Full wwPDB EM Validation Report

Mar 20, 2026 – 09:32 AM UTC

PDB ID	:	8SH9 / pdb_00008sh9
EMDB ID	:	EMD-40481
Title	:	CCT G beta 5 complex best PhLP1 class
Authors	:	Wang, S.; Sass, M.; Willardson, B.M.; Shen, P.S.
Deposited on	:	2023-04-13
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

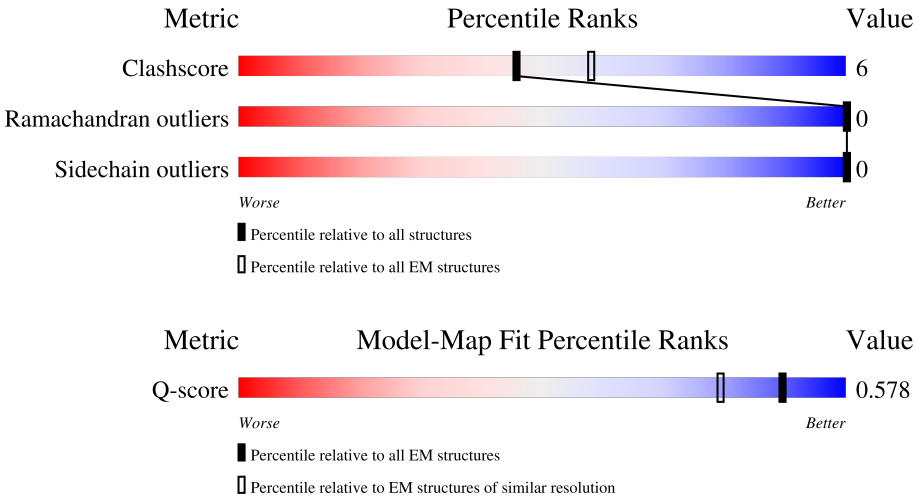
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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 <=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	N	395	10% 89%
2	A	536	84% 16%
2	a	536	83% 16%
3	B	526	86% 14%

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Mol	Chain	Length	Quality of chain
3	b	526	87% 13%
4	D	520	85% 15%
4	d	520	86% 14%
5	E	540	82% 17%
5	e	540	83% 17%
6	G	528	80% 19%
6	g	528	83% 17%
7	H	528	84% 16%
7	h	528	85% 15%
8	Q	538	84% 16%
8	q	538	85% 14%
9	Z	527	86% 14%
9	z	527	86% 14%
10	P	284	60% 17% 23%

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
13	AF3	D	603	-	-	X	-
13	AF3	G	603	-	-	X	-
13	AF3	Z	603	-	-	X	-
13	AF3	d	603	-	-	X	-
13	AF3	e	603	-	-	X	-
13	AF3	g	603	-	-	X	-
13	AF3	h	603	-	-	X	-
13	AF3	q	603	-	-	X	-
13	AF3	z	603	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 67197 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 Guanine nucleotide-binding protein subunit beta-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	43	Total	C	N	O	S	0	0
			322	203	53	62	4		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	535	Total	C	N	O	S	1	0
			4132	2590	719	792	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	540	Total 4169	C 2610	N 724	O 804	S 31	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	526	Total 4089	C 2548	N 726	O 785	S 30	0	0
6	g	528	Total 4102	C 2556	N 729	O 787	S 30	0	0

- Molecule 7 is a protein called T-complex protein 1 subunit eta, N-terminally processed.

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

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

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

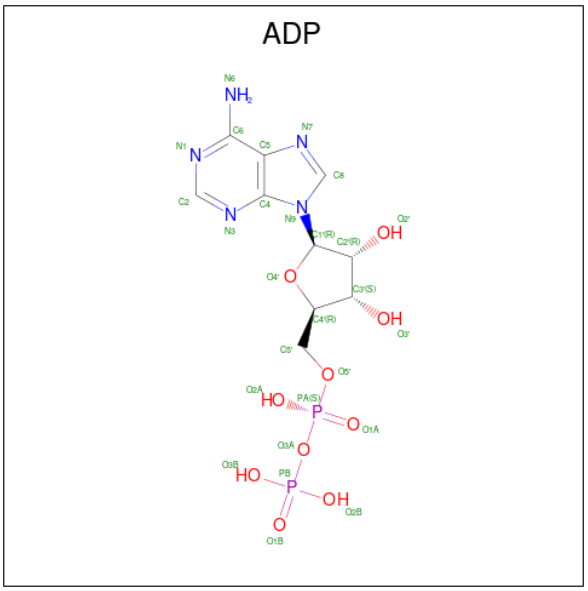
- Molecule 9 is a protein called T-complex protein 1 subunit zeta.

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

- Molecule 10 is a protein called Phosducin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	218	Total 1727	C 1083	N 292	O 339	S 13	0	0

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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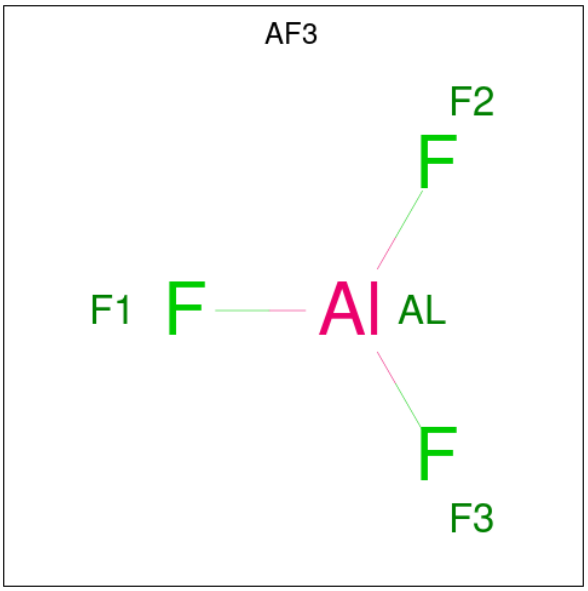
Mol	Chain	Residues	Atoms					AltConf
11	q	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	z	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 13 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



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

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

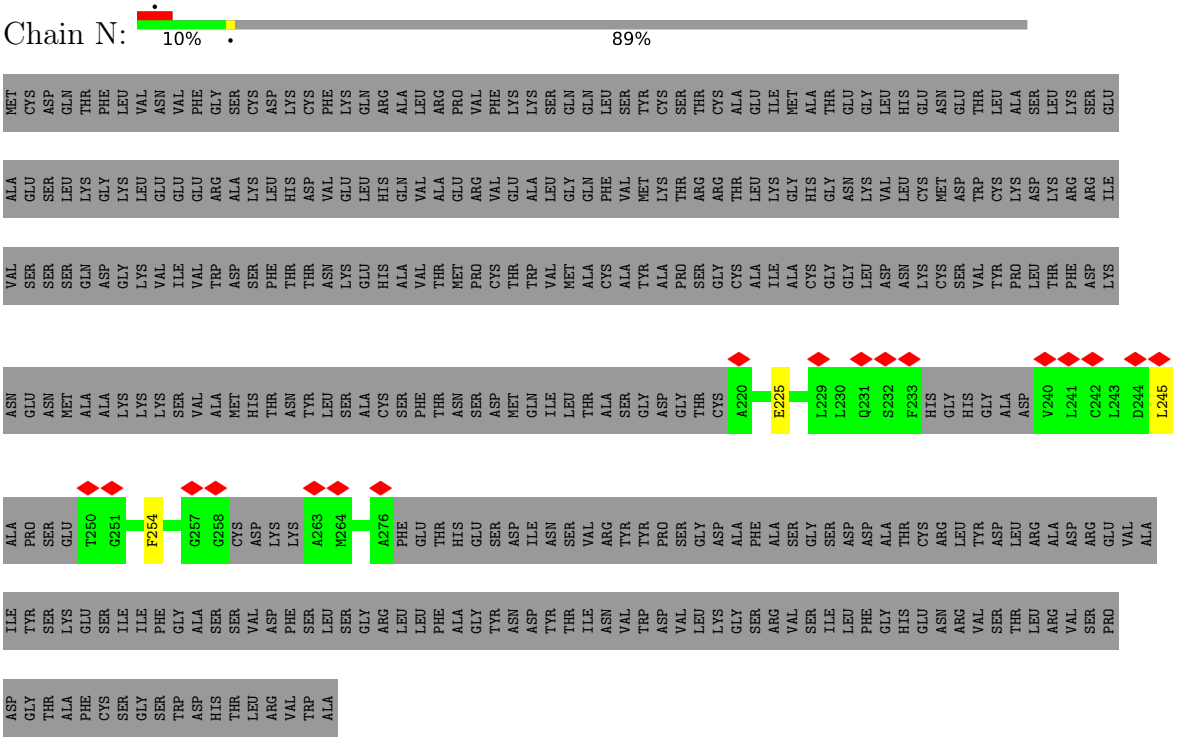
- Molecule 14 is water.

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

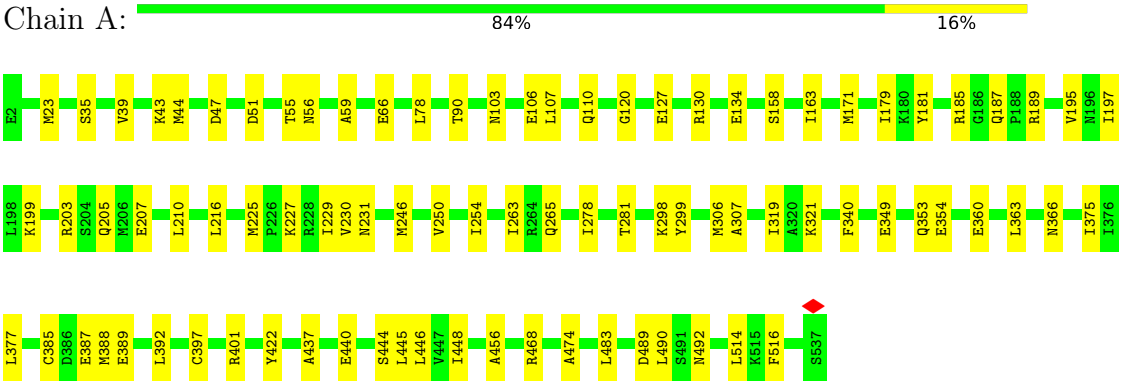
3 Residue-property plots (i)

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: Guanine nucleotide-binding protein subunit beta-5

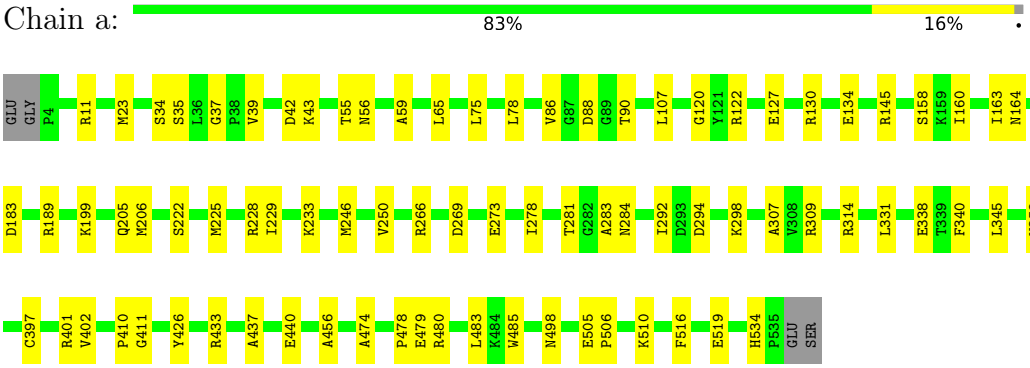


• Molecule 2: T-complex protein 1 subunit alpha



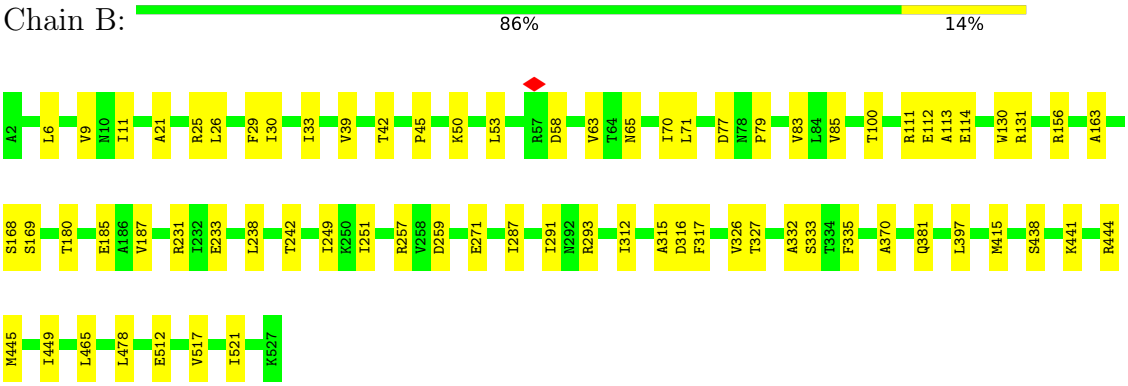
• Molecule 2: T-complex protein 1 subunit alpha

Chain a:



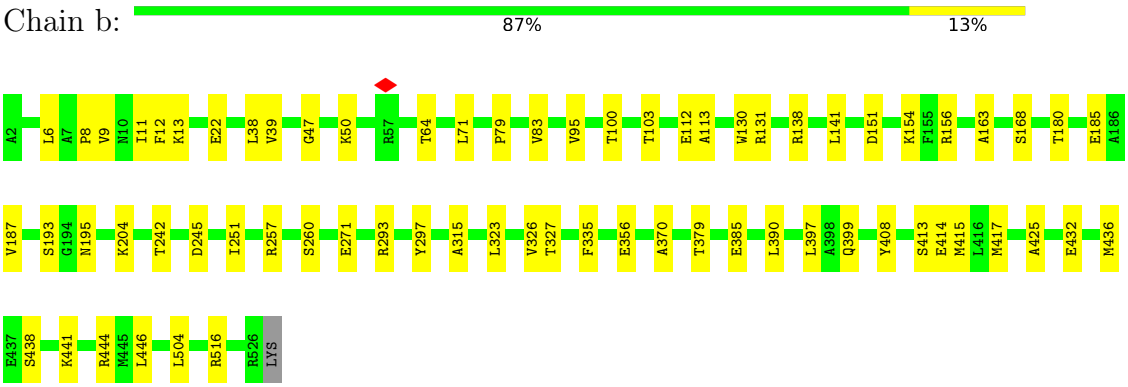
• Molecule 3: T-complex protein 1 subunit beta

Chain B:



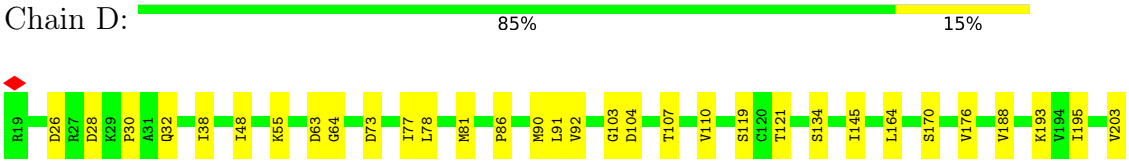
• Molecule 3: T-complex protein 1 subunit beta

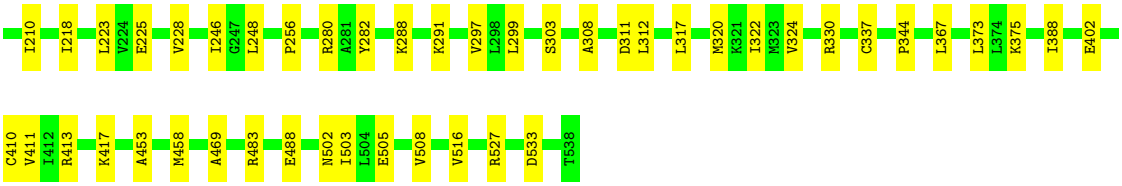
Chain b:



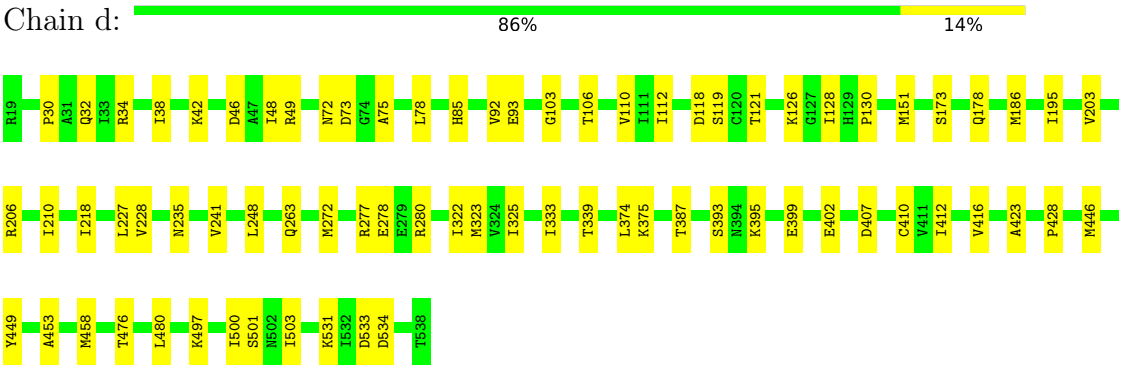
• Molecule 4: T-complex protein 1 subunit delta

Chain D:

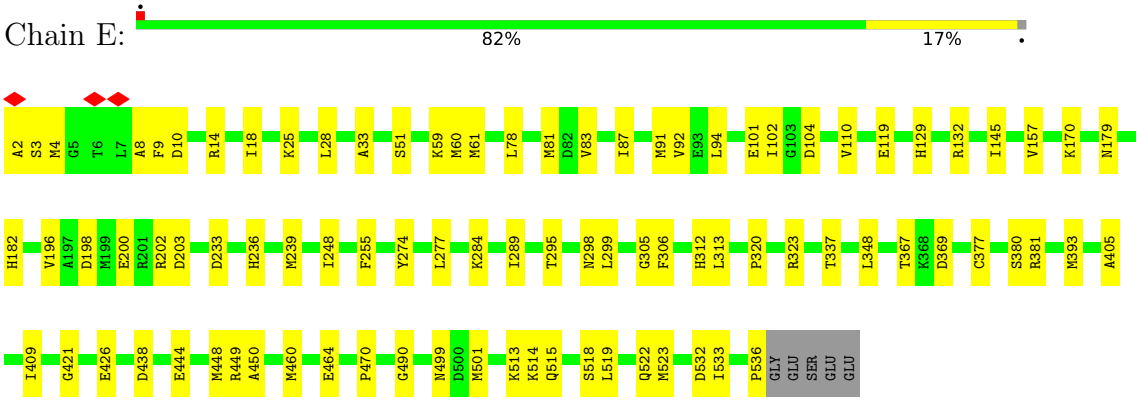




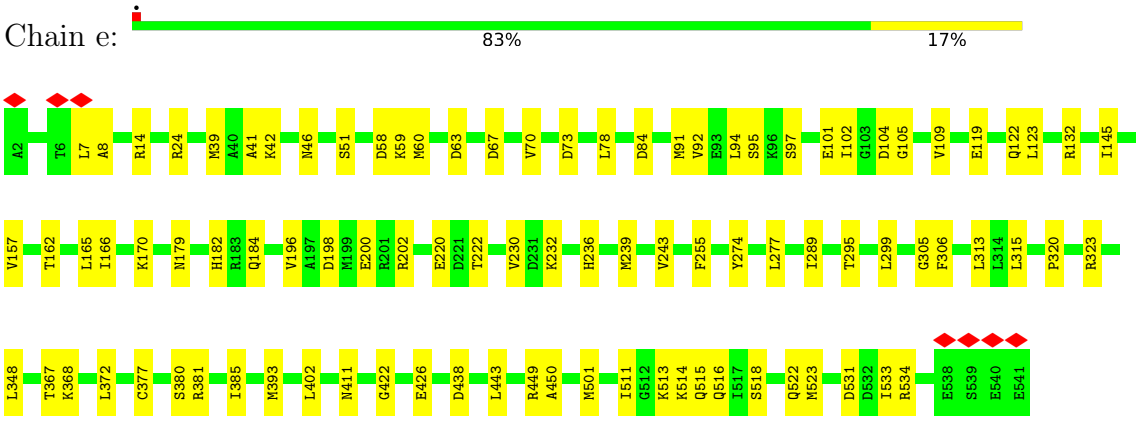
• Molecule 4: T-complex protein 1 subunit delta



• Molecule 5: T-complex protein 1 subunit epsilon

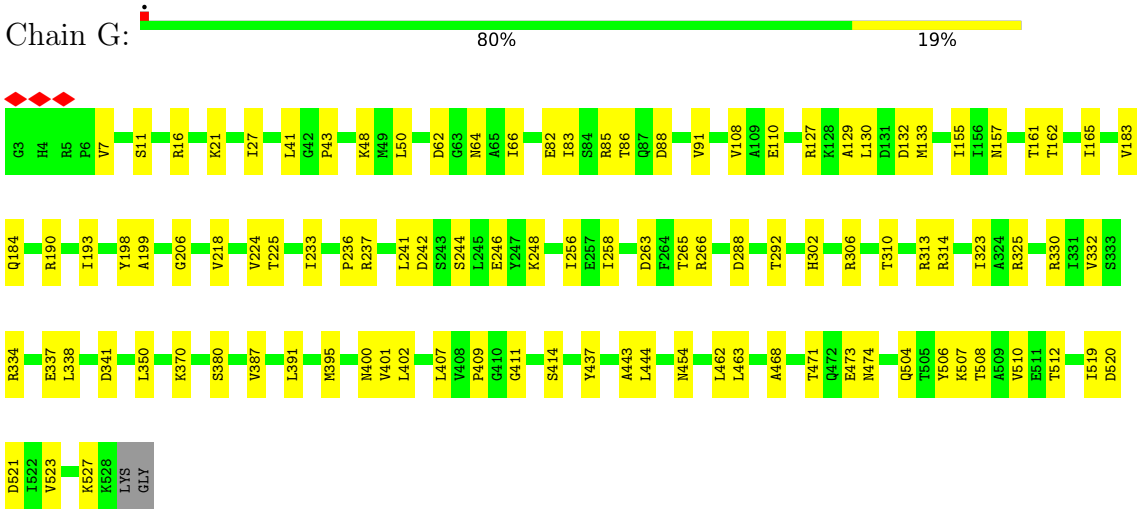


• Molecule 5: T-complex protein 1 subunit epsilon



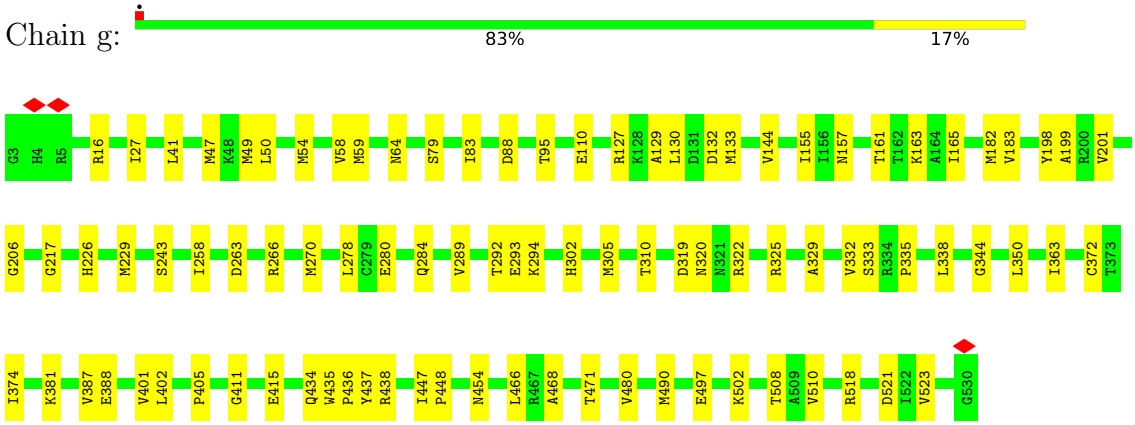
• Molecule 6: T-complex protein 1 subunit gamma

Chain G:



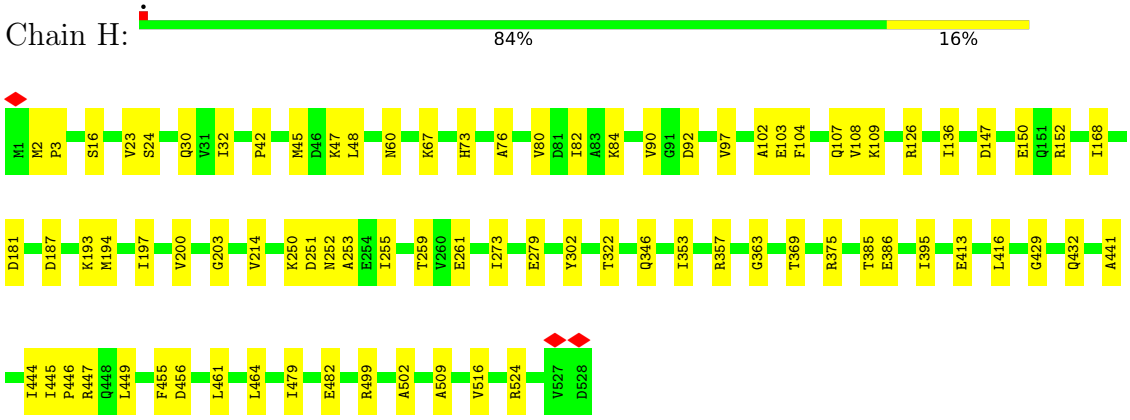
• Molecule 6: T-complex protein 1 subunit gamma

Chain g:



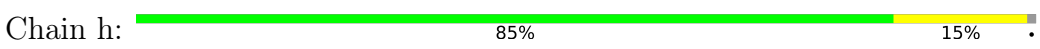
• Molecule 7: T-complex protein 1 subunit eta, N-terminally processed

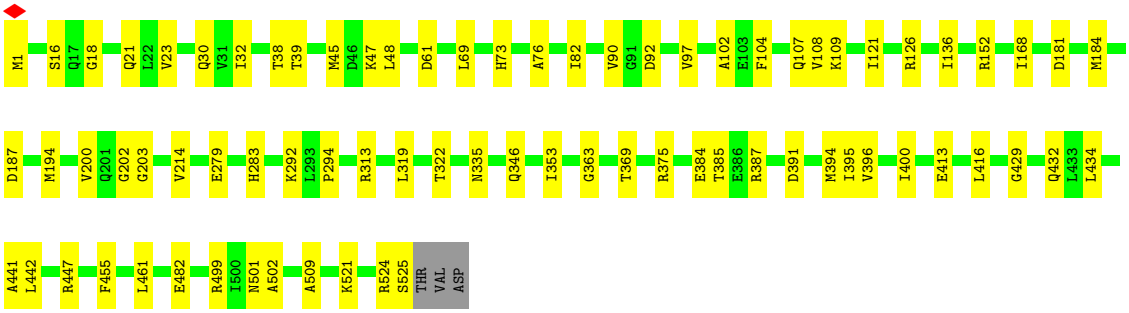
Chain H:



