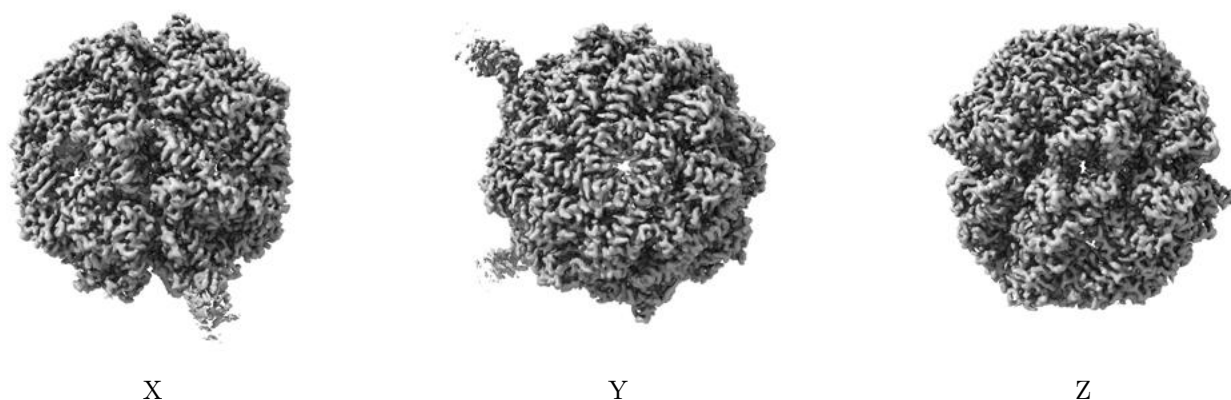
6.5 Orthogonal surface views [i](#)

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.

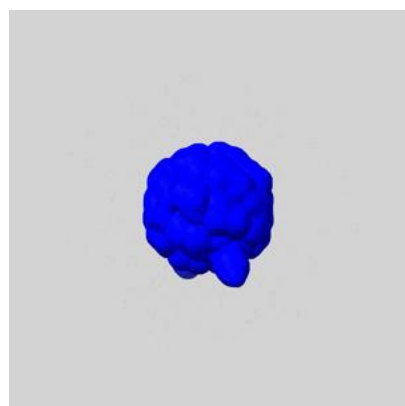
6.6 Mask visualisation [i](#)

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

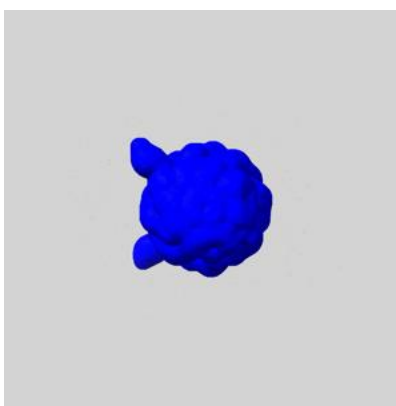
A mask typically either:

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

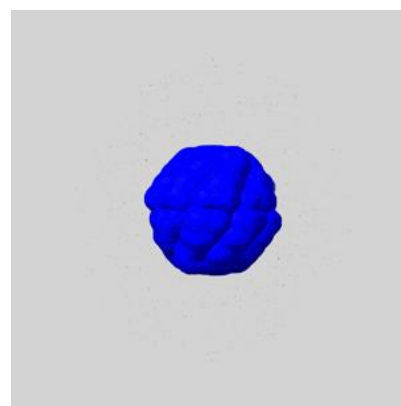
6.6.1 emd_12605_msk_1.map [i](#)



