



Full wwPDB EM Validation Report ⓘ

Apr 26, 2023 – 03:46 pm BST

PDB ID : 8APX
EMDB ID : EMD-15578
Title : CryoEM structure of the Chikungunya virus nsP1 capping pores in covalent complex with a 7GMP cap structure
Authors : Jones, R.; Hons, M.; Reguera, J.
Deposited on : 2022-08-10
Resolution : 3.20 Å(reported)
Based on initial model : 6Z0V

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.dev50
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

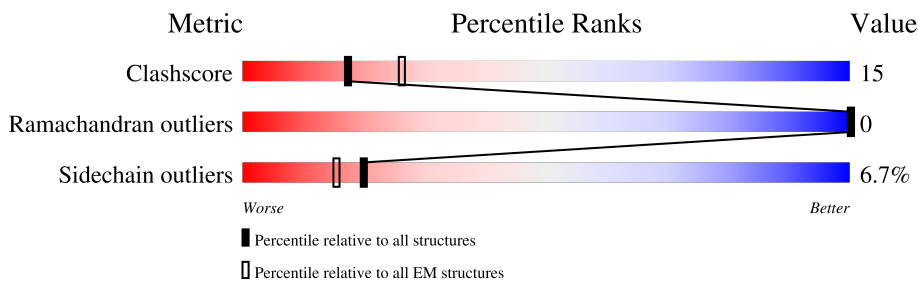
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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






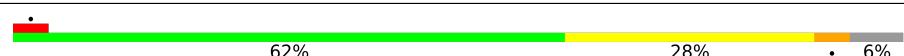
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	469	 63% 28% 6%
1	B	469	 60% 30% 6%
1	C	469	 64% 27% 6%
1	D	469	 64% 28% 6%
1	E	469	 63% 29% 6%
1	F	469	 62% 30% 6%
1	G	469	 59% 31% 6%
1	H	469	 61% 29% 6%

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Mol	Chain	Length	Quality of chain
1	I	469	 60% 30% 6%
1	J	469	 65% 26% 6%
1	K	469	 65% 26% 6%
1	L	469	 62% 28% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 41616 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 Polyprotein P1234.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	A	440	3441	2169	600	645	1	26	0	0
1	B	440	3441	2169	600	645	1	26	0	0
1	C	440	3441	2169	600	645	1	26	0	0
1	D	440	3441	2169	600	645	1	26	0	0
1	E	440	3441	2169	600	645	1	26	0	0
1	F	440	3441	2169	600	645	1	26	0	0
1	G	440	3441	2169	600	645	1	26	0	0
1	H	440	3441	2169	600	645	1	26	0	0
1	I	440	3441	2169	600	645	1	26	0	0
1	J	440	3441	2169	600	645	1	26	0	0
1	K	440	3441	2169	600	645	1	26	0	0
1	L	440	3441	2169	600	645	1	26	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

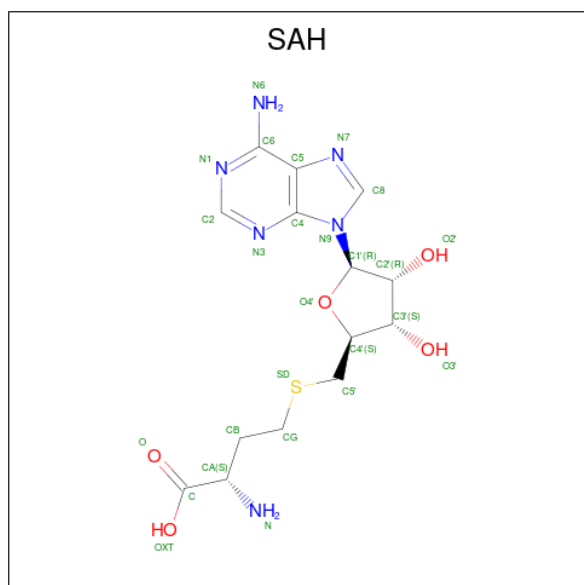
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	D	1	Total	Zn	0
			1	1	
2	E	1	Total	Zn	0
			1	1	
2	F	1	Total	Zn	0
			1	1	
2	G	1	Total	Zn	0
			1	1	
2	H	1	Total	Zn	0
			1	1	
2	I	1	Total	Zn	0
			1	1	
2	J	1	Total	Zn	0
			1	1	
2	K	1	Total	Zn	0
			1	1	
2	L	1	Total	Zn	0
			1	1	

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	B	1	Total	C	N	O	S	0
			26	14	6	5	1	