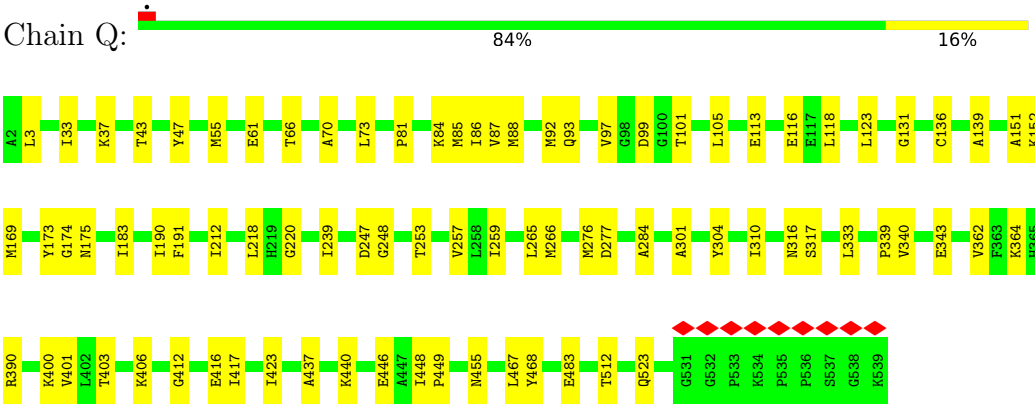
• Molecule 7: T-complex protein 1 subunit eta, N-terminally processed

Chain h:

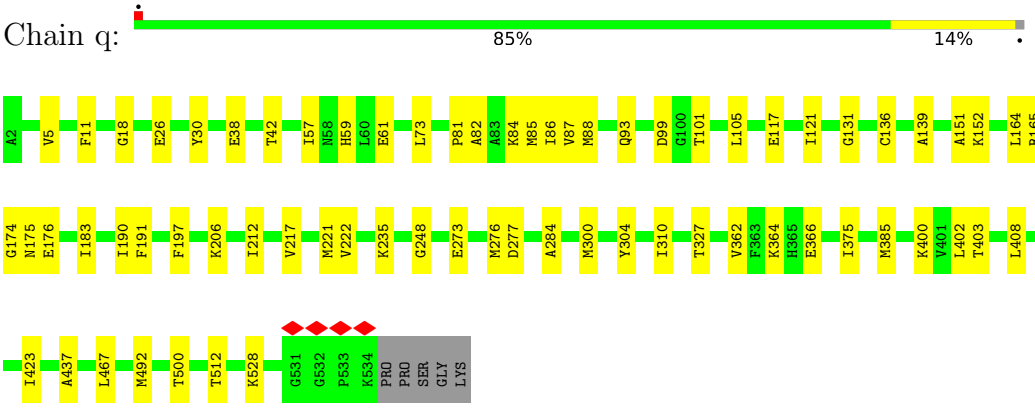




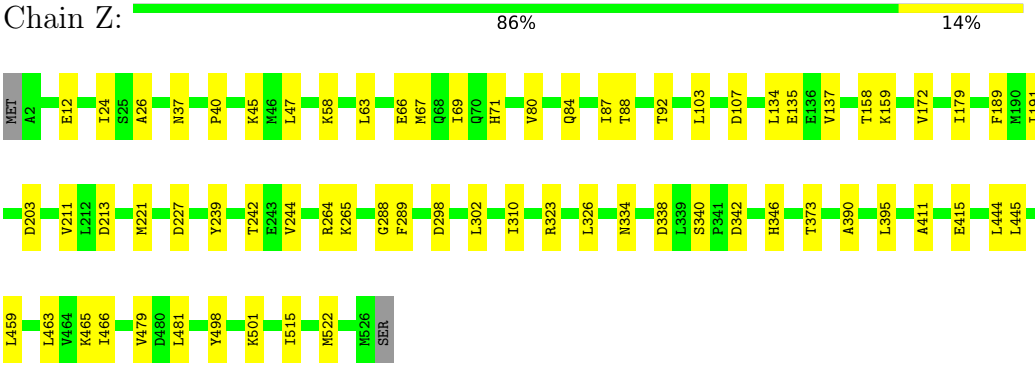
• Molecule 8: T-complex protein 1 subunit theta



• Molecule 8: T-complex protein 1 subunit theta

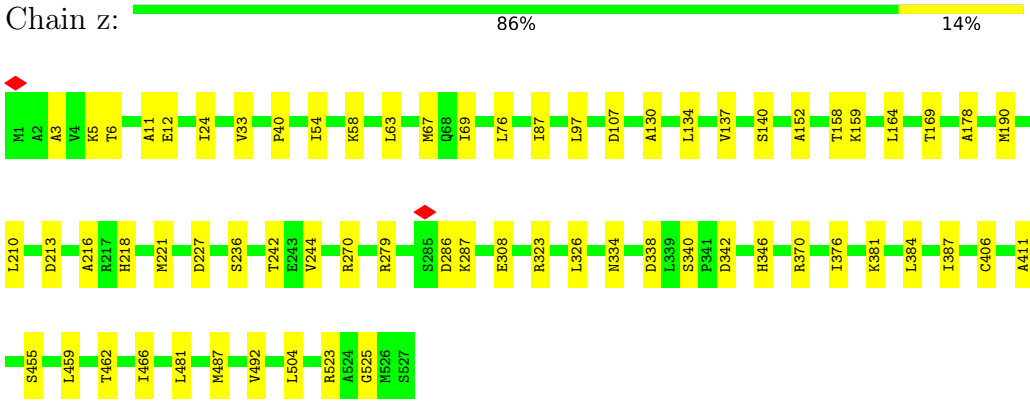


• Molecule 9: T-complex protein 1 subunit zeta



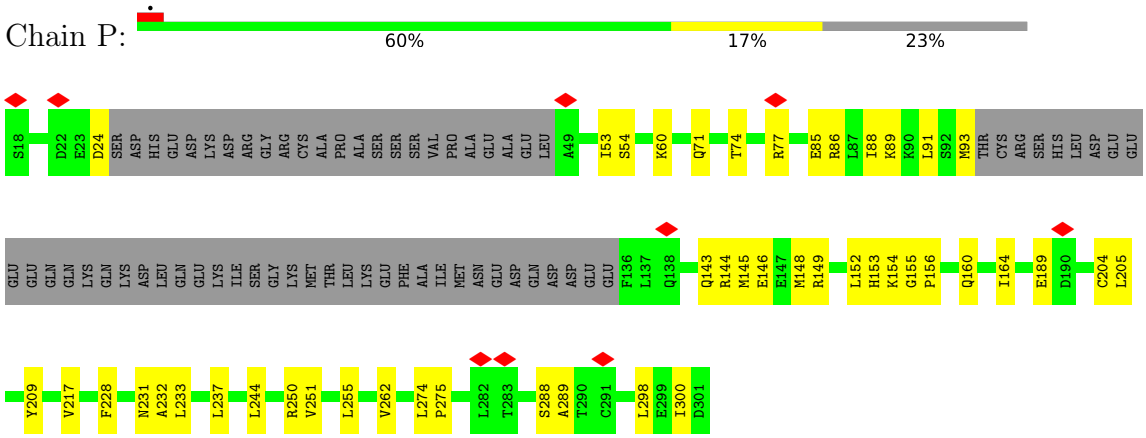
• Molecule 9: T-complex protein 1 subunit zeta

Chain z:



• Molecule 10: Phosducin-like protein

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175869	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 ($e^-/Å^2$)	40.42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.186	Depositor
Minimum map value	-0.376	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.123	Depositor
Map size (Å)	317.4, 317.4, 317.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AF3, ADP

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	N	0.05	0/324	0.17	0/434
2	A	0.13	0/4109	0.25	0/5548
2	a	0.13	0/4081	0.25	0/5510
3	B	0.13	0/3995	0.24	0/5386
3	b	0.13	0/3986	0.25	0/5375
4	D	0.12	0/3955	0.23	0/5338
4	d	0.13	0/3949	0.25	0/5331
5	E	0.13	0/4183	0.26	0/5635
5	e	0.13	0/4220	0.25	0/5684
6	G	0.12	0/4136	0.25	0/5579
6	g	0.12	0/4149	0.24	0/5595
7	H	0.13	0/4111	0.25	0/5550
7	h	0.12	0/4089	0.25	0/5519
8	Q	0.12	0/4147	0.25	0/5606
8	q	0.12	0/4112	0.25	0/5558
9	Z	0.12	0/4069	0.24	0/5486
9	z	0.12	0/4080	0.25	0/5501
10	P	0.12	0/1751	0.35	0/2346
All	All	0.12	0/67446	0.25	0/90981

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

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	N	322	0	306	2	0
2	A	4069	0	4224	58	0
2	a	4041	0	4205	68	0
3	B	3952	0	4070	50	0
3	b	3943	0	4057	52	0
4	D	3923	0	4131	45	0
4	d	3917	0	4120	54	0
5	E	4132	0	4246	69	0
5	e	4169	0	4272	68	0
6	G	4089	0	4224	72	0
6	g	4102	0	4240	58	0
7	H	4054	0	4160	56	0
7	h	4032	0	4140	55	0
8	Q	4086	0	4160	54	0
8	q	4053	0	4125	50	0
9	Z	4022	0	4161	49	0
9	z	4033	0	4171	46	0
10	P	1727	0	1701	37	0
11	A	27	0	12	1	0
11	B	27	0	12	3	0
11	D	27	0	12	1	0
11	E	27	0	12	0	0
11	G	27	0	12	2	0
11	H	27	0	12	1	0
11	Q	27	0	12	3	0
11	Z	27	0	12	2	0
11	a	27	0	12	3	0
11	b	27	0	12	2	0
11	d	27	0	12	2	0
11	e	27	0	12	1	0
11	g	27	0	12	2	0
11	h	27	0	12	2	0
11	q	27	0	12	2	0
11	z	27	0	12	3	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
12	E	1	0	0	0	0
12	G	1	0	0	0	0
12	H	1	0	0	0	0
12	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1	0	0	0	0
12	a	1	0	0	0	0
12	b	1	0	0	0	0
12	d	1	0	0	0	0
12	e	1	0	0	0	0
12	g	1	0	0	0	0
12	h	1	0	0	0	0
12	q	1	0	0	0	0
12	z	1	0	0	0	0
13	A	4	0	0	1	0
13	B	4	0	0	0	0
13	D	4	0	0	3	0
13	E	4	0	0	0	0
13	G	4	0	0	2	0
13	H	4	0	0	0	0
13	Q	4	0	0	1	0
13	Z	4	0	0	2	0
13	a	4	0	0	1	0
13	b	4	0	0	1	0
13	d	4	0	0	2	0
13	e	4	0	0	2	0
13	g	4	0	0	3	0
13	h	4	0	0	3	0
13	q	4	0	0	2	0
13	z	4	0	0	2	0
14	A	2	0	0	0	0
14	B	2	0	0	0	0
14	D	1	0	0	0	0
14	E	1	0	0	0	0
14	G	1	0	0	0	0
14	H	1	0	0	0	0
14	Q	1	0	0	0	0
14	Z	1	0	0	0	0
14	a	2	0	0	0	0
14	b	1	0	0	0	0
14	d	1	0	0	1	0
14	e	1	0	0	0	0
14	g	1	0	0	0	0
14	h	1	0	0	0	0
14	q	1	0	0	0	0
14	z	1	0	0	0	0
All	All	67197	0	68905	838	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 6.