X



Y

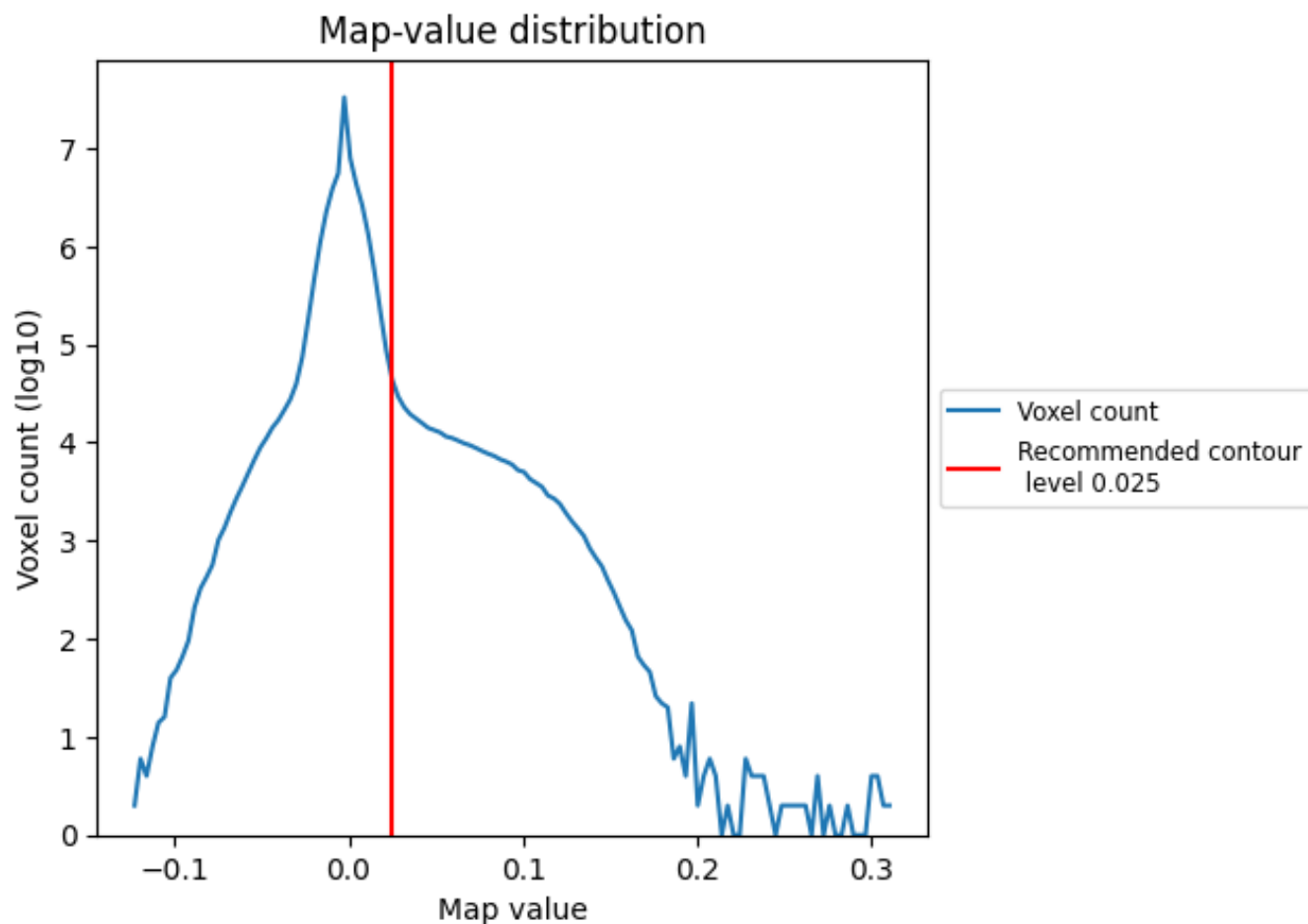


Z

7 Map analysis [i](#)

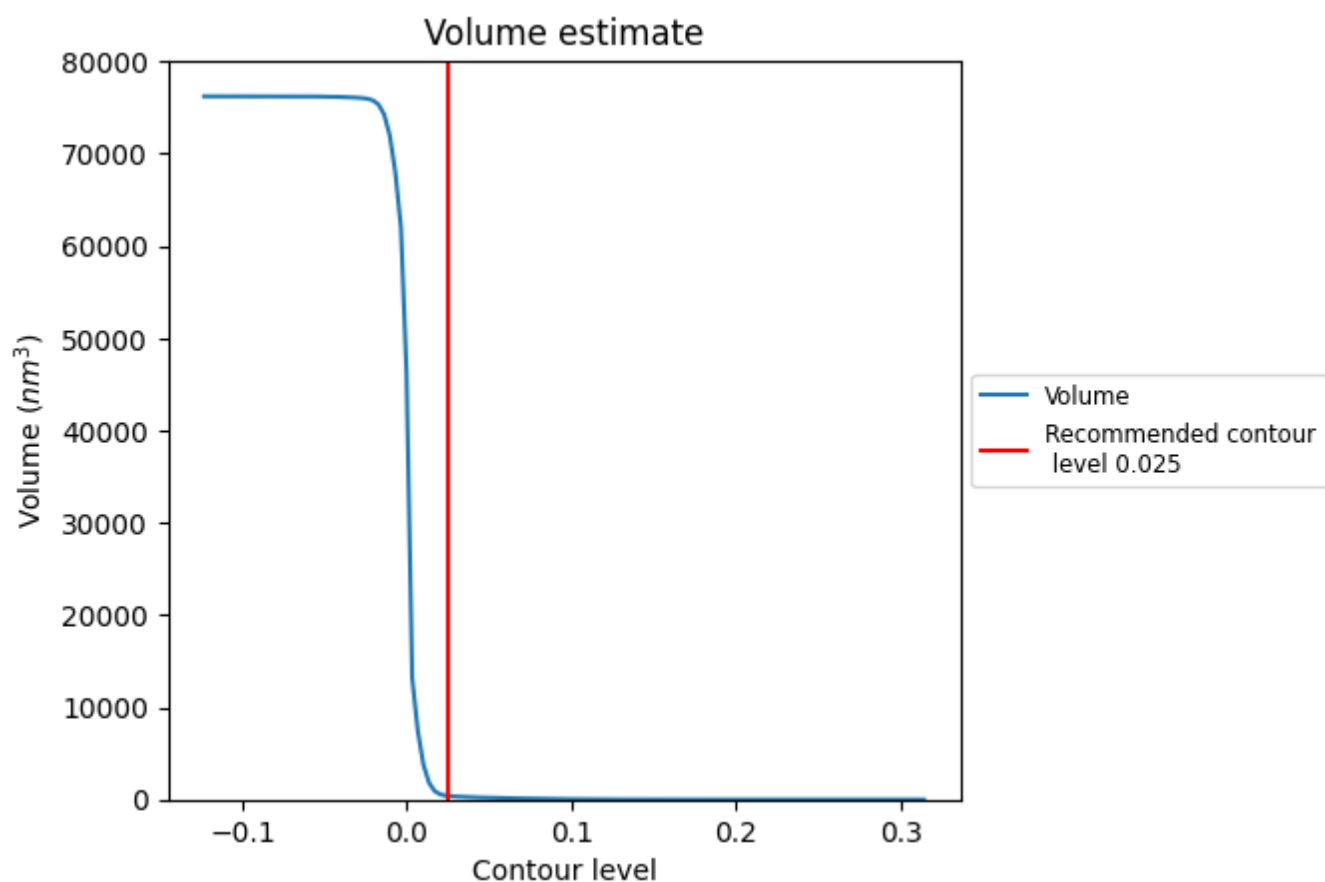
This section contains the results of statistical analysis of the map.

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.