All (838) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:79:PRO:HB2	5:e:60:MET:HE2	1.53	0.90
5:E:305:GLY:HA2	5:E:323:ARG:HB2	1.64	0.79
2:a:228:ARG:HG3	2:a:352:VAL:HG22	1.66	0.77
7:h:292:LYS:HG3	7:h:319:LEU:HD12	1.65	0.77
5:E:515:GLN:HE22	7:H:203:GLY:H	1.34	0.75
6:g:27:ILE:HD13	6:g:110:GLU:HB2	1.68	0.75
2:A:353:GLN:HE21	2:A:360:GLU:HB3	1.51	0.74
3:B:53:LEU:HD21	4:D:86:PRO:HG3	1.70	0.73
10:P:149:ARG:HA	10:P:152:LEU:HG	1.69	0.73
3:B:39:VAL:HG22	3:B:100:THR:HG23	1.71	0.72
10:P:145:MET:SD	10:P:149:ARG:NH1	2.62	0.72
6:g:289:VAL:HG21	6:g:350:LEU:HD13	1.70	0.72
9:Z:242:THR:HG22	9:Z:244:VAL:H	1.55	0.72
8:Q:175:ASN:HD21	8:Q:212:ILE:HD11	1.55	0.71
10:P:189:GLU:HB2	10:P:233:LEU:HD11	1.71	0.71
7:h:82:ILE:HG21	7:h:509:ALA:HB2	1.73	0.71
6:G:233:ILE:HD12	6:G:350:LEU:HD23	1.71	0.71
6:g:183:VAL:HG21	6:g:199:ALA:HB2	1.74	0.70
2:A:474:ALA:HB2	2:A:483:LEU:HB2	1.74	0.70
4:D:28:ASP:N	3:b:22:GLU:OE2	2.24	0.70
4:d:38:ILE:HG21	4:d:121:THR:HB	1.74	0.70
2:a:338:GLU:OE1	4:d:280:ARG:NH1	2.25	0.70
4:d:78:LEU:HB3	4:d:92:VAL:HG22	1.74	0.69
5:E:367:THR:HG23	5:E:369:ASP:H	1.57	0.69
7:H:346:GLN:HB2	7:H:363:GLY:HA3	1.72	0.69
4:D:30:PRO:HB3	4:D:533:ASP:HB2	1.75	0.69
3:B:517:VAL:HG21	5:E:60:MET:HE3	1.75	0.68
7:H:82:ILE:HG21	7:H:509:ALA:HB2	1.75	0.68
3:b:39:VAL:HG22	3:b:100:THR:HG23	1.75	0.68
4:D:502:ASN:HD22	4:D:505:GLU:HG2	1.58	0.68
4:D:193:LYS:NZ	4:D:225:GLU:OE2	2.26	0.68
9:z:242:THR:HG22	9:z:244:VAL:H	1.59	0.68
3:B:415:MET:HE1	3:B:444:ARG:HG3	1.75	0.68
5:E:198:ASP:HB3	5:E:202:ARG:HB2	1.76	0.68
9:Z:189:PHE:O	9:Z:323:ARG:NH1	2.26	0.67
7:H:67:LYS:HG2	7:H:84:LYS:HE2	1.77	0.67
2:a:59:ALA:HB2	2:a:90:THR:HG21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:g:47:MET:HE2	6:g:59:MET:HG2	1.76	0.67
6:g:292:THR:HG22	6:g:294:LYS:H	1.60	0.67
4:d:30:PRO:HB3	4:d:533:ASP:HB2	1.75	0.67
5:E:200:GLU:HG2	5:E:202:ARG:HG3	1.76	0.67
8:Q:169:MET:SD	11:Q:601:ADP:N6	2.67	0.67
5:e:60:MET:HG3	5:e:70:VAL:HG22	1.77	0.67
9:z:218:HIS:HB3	9:z:221:MET:HG2	1.77	0.67
6:G:218:VAL:HG21	6:G:323:ILE:HG12	1.78	0.66
3:b:417:MET:HE2	3:b:504:LEU:HD22	1.77	0.66
11:b:601:ADP:PB	13:b:603:AF3:F1	2.42	0.66
2:a:164:ASN:ND2	2:a:206:MET:SD	2.68	0.66
5:e:305:GLY:HA2	5:e:323:ARG:HB2	1.77	0.66
4:d:151:MET:HE1	4:d:428:PRO:HA	1.77	0.66
3:B:112:GLU:HB3	3:B:438:SER:HB3	1.78	0.66
7:H:2:MET:HE3	7:H:3:PRO:HD2	1.77	0.66
8:Q:253:THR:OG1	9:Z:239:TYR:OH	2.13	0.66
2:a:56:ASN:ND2	2:a:158:SER:O	2.29	0.66
2:A:353:GLN:O	6:G:190:ARG:NH1	2.28	0.65
5:e:198:ASP:HB3	5:e:202:ARG:HB2	1.78	0.64
6:G:21:LYS:HB3	7:h:1:MET:HE3	1.79	0.64
6:G:83:ILE:HD13	6:G:512:THR:HG21	1.80	0.64
2:a:222:SER:H	2:a:225:MET:HE3	1.62	0.64
6:g:64:ASN:ND2	6:g:88:ASP:OD2	2.31	0.64
2:a:246:MET:HE3	2:a:250:VAL:HG11	1.79	0.63
2:A:103:ASN:ND2	2:A:444:SER:OG	2.29	0.63
4:d:34:ARG:NH1	4:d:130:PRO:HG3	2.12	0.63
7:h:294:PRO:HG3	7:h:313:ARG:HE	1.63	0.63
6:G:132:ASP:OD2	6:G:437:TYR:OH	2.16	0.63
9:Z:135:GLU:OE2	9:Z:498:TYR:OH	2.17	0.63
3:B:156:ARG:NH2	3:B:185:GLU:OE2	2.30	0.63
6:G:302:HIS:HB2	9:Z:334:ASN:HB2	1.79	0.62
4:D:210:ILE:HG21	4:D:402:GLU:HG3	1.81	0.62
3:b:112:GLU:HB3	3:b:438:SER:HB3	1.81	0.62
6:g:129:ALA:O	6:g:133:MET:HG3	1.99	0.62
2:A:59:ALA:HB2	2:A:90:THR:HG21	1.81	0.62
8:q:222:VAL:HG22	8:q:362:VAL:HG22	1.81	0.62
6:g:293:GLU:HG3	6:g:320:ASN:HD22	1.65	0.62
3:B:131:ARG:NH2	3:B:512:GLU:OE2	2.33	0.62
10:P:232:ALA:HA	10:P:250:ARG:HD3	1.80	0.62
2:a:182:THR:H	10:P:300:ILE:HG13	1.64	0.62
8:q:81:PRO:HA	8:q:84:LYS:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:56:ASN:ND2	2:A:158:SER:O	2.33	0.61
9:Z:24:ILE:HD13	9:Z:107:ASP:HB2	1.82	0.61
5:e:51:SER:OG	5:e:59:LYS:NZ	2.30	0.61
5:e:422:GLY:HA3	5:e:501:MET:HE2	1.81	0.61
3:B:316:ASP:OD1	3:B:317:PHE:N	2.32	0.61
2:A:106:GLU:OE2	2:A:110:GLN:NE2	2.34	0.61
4:D:458:MET:HE3	4:D:458:MET:HA	1.81	0.61
7:H:32:ILE:HG13	7:H:76:ALA:HB1	1.83	0.61
3:b:156:ARG:NH2	3:b:185:GLU:OE2	2.34	0.61
5:e:426:GLU:OE2	5:e:513:LYS:NZ	2.31	0.61
7:h:32:ILE:HG13	7:h:76:ALA:HB1	1.82	0.61
9:z:236:SER:O	9:z:270:ARG:NH2	2.34	0.61
8:q:217:VAL:HG22	8:q:375:ILE:HG12	1.83	0.61
9:z:449:LYS:HD3	9:z:459:LEU:HD21	1.82	0.61
5:E:426:GLU:OE2	5:E:513:LYS:NZ	2.33	0.61
6:g:434:GLN:OE1	6:g:438:ARG:NH2	2.33	0.61
9:z:525:GLY:O	10:P:160:GLN:NE2	2.33	0.61
10:P:86:ARG:HB2	10:P:244:LEU:HD11	1.82	0.60
6:G:155:ILE:HG21	6:G:401:VAL:HG21	1.81	0.60
9:Z:40:PRO:HD3	9:Z:158:THR:HG22	1.83	0.60
6:g:411:GLY:HA3	6:g:490:MET:HE3	1.83	0.60
2:a:39:VAL:HG21	2:a:456:ALA:HB2	1.84	0.60
3:b:193:SER:OG	3:b:195:ASN:OD1	2.18	0.60
6:G:64:ASN:ND2	6:G:88:ASP:OD2	2.33	0.60
9:Z:340:SER:OG	9:Z:342:ASP:OD1	2.18	0.60
8:Q:416:GLU:HG2	8:Q:448:ILE:HG13	1.82	0.60
2:a:474:ALA:HB2	2:a:483:LEU:HB2	1.83	0.60
2:a:534:HIS:HE1	10:P:71:GLN:HG2	1.67	0.60
4:d:112:ILE:HG23	4:d:458:MET:HE1	1.84	0.60
9:z:216:ALA:HB1	9:z:221:MET:HG3	1.83	0.60
9:z:279:ARG:NH1	9:z:308:GLU:OE2	2.34	0.60
4:d:103:GLY:HA3	4:d:410:CYS:HB3	1.84	0.60
7:h:525:SER:HB2	8:q:59:HIS:HB2	1.84	0.60
3:B:65:ASN:ND2	3:B:169:SER:O	2.35	0.59
5:E:2:ALA:N	2:a:11:ARG:O	2.35	0.59
4:d:75:ALA:HB2	4:d:106:THR:HG21	1.83	0.59
5:e:236:HIS:H	5:e:239:MET:HE2	1.66	0.59
6:g:64:ASN:HB2	6:g:95:THR:HG21	1.84	0.59
2:A:298:LYS:NZ	6:G:242:ASP:OD2	2.35	0.59
8:Q:417:ILE:HG13	8:Q:467:LEU:HD13	1.84	0.59
4:d:446:MET:HA	4:d:449:TYR:HD1	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:g:381:LYS:HE3	10:P:148:MET:HE1	1.82	0.59
8:q:84:LYS:O	8:q:88:MET:HG3	2.02	0.59
4:D:195:ILE:HG21	4:D:203:VAL:HG22	1.85	0.59
11:z:601:ADP:O2B	13:z:603:AF3:F3	2.11	0.59
10:P:93:MET:SD	10:P:93:MET:N	2.76	0.59
4:D:119:SER:HB3	4:D:453:ALA:HB1	1.85	0.59
9:z:340:SER:OG	9:z:342:ASP:OD1	2.20	0.59
7:H:429:GLY:HA2	7:H:432:GLN:HB3	1.85	0.59
7:H:455:PHE:CE1	7:H:482:GLU:HG2	2.38	0.59
11:Q:601:ADP:O1B	13:Q:603:AF3:F2	2.11	0.59
2:a:229:ILE:HD13	2:a:284:ASN:HB3	1.83	0.59
8:q:284:ALA:HB2	8:q:310:ILE:HD11	1.83	0.59
7:H:45:MET:O	7:H:60:ASN:ND2	2.36	0.58
4:D:55:LYS:HG3	4:D:469:ALA:HA	1.84	0.58
8:Q:417:ILE:HD11	8:Q:449:PRO:HG3	1.85	0.58
6:G:50:LEU:HD13	9:Z:522:MET:HB2	1.84	0.58
5:e:230:VAL:HB	5:e:372:LEU:HB2	1.86	0.58
11:G:601:ADP:O1B	13:G:603:AF3:F1	2.11	0.58
9:Z:445:LEU:HD22	9:Z:463:LEU:HD11	1.86	0.58
3:B:131:ARG:NH2	5:E:179:ASN:OD1	2.36	0.58
1:N:225:GLU:OE2	4:D:330:ARG:NH2	2.36	0.58
4:d:497:LYS:HE2	4:d:501:SER:HB3	1.85	0.58
7:h:194:MET:O	7:h:369:THR:OG1	2.17	0.58
8:Q:92:MET:HE1	9:Z:198:HIS:HA	1.86	0.58
6:G:468:ALA:O	6:G:471:THR:OG1	2.22	0.58
11:Z:601:ADP:O1B	13:Z:603:AF3:F1	2.12	0.58
6:g:41:LEU:O	6:g:454:ASN:ND2	2.33	0.58
8:q:417:ILE:HG13	8:q:467:LEU:HD13	1.85	0.58
6:g:319:ASP:OD1	6:g:322:ARG:NH1	2.36	0.57
6:G:130:LEU:HB2	6:G:510:VAL:HG11	1.86	0.57
6:g:79:SER:O	6:g:83:ILE:HG12	2.04	0.57
7:H:456:ASP:OD2	2:a:433:ARG:NH2	2.37	0.57
8:Q:93:GLN:NE2	8:Q:99:ASP:O	2.37	0.57
4:d:195:ILE:HG21	4:d:203:VAL:HG22	1.85	0.57
3:b:38:LEU:O	3:b:50:LYS:NZ	2.31	0.57
6:G:313:ARG:HG2	6:G:314:ARG:HG3	1.87	0.57
6:g:130:LEU:HB2	6:g:510:VAL:HG11	1.87	0.57
6:g:468:ALA:O	6:g:471:THR:OG1	2.23	0.57
7:h:97:VAL:HG12	7:h:502:ALA:HA	1.87	0.57
7:h:346:GLN:HB2	7:h:363:GLY:HA3	1.86	0.57
4:D:32:GLN:HB3	3:b:6:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:228:VAL:HG22	4:D:375:LYS:HG2	1.87	0.57
4:D:311:ASP:OD1	4:D:312:LEU:N	2.38	0.57
9:Z:455:SER:OG	9:Z:481:LEU:O	2.23	0.57
7:h:521:LYS:HG2	8:q:57:ILE:HD12	1.85	0.57
3:B:83:VAL:HG22	5:E:393:MET:HE3	1.85	0.57
7:H:107:GLN:HG3	7:H:441:ALA:HB2	1.87	0.57
9:z:198:HIS:CE1	9:z:199:LYS:HG2	2.40	0.57
6:G:206:GLY:HA3	9:Z:87:ILE:HG13	1.86	0.56
8:Q:316:ASN:OD1	8:Q:317:SER:N	2.37	0.56
11:z:601:ADP:O2B	13:z:603:AF3:F1	2.12	0.56
2:A:171:MET:HG3	2:A:210:LEU:HB2	1.86	0.56
5:E:289:ILE:HG13	5:E:313:LEU:HB3	1.87	0.56
7:H:97:VAL:HG12	7:H:502:ALA:HA	1.87	0.56
8:Q:173:TYR:OH	8:Q:483:GLU:OE2	2.21	0.56
8:Q:190:ILE:HG22	8:Q:191:PHE:H	1.70	0.56
11:g:601:ADP:O2B	13:g:603:AF3:F3	2.13	0.56
5:E:295:THR:HG21	5:E:348:LEU:HG	1.87	0.56
6:G:7:VAL:HG12	5:e:7:LEU:HD23	1.87	0.56
2:a:163:ILE:HB	6:g:127:ARG:HH11	1.69	0.56
9:z:5:LYS:NZ	9:z:11:ALA:O	2.38	0.56
11:a:601:ADP:O2B	13:a:603:AF3:F3	2.14	0.56
2:A:216:LEU:HD21	2:A:319:ILE:HD11	1.88	0.56
7:h:107:GLN:HG3	7:h:441:ALA:HB2	1.87	0.56
8:q:364:LYS:NZ	8:q:366:GLU:OE2	2.38	0.56
5:E:438:ASP:OD1	5:E:449:ARG:NH2	2.38	0.56
4:d:210:ILE:HG21	4:d:402:GLU:HG3	1.87	0.56
9:z:24:ILE:HD13	9:z:107:ASP:HB2	1.88	0.56
4:D:170:SER:HB2	4:D:411:VAL:HG21	1.86	0.56
6:G:129:ALA:O	6:G:133:MET:HG3	2.05	0.56
6:G:473:GLU:HG2	6:G:474:ASN:N	2.21	0.56
7:h:23:VAL:HG13	7:h:109:LYS:HE3	1.87	0.56
5:E:25:LYS:HG2	5:E:536:PRO:HA	1.88	0.56
3:b:168:SER:OG	11:b:601:ADP:N7	2.39	0.56
6:g:280:GLU:OE2	6:g:284:GLN:NE2	2.36	0.56
2:A:44:MET:HG3	6:G:519:ILE:HG21	1.87	0.55
6:G:265:THR:HG21	9:Z:265:LYS:HB3	1.88	0.55
7:H:168:ILE:HG21	7:H:385:THR:HG23	1.87	0.55
3:b:356:GLU:O	4:d:206:ARG:NH2	2.39	0.55
4:d:118:ASP:O	4:d:121:THR:HG22	2.06	0.55
4:D:303:SER:HB3	4:D:308:ALA:HB2	1.87	0.55
5:E:28:LEU:HB3	5:E:33:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:27:ILE:HD13	6:G:110:GLU:HB2	1.89	0.55
4:d:235:ASN:ND2	4:d:322:ILE:O	2.38	0.55
2:A:179:ILE:HG21	2:A:195:VAL:HG22	1.89	0.55
6:G:91:VAL:O	6:G:400:ASN:ND2	2.39	0.55
3:b:9:VAL:HG13	3:b:11:ILE:HD11	1.88	0.55
3:b:415:MET:HE1	3:b:444:ARG:HG3	1.87	0.55
7:H:30:GLN:NE2	7:H:102:ALA:O	2.38	0.55
8:Q:239:ILE:HD12	8:Q:239:ILE:H	1.72	0.55
10:P:231:ASN:O	10:P:250:ARG:NH1	2.40	0.55
3:b:163:ALA:HB3	3:b:180:THR:HG23	1.87	0.55
11:q:601:ADP:O2B	13:q:603:AF3:F2	2.14	0.55
5:e:230:VAL:HG12	5:e:232:LYS:H	1.70	0.55
6:g:497:GLU:OE1	6:g:502:LYS:HD3	2.07	0.55
3:B:163:ALA:HB3	3:B:180:THR:HG23	1.89	0.54
6:G:411:GLY:N	11:G:601:ADP:O2'	2.37	0.54
8:Q:523:GLN:HB2	9:Z:45:LYS:HG3	1.87	0.54
5:E:532:ASP:HB2	7:H:47:LYS:HD2	1.90	0.54
6:g:182:MET:SD	6:g:372:CYS:HB3	2.47	0.54
9:Z:84:GLN:OE1	9:Z:88:THR:OG1	2.21	0.54
5:e:200:GLU:HG2	5:e:202:ARG:HG3	1.88	0.54
7:h:200:VAL:HG11	7:h:353:ILE:HG22	1.90	0.54
3:B:63:VAL:HG12	3:B:381:GLN:HB3	1.88	0.54
4:D:248:LEU:HD23	4:D:299:LEU:HB2	1.87	0.54
6:G:183:VAL:HG21	6:G:199:ALA:HB2	1.89	0.54
7:H:447:ARG:HB2	7:H:461:LEU:HD11	1.88	0.54
6:G:16:ARG:HG3	6:G:523:VAL:HG22	1.90	0.54
3:B:9:VAL:HG13	3:B:11:ILE:HD11	1.89	0.54
4:d:277:ARG:O	4:d:280:ARG:HG2	2.08	0.54
6:g:132:ASP:OD2	6:g:437:TYR:OH	2.19	0.54
2:a:266:ARG:NH1	2:a:273:GLU:OE2	2.38	0.54
11:h:601:ADP:O3B	13:h:603:AF3:F3	2.16	0.54
3:B:326:VAL:HG13	3:B:327:THR:HG23	1.90	0.54
4:d:119:SER:HB2	4:d:453:ALA:HB1	1.89	0.54
6:g:49:MET:HE3	9:z:76:LEU:HD11	1.89	0.54
1:N:245:LEU:HD13	1:N:254:PHE:HB3	1.90	0.54
7:H:152:ARG:NH2	7:H:181:ASP:OD1	2.41	0.54
7:H:446:PRO:HA	7:H:449:LEU:HD12	1.89	0.54
2:a:145:ARG:NH2	2:a:174:ASP:OD1	2.41	0.54
3:b:138:ARG:NH2	5:e:220:GLU:OE2	2.35	0.53
3:b:432:GLU:O	3:b:436:MET:HG3	2.08	0.53
8:Q:70:ALA:HB2	8:Q:101:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:50:LYS:HD3	4:d:534:ASP:HB3	1.91	0.53
5:e:438:ASP:OD1	5:e:449:ARG:NH2	2.42	0.53
3:B:33:ILE:HD11	3:B:111:ARG:HB2	1.90	0.53
5:E:377:CYS:HB2	5:E:380:SER:HB2	1.91	0.53
8:Q:220:GLY:O	8:Q:374:THR:OG1	2.26	0.53
4:D:291:LYS:HD3	4:D:322:ILE:HD11	1.91	0.53
5:E:78:LEU:HB3	5:E:92:VAL:HG22	1.90	0.53
9:Z:172:VAL:HG13	9:Z:395:LEU:HD23	1.91	0.53
6:g:243:SER:OG	6:g:333:SER:O	2.20	0.53
7:h:73:HIS:HB3	7:h:76:ALA:HB3	1.91	0.53
7:h:90:VAL:HG12	7:h:92:ASP:H	1.74	0.53
5:E:236:HIS:HB2	5:E:239:MET:HE3	1.90	0.53
5:e:295:THR:HG21	5:e:348:LEU:HG	1.91	0.53
2:A:163:ILE:HB	6:G:127:ARG:HD2	1.91	0.53
3:b:83:VAL:HG22	5:e:393:MET:SD	2.48	0.53
4:D:38:ILE:HG21	4:D:121:THR:OG1	2.09	0.53
5:E:515:GLN:HE22	7:H:203:GLY:N	2.05	0.53
6:G:306:ARG:NH1	9:Z:338:ASP:OD2	2.42	0.53
7:H:193:LYS:HG3	7:H:194:MET:HE2	1.91	0.53
6:g:155:ILE:HG21	6:g:401:VAL:HG21	1.92	0.53
4:d:228:VAL:HG22	4:d:387:THR:HG21	1.91	0.52
4:d:325:ILE:HD13	4:d:374:LEU:HD21	1.90	0.52
7:h:61:ASP:OD1	13:h:603:AF3:F2	2.17	0.52
8:q:277:ASP:HB2	8:q:304:TYR:CZ	2.43	0.52
2:A:227:LYS:HD3	2:A:353:GLN:HG2	1.89	0.52
6:G:184:GLN:HG3	6:G:193:ILE:HG12	1.90	0.52
8:q:190:ILE:HG22	8:q:191:PHE:H	1.75	0.52
5:E:170:LYS:O	5:E:182:HIS:NE2	2.35	0.52
6:G:244:SER:HB3	6:G:246:GLU:HG2	1.90	0.52
9:z:3:ALA:O	9:z:6:THR:OG1	2.26	0.52
2:A:47:ASP:HB2	2:A:51:ASP:HB2	1.90	0.52
2:a:402:VAL:HG23	2:a:506:PRO:HG3	1.90	0.52
5:e:42:LYS:O	5:e:46:ASN:ND2	2.42	0.52
7:H:90:VAL:HG12	7:H:92:ASP:H	1.75	0.52
2:a:278:ILE:O	2:a:281:THR:HG22	2.09	0.52
5:e:239:MET:SD	5:e:320:PRO:HA	2.50	0.52
7:H:251:ASP:OD1	7:H:252:ASN:N	2.43	0.52
2:a:34:SER:OG	2:a:43:LYS:NZ	2.42	0.52
4:d:46:ASP:HA	4:d:49:ARG:HD3	1.92	0.52
5:e:533:ILE:HD13	7:h:48:LEU:HB3	1.91	0.52
4:D:86:PRO:O	4:D:90:MET:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:255:PHE:HB2	5:e:306:PHE:HB2	1.92	0.52
4:d:228:VAL:HG12	4:d:375:LYS:HG2	1.92	0.52
5:E:239:MET:SD	5:E:320:PRO:HA	2.49	0.51
5:E:515:GLN:NE2	7:H:203:GLY:H	2.07	0.51
5:e:102:ILE:HG22	5:e:104:ASP:H	1.75	0.51
8:q:18:GLY:HA3	8:q:528:LYS:HG3	1.91	0.51
10:P:24:ASP:OD1	10:P:24:ASP:N	2.43	0.51
5:E:51:SER:OG	5:E:59:LYS:NZ	2.35	0.51
5:e:518:SER:O	5:e:522:GLN:HG2	2.10	0.51
2:A:278:ILE:O	2:A:281:THR:HG22	2.10	0.51
5:E:255:PHE:HB2	5:E:306:PHE:HB3	1.91	0.51
6:G:409:PRO:O	6:G:414:SER:OG	2.28	0.51
2:A:181:TYR:HH	2:A:189:ARG:HH22	1.57	0.51
8:Q:276:MET:HE2	8:Q:301:ALA:HB2	1.93	0.51
5:e:236:HIS:HB3	5:e:239:MET:HG3	1.92	0.51
4:d:227:LEU:HB3	4:d:339:THR:HG21	1.93	0.51
4:D:223:LEU:HD12	4:D:388:ILE:HG12	1.92	0.51
7:H:197:ILE:HG21	7:H:386:GLU:HG3	1.93	0.51
9:Z:338:ASP:OD1	9:Z:338:ASP:N	2.44	0.51
2:a:163:ILE:HB	6:g:127:ARG:HD2	1.92	0.51
5:e:411:ASN:HB3	5:e:511:ILE:HD11	1.93	0.51
6:g:144:VAL:HG12	6:g:405:PRO:O	2.11	0.51
6:g:258:ILE:HG23	6:g:263:ASP:HB2	1.93	0.51
6:G:133:MET:HE2	6:G:506:TYR:CD2	2.46	0.51
7:H:499:ARG:NH2	11:H:601:ADP:O3'	2.43	0.51
3:b:251:ILE:HG13	5:e:277:LEU:HD11	1.93	0.51
9:z:40:PRO:HA	9:z:158:THR:HA	1.92	0.51
2:A:225:MET:HE1	2:A:307:ALA:HB3	1.91	0.51
5:e:306:PHE:CE1	5:e:323:ARG:HB3	2.46	0.51
10:P:85:GLU:O	10:P:89:LYS:NZ	2.32	0.51
2:A:229:ILE:HG12	2:A:306:MET:HE3	1.92	0.50
8:q:175:ASN:ND2	8:q:212:ILE:HD11	2.25	0.50
7:H:73:HIS:HB3	7:H:76:ALA:HB3	1.93	0.50
7:h:202:GLY:O	7:h:375:ARG:NH2	2.44	0.50
2:A:230:VAL:HG23	2:A:231:ASN:H	1.76	0.50
7:h:279:GLU:OE1	7:h:283:HIS:NE2	2.45	0.50
8:q:151:ALA:O	8:q:152:LYS:HG2	2.11	0.50
2:A:489:ASP:OD2	2:A:492:ASN:ND2	2.45	0.50
8:Q:277:ASP:HB2	8:Q:304:TYR:CZ	2.46	0.50
8:Q:284:ALA:HB2	8:Q:310:ILE:HD11	1.93	0.50
3:b:151:ASP:HB3	3:b:154:LYS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:153:HIS:C	10:P:154:LYS:HD2	2.35	0.50
4:D:288:LYS:HG2	4:D:320:MET:HE1	1.94	0.50
4:d:34:ARG:HH11	4:d:130:PRO:HG3	1.76	0.50
7:h:429:GLY:HA2	7:h:432:GLN:HB3	1.94	0.50
8:q:402:LEU:HD21	8:q:408:LEU:HD21	1.92	0.50
2:a:78:LEU:HD11	2:a:516:PHE:HB3	1.93	0.50
7:h:187:ASP:OD1	7:h:187:ASP:N	2.44	0.50
8:Q:364:LYS:NZ	8:Q:366:GLU:OE2	2.45	0.50
6:g:266:ARG:O	6:g:270:MET:HG3	2.12	0.50
9:z:286:ASP:OD1	9:z:287:LYS:N	2.45	0.50
3:B:251:ILE:HG13	5:E:277:LEU:HD11	1.92	0.49
3:b:326:VAL:HG13	3:b:327:THR:HG23	1.93	0.49
3:b:516:ARG:NH2	5:e:58:ASP:OD1	2.45	0.49
6:G:82:GLU:O	6:G:86:THR:HG23	2.12	0.49
3:b:187:VAL:HG21	3:b:397:LEU:HB2	1.95	0.49
4:d:241:VAL:HG23	4:d:323:MET:HE3	1.94	0.49
2:A:171:MET:HE3	2:A:375:ILE:HD13	1.93	0.49
3:B:79:PRO:HB2	5:E:60:MET:SD	2.53	0.49
9:z:338:ASP:N	9:z:338:ASP:OD1	2.45	0.49
5:E:518:SER:O	5:E:522:GLN:HG2	2.12	0.49
7:H:250:LYS:HB2	7:H:253:ALA:HB2	1.93	0.49
6:g:83:ILE:HG23	6:g:508:THR:HG22	1.94	0.49
2:A:130:ARG:NH1	2:A:134:GLU:OE1	2.45	0.49
4:D:48:ILE:HD12	4:D:107:THR:HG23	1.94	0.49
5:e:14:ARG:NH1	7:h:16:SER:OG	2.39	0.49
6:g:206:GLY:HA3	9:z:87:ILE:HG13	1.94	0.49
2:A:354:GLU:HG3	2:A:363:LEU:HD12	1.94	0.49
7:H:259:THR:HG22	7:H:261:GLU:H	1.77	0.49
9:Z:213:ASP:N	9:Z:213:ASP:OD1	2.42	0.49
5:e:184:GLN:NE2	5:e:222:THR:O	2.46	0.49
4:D:63:ASP:OD2	4:D:64:GLY:N	2.46	0.49
6:G:82:GLU:OE1	6:G:85:ARG:NH2	2.41	0.49
6:G:133:MET:HE3	6:G:444:LEU:HD22	1.95	0.49
7:H:136:ILE:HD11	7:H:416:LEU:HD11	1.95	0.49
6:g:226:HIS:CG	6:g:305:MET:HE1	2.47	0.49
8:q:248:GLY:N	8:q:276:MET:HE1	2.27	0.49
9:z:12:GLU:OE2	9:z:523:ARG:NH1	2.39	0.49
4:D:78:LEU:HB3	4:D:92:VAL:HG22	1.94	0.49
4:D:145:ILE:HD12	4:D:516:VAL:HG13	1.95	0.49
7:h:126:ARG:NH1	8:q:174:GLY:HA3	2.27	0.49
8:q:412:GLY:HA3	8:q:492:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:176:VAL:HG12	4:D:218:ILE:HD13	1.95	0.49
4:D:503:ILE:HG13	4:D:508:VAL:HB	1.95	0.49
5:e:24:ARG:HG2	5:e:24:ARG:HH11	1.78	0.49
2:A:66:GLU:HB3	6:G:11:SER:HB3	1.95	0.48
3:B:249:ILE:HG21	5:E:277:LEU:HG	1.96	0.48
4:D:26:ASP:OD1	4:D:26:ASP:N	2.44	0.48
3:b:271:GLU:HG2	5:e:274:TYR:CZ	2.48	0.48
5:e:289:ILE:HG13	5:e:313:LEU:HB3	1.95	0.48
5:E:444:GLU:O	5:E:448:MET:HG3	2.13	0.48
8:Q:333:LEU:HD11	8:Q:339:PRO:HB3	1.95	0.48
5:e:531:ASP:HB3	7:h:45:MET:HE3	1.94	0.48
5:e:145:ILE:HG23	5:e:514:LYS:HD2	1.94	0.48
6:G:473:GLU:HG2	6:G:474:ASN:H	1.77	0.48
9:Z:159:LYS:HG2	9:Z:390:ALA:HA	1.95	0.48
2:a:127:GLU:HG3	2:a:426:TYR:CZ	2.48	0.48
11:g:601:ADP:O2B	13:g:603:AF3:F1	2.21	0.48
3:B:58:ASP:OD1	3:B:58:ASP:N	2.46	0.48
3:B:168:SER:OG	11:B:601:ADP:N7	2.45	0.48
5:E:196:VAL:HG12	5:E:381:ARG:O	2.13	0.48
2:a:294:ASP:O	2:a:298:LYS:HG2	2.13	0.48
8:q:221:MET:HG3	8:q:327:THR:HG21	1.94	0.48
11:A:601:ADP:O2B	13:A:603:AF3:F3	2.21	0.48
2:A:299:TYR:OH	6:G:337:GLU:OE2	2.22	0.48
7:H:279:GLU:OE1	7:H:302:TYR:OH	2.29	0.48
9:Z:221:MET:HE1	9:Z:302:LEU:HD22	1.95	0.48
4:d:423:ALA:HB1	4:d:503:ILE:HD11	1.95	0.48
2:A:265:GLN:OE1	6:G:334:ARG:NH2	2.46	0.48
3:B:77:ASP:OD2	3:B:77:ASP:N	2.43	0.48
2:a:205:GLN:OE1	6:g:127:ARG:NH2	2.46	0.48
8:q:11:PHE:CE1	9:z:69:ILE:HD11	2.49	0.48
5:E:10:ASP:OD2	7:H:24:SER:OG	2.30	0.48
3:b:379:THR:HG23	4:d:93:GLU:HB2	1.95	0.48
5:e:157:VAL:HG12	5:e:157:VAL:O	2.14	0.48
9:z:152:ALA:HB3	9:z:169:THR:HG23	1.96	0.48
2:A:23:MET:HE2	5:e:8:ALA:HA	1.95	0.47
4:d:48:ILE:HD11	4:d:110:VAL:HG11	1.94	0.47
8:q:139:ALA:HB2	8:q:423:ILE:HD11	1.96	0.47
6:G:225:THR:HG22	6:G:313:ARG:HB2	1.96	0.47
6:G:504:GLN:NE2	6:G:508:THR:OG1	2.47	0.47
7:H:103:GLU:HG2	7:H:444:ILE:HB	1.96	0.47
7:H:413:GLU:OE1	7:H:445:ILE:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:47:TYR:O	8:Q:455:ASN:ND2	2.38	0.47
9:Z:289:PHE:HB3	9:Z:310:ILE:HG12	1.96	0.47
9:Z:411:ALA:N	11:Z:601:ADP:O2'	2.43	0.47
3:b:245:ASP:HB2	3:b:297:TYR:CZ	2.50	0.47
5:e:41:ALA:HB1	5:e:91:MET:HE3	1.96	0.47
6:g:157:ASN:O	6:g:161:THR:HG23	2.15	0.47
4:D:73:ASP:OD1	13:D:603:AF3:F3	2.22	0.47
7:h:38:THR:OG1	7:h:47:LYS:NZ	2.38	0.47
7:h:168:ILE:HG21	7:h:385:THR:HG23	1.95	0.47
9:z:159:LYS:HD3	9:z:159:LYS:HA	1.55	0.47
3:B:445:MET:HE3	3:B:449:ILE:HG13	1.96	0.47
2:a:120:GLY:HA3	2:a:437:ALA:HB3	1.96	0.47
2:a:411:GLY:O	2:a:498:ASN:ND2	2.39	0.47
6:g:163:LYS:NZ	13:g:603:AF3:F1	2.36	0.47
9:z:210:LEU:HD11	9:z:323:ARG:HB3	1.96	0.47
9:z:455:SER:OG	9:z:481:LEU:O	2.31	0.47
2:A:246:MET:HB3	2:A:250:VAL:HB	1.95	0.47
6:G:62:ASP:OD1	13:G:603:AF3:F3	2.23	0.47
7:H:80:VAL:HG12	7:H:84:LYS:HE3	1.96	0.47
8:Q:400:LYS:O	8:Q:403:THR:OG1	2.27	0.47
8:Q:412:GLY:N	11:Q:601:ADP:O2'	2.38	0.47
8:q:131:GLY:HA3	8:q:437:ALA:HB3	1.95	0.47
8:q:400:LYS:O	8:q:403:THR:OG1	2.25	0.47
3:B:326:VAL:HB	3:B:370:ALA:HB3	1.96	0.47
5:E:81:MET:HG2	5:E:83:VAL:HG13	1.96	0.47
5:E:102:ILE:HG22	5:E:104:ASP:H	1.80	0.47
2:a:65:LEU:HD21	6:g:523:VAL:HG11	1.96	0.47
3:b:242:THR:HG21	3:b:335:PHE:CE2	2.49	0.47
3:b:408:TYR:O	3:b:413:SER:OG	2.30	0.47
4:d:85:HIS:CD2	10:P:60:LYS:HE3	2.50	0.47
7:h:396:VAL:O	7:h:400:ILE:HG12	2.15	0.47
9:z:462:THR:O	9:z:466:ILE:HG12	2.15	0.47
9:z:487:MET:HE2	9:z:492:VAL:HG21	1.97	0.47
5:E:306:PHE:CE2	5:E:323:ARG:HB3	2.50	0.47
8:Q:37:LYS:NZ	8:Q:113:GLU:OE2	2.37	0.47
8:Q:446:GLU:OE2	8:Q:468:TYR:OH	2.28	0.47