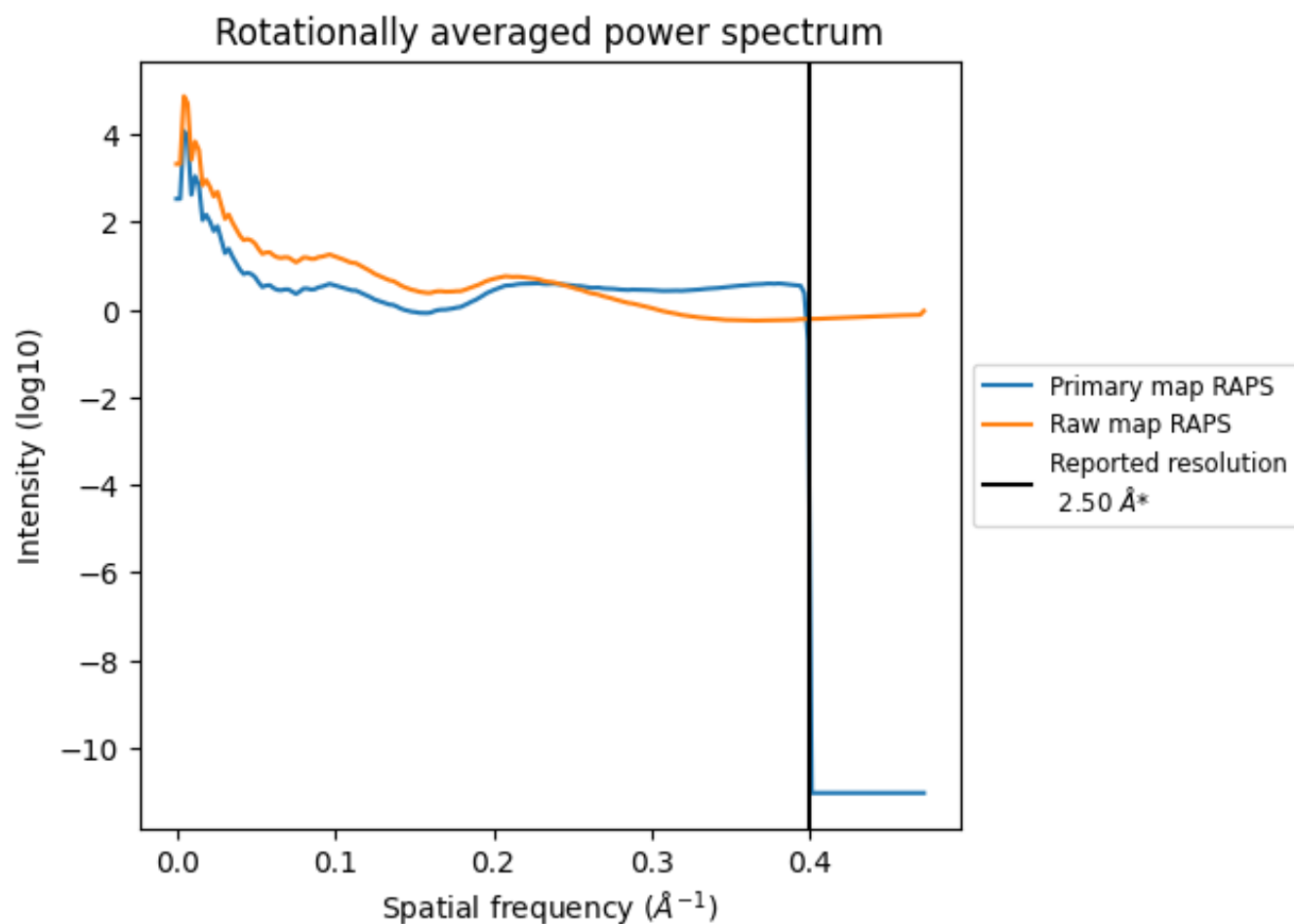
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 399 nm^3 ; this corresponds to an approximate mass of 361 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 ⓘ

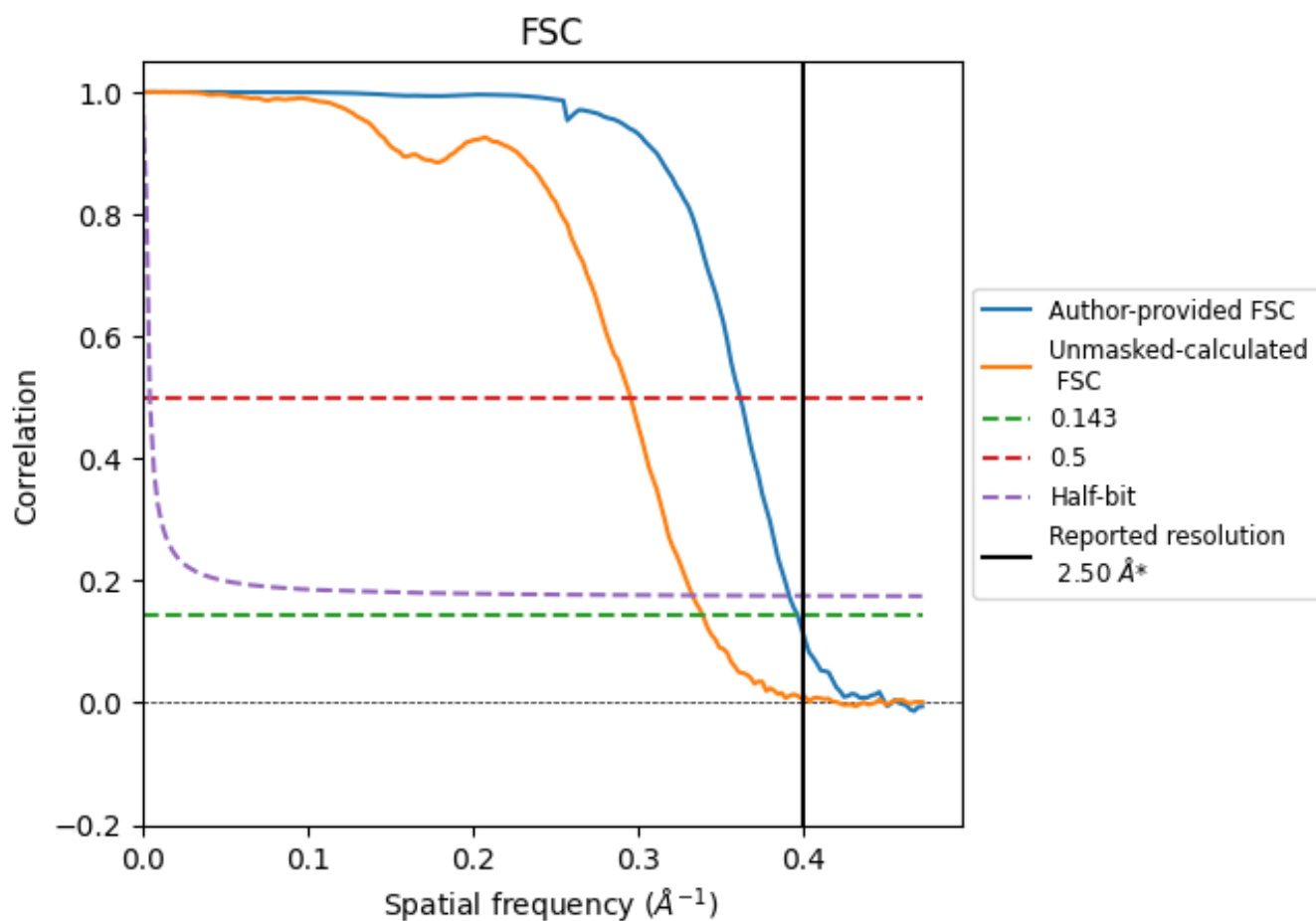


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates

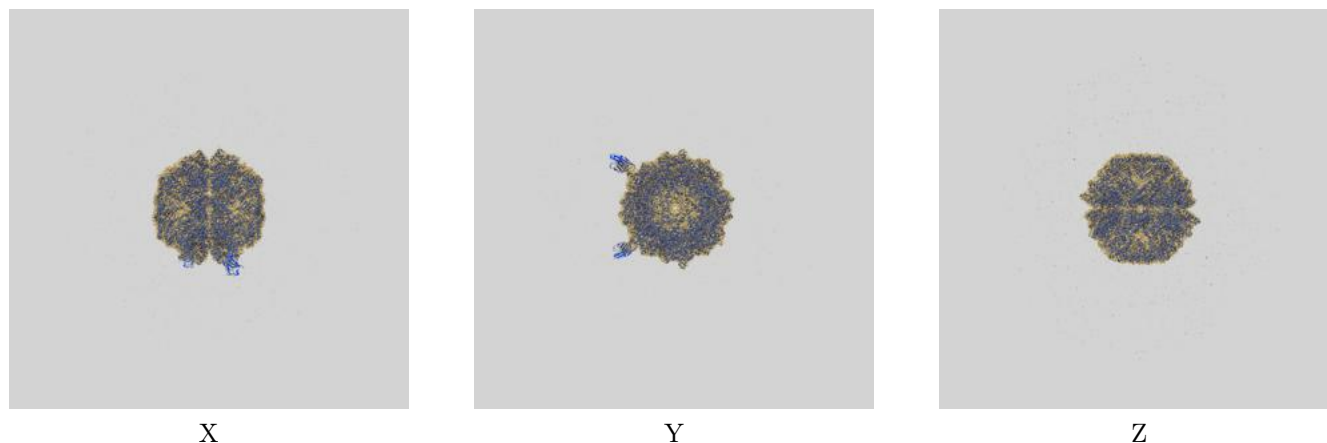
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.52	2.76	2.56
Unmasked-calculated*	2.95	3.39	3.00