9:Z:449:LYS:HB3	9:Z:459:LEU:HD23	1.97	0.47
3:B:45:PRO:HG3	11:B:601:ADP:C5	2.49	0.47
6:G:198:TYR:CE1	6:G:325:ARG:HG3	2.49	0.47
7:H:214:VAL:HG11	7:H:322:THR:HA	1.97	0.47
8:Q:73:LEU:HD13	8:Q:87:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:291:ILE:HG13	3:B:312:ILE:HB	1.96	0.47
8:Q:73:LEU:HD11	8:Q:105:LEU:HD22	1.97	0.47
2:a:122:ARG:HG3	4:d:178:GLN:HG3	1.97	0.47
7:h:524:ARG:NH1	8:q:61:GLU:OE2	2.48	0.47
8:q:86:ILE:HG22	8:q:105:LEU:HD12	1.97	0.47
5:E:255:PHE:HB2	5:E:306:PHE:CB	2.46	0.46
5:E:533:ILE:HD13	7:H:48:LEU:HB3	1.98	0.46
9:Z:415:GLU:OE1	9:Z:501:LYS:NZ	2.47	0.46
2:a:505:GLU:OE1	2:a:510:LYS:NZ	2.36	0.46
4:d:173:SER:OG	11:d:601:ADP:O2A	2.29	0.46
5:e:196:VAL:HG12	5:e:381:ARG:O	2.15	0.46
8:q:85:MET:HE2	9:z:54:ILE:HG21	1.96	0.46
9:z:178:ALA:O	9:z:370:ARG:NH1	2.47	0.46
10:P:144:ARG:O	10:P:148:MET:HG2	2.15	0.46
3:B:293:ARG:HA	3:B:315:ALA:O	2.15	0.46
8:Q:139:ALA:HB2	8:Q:423:ILE:HD11	1.97	0.46
4:d:73:ASP:OD1	13:d:603:AF3:F2	2.23	0.46
3:B:231:ARG:NH1	3:B:233:GLU:OE2	2.39	0.46
6:G:332:VAL:HG21	6:G:338:LEU:HD13	1.98	0.46
6:G:520:ASP:OD1	6:G:521:ASP:N	2.49	0.46
8:Q:218:LEU:HD21	8:Q:362:VAL:HG13	1.97	0.46
9:Z:227:ASP:O	9:Z:288:GLY:N	2.33	0.46
3:b:260:SER:HB2	4:d:278:GLU:OE1	2.15	0.46
3:b:293:ARG:HA	3:b:315:ALA:O	2.14	0.46
5:e:170:LYS:O	5:e:182:HIS:NE2	2.47	0.46
6:g:415:GLU:OE2	6:g:502:LYS:NZ	2.27	0.46
3:B:465:LEU:HD11	3:B:478:LEU:HG	1.95	0.46
3:b:113:ALA:HB2	3:b:130:TRP:CH2	2.49	0.46
11:d:601:ADP:O2B	13:d:603:AF3:F3	2.23	0.46
10:P:74:THR:HA	10:P:77:ARG:HE	1.81	0.46
3:B:521:ILE:HB	5:E:61:MET:SD	2.55	0.46
6:G:157:ASN:O	6:G:161:THR:HG23	2.16	0.46
5:e:119:GLU:HB3	5:e:450:ALA:HB1	1.97	0.46
8:Q:247:ASP:OD1	8:Q:248:GLY:N	2.47	0.46
3:b:326:VAL:HB	3:b:370:ALA:HB3	1.96	0.46
10:P:231:ASN:OD1	10:P:232:ALA:N	2.48	0.46
2:A:205:GLN:OE1	6:G:127:ARG:NH2	2.48	0.46
7:H:147:ASP:HB3	7:H:150:GLU:HB2	1.96	0.46
5:e:73:ASP:OD1	13:e:603:AF3:F2	2.24	0.46
8:q:82:ALA:O	8:q:86:ILE:HG12	2.15	0.46
8:q:165:ARG:O	8:q:169:MET:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:104:ASP:OD1	13:D:603:AF3:F2	2.24	0.46
6:G:41:LEU:O	6:G:454:ASN:ND2	2.37	0.46
6:G:246:GLU:HG3	6:G:248:LYS:HE2	1.97	0.46
6:g:447:ILE:HB	6:g:448:PRO:HD3	1.98	0.46
5:E:129:HIS:HB3	5:E:132:ARG:HG2	1.97	0.46
8:Q:151:ALA:HB3	8:Q:406:LYS:HE2	1.98	0.46
6:g:302:HIS:HB2	9:z:334:ASN:HB2	1.97	0.46
10:P:205:LEU:O	10:P:209:TYR:N	2.49	0.46
3:B:113:ALA:HB2	3:B:130:TRP:CH2	2.50	0.46
3:B:257:ARG:HA	3:B:257:ARG:HD3	1.75	0.46
2:a:397:CYS:O	2:a:401:ARG:HG2	2.16	0.46
8:q:206:LYS:HD2	8:q:385:MET:HB3	1.98	0.46
2:A:39:VAL:HG21	2:A:456:ALA:HB2	1.98	0.45
5:e:94:LEU:HD13	5:e:523:MET:HG3	1.98	0.45
11:e:601:ADP:O3B	13:e:603:AF3:F3	2.25	0.45
6:g:50:LEU:HB2	6:g:58:VAL:HB	1.97	0.45
8:Q:259:ILE:HG21	8:Q:265:LEU:HB2	1.98	0.45
5:e:157:VAL:HA	5:e:165:LEU:HD11	1.97	0.45
3:B:271:GLU:HG2	5:E:274:TYR:CZ	2.52	0.45
5:E:8:ALA:HB1	2:a:23:MET:HG3	1.98	0.45
5:E:94:LEU:HD13	5:E:523:MET:HG3	1.98	0.45
7:H:23:VAL:HG13	7:H:109:LYS:HE3	1.99	0.45
9:Z:200:SER:OG	9:Z:203:ASP:OD2	2.29	0.45
4:d:476:THR:HG23	4:d:500:ILE:HD11	1.98	0.45
5:e:243:VAL:HG21	5:e:299:LEU:HD12	1.97	0.45
7:h:30:GLN:NE2	7:h:102:ALA:O	2.39	0.45
7:h:136:ILE:HD11	7:h:416:LEU:HD11	1.98	0.45
7:h:442:LEU:HD23	7:h:442:LEU:HA	1.85	0.45
2:a:181:TYR:CE2	10:P:298:LEU:HD23	2.51	0.45
2:A:78:LEU:HD11	2:A:516:PHE:HB3	1.98	0.45
3:B:242:THR:HG21	3:B:335:PHE:CE2	2.52	0.45
11:D:601:ADP:O1B	13:D:603:AF3:F1	2.24	0.45
6:G:43:PRO:HA	6:G:162:THR:HA	1.99	0.45
6:G:108:VAL:HG11	6:G:443:ALA:HB2	1.98	0.45
8:Q:43:THR:HB	8:Q:105:LEU:HD23	1.99	0.45
2:a:519:GLU:OE1	4:d:393:SER:OG	2.25	0.45
2:A:446:LEU:HD11	2:A:468:ARG:HD2	1.98	0.45
3:B:26:LEU:O	3:B:30:ILE:HG12	2.16	0.45
3:b:71:LEU:HD11	3:b:103:THR:HG21	1.99	0.45
3:B:259:ASP:OD1	3:B:259:ASP:N	2.48	0.45
4:D:134:SER:HB2	4:D:527:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:165:ILE:HD12	6:G:387:VAL:HG13	1.99	0.45
4:d:128:ILE:HD13	4:d:446:MET:HB3	1.99	0.45
5:e:101:GLU:HG2	5:e:515:GLN:NE2	2.31	0.45
5:e:109:VAL:HG13	5:e:516:GLN:HG2	1.99	0.45
5:e:236:HIS:H	5:e:239:MET:CE	2.30	0.45
8:q:38:GLU:O	8:q:42:THR:HG23	2.16	0.45
5:E:490:GLY:O	5:E:499:ASN:ND2	2.43	0.44
8:Q:97:VAL:HG13	8:Q:401:VAL:HG21	1.98	0.44
2:a:534:HIS:CE1	10:P:71:GLN:HG2	2.49	0.44
3:b:257:ARG:HD3	4:d:263:GLN:HE21	1.82	0.44
3:B:71:LEU:HB3	3:B:85:VAL:HG22	1.98	0.44
7:H:126:ARG:NH1	8:Q:174:GLY:HA3	2.32	0.44
2:a:199:LYS:HZ2	10:P:288:SER:HB3	1.83	0.44
2:a:225:MET:SD	2:a:307:ALA:N	2.88	0.44
3:b:441:LYS:HB2	3:b:441:LYS:HE3	1.68	0.44
4:d:42:LYS:HE2	4:d:46:ASP:OD2	2.17	0.44
4:D:483:ARG:NE	4:D:488:GLU:OE2	2.37	0.44
5:E:18:ILE:HA	7:H:73:HIS:HB2	1.98	0.44
8:Q:131:GLY:HA3	8:Q:437:ALA:HB3	1.99	0.44
9:Z:326:LEU:HD23	9:Z:326:LEU:HA	1.86	0.44
7:h:335:ASN:ND2	8:q:273:GLU:OE2	2.50	0.44
5:E:248:ILE:HD12	5:E:337:THR:HG21	1.99	0.44
6:G:48:LYS:HD2	6:G:66:ILE:HD13	2.00	0.44
6:g:198:TYR:CE1	6:g:325:ARG:HG3	2.53	0.44
7:h:152:ARG:NH2	7:h:181:ASP:OD1	2.35	0.44
8:q:416:GLU:OE1	8:q:416:GLU:N	2.47	0.44
9:z:140:SER:HA	9:z:406:CYS:HA	1.99	0.44
10:P:86:ARG:HG3	10:P:237:LEU:HD11	2.00	0.44
2:A:349:GLU:HB2	2:A:366:ASN:HB2	1.99	0.44
4:D:77:ILE:O	4:D:81:MET:HG2	2.17	0.44
5:e:78:LEU:HB3	5:e:92:VAL:HG22	2.00	0.44
8:q:136:CYS:HB2	8:q:512:THR:HG21	2.00	0.44
9:z:97:LEU:HD13	9:z:450:VAL:HG21	2.00	0.44
2:a:206:MET:HE3	2:a:206:MET:HB3	1.83	0.44
6:g:466:LEU:HD22	6:g:480:VAL:HG13	2.00	0.44
9:Z:37:ASN:O	9:Z:58:LYS:NZ	2.37	0.44
8:q:164:LEU:O	8:q:168:ILE:HG12	2.17	0.44
3:B:238:LEU:HB2	3:B:287:ILE:HG21	1.99	0.44
6:G:237:ARG:H	6:G:288:ASP:HB2	1.83	0.44
2:a:160:ILE:HD12	6:g:518:ARG:HD3	1.99	0.44
4:d:395:LYS:O	4:d:399:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:104:ASP:OD1	5:e:105:GLY:N	2.48	0.44
6:g:278:LEU:HD22	6:g:335:PRO:HG2	1.99	0.44
8:q:235:LYS:HD3	8:q:235:LYS:HA	1.78	0.44
9:z:33:VAL:HG11	9:z:67:MET:SD	2.57	0.44
3:B:6:LEU:HD23	4:d:32:GLN:HB3	1.99	0.44
6:G:330:ARG:NH1	6:G:341:ASP:OD2	2.50	0.44
7:H:524:ARG:HD3	8:Q:61:GLU:OE2	2.17	0.44
4:d:72:ASN:ND2	4:d:173:SER:O	2.51	0.44
7:h:384:GLU:OE1	7:h:387:ARG:NH1	2.42	0.44
8:q:73:LEU:HD11	8:q:105:LEU:HD22	1.99	0.44
8:q:168:ILE:HD13	8:q:183:ILE:HD12	2.00	0.44
10:P:53:ILE:HG13	10:P:54:SER:N	2.32	0.44
2:A:181:TYR:OH	2:A:321:LYS:NZ	2.42	0.43
9:Z:92:THR:N	13:Z:603:AF3:F3	2.33	0.43
2:a:266:ARG:HA	2:a:269:ASP:HB2	2.00	0.43
2:a:519:GLU:OE2	4:d:218:ILE:HG13	2.18	0.43
5:e:162:THR:O	5:e:166:ILE:HG12	2.18	0.43
2:a:158:SER:O	6:g:518:ARG:NH2	2.52	0.43
5:e:236:HIS:CE1	5:e:315:LEU:HD22	2.53	0.43
7:h:92:ASP:HB3	7:h:395:ILE:HD11	2.00	0.43
8:q:93:GLN:NE2	8:q:99:ASP:O	2.42	0.43
2:A:107:LEU:HG	2:A:440:GLU:HG3	2.01	0.43
9:Z:465:LYS:HB2	9:Z:465:LYS:HE3	1.83	0.43
2:a:37:GLY:N	11:a:601:ADP:H5'1	2.34	0.43
6:g:332:VAL:HG21	6:g:338:LEU:HD23	2.01	0.43
10:P:251:VAL:O	10:P:255:LEU:HB2	2.19	0.43
5:E:298:ASN:O	5:E:320:PRO:HD2	2.18	0.43
6:G:391:LEU:HD23	6:G:391:LEU:HA	1.83	0.43
8:Q:340:VAL:HG22	8:Q:343:GLU:CD	2.42	0.43
2:a:75:LEU:HD23	2:a:75:LEU:HA	1.85	0.43
4:d:30:PRO:O	4:d:34:ARG:NE	2.43	0.43
8:q:165:ARG:HG3	8:q:176:GLU:HG3	2.01	0.43
5:E:203:ASP:OD2	7:H:357:ARG:NH2	2.36	0.43
6:G:463:LEU:HD12	6:G:463:LEU:HA	1.86	0.43
2:a:183:ASP:OD2	2:a:189:ARG:NH1	2.51	0.43
5:e:367:THR:O	5:e:368:LYS:HG2	2.19	0.43
9:z:195:GLU:OE1	9:z:381:LYS:NZ	2.41	0.43
9:z:199:LYS:HA	9:z:199:LYS:HD3	1.78	0.43
6:G:462:LEU:HD23	6:G:462:LEU:HA	1.85	0.43
8:Q:33:ILE:HD13	8:Q:116:GLU:HB2	1.99	0.43
8:Q:81:PRO:O	8:Q:85:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:164:LEU:O	8:Q:168:ILE:HG12	2.18	0.43
2:a:480:ARG:HA	2:a:480:ARG:HD2	1.83	0.43
6:g:266:ARG:HD2	6:g:266:ARG:HA	1.79	0.43
8:Q:151:ALA:O	8:Q:152:LYS:HG2	2.19	0.43
4:d:412:ILE:O	4:d:416:VAL:HG23	2.18	0.43
7:h:104:PHE:O	7:h:108:VAL:HG22	2.19	0.43
7:h:499:ARG:HA	7:h:499:ARG:HD3	1.72	0.43
8:q:408:LEU:HD23	8:q:500:THR:HA	2.01	0.43
9:z:63:LEU:O	9:z:67:MET:HG3	2.18	0.43
2:A:281:THR:HG21	2:A:340:PHE:CE1	2.53	0.43
2:a:23:MET:HE3	2:a:23:MET:HB3	1.94	0.43
2:a:37:GLY:H	11:a:601:ADP:H5'1	1.83	0.43
2:a:281:THR:HG21	2:a:340:PHE:CE1	2.54	0.43
4:d:30:PRO:C	4:d:34:ARG:HE	2.26	0.43
5:e:385:ILE:HG21	5:e:402:LEU:HD13	2.01	0.43
6:g:16:ARG:NH2	6:g:521:ASP:OD2	2.52	0.43
7:h:447:ARG:HB2	7:h:461:LEU:HD11	2.01	0.43
9:z:164:LEU:HD21	9:z:387:ILE:HG12	2.00	0.43
10:P:274:LEU:HD12	10:P:275:PRO:HD2	2.01	0.43
5:E:145:ILE:HG23	5:E:514:LYS:HD2	2.00	0.43
7:H:516:VAL:HG11	8:Q:55:MET:HG3	2.01	0.43
2:a:199:LYS:HB3	2:a:385:CYS:HB3	2.00	0.43
3:b:47:GLY:O	4:d:531:LYS:NZ	2.51	0.43
5:e:377:CYS:HB2	5:e:380:SER:HB2	2.01	0.43
8:q:73:LEU:HD13	8:q:87:VAL:HG22	2.01	0.43
8:q:101:THR:N	13:q:603:AF3:F1	2.34	0.43
9:z:190:MET:SD	9:z:326:LEU:HD12	2.59	0.43
10:P:155:GLY:H	10:P:156:PRO:HD2	1.84	0.43
2:A:127:GLU:HG3	2:A:422:TYR:HE2	1.84	0.42
4:D:103:GLY:HA3	4:D:410:CYS:HB3	2.00	0.42
5:E:3:SER:OG	5:E:4:MET:N	2.51	0.42
7:H:187:ASP:OD1	7:H:187:ASP:N	2.48	0.42
9:Z:134:LEU:HA	9:Z:137:VAL:HG12	2.01	0.42
6:g:217:GLY:HA3	6:g:363:ILE:O	2.19	0.42
8:q:11:PHE:HE1	9:z:69:ILE:HD11	1.84	0.42
8:q:248:GLY:H	8:q:276:MET:HE1	1.84	0.42
10:P:143:GLN:HG3	10:P:262:VAL:HG21	2.01	0.42
2:A:397:CYS:O	2:A:401:ARG:HG2	2.19	0.42
3:B:332:ALA:HA	5:E:312:HIS:CD2	2.55	0.42
9:Z:63:LEU:O	9:Z:67:MET:HG3	2.18	0.42
2:a:107:LEU:HG	2:a:440:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:186:MET:HE3	4:d:186:MET:HB2	1.87	0.42
5:e:123:LEU:HD23	5:e:123:LEU:HA	1.87	0.42
4:D:256:PRO:HD3	4:D:282:TYR:CD2	2.54	0.42
5:E:101:GLU:OE1	7:H:375:ARG:NH2	2.49	0.42
7:H:194:MET:O	7:H:369:THR:OG1	2.25	0.42
7:H:395:ILE:HD13	7:H:395:ILE:HA	1.94	0.42
2:a:281:THR:HG23	2:a:345:LEU:HD11	2.00	0.42
7:h:214:VAL:HG11	7:h:322:THR:HA	2.01	0.42
7:h:394:MET:HE3	7:h:394:MET:HB3	1.82	0.42
9:z:130:ALA:HB1	9:z:418:MET:SD	2.60	0.42
9:z:411:ALA:N	11:z:601:ADP:O2'	2.50	0.42
10:P:88:ILE:HD13	10:P:91:LEU:HD23	1.99	0.42
10:P:209:TYR:CE1	10:P:274:LEU:HD21	2.53	0.42
4:D:280:ARG:HG2	4:D:312:LEU:HD21	2.02	0.42
5:E:78:LEU:HD11	5:E:110:VAL:HG21	2.02	0.42
9:Z:40:PRO:HA	9:Z:158:THR:HA	2.01	0.42
3:b:131:ARG:NH2	5:e:179:ASN:OD1	2.48	0.42
3:b:425:ALA:HB2	3:b:436:MET:HB2	2.01	0.42
7:h:391:ASP:OD2	13:h:603:AF3:F2	2.27	0.42
9:z:227:ASP:OD1	9:z:346:HIS:NE2	2.48	0.42
10:P:60:LYS:O	10:P:60:LYS:NZ	2.29	0.42
3:B:441:LYS:HE3	3:B:441:LYS:HB2	1.82	0.42
7:H:255:ILE:HG12	8:Q:259:ILE:HB	2.00	0.42
2:a:246:MET:CE	4:d:272:MET:HG3	2.49	0.42
4:d:407:ASP:OD1	14:d:701:HOH:O	2.22	0.42
5:e:132:ARG:NH2	5:e:443:LEU:HD22	2.35	0.42
9:z:58:LYS:HB3	9:z:58:LYS:HE2	1.76	0.42
7:H:104:PHE:O	7:H:108:VAL:HG22	2.19	0.42
8:Q:136:CYS:HB2	8:Q:512:THR:HG21	2.02	0.42
2:a:410:PRO:HG3	2:a:485:TRP:HE3	1.85	0.42
7:h:18:GLY:O	7:h:21:GLN:HG3	2.19	0.42
7:h:39:THR:CG2	7:h:47:LYS:HZ3	2.33	0.42
3:B:100:THR:HB	11:B:601:ADP:O3B	2.20	0.42
4:D:246:ILE:HG13	4:D:297:VAL:HB	2.02	0.42
4:D:367:LEU:HD11	4:D:373:LEU:HG	2.01	0.42
5:E:119:GLU:HB3	5:E:450:ALA:HB1	2.02	0.42
9:Z:103:LEU:HD21	9:Z:515:ILE:HG21	2.01	0.42
3:b:79:PRO:O	3:b:83:VAL:HG23	2.19	0.42
6:g:435:TRP:HB2	6:g:436:PRO:HD3	2.02	0.42
9:z:195:GLU:HB3	9:z:384:LEU:HD13	2.01	0.42
2:A:35:SER:HB3	2:A:56:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:197:ILE:HG21	2:A:389:GLU:HG3	2.01	0.42
9:Z:227:ASP:OD1	9:Z:346:HIS:NE2	2.53	0.42
2:a:233:LYS:HB2	2:a:283:ALA:HA	2.02	0.42
7:h:121:ILE:HA	7:h:434:LEU:HD13	2.01	0.42
2:A:66:GLU:OE2	6:G:527:LYS:N	2.40	0.42
3:B:333:SER:H	5:E:312:HIS:CG	2.38	0.42
6:G:256:ILE:HD11	9:Z:244:VAL:HB	2.01	0.42
2:a:266:ARG:HA	2:a:266:ARG:HD2	1.82	0.42
4:d:458:MET:HA	4:d:458:MET:HE2	2.02	0.42
8:q:412:GLY:N	11:q:601:ADP:O2'	2.36	0.42
2:A:120:GLY:HA3	2:A:437:ALA:HB3	2.02	0.41
2:A:456:ALA:HB2	2:A:490:LEU:HD12	2.02	0.41
5:E:233:ASP:OD1	5:E:233:ASP:N	2.51	0.41
7:H:200:VAL:HG11	7:H:353:ILE:HG22	2.02	0.41
3:b:13:LYS:HG2	5:e:84:ASP:OD1	2.20	0.41
3:b:245:ASP:HB2	3:b:297:TYR:CE2	2.55	0.41
2:A:377:LEU:HD21	2:A:392:LEU:HD22	2.00	0.41
3:B:187:VAL:HG21	3:B:397:LEU:HB2	2.02	0.41
6:G:224:VAL:HG12	6:G:310:THR:HG23	2.02	0.41
6:G:258:ILE:HG23	6:G:263:ASP:HB2	2.02	0.41
9:Z:47:LEU:HD13	9:Z:66:GLU:HB2	2.00	0.41
9:Z:67:MET:HB3	9:Z:69:ILE:HG12	2.01	0.41
9:Z:179:ILE:HD13	9:Z:191:ILE:HG13	2.03	0.41
3:b:11:ILE:O	3:b:12:PHE:CG	2.73	0.41
6:g:201:VAL:HG11	6:g:388:GLU:HG3	2.01	0.41
7:h:413:GLU:OE2	7:h:499:ARG:NE	2.48	0.41
3:B:21:ALA:HB1	3:B:25:ARG:NH2	2.35	0.41
4:D:413:ARG:HD2	4:D:417:LYS:HE2	2.01	0.41
5:E:8:ALA:HA	2:a:23:MET:HE2	2.02	0.41
5:E:157:VAL:HG12	5:E:157:VAL:O	2.21	0.41
8:Q:86:ILE:HG22	8:Q:105:LEU:HD12	2.01	0.41
9:Z:466:ILE:HD13	9:Z:479:VAL:HG22	2.02	0.41
3:b:323:LEU:HA	3:b:326:VAL:HG12	2.02	0.41
5:e:255:PHE:HB2	5:e:306:PHE:CB	2.50	0.41
8:q:117:GLU:O	8:q:121:ILE:HG23	2.20	0.41
5:E:405:ALA:O	5:E:409:ILE:HG12	2.21	0.41
5:E:501:MET:HA	5:E:501:MET:HE2	2.01	0.41
6:G:155:ILE:HG12	6:G:407:LEU:HD11	2.02	0.41
8:Q:440:LYS:HA	8:Q:440:LYS:HD3	1.83	0.41
5:e:515:GLN:HE22	7:h:203:GLY:HA2	1.85	0.41
7:h:214:VAL:HG11	7:h:322:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:z:376:ILE:HG22	9:z:384:LEU:HD22	2.02	0.41
9:z:504:LEU:HD23	9:z:504:LEU:HA	1.93	0.41
2:A:385:CYS:HA	2:A:388:MET:HE3	2.02	0.41
5:E:284:LYS:HA	5:E:284:LYS:HD2	1.78	0.41
9:z:213:ASP:OD1	9:z:213:ASP:N	2.53	0.41
2:A:55:THR:HA	2:A:387:GLU:OE1	2.20	0.41
4:D:317:LEU:HD13	4:D:324:VAL:HG21	2.01	0.41
9:Z:264:ARG:NH1	9:Z:298:ASP:OD2	2.54	0.41
3:b:9:VAL:HG12	5:e:39:MET:HE3	2.01	0.41
5:e:63:ASP:OD1	5:e:67:ASP:N	2.54	0.41
6:g:201:VAL:HG22	6:g:374:ILE:HB	2.03	0.41
8:q:300:MET:HE2	8:q:300:MET:HB2	1.89	0.41
2:A:514:LEU:HD23	2:A:514:LEU:HA	1.94	0.41
4:D:164:LEU:HD23	4:D:188:VAL:HG21	2.02	0.41
5:E:87:ILE:O	5:E:91:MET:HG2	2.21	0.41
5:E:519:LEU:HD23	5:E:519:LEU:HA	1.94	0.41
9:Z:211:VAL:HG23	9:Z:373:THR:HG21	2.02	0.41
9:Z:444:LEU:HD23	9:Z:444:LEU:HA	1.91	0.41
2:a:35:SER:HB3	2:a:56:ASN:OD1	2.20	0.41
3:b:323:LEU:O	3:b:327:THR:OG1	2.31	0.41
6:g:402:LEU:HD23	6:g:402:LEU:HA	1.92	0.41
7:h:294:PRO:HA	7:h:313:ARG:HD2	2.01	0.41
2:A:254:ILE:HD11	2:A:263:ILE:HD12	2.01	0.41
5:E:299:LEU:HD12	5:E:320:PRO:O	2.21	0.41
5:E:460:MET:HE1	4:d:126:LYS:HG2	2.01	0.41
6:G:380:SER:HB3	9:Z:80:VAL:HG22	2.02	0.41
2:a:130:ARG:NH1	2:a:134:GLU:OE1	2.54	0.41
2:a:199:LYS:NZ	10:P:288:SER:HB3	2.36	0.41
2:a:331:LEU:O	2:a:338:GLU:HA	2.21	0.41
3:b:8:PRO:HB2	5:e:39:MET:HE1	2.03	0.41
5:e:97:SER:HB3	7:h:202:GLY:HA2	2.01	0.41
5:e:515:GLN:NE2	7:h:203:GLY:HA2	2.35	0.41
7:h:499:ARG:NH2	11:h:601:ADP:O3'	2.54	0.41
8:q:191:PHE:HB2	8:q:197:PHE:HD1	1.86	0.41
9:z:134:LEU:HA	9:z:137:VAL:HG12	2.02	0.41
2:A:445:LEU:HD23	2:A:445:LEU:HA	1.85	0.41
4:D:91:LEU:HD13	4:D:110:VAL:HG13	2.03	0.41
5:E:464:GLU:HB2	5:E:470:PRO:HG3	2.03	0.41
6:G:370:LYS:HA	6:G:370:LYS:HD2	1.90	0.41
7:H:32:ILE:HD13	7:H:32:ILE:HA	1.91	0.41
7:H:42:PRO:HG2	7:H:479:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:464:LEU:HD23	7:H:464:LEU:HA	1.95	0.41
8:Q:66:THR:HB	8:Q:390:ARG:NH1	2.36	0.41
8:Q:168:ILE:HD13	8:Q:183:ILE:HD12	2.02	0.41
2:a:55:THR:HA	2:a:387:GLU:OE1	2.21	0.41
2:a:86:VAL:HG12	2:a:88:ASP:H	1.86	0.41
3:b:64:THR:HA	3:b:385:GLU:OE1	2.21	0.41
3:b:204:LYS:HA	3:b:204:LYS:HD2	1.91	0.41
5:e:78:LEU:HD12	5:e:95:SER:OG	2.21	0.41
6:g:54:MET:HG2	10:P:204:CYS:SG	2.61	0.41
7:h:152:ARG:HH21	7:h:184:MET:HE2	1.86	0.41
10:P:91:LEU:HD13	10:P:228:PHE:HD1	1.86	0.41
2:A:207:GLU:OE2	6:G:507:LYS:NZ	2.32	0.41
3:B:50:LYS:HD2	3:B:70:ILE:HD13	2.02	0.41
6:G:266:ARG:HA	6:G:266:ARG:HD2	1.86	0.41
9:Z:26:ALA:HB2	9:Z:71:HIS:CE1	2.56	0.41
7:h:455:PHE:CZ	7:h:482:GLU:HA	2.56	0.41
2:A:163:ILE:HB	6:G:127:ARG:HH11	1.86	0.40
2:A:199:LYS:HB3	2:A:385:CYS:HB3	2.03	0.40
5:E:14:ARG:NH1	7:H:16:SER:OG	2.47	0.40
6:G:236:PRO:HG3	6:G:350:LEU:HB2	2.03	0.40
6:G:241:LEU:HB2	6:G:292:THR:HB	2.02	0.40
7:H:273:ILE:HD11	8:Q:266:MET:HA	2.03	0.40
9:Z:47:LEU:HD13	9:Z:66:GLU:CB	2.51	0.40
2:a:478:PRO:HD2	2:a:479:GLU:OE1	2.22	0.40
3:b:95:VAL:HG12	3:b:399:GLN:HG3	2.03	0.40
6:g:165:ILE:HD12	6:g:387:VAL:HG13	2.02	0.40
10:P:164:ILE:HB	10:P:217:VAL:HB	2.03	0.40
4:D:91:LEU:HD23	4:D:91:LEU:HA	1.91	0.40
5:E:421:GLY:O	5:E:501:MET:HG3	2.21	0.40
8:Q:3:LEU:HD23	8:Q:3:LEU:HA	1.93	0.40
2:a:314:ARG:NH2	10:P:289:ALA:HB3	2.37	0.40
4:d:248:LEU:HD21	4:d:333:ILE:HD12	2.03	0.40
6:g:329:ALA:HB2	6:g:344:GLY:HA3	2.02	0.40
7:h:501:ASN:C	7:h:501:ASN:HD22	2.28	0.40
10:P:146:GLU:HA	10:P:149:ARG:NH1	2.36	0.40
2:A:43:LYS:HG2	6:G:521:ASP:HB3	2.03	0.40
2:A:185:ARG:HG3	2:A:187:GLN:HG2	2.03	0.40
2:A:448:ILE:HD13	2:A:448:ILE:HA	1.91	0.40
3:B:50:LYS:O	3:B:63:VAL:HA	2.21	0.40
7:H:253:ALA:HA	8:Q:257:VAL:HB	2.02	0.40
8:Q:84:LYS:O	8:Q:88:MET:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:12:GLU:HB3	8:q:5:VAL:HB	2.03	0.40
2:a:222:SER:N	2:a:225:MET:HE3	2.34	0.40
2:a:292:ILE:O	2:a:309:ARG:NH1	2.54	0.40
3:b:141:LEU:HD13	3:b:417:MET:HE3	2.03	0.40
3:b:390:LEU:HD12	3:b:390:LEU:HA	1.90	0.40
6:g:229:MET:SD	6:g:310:THR:HA	2.61	0.40
2:A:203:ARG:NE	2:A:207:GLU:OE1	2.39	0.40
2:A:353:GLN:NE2	2:A:360:GLU:HB3	2.28	0.40
3:B:42:THR:HB	3:B:65:ASN:OD1	2.21	0.40
3:B:517:VAL:HG21	5:E:60:MET:HB2	2.03	0.40
5:E:9[C]:PHE:HD1	5:E:9[C]:PHE:HA	1.75	0.40
6:G:402:LEU:HD23	6:G:402:LEU:HA	1.93	0.40
2:a:42:ASP:CG	6:g:518:ARG:HE	2.29	0.40
3:b:414:GLU:HG2	3:b:446:LEU:HD23	2.03	0.40
8:q:26:GLU:HA	8:q:30:TYR:CD2	2.56	0.40
3:B:29:PHE:CD2	3:B:114:GLU:HB2	2.56	0.40
4:D:337:CYS:SG	4:D:344:PRO:HD3	2.61	0.40
6:G:391:LEU:O	6:G:395:MET:HG3	2.22	0.40
8:Q:118:LEU:HD22	8:Q:123:LEU:HD12	2.03	0.40
4:d:480:LEU:HD23	4:d:480:LEU:HA	1.97	0.40
5:e:119:GLU:O	5:e:122:GLN:HG3	2.22	0.40
5:e:534:ARG:HD3	7:h:69:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	35/395 (9%)	35 (100%)	0	0	100	100
2	A	534/536 (100%)	513 (96%)	21 (4%)	0	100	100
2	a	530/536 (99%)	510 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	524/526 (100%)	506 (97%)	18 (3%)	0	100	100
3	b	523/526 (99%)	508 (97%)	15 (3%)	0	100	100
4	D	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
4	d	518/520 (100%)	491 (95%)	27 (5%)	0	100	100
5	E	534/540 (99%)	518 (97%)	16 (3%)	0	100	100
5	e	539/540 (100%)	522 (97%)	17 (3%)	0	100	100
6	G	524/528 (99%)	509 (97%)	15 (3%)	0	100	100
6	g	526/528 (100%)	513 (98%)	13 (2%)	0	100	100
7	H	526/528 (100%)	508 (97%)	18 (3%)	0	100	100
7	h	523/528 (99%)	507 (97%)	16 (3%)	0	100	100
8	Q	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
8	q	531/538 (99%)	510 (96%)	21 (4%)	0	100	100
9	Z	523/527 (99%)	508 (97%)	15 (3%)	0	100	100
9	z	525/527 (100%)	510 (97%)	15 (3%)	0	100	100
10	P	212/284 (75%)	193 (91%)	19 (9%)	0	100	100
All	All	8681/9165 (95%)	8389 (97%)	292 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	N	35/334 (10%)	35 (100%)	0	100	100
2	A	447/447 (100%)	447 (100%)	0	100	100
2	a	444/447 (99%)	444 (100%)	0	100	100
3	B	418/418 (100%)	418 (100%)	0	100	100
3	b	417/418 (100%)	417 (100%)	0	100	100
4	D	442/442 (100%)	442 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	441/442 (100%)	441 (100%)	0	100	100
5	E	452/455 (99%)	452 (100%)	0	100	100
5	e	456/455 (100%)	456 (100%)	0	100	100
6	G	456/457 (100%)	456 (100%)	0	100	100
6	g	457/457 (100%)	457 (100%)	0	100	100
7	H	435/435 (100%)	435 (100%)	0	100	100
7	h	432/435 (99%)	432 (100%)	0	100	100
8	Q	442/442 (100%)	442 (100%)	0	100	100
8	q	438/442 (99%)	438 (100%)	0	100	100
9	Z	437/439 (100%)	437 (100%)	0	100	100
9	z	438/439 (100%)	438 (100%)	0	100	100
10	P	191/250 (76%)	191 (100%)	0	100	100
All	All	7278/7654 (95%)	7278 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	231	GLN
2	A	135	ASN
2	A	170	ASN
2	A	193	ASN
2	A	353	GLN
2	A	393	HIS
3	B	288	ASN
3	B	337	HIS
3	B	380	GLN
3	B	464	GLN
4	D	25	GLN
4	D	125	GLN
4	D	301	GLN
4	D	350	GLN
5	E	55	ASN
5	E	469	ASN
5	E	495	HIS
5	E	515	GLN
6	G	71	GLN