*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 2.95 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

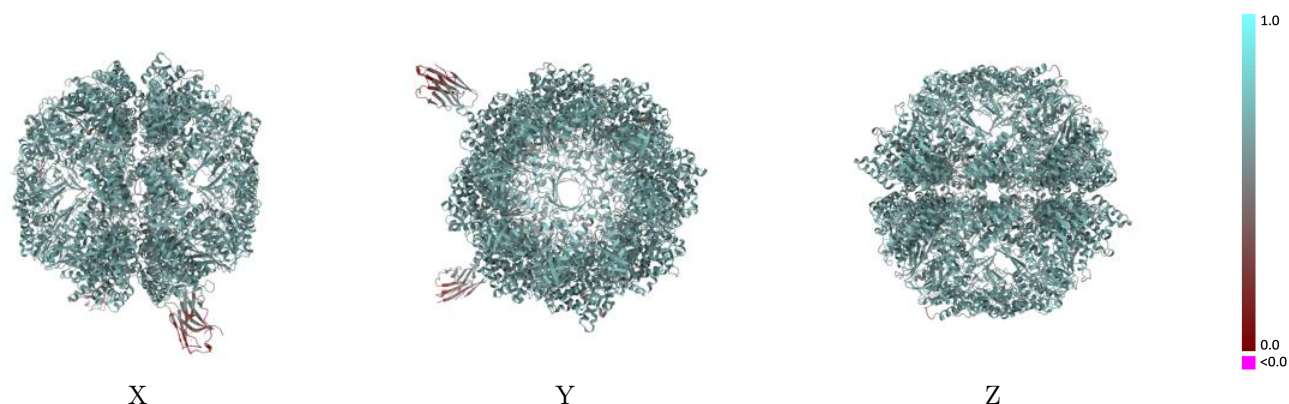
This section contains information regarding the fit between EMDB map EMD-12605 and PDB model 7NVL. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



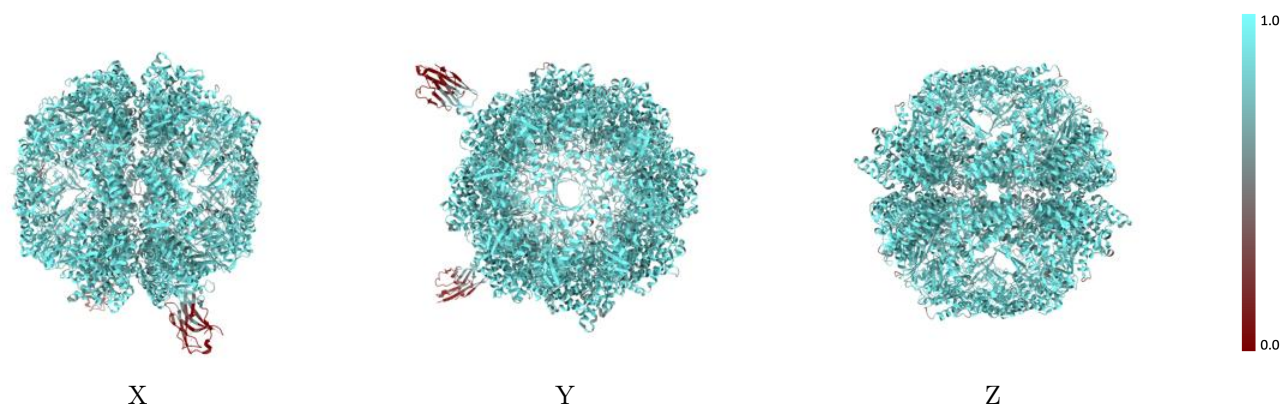
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