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Mol	Chain	Res	Type
6	G	74	HIS
6	G	390	ASN
6	G	396	GLN
6	G	406	GLN
6	G	420	HIS
6	G	481	ASN
7	H	17	GLN
7	H	60	ASN
7	H	107	GLN
7	H	130	GLN
7	H	264	GLN
7	H	335	ASN
7	H	359	ASN
7	H	448	GLN
7	H	501	ASN
8	Q	145	ASN
8	Q	172	GLN
8	Q	175	ASN
8	Q	365	HIS
2	a	139	ASN
2	a	193	ASN
2	a	450	ASN
3	b	65	ASN
3	b	157	GLN
3	b	464	GLN
4	d	250	GLN
4	d	262	ASN
5	e	403	HIS
5	e	495	HIS
5	e	515	GLN
6	g	26	ASN
6	g	74	HIS
6	g	111	HIS
6	g	235	ASN
6	g	390	ASN
6	g	420	HIS
7	h	151	GLN
7	h	201	GLN
7	h	331	GLN
7	h	359	ASN
7	h	431	GLN
7	h	448	GLN

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Mol	Chain	Res	Type
8	q	4	HIS
8	q	32	ASN
8	q	53	ASN
8	q	80	HIS
8	q	140	HIS
8	q	475	ASN
9	z	218	HIS
9	z	294	GLN
9	z	380	ASN
10	P	56	ASN
10	P	292	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
13	AF3	a	603	-	0,3,3	-	-	-		
11	ADP	D	601	12	28,29,29	1.41	4 (14%)	43,45,45	1.83	8 (18%)
13	AF3	h	603	-	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	ADP	G	601	12	28,29,29	1.39	5 (17%)	43,45,45	1.82	10 (23%)
13	AF3	A	603	-	0,3,3	-	-	-		
13	AF3	B	603	-	0,3,3	-	-	-		
13	AF3	D	603	-	0,3,3	-	-	-		
11	ADP	d	601	12	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)
11	ADP	A	601	12	28,29,29	1.39	4 (14%)	43,45,45	1.80	9 (20%)
13	AF3	z	603	-	0,3,3	-	-	-		
11	ADP	H	601	12	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)
13	AF3	G	603	-	0,3,3	-	-	-		
11	ADP	Z	601	12	28,29,29	1.39	4 (14%)	43,45,45	1.85	8 (18%)
13	AF3	Z	603	-	0,3,3	-	-	-		
11	ADP	h	601	12	28,29,29	1.40	4 (14%)	43,45,45	1.82	9 (20%)
13	AF3	E	603	-	0,3,3	-	-	-		
13	AF3	Q	603	-	0,3,3	-	-	-		
11	ADP	Q	601	12	28,29,29	1.39	4 (14%)	43,45,45	1.85	10 (23%)
11	ADP	E	601	12	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
11	ADP	b	601	12	28,29,29	1.39	4 (14%)	43,45,45	1.85	11 (25%)
11	ADP	e	601	12	28,29,29	1.40	4 (14%)	43,45,45	1.81	9 (20%)
13	AF3	b	603	-	0,3,3	-	-	-		
13	AF3	d	603	-	0,3,3	-	-	-		
13	AF3	g	603	-	0,3,3	-	-	-		
11	ADP	g	601	12	28,29,29	1.40	5 (17%)	43,45,45	1.82	10 (23%)
11	ADP	z	601	12	28,29,29	1.39	4 (14%)	43,45,45	1.84	9 (20%)
11	ADP	B	601	12	28,29,29	1.40	4 (14%)	43,45,45	1.84	10 (23%)
13	AF3	e	603	-	0,3,3	-	-	-		
11	ADP	q	601	12	28,29,29	1.38	5 (17%)	43,45,45	1.82	9 (20%)
13	AF3	q	603	-	0,3,3	-	-	-		
11	ADP	a	601	12	28,29,29	1.38	4 (14%)	43,45,45	1.83	10 (23%)
13	AF3	H	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
11	ADP	D	601	12	-	0/16/32/32	0/3/3/3
11	ADP	g	601	12	-	5/16/32/32	0/3/3/3
11	ADP	z	601	12	-	6/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ADP	H	601	12	-	0/16/32/32	0/3/3/3
11	ADP	B	601	12	-	3/16/32/32	0/3/3/3
11	ADP	E	601	12	-	0/16/32/32	0/3/3/3
11	ADP	Q	601	12	-	5/16/32/32	0/3/3/3
11	ADP	b	601	12	-	3/16/32/32	0/3/3/3
11	ADP	q	601	12	-	6/16/32/32	0/3/3/3
11	ADP	a	601	12	-	4/16/32/32	0/3/3/3
11	ADP	Z	601	12	-	6/16/32/32	0/3/3/3
11	ADP	h	601	12	-	0/16/32/32	0/3/3/3
11	ADP	G	601	12	-	1/16/32/32	0/3/3/3
11	ADP	e	601	12	-	0/16/32/32	0/3/3/3
11	ADP	d	601	12	-	1/16/32/32	0/3/3/3
11	ADP	A	601	12	-	5/16/32/32	0/3/3/3

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	z	601	ADP	C5-C4	4.59	1.47	1.39
11	g	601	ADP	C5-C4	4.58	1.47	1.39
11	G	601	ADP	C5-C4	4.57	1.47	1.39
11	A	601	ADP	C5-C4	4.56	1.47	1.39
11	Z	601	ADP	C5-C4	4.56	1.47	1.39
11	D	601	ADP	C5-C4	4.56	1.47	1.39
11	d	601	ADP	C5-C4	4.55	1.47	1.39
11	e	601	ADP	C5-C4	4.54	1.47	1.39
11	Q	601	ADP	C5-C4	4.54	1.47	1.39
11	q	601	ADP	C5-C4	4.54	1.47	1.39
11	a	601	ADP	C5-C4	4.54	1.47	1.39
11	B	601	ADP	C5-C4	4.51	1.47	1.39
11	H	601	ADP	C5-C4	4.51	1.47	1.39
11	E	601	ADP	C5-C4	4.50	1.47	1.39
11	b	601	ADP	C5-C4	4.50	1.47	1.39
11	h	601	ADP	C5-C4	4.48	1.47	1.39
11	H	601	ADP	C5-C6	2.70	1.48	1.41
11	D	601	ADP	C5-C6	2.69	1.48	1.41
11	a	601	ADP	C5-C6	2.68	1.48	1.41
11	E	601	ADP	C5-C6	2.68	1.48	1.41
11	h	601	ADP	C5-C6	2.68	1.48	1.41
11	b	601	ADP	C5-C6	2.67	1.48	1.41
11	e	601	ADP	C5-C6	2.67	1.48	1.41
11	A	601	ADP	C5-C6	2.67	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Q	601	ADP	C5-C6	2.67	1.48	1.41
11	B	601	ADP	C5-C6	2.67	1.48	1.41
11	z	601	ADP	C5-C6	2.66	1.48	1.41
11	d	601	ADP	C5-C6	2.66	1.48	1.41
11	Z	601	ADP	C5-C6	2.65	1.48	1.41
11	q	601	ADP	C5-C6	2.65	1.48	1.41
11	g	601	ADP	C5-C6	2.64	1.48	1.41
11	G	601	ADP	C5-C6	2.63	1.48	1.41
11	Z	601	ADP	C5-N7	-2.39	1.34	1.39
11	Q	601	ADP	C5-N7	-2.36	1.34	1.39
11	D	601	ADP	C5-N7	-2.35	1.34	1.39
11	z	601	ADP	C5-N7	-2.35	1.34	1.39
11	E	601	ADP	C5-N7	-2.34	1.34	1.39
11	B	601	ADP	C5-N7	-2.34	1.34	1.39
11	e	601	ADP	C8-N7	2.34	1.36	1.31
11	A	601	ADP	C5-N7	-2.33	1.34	1.39
11	g	601	ADP	C5-N7	-2.33	1.34	1.39
11	E	601	ADP	C8-N7	2.33	1.36	1.31
11	G	601	ADP	C5-N7	-2.33	1.34	1.39
11	h	601	ADP	C8-N7	2.32	1.36	1.31
11	A	601	ADP	C8-N7	2.32	1.36	1.31
11	d	601	ADP	C5-N7	-2.32	1.34	1.39
11	h	601	ADP	C5-N7	-2.32	1.34	1.39
11	b	601	ADP	C8-N7	2.31	1.36	1.31
11	B	601	ADP	C8-N7	2.31	1.36	1.31
11	d	601	ADP	C8-N7	2.31	1.36	1.31
11	q	601	ADP	C5-N7	-2.31	1.34	1.39
11	a	601	ADP	C8-N7	2.30	1.36	1.31
11	D	601	ADP	C8-N7	2.30	1.36	1.31
11	e	601	ADP	C5-N7	-2.30	1.34	1.39
11	Q	601	ADP	C8-N7	2.30	1.36	1.31
11	b	601	ADP	C5-N7	-2.29	1.34	1.39
11	g	601	ADP	C8-N7	2.29	1.36	1.31
11	a	601	ADP	C5-N7	-2.28	1.34	1.39
11	H	601	ADP	C5-N7	-2.27	1.34	1.39
11	q	601	ADP	C8-N7	2.27	1.36	1.31
11	H	601	ADP	C8-N7	2.27	1.36	1.31
11	z	601	ADP	C8-N7	2.25	1.36	1.31
11	Z	601	ADP	C8-N7	2.23	1.36	1.31
11	G	601	ADP	C8-N7	2.23	1.36	1.31
11	g	601	ADP	C4-N9	-2.12	1.33	1.37
11	q	601	ADP	C4-N9	-2.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	601	ADP	C4-N9	-2.05	1.33	1.37

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	601	ADP	C5-C4-N3	-5.90	118.59	126.72
11	d	601	ADP	C5-C4-N3	-5.86	118.65	126.72
11	H	601	ADP	C5-C4-N3	-5.85	118.66	126.72
11	Z	601	ADP	C5-C4-N3	-5.85	118.67	126.72
11	b	601	ADP	C5-C4-N3	-5.84	118.67	126.72
11	E	601	ADP	C5-C4-N3	-5.84	118.68	126.72
11	z	601	ADP	C5-C4-N3	-5.82	118.70	126.72
11	e	601	ADP	C5-C4-N3	-5.80	118.73	126.72
11	h	601	ADP	C5-C4-N3	-5.77	118.77	126.72
11	A	601	ADP	C5-C4-N3	-5.77	118.77	126.72
11	B	601	ADP	C5-C4-N3	-5.75	118.80	126.72
11	a	601	ADP	C5-C4-N3	-5.74	118.82	126.72
11	Q	601	ADP	C5-C4-N3	-5.71	118.85	126.72
11	G	601	ADP	C5-C4-N3	-5.65	118.94	126.72
11	q	601	ADP	C5-C4-N3	-5.61	118.99	126.72
11	g	601	ADP	C5-C4-N3	-5.58	119.03	126.72
11	Z	601	ADP	N3-C4-N9	4.66	135.09	127.17
11	z	601	ADP	N3-C4-N9	4.64	135.06	127.17
11	D	601	ADP	N3-C4-N9	4.59	134.97	127.17
11	a	601	ADP	N3-C4-N9	4.58	134.95	127.17
11	E	601	ADP	N3-C4-N9	4.57	134.94	127.17
11	A	601	ADP	N3-C4-N9	4.56	134.92	127.17
11	b	601	ADP	N3-C4-N9	4.55	134.91	127.17
11	H	601	ADP	N3-C4-N9	4.55	134.90	127.17
11	d	601	ADP	N3-C4-N9	4.53	134.88	127.17
11	B	601	ADP	N3-C4-N9	4.52	134.86	127.17
11	Q	601	ADP	N3-C4-N9	4.52	134.85	127.17
11	h	601	ADP	N3-C4-N9	4.51	134.83	127.17
11	e	601	ADP	N3-C4-N9	4.50	134.81	127.17
11	G	601	ADP	N3-C4-N9	4.46	134.75	127.17
11	q	601	ADP	N3-C4-N9	4.39	134.63	127.17
11	g	601	ADP	N3-C4-N9	4.36	134.58	127.17
11	H	601	ADP	C2-N3-C4	3.75	120.98	111.83
11	E	601	ADP	C2-N3-C4	3.73	120.94	111.83
11	d	601	ADP	C2-N3-C4	3.73	120.94	111.83
11	D	601	ADP	C2-N3-C4	3.73	120.93	111.83
11	b	601	ADP	C2-N3-C4	3.72	120.92	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	z	601	ADP	C2-N3-C4	3.71	120.89	111.83
11	Q	601	ADP	C2-N3-C4	3.71	120.89	111.83
11	B	601	ADP	C2-N3-C4	3.71	120.88	111.83
11	A	601	ADP	C2-N3-C4	3.70	120.88	111.83
11	h	601	ADP	C2-N3-C4	3.70	120.88	111.83
11	a	601	ADP	C2-N3-C4	3.68	120.83	111.83
11	Z	601	ADP	C2-N3-C4	3.68	120.81	111.83
11	e	601	ADP	C2-N3-C4	3.68	120.81	111.83
11	q	601	ADP	C2-N3-C4	3.65	120.75	111.83
11	G	601	ADP	C2-N3-C4	3.60	120.61	111.83
11	d	601	ADP	C4-C5-N7	-3.59	106.47	110.58
11	e	601	ADP	C4-C5-N7	-3.58	106.49	110.58
11	g	601	ADP	C2-N3-C4	3.58	120.56	111.83
11	D	601	ADP	C4-C5-N7	-3.57	106.50	110.58
11	b	601	ADP	C4-C5-N7	-3.56	106.52	110.58
11	g	601	ADP	C4-C5-N7	-3.55	106.53	110.58
11	q	601	ADP	C4-C5-N7	-3.54	106.53	110.58
11	H	601	ADP	C4-C5-N7	-3.54	106.53	110.58
11	h	601	ADP	C4-C5-N7	-3.54	106.54	110.58
11	Q	601	ADP	C4-C5-N7	-3.52	106.56	110.58
11	G	601	ADP	C4-C5-N7	-3.51	106.57	110.58
11	A	601	ADP	C4-C5-N7	-3.50	106.58	110.58
11	E	601	ADP	C4-C5-N7	-3.49	106.59	110.58
11	a	601	ADP	C4-C5-N7	-3.49	106.59	110.58
11	B	601	ADP	C4-C5-N7	-3.48	106.60	110.58
11	z	601	ADP	C4-C5-N7	-3.43	106.66	110.58
11	Z	601	ADP	C4-C5-N7	-3.39	106.71	110.58
11	Q	601	ADP	N3-C2-N1	-3.31	123.57	128.58
11	B	601	ADP	N3-C2-N1	-3.28	123.62	128.58
11	a	601	ADP	N3-C2-N1	-3.27	123.63	128.58
11	H	601	ADP	N3-C2-N1	-3.27	123.64	128.58
11	q	601	ADP	N3-C2-N1	-3.26	123.64	128.58
11	b	601	ADP	N3-C2-N1	-3.26	123.65	128.58
11	h	601	ADP	N3-C2-N1	-3.26	123.65	128.58
11	A	601	ADP	N3-C2-N1	-3.24	123.68	128.58
11	E	601	ADP	N3-C2-N1	-3.24	123.68	128.58
11	d	601	ADP	N3-C2-N1	-3.23	123.69	128.58
11	D	601	ADP	N3-C2-N1	-3.23	123.70	128.58
11	z	601	ADP	N3-C2-N1	-3.21	123.73	128.58
11	e	601	ADP	N3-C2-N1	-3.18	123.77	128.58
11	Z	601	ADP	N3-C2-N1	-3.17	123.78	128.58
11	g	601	ADP	N3-C2-N1	-3.10	123.88	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	601	ADP	N3-C2-N1	-3.10	123.89	128.58
11	a	601	ADP	C4-N9-C8	2.87	108.75	105.74
11	g	601	ADP	C4-N9-C8	2.78	108.65	105.74
11	Q	601	ADP	C4-N9-C8	2.76	108.64	105.74
11	q	601	ADP	C4-N9-C8	2.76	108.64	105.74
11	A	601	ADP	C4-N9-C8	2.74	108.62	105.74
11	G	601	ADP	C4-N9-C8	2.74	108.62	105.74
11	h	601	ADP	C4-N9-C8	2.71	108.58	105.74
11	z	601	ADP	C4-N9-C8	2.70	108.58	105.74
11	B	601	ADP	C4-N9-C8	2.68	108.55	105.74
11	b	601	ADP	C4-N9-C8	2.66	108.53	105.74
11	E	601	ADP	C4-N9-C8	2.65	108.53	105.74
11	e	601	ADP	C4-N9-C8	2.64	108.51	105.74
11	H	601	ADP	C4-N9-C8	2.61	108.48	105.74
11	d	601	ADP	C4-N9-C8	2.61	108.47	105.74
11	Q	601	ADP	C5-N7-C8	2.61	107.55	103.45
11	d	601	ADP	C5-N7-C8	2.59	107.52	103.45
11	h	601	ADP	C5-N7-C8	2.59	107.52	103.45
11	Z	601	ADP	C4-N9-C8	2.59	108.46	105.74
11	D	601	ADP	C5-N7-C8	2.58	107.50	103.45
11	D	601	ADP	C4-N9-C8	2.57	108.44	105.74
11	b	601	ADP	C5-N7-C8	2.57	107.49	103.45
11	a	601	ADP	C5-N7-C8	2.56	107.48	103.45
11	e	601	ADP	C5-N7-C8	2.56	107.48	103.45
11	B	601	ADP	C5-N7-C8	2.56	107.47	103.45
11	E	601	ADP	C5-N7-C8	2.56	107.47	103.45
11	q	601	ADP	C5-N7-C8	2.56	107.47	103.45
11	H	601	ADP	C5-N7-C8	2.55	107.46	103.45
11	A	601	ADP	C5-N7-C8	2.55	107.46	103.45
11	g	601	ADP	C5-N7-C8	2.53	107.43	103.45
11	G	601	ADP	C5-N7-C8	2.51	107.40	103.45
11	z	601	ADP	C5-N7-C8	2.51	107.40	103.45
11	Z	601	ADP	C5-N7-C8	2.46	107.32	103.45
11	B	601	ADP	C3'-C2'-C1'	2.29	105.79	101.46
11	q	601	ADP	C6-C5-N7	2.23	136.39	132.09
11	Z	601	ADP	C3'-C2'-C1'	2.23	105.67	101.46
11	g	601	ADP	C6-C5-N7	2.22	136.37	132.09
11	Q	601	ADP	C6-C5-N7	2.21	136.35	132.09
11	d	601	ADP	C6-C5-N7	2.18	136.29	132.09
11	H	601	ADP	C6-C5-N7	2.15	136.23	132.09
11	e	601	ADP	C6-C5-N7	2.14	136.22	132.09
11	A	601	ADP	C6-C5-N7	2.14	136.21	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	z	601	ADP	C3'-C2'-C1'	2.14	105.51	101.46
11	b	601	ADP	O4'-C1'-N9	2.14	112.20	108.09
11	G	601	ADP	C6-C5-N7	2.14	136.21	132.09
11	b	601	ADP	C6-C5-N7	2.14	136.21	132.09
11	h	601	ADP	C6-C5-N7	2.14	136.21	132.09
11	D	601	ADP	C6-C5-N7	2.13	136.20	132.09
11	B	601	ADP	C6-C5-N7	2.13	136.19	132.09
11	a	601	ADP	C6-C5-N7	2.12	136.18	132.09
11	G	601	ADP	C3'-C2'-C1'	2.11	105.45	101.46
11	a	601	ADP	N9-C8-N7	-2.11	110.94	113.94
11	h	601	ADP	N9-C8-N7	-2.10	110.96	113.94
11	Q	601	ADP	N9-C8-N7	-2.09	110.97	113.94
11	E	601	ADP	C6-C5-N7	2.09	136.12	132.09
11	q	601	ADP	N9-C8-N7	-2.08	110.98	113.94
11	Q	601	ADP	C3'-C2'-C1'	2.08	105.39	101.46
11	z	601	ADP	C6-C5-N7	2.08	136.10	132.09
11	a	601	ADP	C3'-C2'-C1'	2.08	105.39	101.46
11	g	601	ADP	C3'-C2'-C1'	2.07	105.38	101.46
11	g	601	ADP	N9-C8-N7	-2.06	111.01	113.94
11	B	601	ADP	N9-C8-N7	-2.05	111.03	113.94
11	E	601	ADP	N9-C8-N7	-2.04	111.03	113.94
11	A	601	ADP	N9-C8-N7	-2.04	111.04	113.94
11	b	601	ADP	N9-C8-N7	-2.04	111.04	113.94
11	d	601	ADP	N9-C8-N7	-2.03	111.06	113.94
11	e	601	ADP	N9-C8-N7	-2.03	111.06	113.94
11	b	601	ADP	C3'-C2'-C1'	2.01	105.27	101.46
11	G	601	ADP	N9-C8-N7	-2.00	111.09	113.94
11	H	601	ADP	N9-C8-N7	-2.00	111.10	113.94

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	601	ADP	C5'-O5'-PA-O1A
11	A	601	ADP	C5'-O5'-PA-O2A
11	A	601	ADP	C5'-O5'-PA-O3A
11	B	601	ADP	PB-O3A-PA-O5'
11	B	601	ADP	C5'-O5'-PA-O2A
11	Q	601	ADP	C5'-O5'-PA-O1A
11	Q	601	ADP	C5'-O5'-PA-O3A
11	Z	601	ADP	C5'-O5'-PA-O1A
11	Z	601	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
11	a	601	ADP	C5'-O5'-PA-O1A
11	a	601	ADP	C5'-O5'-PA-O2A
11	a	601	ADP	C5'-O5'-PA-O3A
11	b	601	ADP	PA-O3A-PB-O2B
11	g	601	ADP	C5'-O5'-PA-O2A
11	q	601	ADP	C5'-O5'-PA-O2A
11	q	601	ADP	C5'-O5'-PA-O3A
11	z	601	ADP	C5'-O5'-PA-O2A
11	Z	601	ADP	C3'-C4'-C5'-O5'
11	b	601	ADP	PB-O3A-PA-O5'
11	d	601	ADP	PB-O3A-PA-O5'
11	b	601	ADP	PA-O3A-PB-O3B
11	g	601	ADP	PB-O3A-PA-O2A
11	Q	601	ADP	C3'-C4'-C5'-O5'
11	B	601	ADP	C5'-O5'-PA-O3A
11	Q	601	ADP	C5'-O5'-PA-O2A
11	Z	601	ADP	C5'-O5'-PA-O2A
11	g	601	ADP	C5'-O5'-PA-O1A
11	g	601	ADP	C5'-O5'-PA-O3A
11	q	601	ADP	C5'-O5'-PA-O1A
11	z	601	ADP	C5'-O5'-PA-O1A
11	z	601	ADP	C5'-O5'-PA-O3A
11	q	601	ADP	PB-O3A-PA-O2A
11	z	601	ADP	PB-O3A-PA-O2A
11	q	601	ADP	C3'-C4'-C5'-O5'
11	z	601	ADP	C3'-C4'-C5'-O5'
11	A	601	ADP	PB-O3A-PA-O1A
11	A	601	ADP	PB-O3A-PA-O2A
11	G	601	ADP	PB-O3A-PA-O2A
11	Z	601	ADP	PB-O3A-PA-O1A
11	g	601	ADP	PB-O3A-PA-O1A
11	q	601	ADP	PB-O3A-PA-O1A
11	z	601	ADP	PB-O3A-PA-O1A
11	Z	601	ADP	O4'-C4'-C5'-O5'
11	Q	601	ADP	PB-O3A-PA-O2A
11	a	601	ADP	PB-O3A-PA-O2A

There are no ring outliers.

28 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	a	603	AF3	1	0

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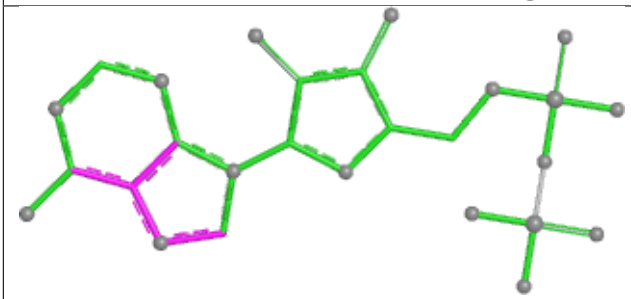
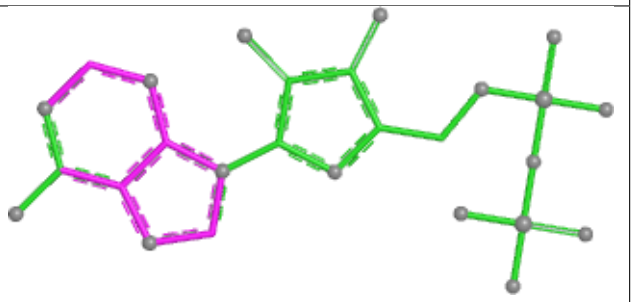
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	601	ADP	1	0
13	h	603	AF3	3	0
11	G	601	ADP	2	0
13	A	603	AF3	1	0
13	D	603	AF3	3	0
11	d	601	ADP	2	0
11	A	601	ADP	1	0
13	z	603	AF3	2	0
11	H	601	ADP	1	0
13	G	603	AF3	2	0
11	Z	601	ADP	2	0
13	Z	603	AF3	2	0
11	h	601	ADP	2	0
13	Q	603	AF3	1	0
11	Q	601	ADP	3	0
11	b	601	ADP	2	0
11	e	601	ADP	1	0
13	b	603	AF3	1	0
13	d	603	AF3	2	0
13	g	603	AF3	3	0
11	g	601	ADP	2	0
11	z	601	ADP	3	0
11	B	601	ADP	3	0
13	e	603	AF3	2	0
11	q	601	ADP	2	0
13	q	603	AF3	2	0
11	a	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 then 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.