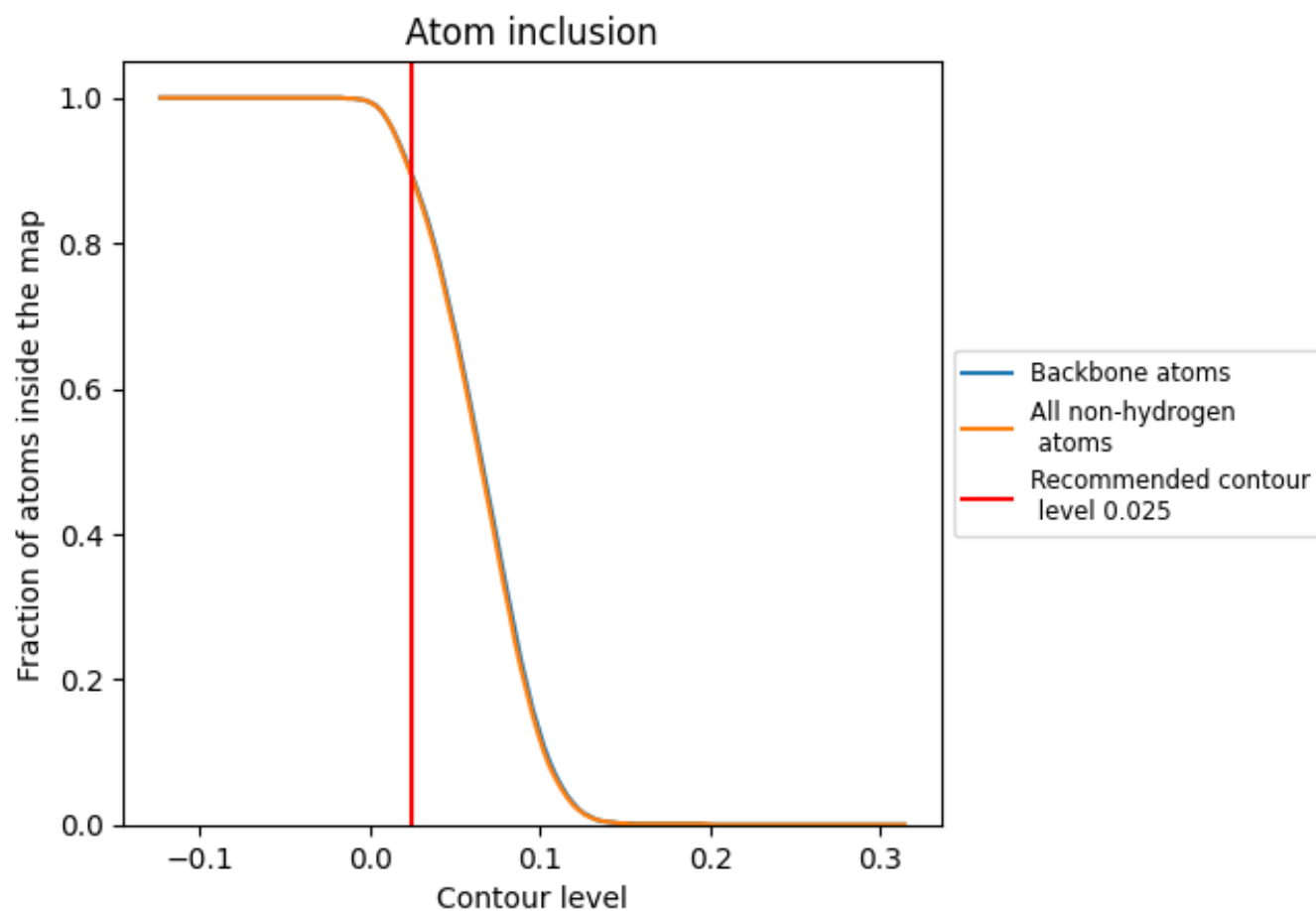
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 89% of all backbone atoms, 89% 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	 0.8890	 0.6310
A	 0.8950	 0.6330
B	 0.9050	 0.6370
D	 0.9030	 0.6380
E	 0.9120	 0.6370
G	 0.9100	 0.6400
H	 0.9160	 0.6410
N	 0.3120	 0.4030
Q	 0.9010	 0.6380
Z	 0.9000	 0.6330
a	 0.8960	 0.6330
b	 0.9050	 0.6360
d	 0.9030	 0.6380
e	 0.9110	 0.6370
g	 0.9110	 0.6420
h	 0.9170	 0.6410
n	 0.3140	 0.3980
q	 0.9010	 0.6370
z	 0.9010	 0.6320