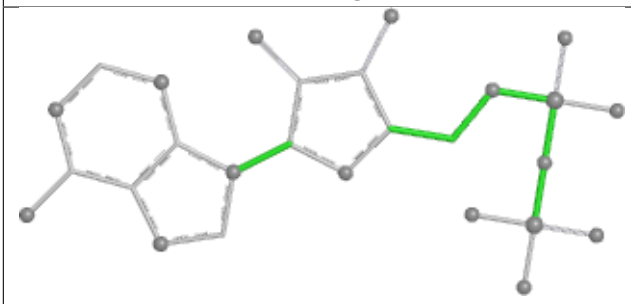
Ligand ADP D 601



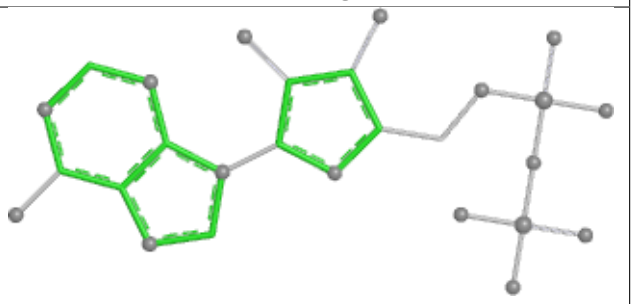
Bond lengths



Bond angles

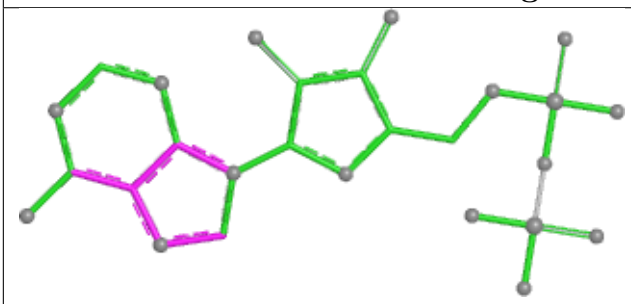


Torsions



Rings

Ligand ADP G 601



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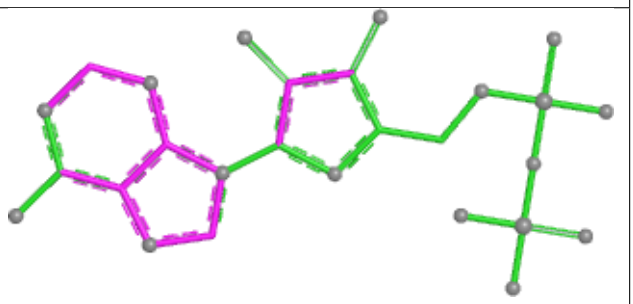

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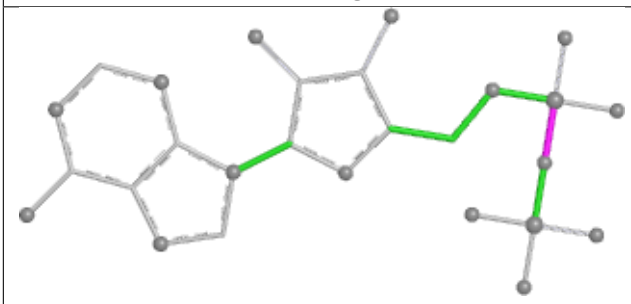

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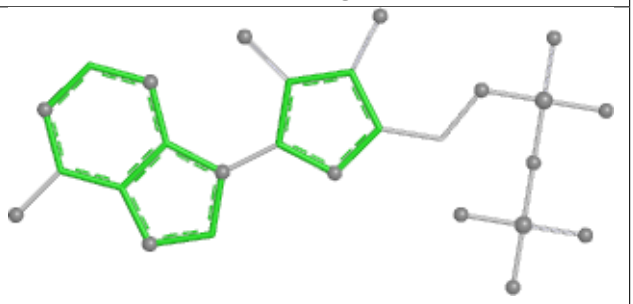

Rings

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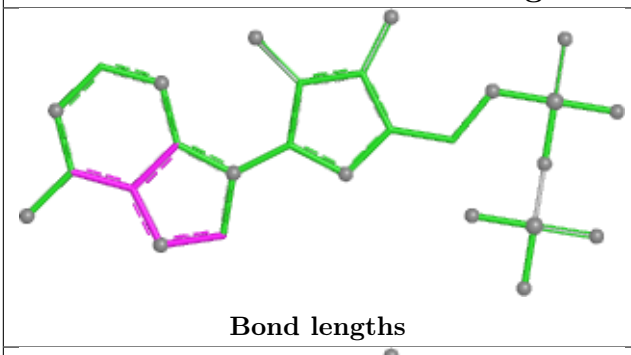

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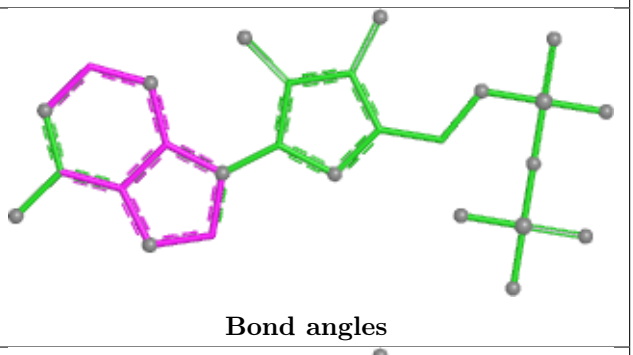

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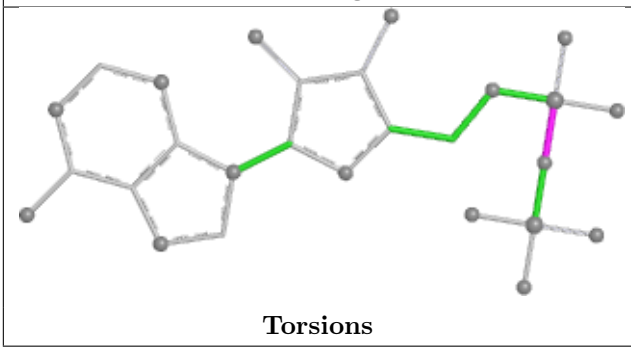

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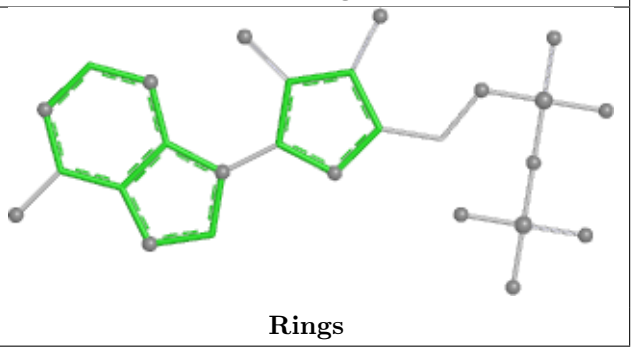

Rings

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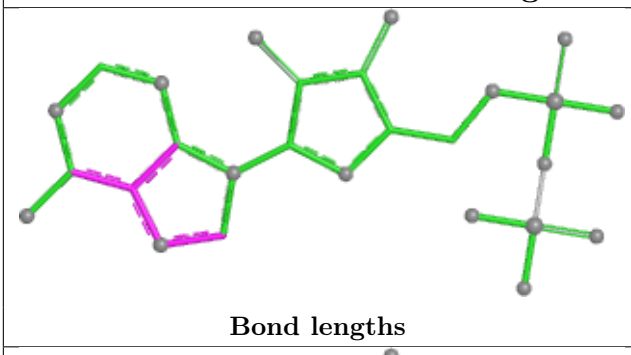

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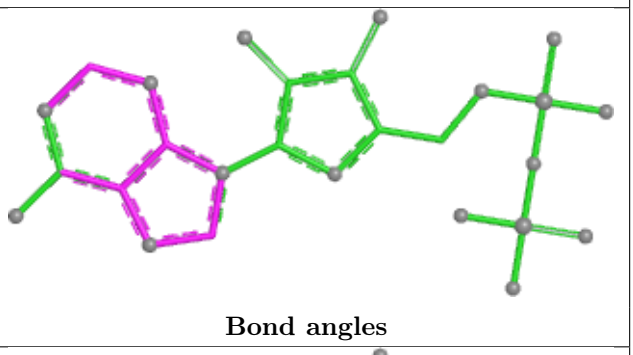

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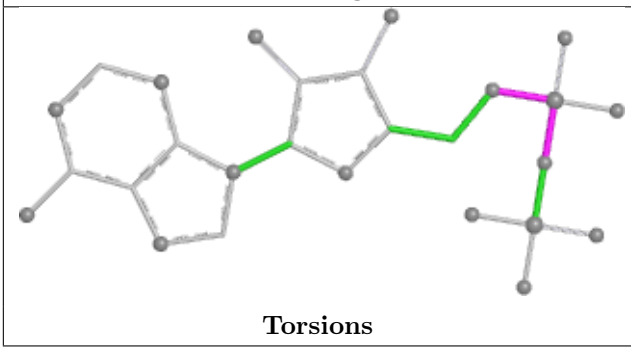

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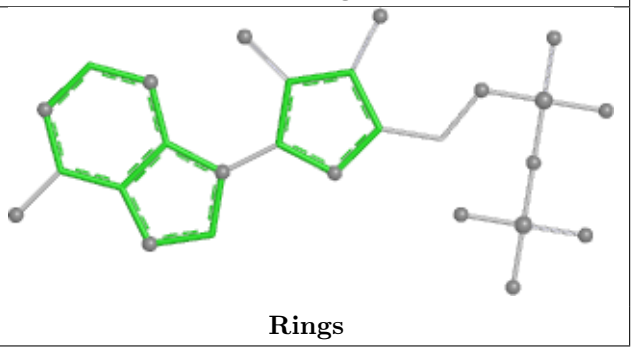

Rings

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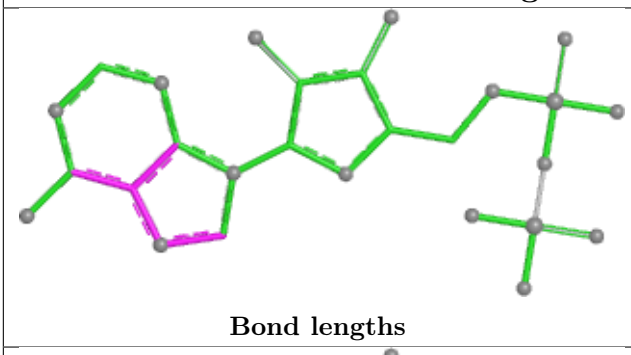

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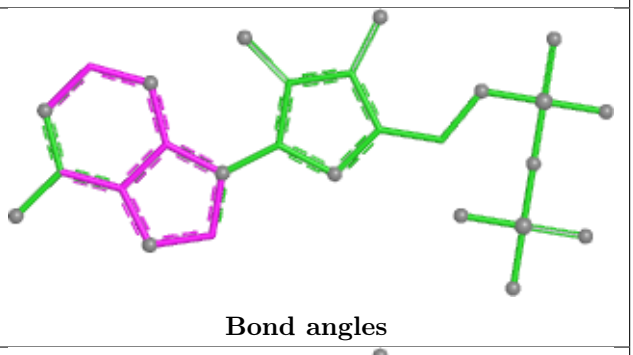

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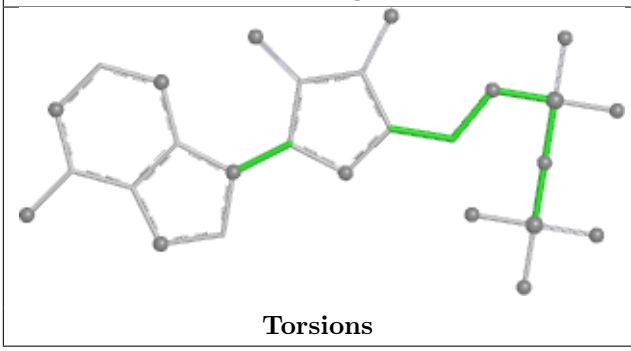

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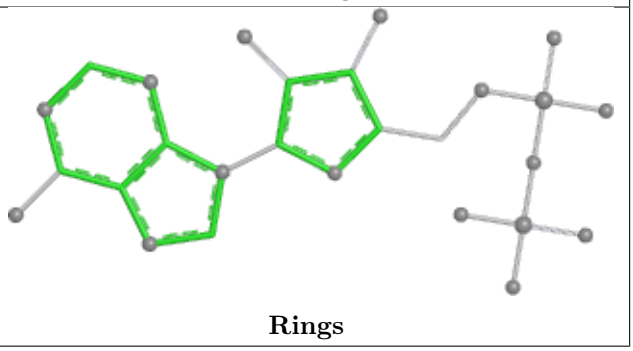

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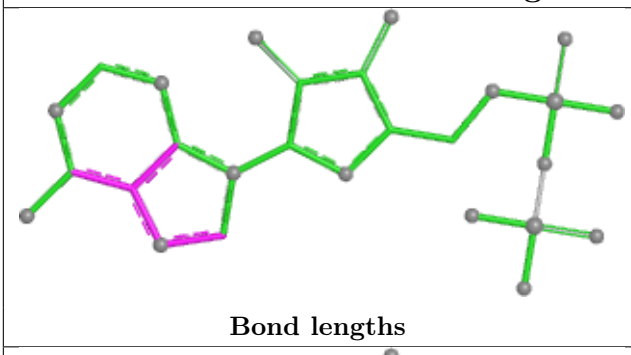

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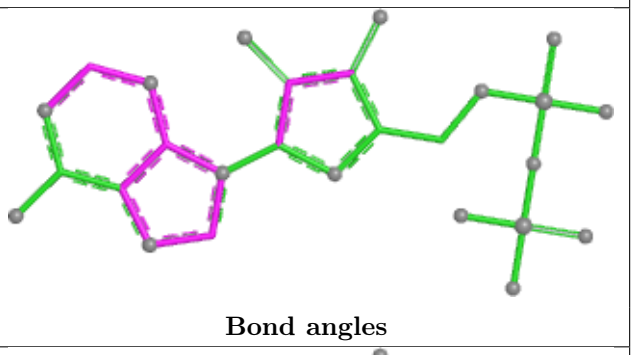

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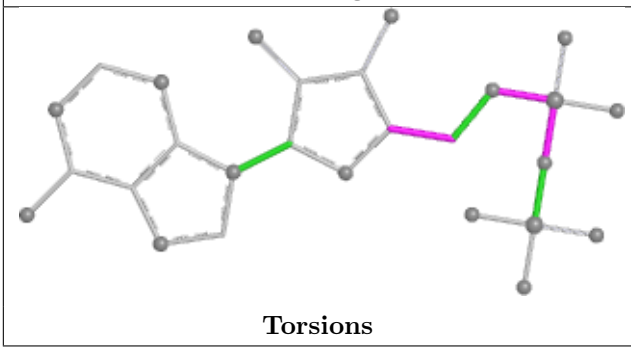

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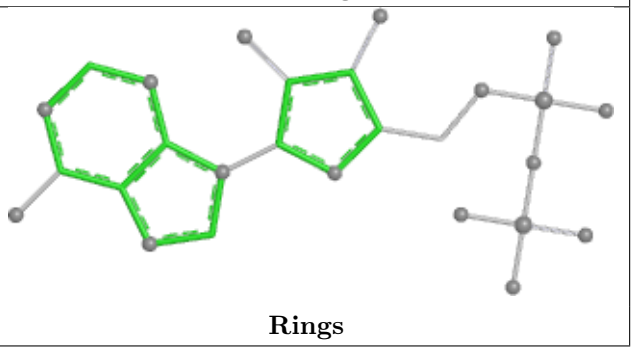

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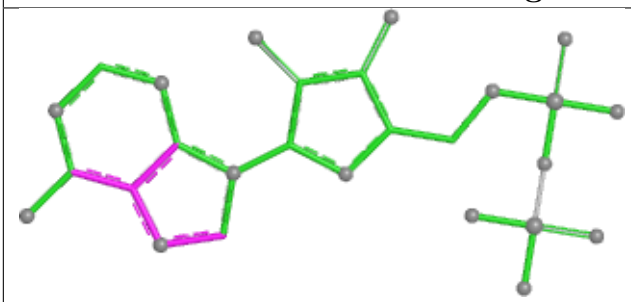

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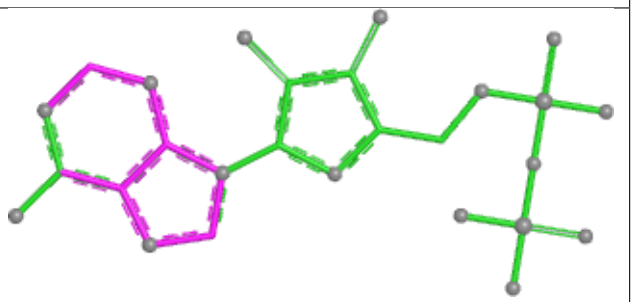

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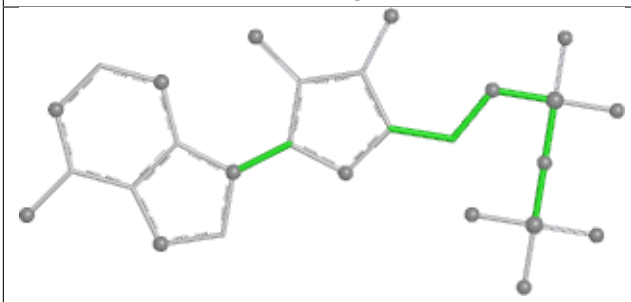

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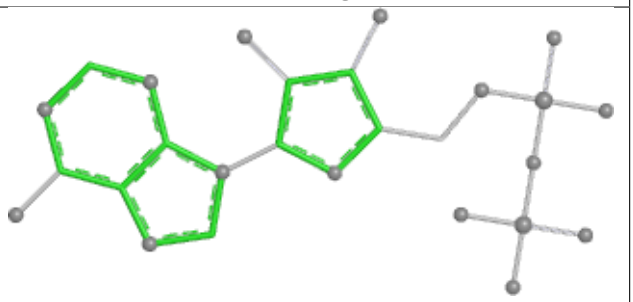

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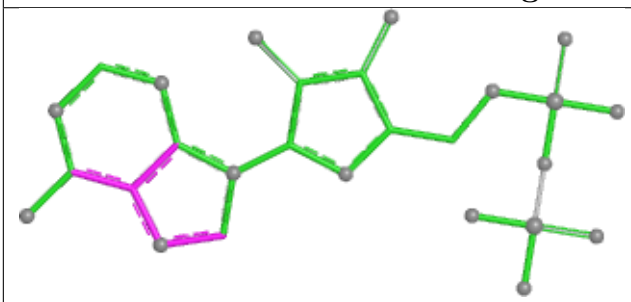

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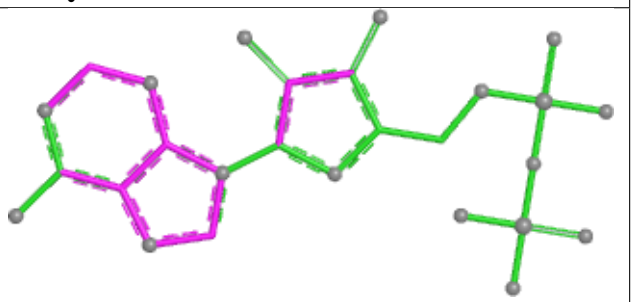

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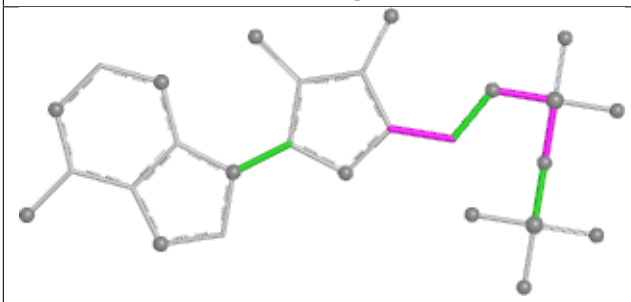

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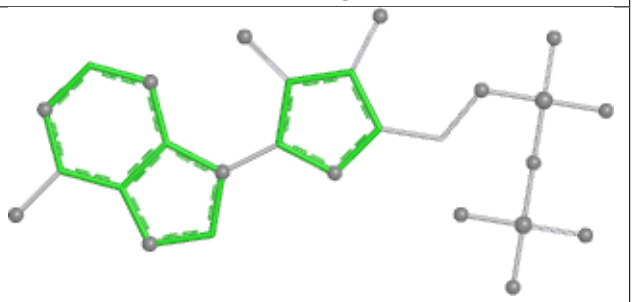

Rings

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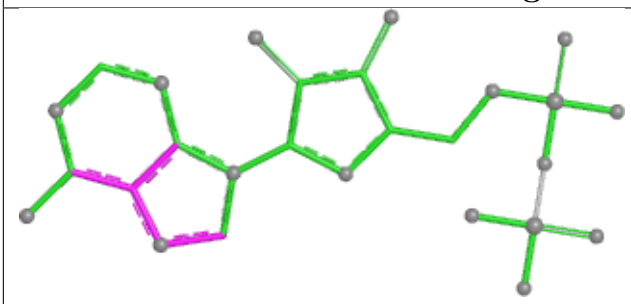

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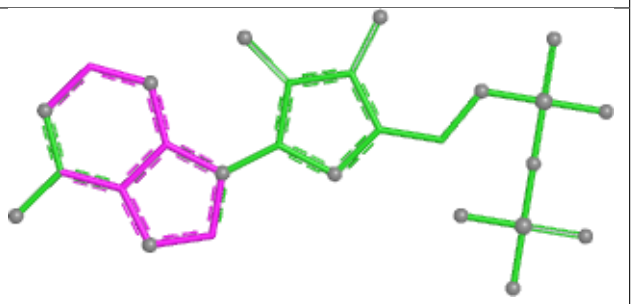

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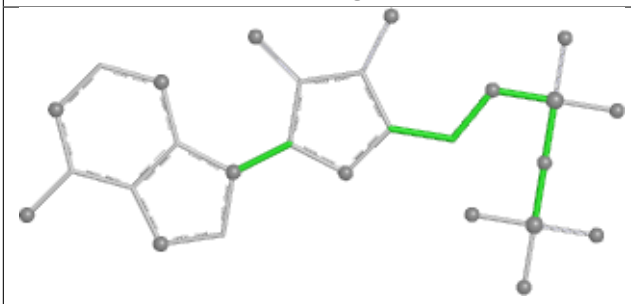

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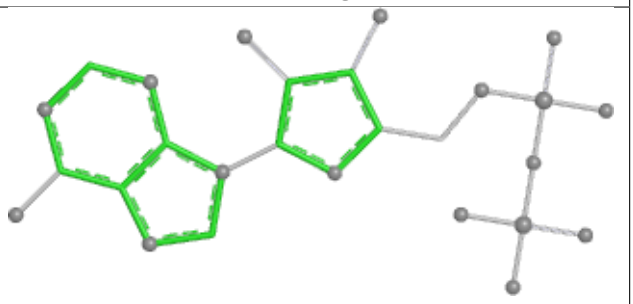
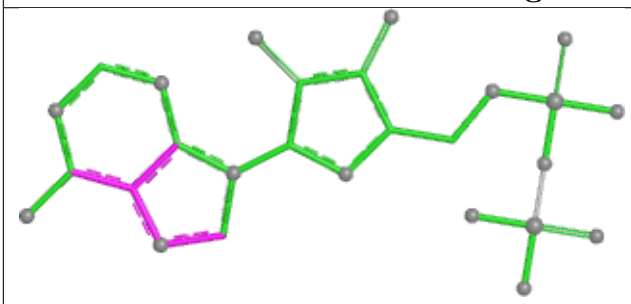


Rings

Ligand ADP b 601



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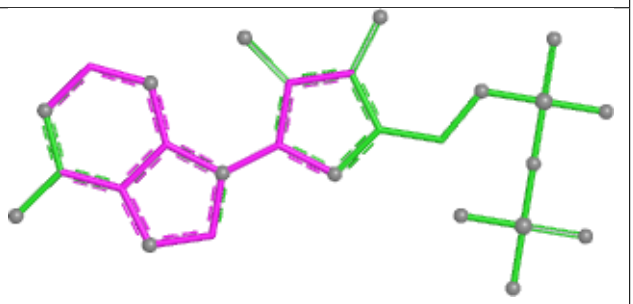

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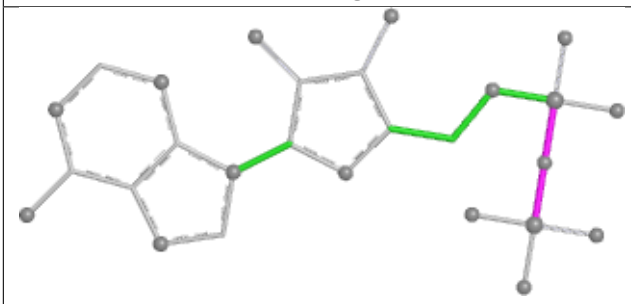

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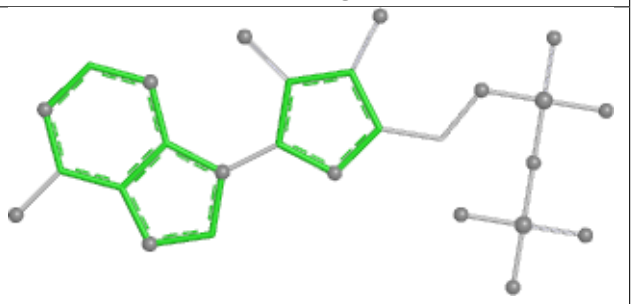
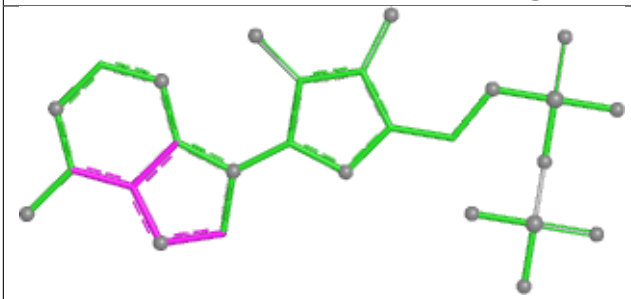


Rings

Ligand ADP e 601



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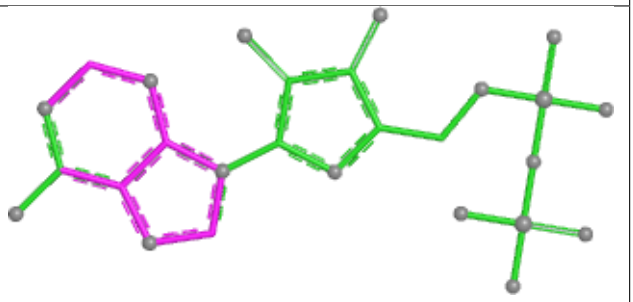

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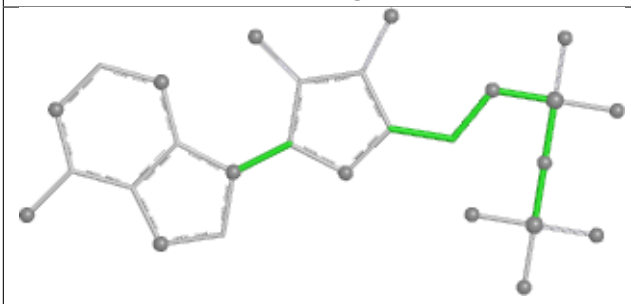

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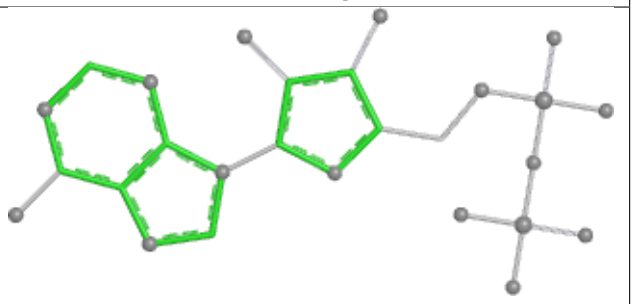

Rings

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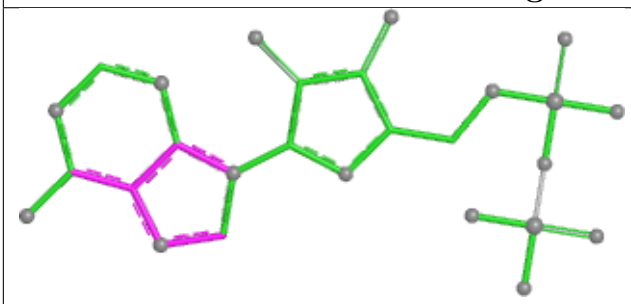
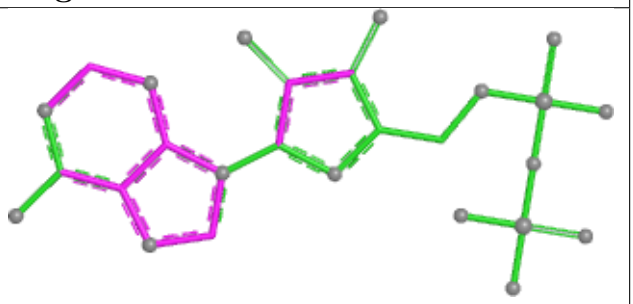
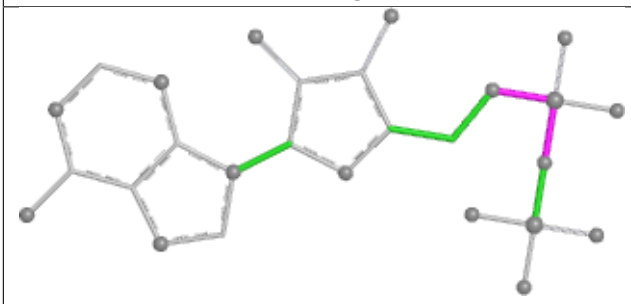


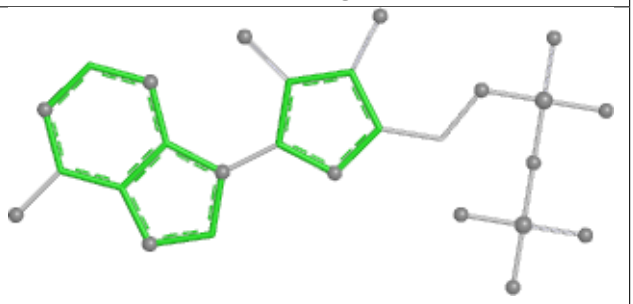
Bond lengths



Bond angles

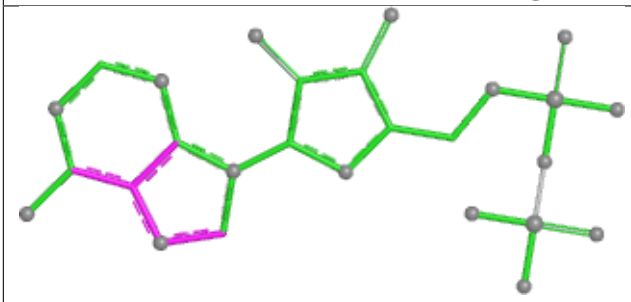


Torsions

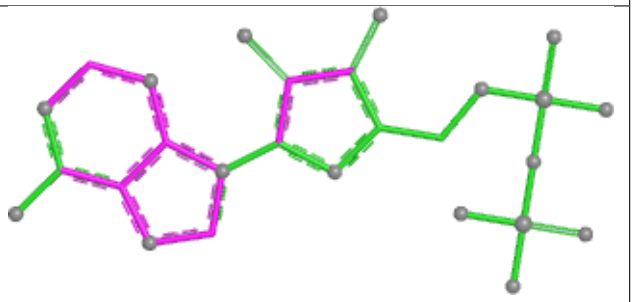


Rings

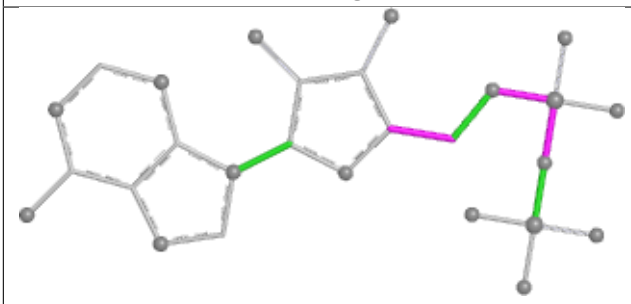
Ligand ADP z 601



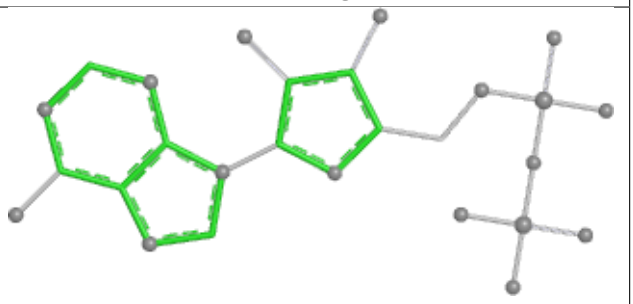
Bond lengths



Bond angles

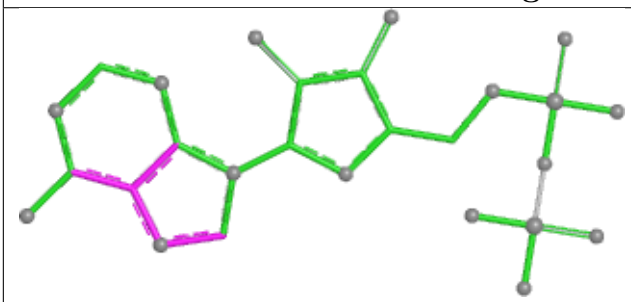


Torsions

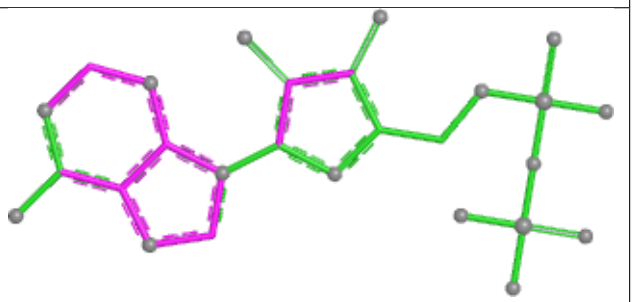


Rings

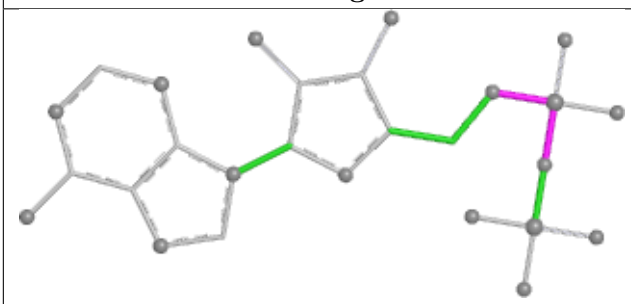
Ligand ADP B 601



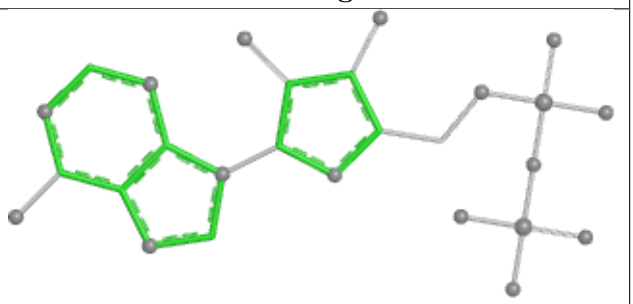
Bond lengths



Bond angles

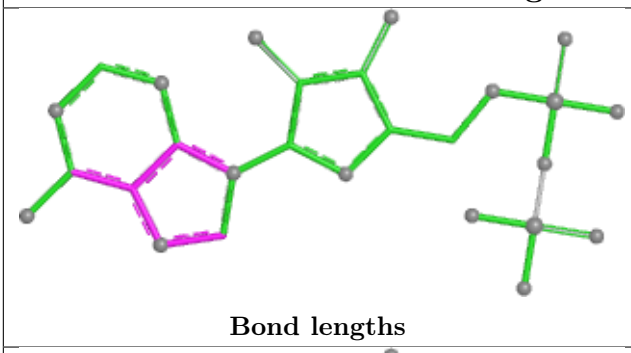


Torsions

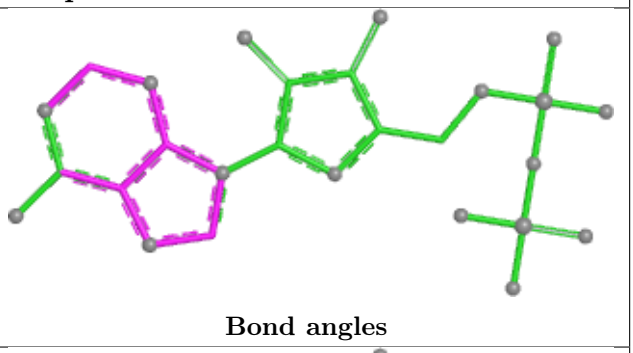


Rings

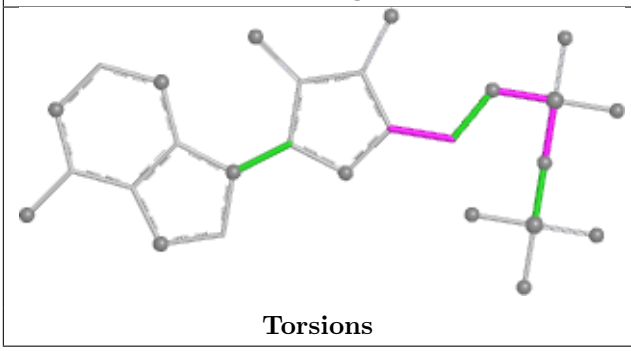
Ligand ADP q 601



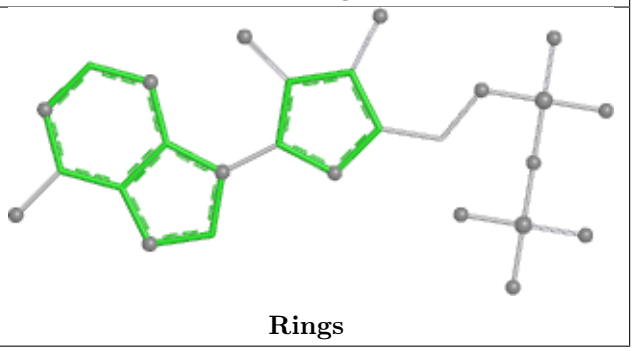
Bond lengths



Bond angles

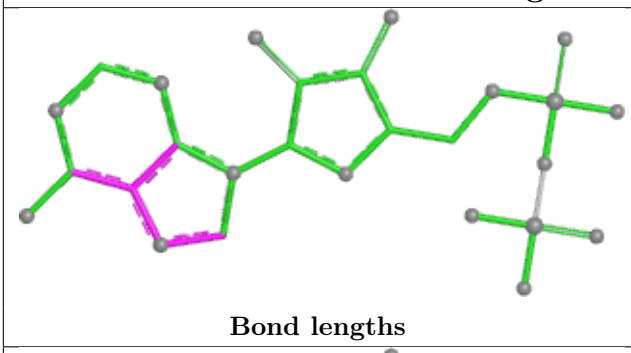


Torsions

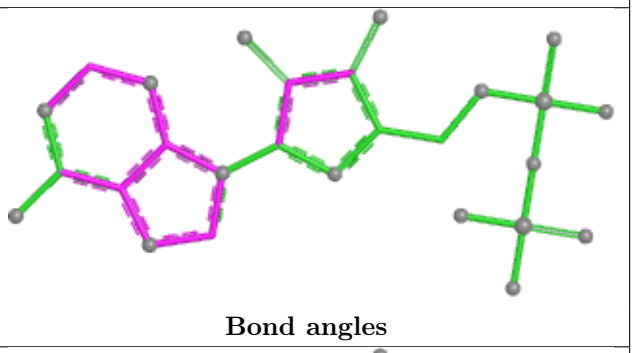


Rings

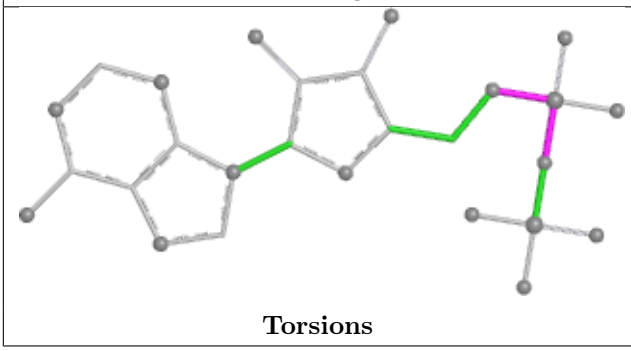
Ligand ADP a 601



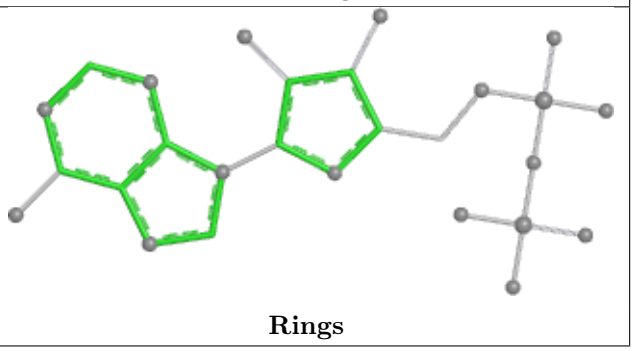
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

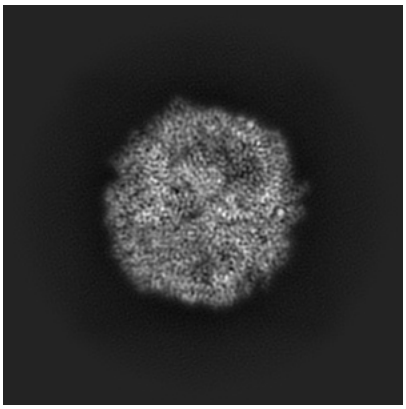
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40481. These allow visual inspection of the internal detail of the map and identification of artifacts.

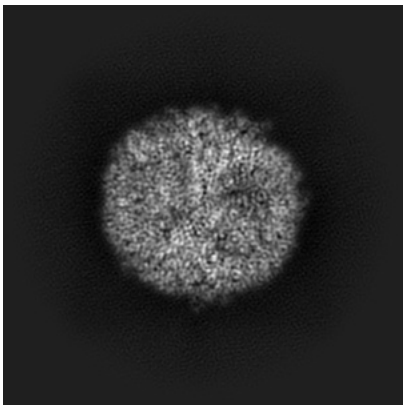
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

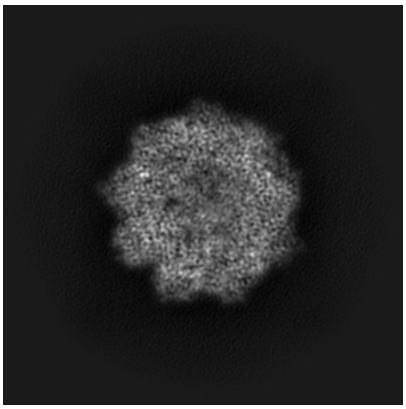
6.1.1 Primary map



X

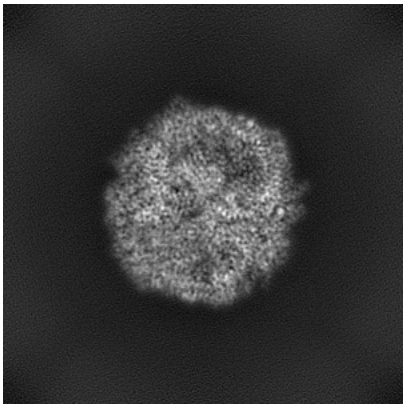


Y

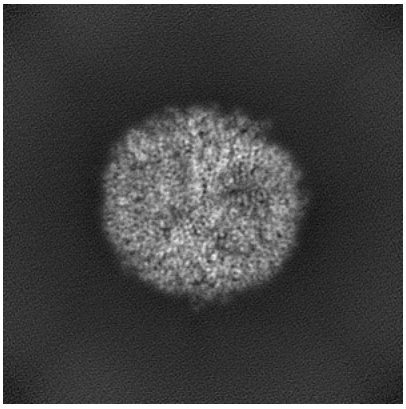


Z

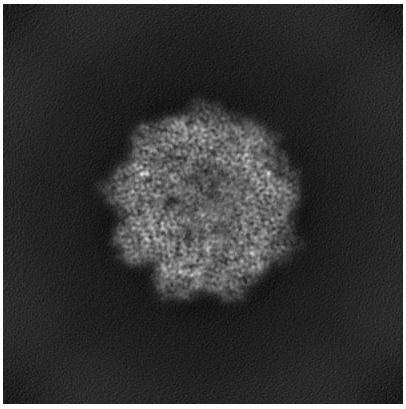
6.1.2 Raw map



X



Y

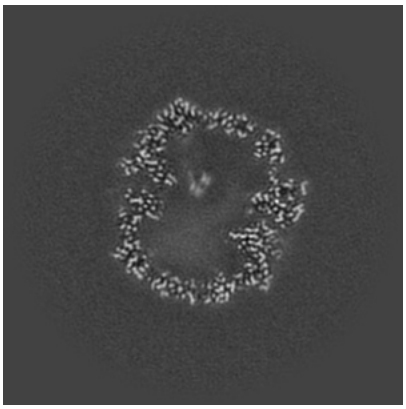


Z

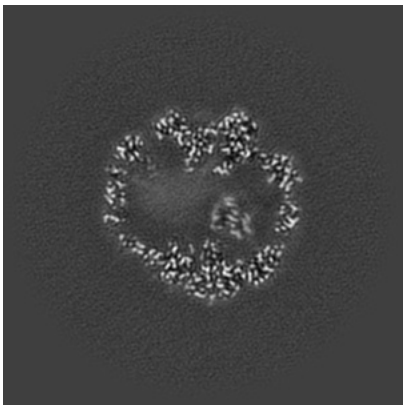
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

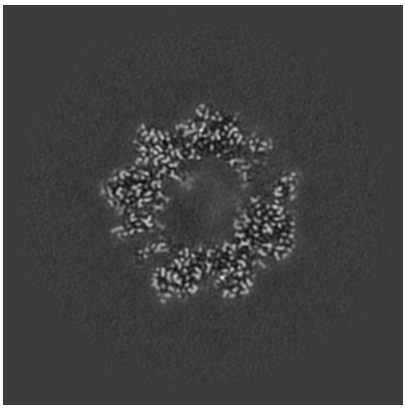
6.2.1 Primary map



X Index: 150

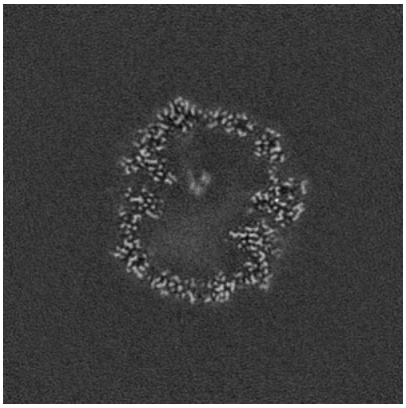


Y Index: 150

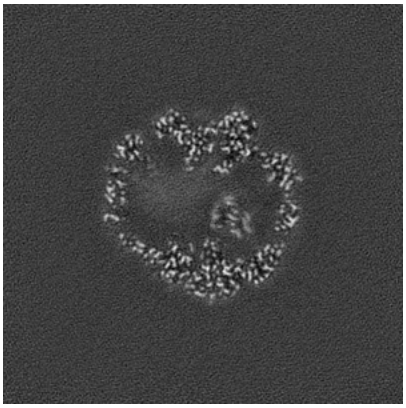


Z Index: 150

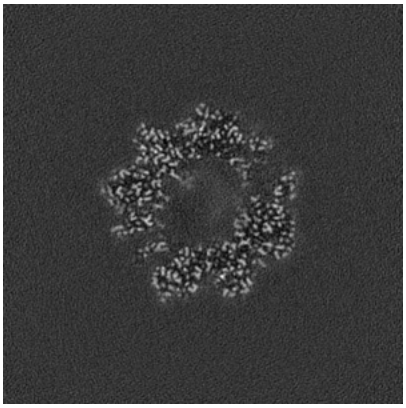
6.2.2 Raw map



X Index: 150



Y Index: 150

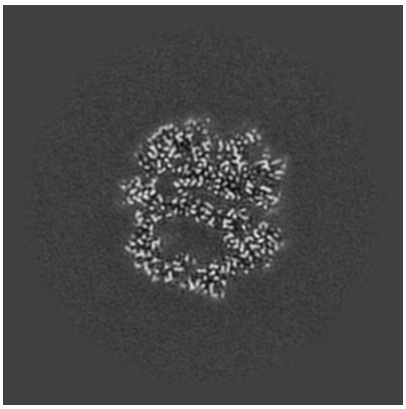


Z Index: 150

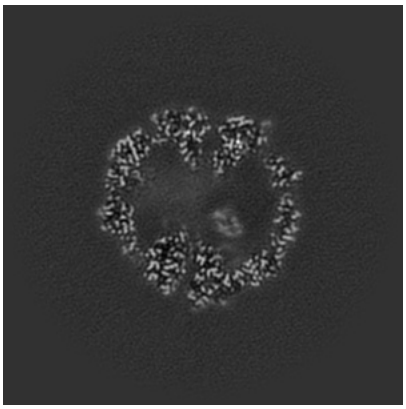
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

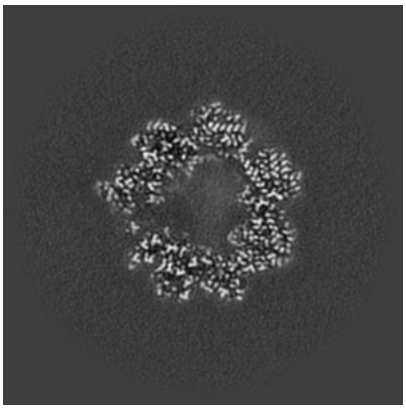
6.3.1 Primary map



X Index: 187

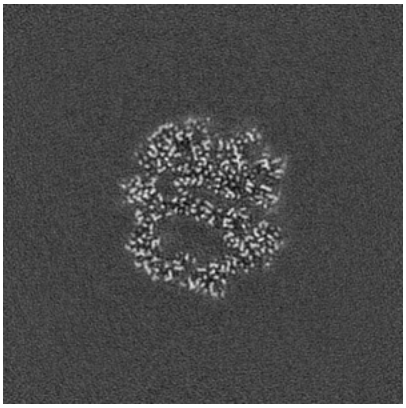


Y Index: 158

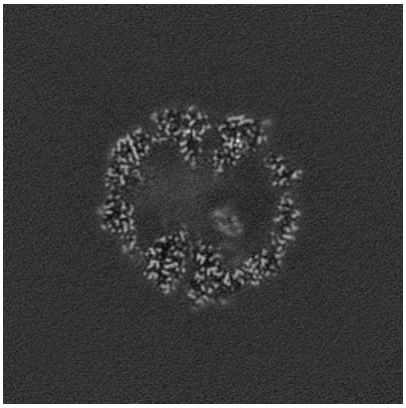


Z Index: 143

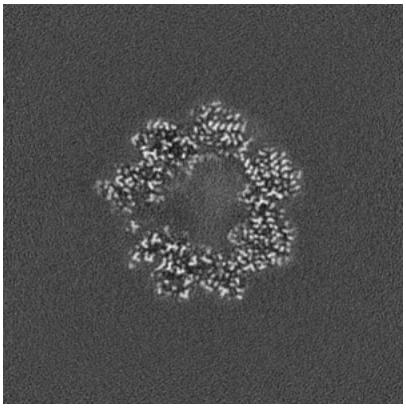
6.3.2 Raw map



X Index: 187



Y Index: 158

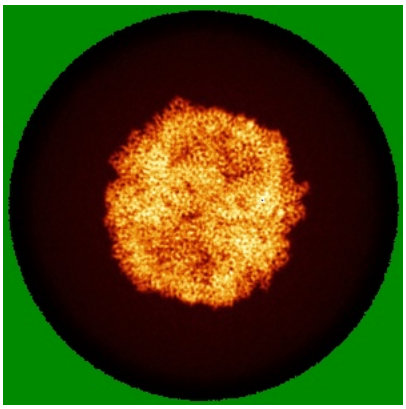


Z Index: 143

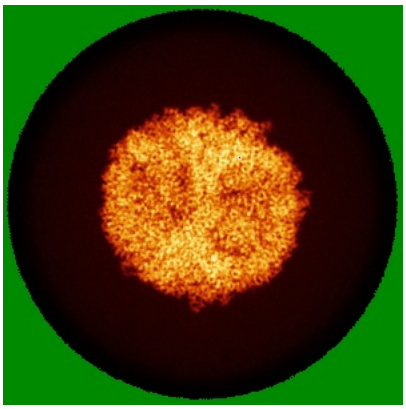
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

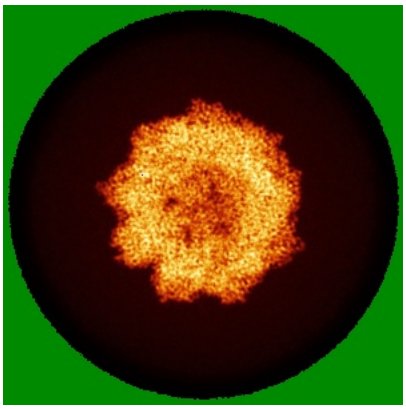
6.4.1 Primary map



X

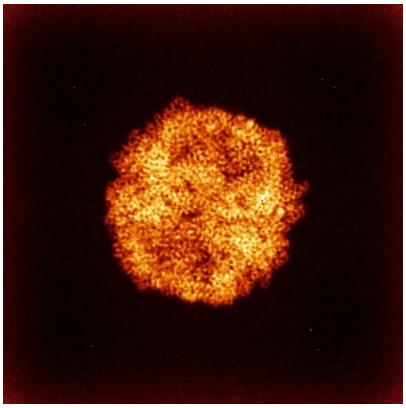


Y

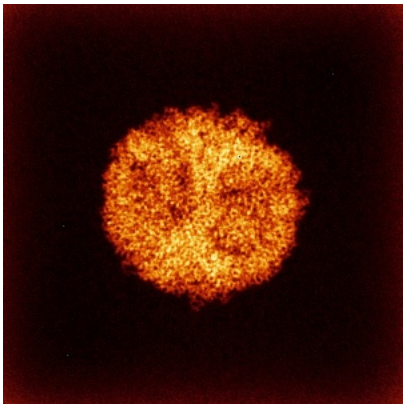


Z

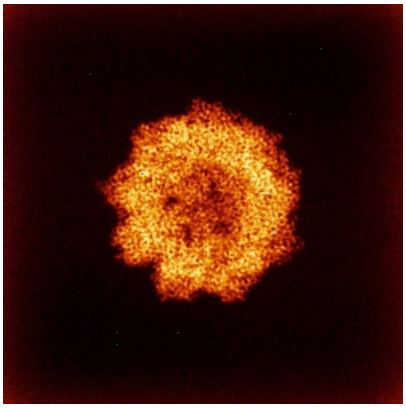
6.4.2 Raw map



X



Y

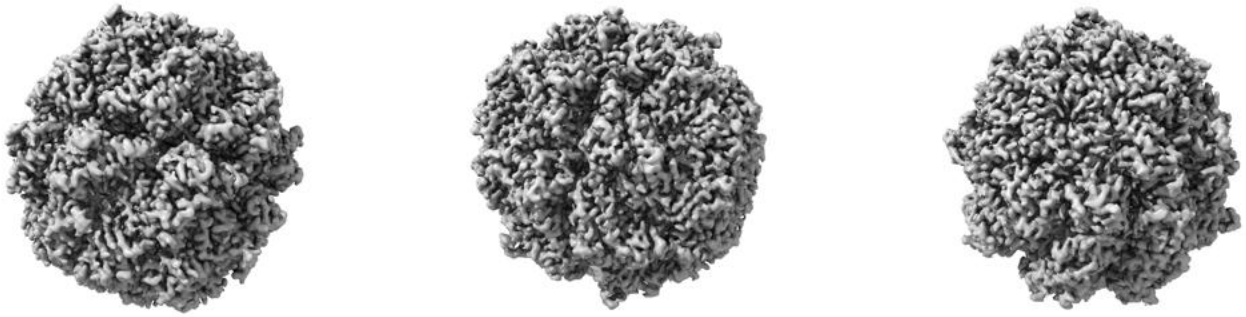


Z

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)

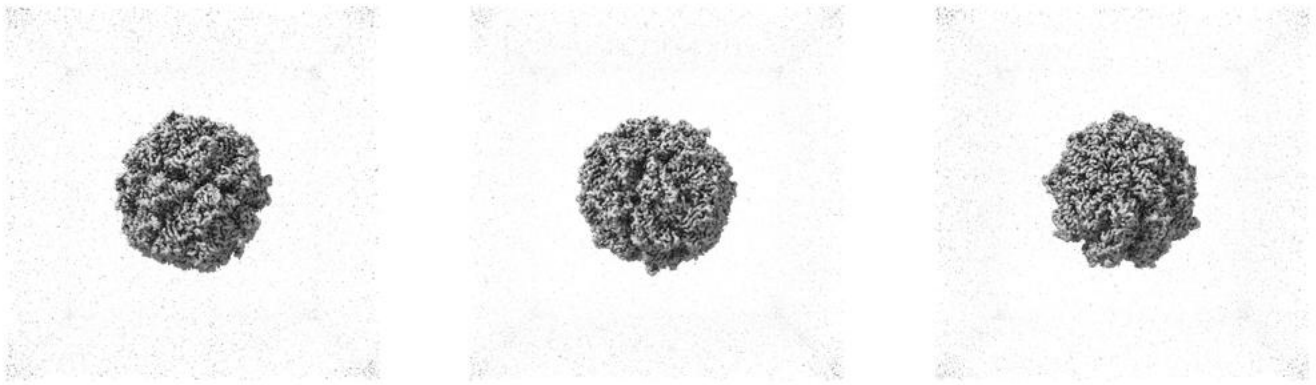
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.123. 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



X Y Z

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

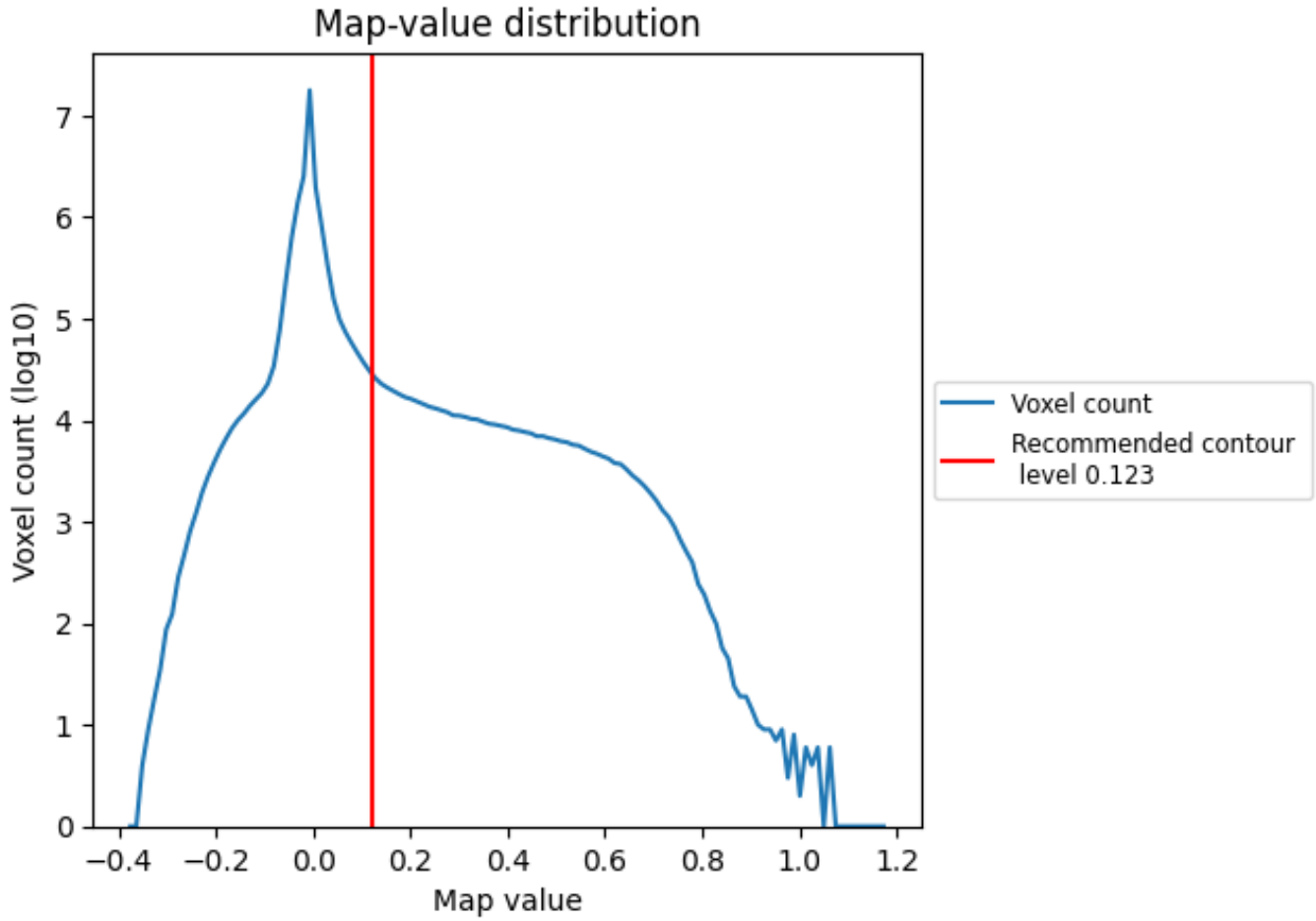
6.6 Mask visualisation (i)

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

7 Map analysis

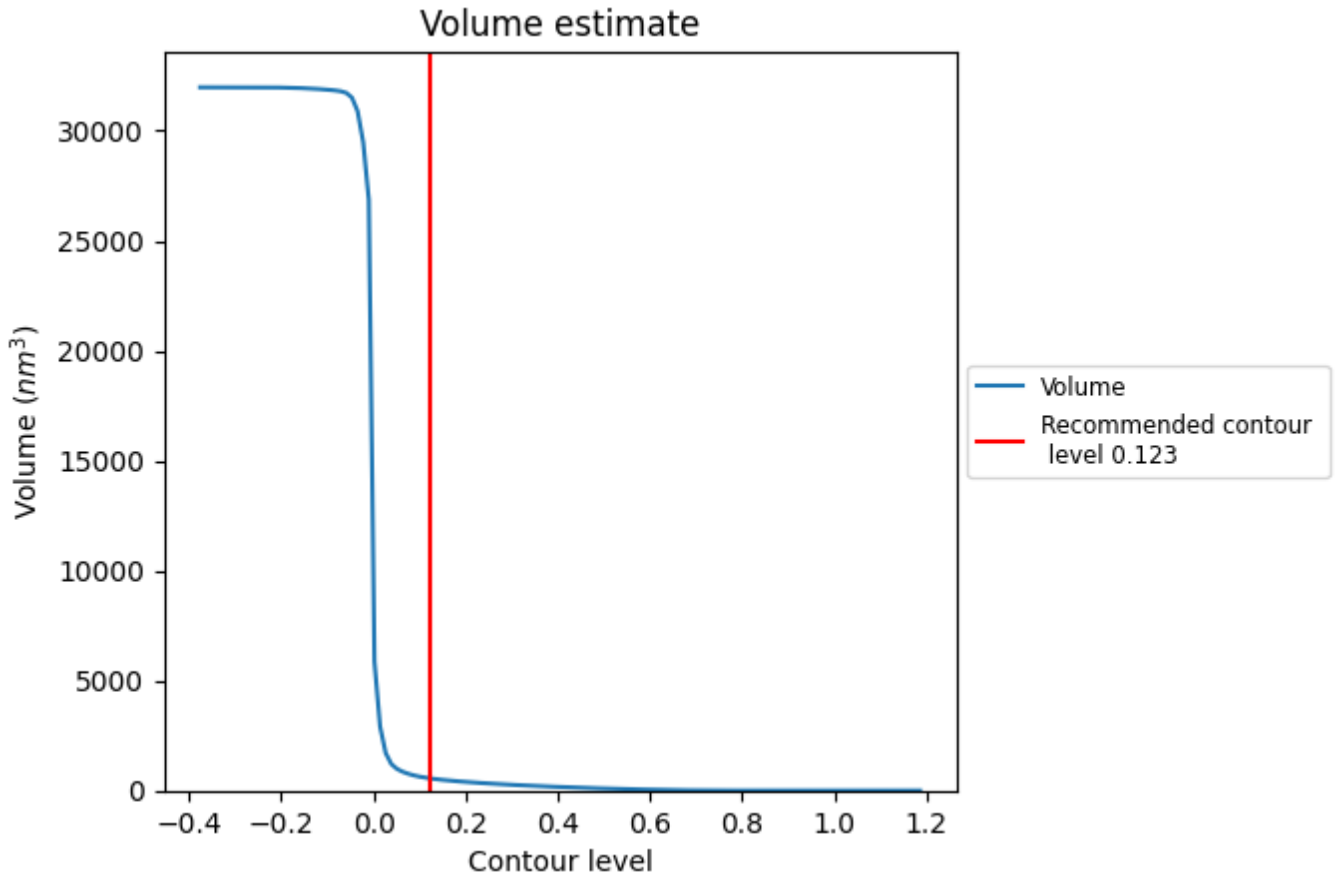
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

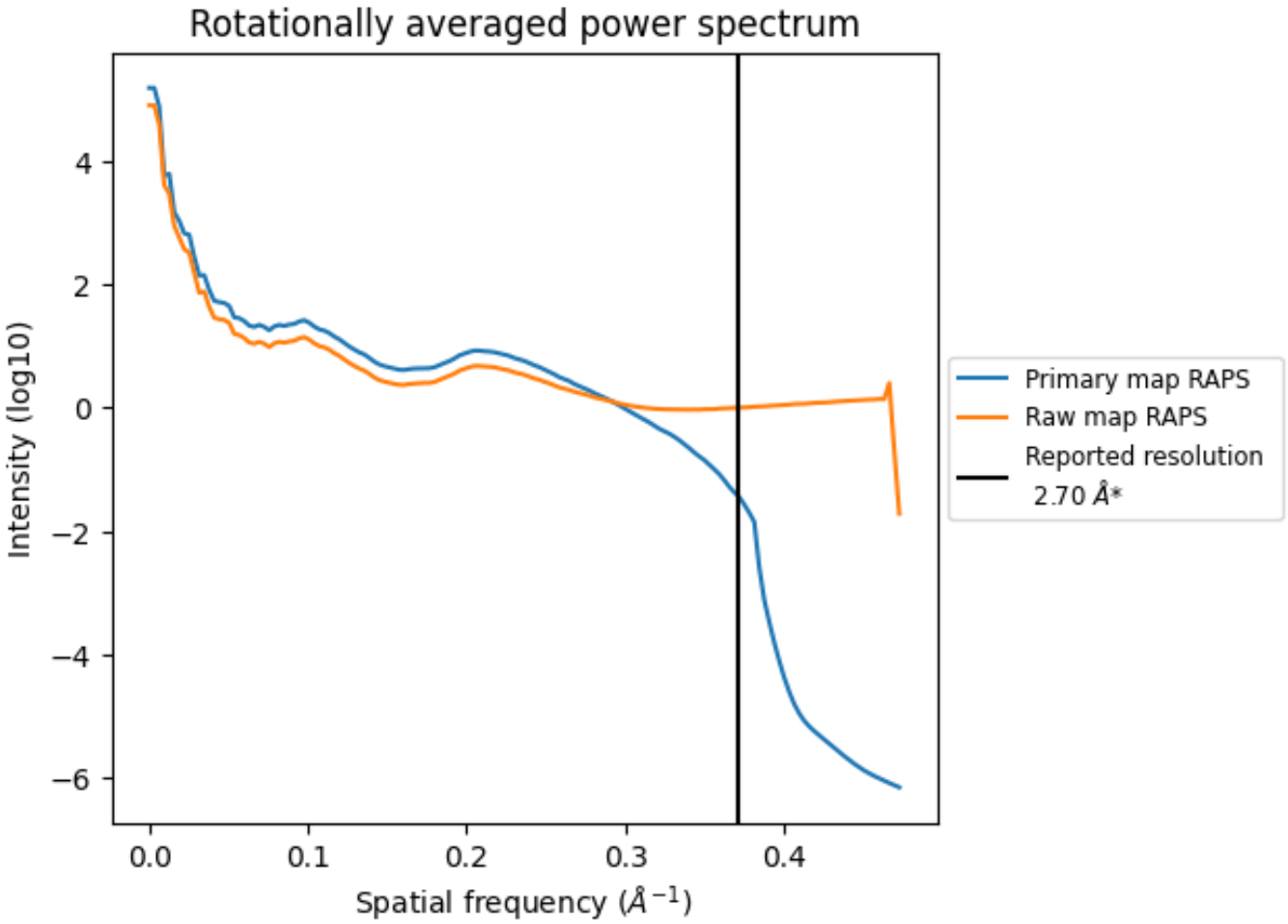
7.2 Volume estimate



The volume at the recommended contour level is 552 nm^3; this corresponds to an approximate mass of 499 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 (i)

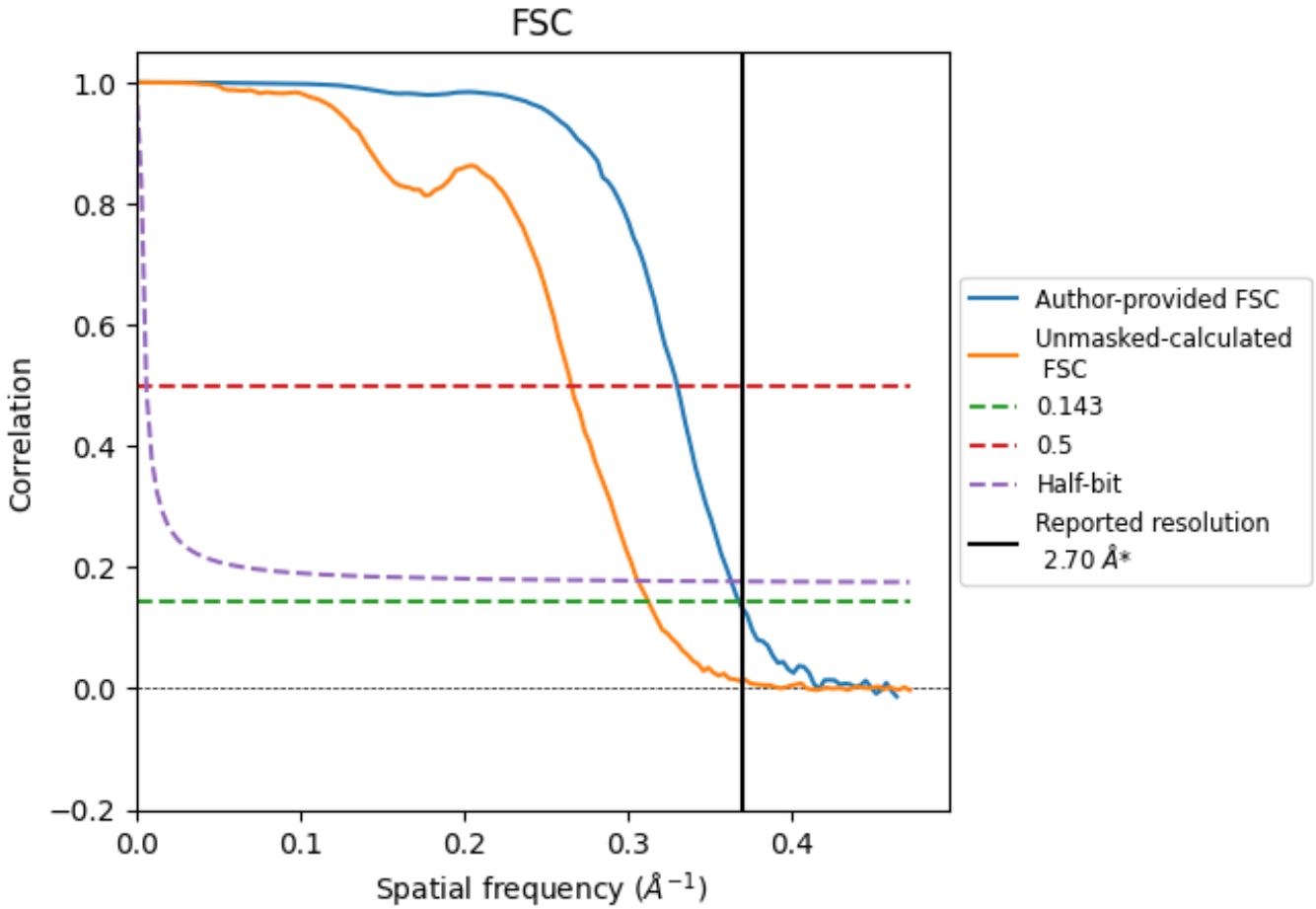


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

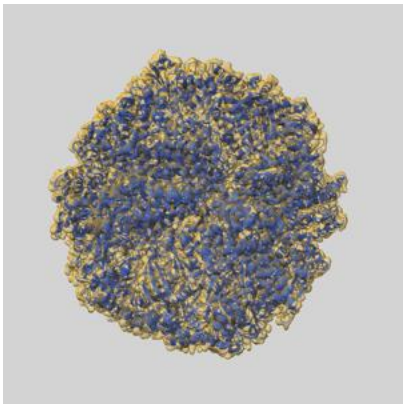
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	3.03	2.75
Unmasked-calculated*	3.19	3.76	3.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.19 differs from the reported value 2.7 by more than 10 %

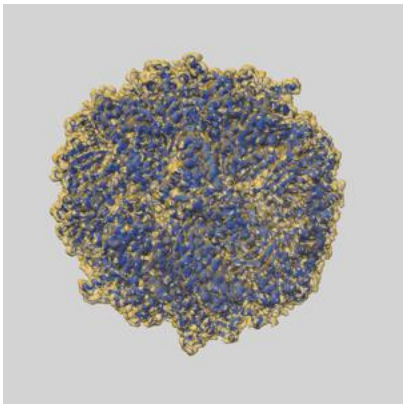
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40481 and PDB model 8SH9. Per-residue inclusion information can be found in section 3 on page 10.

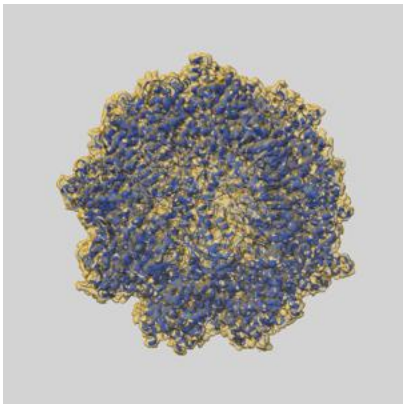
9.1 Map-model overlay



X



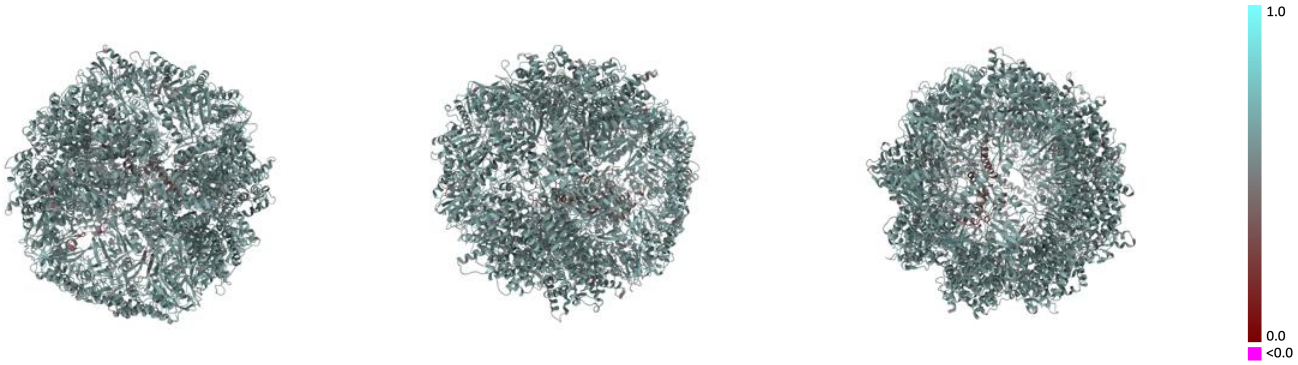
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.123 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.

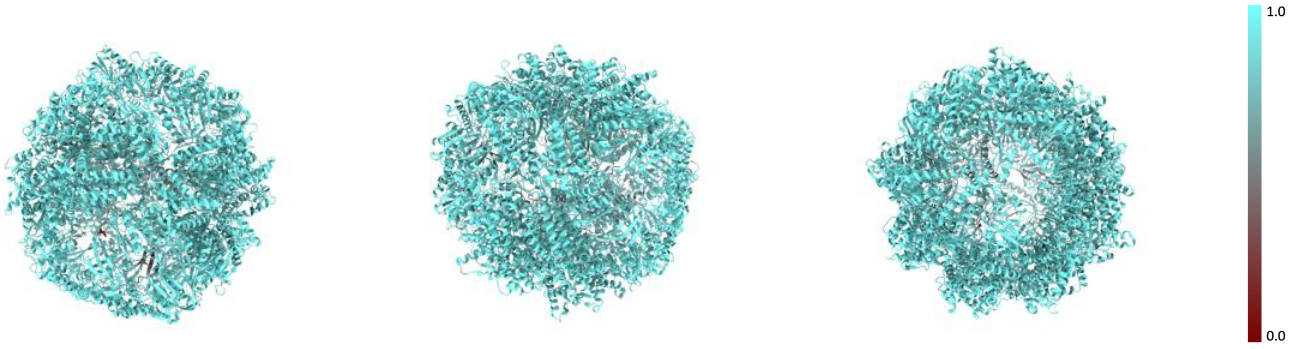
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

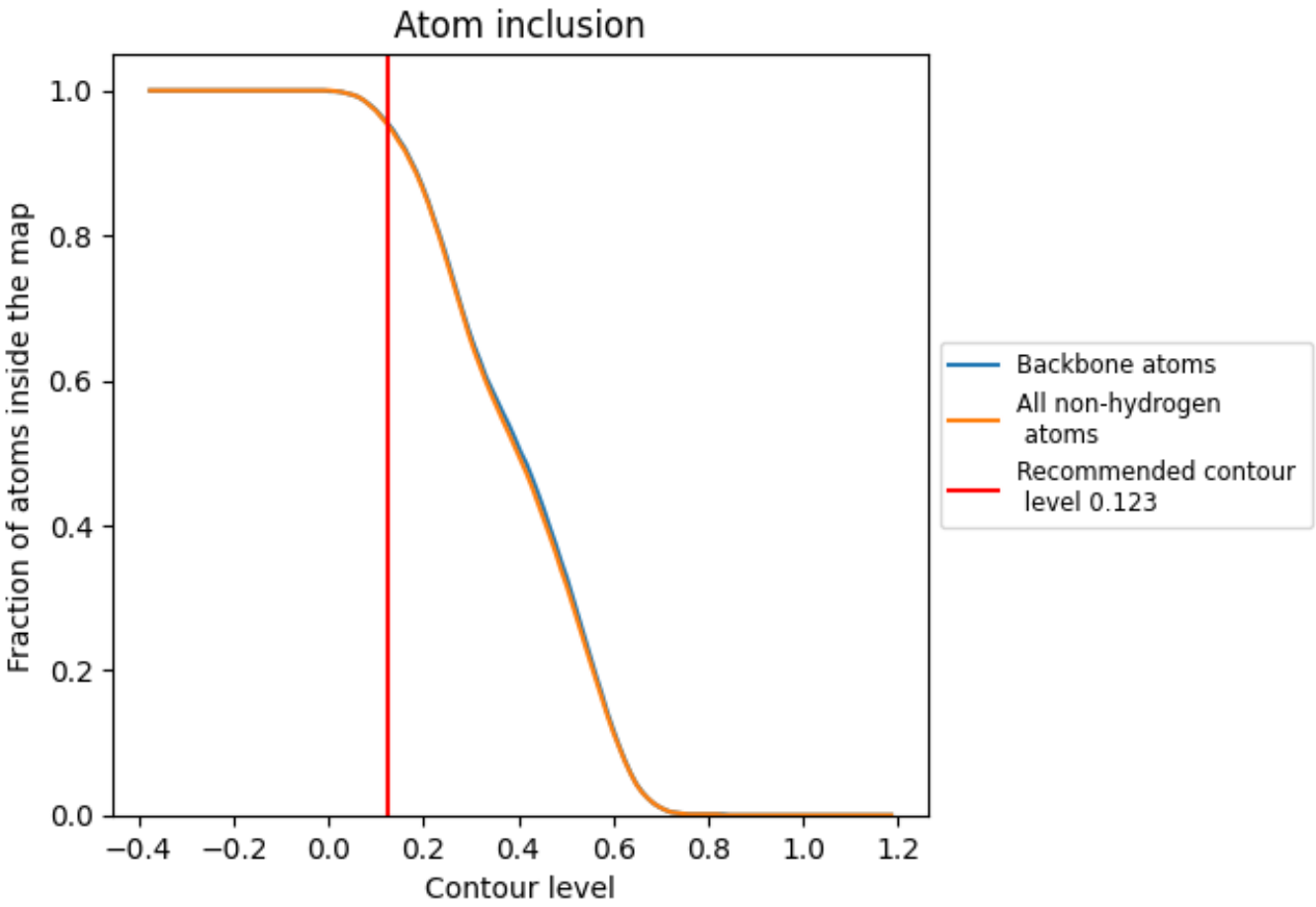
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.123).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.123) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9540	0.5780
A	0.9560	0.5730
B	0.9690	0.5880
D	0.9690	0.5840
E	0.9590	0.5830
G	0.9610	0.5840
H	0.9610	0.5850
N	0.4840	0.5110
P	0.7980	0.4120
Q	0.9500	0.5770
Z	0.9610	0.5820
a	0.9620	0.5850
b	0.9700	0.5900
d	0.9650	0.5840
e	0.9520	0.5780
g	0.9620	0.5880
h	0.9620	0.5860
q	0.9560	0.5810
z	0.9610	0.5810