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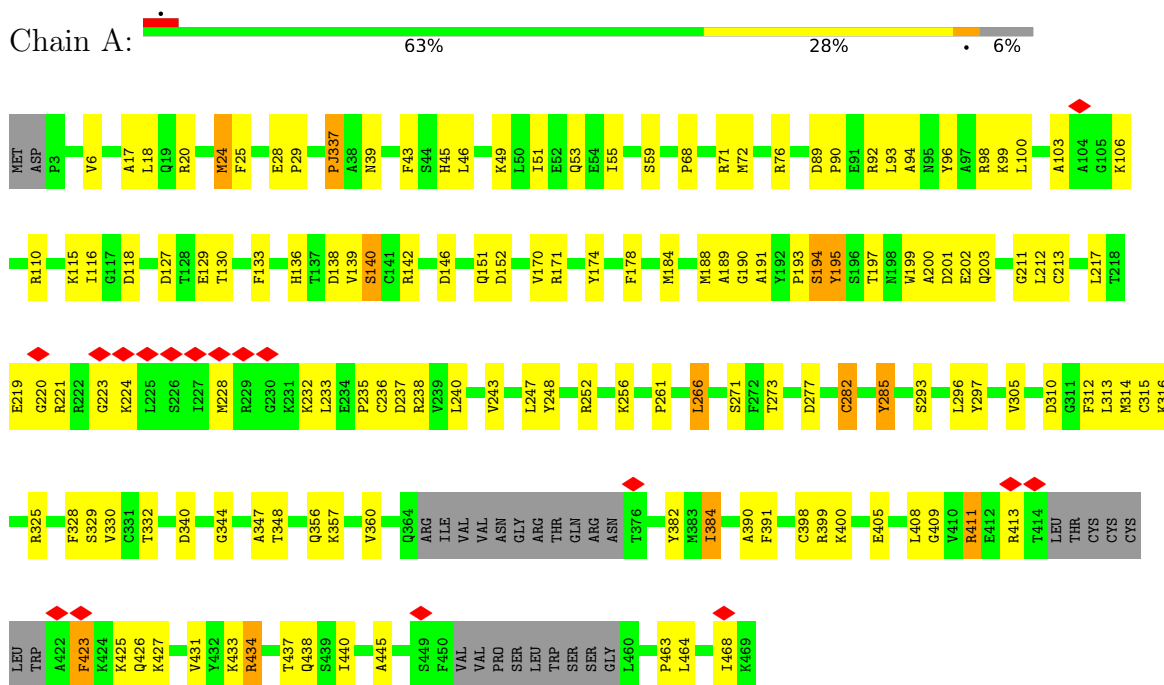
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Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	D	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	E	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	F	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	G	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	H	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	I	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	J	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	K	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	L	1	Total	C	N	O	S	0
			26	14	6	5	1	

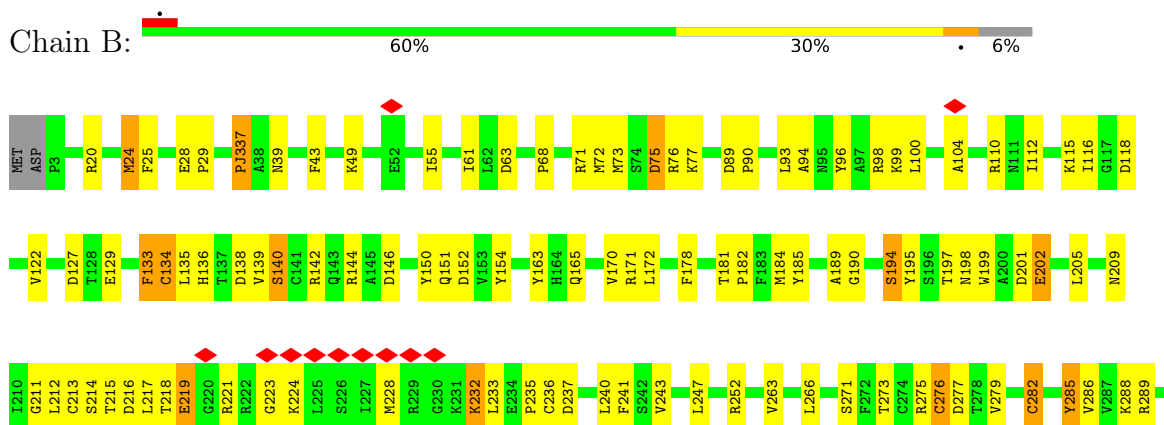
3 Residue-property plots

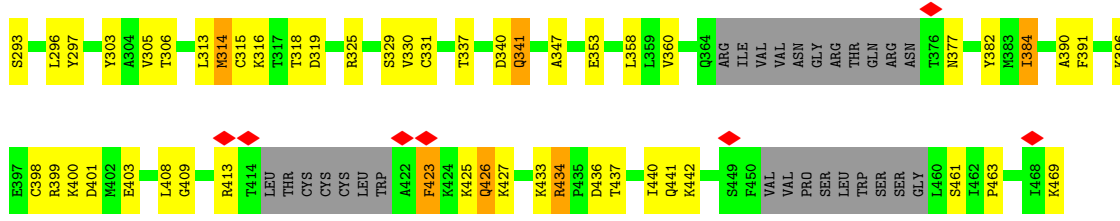
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Polyprotein P1234

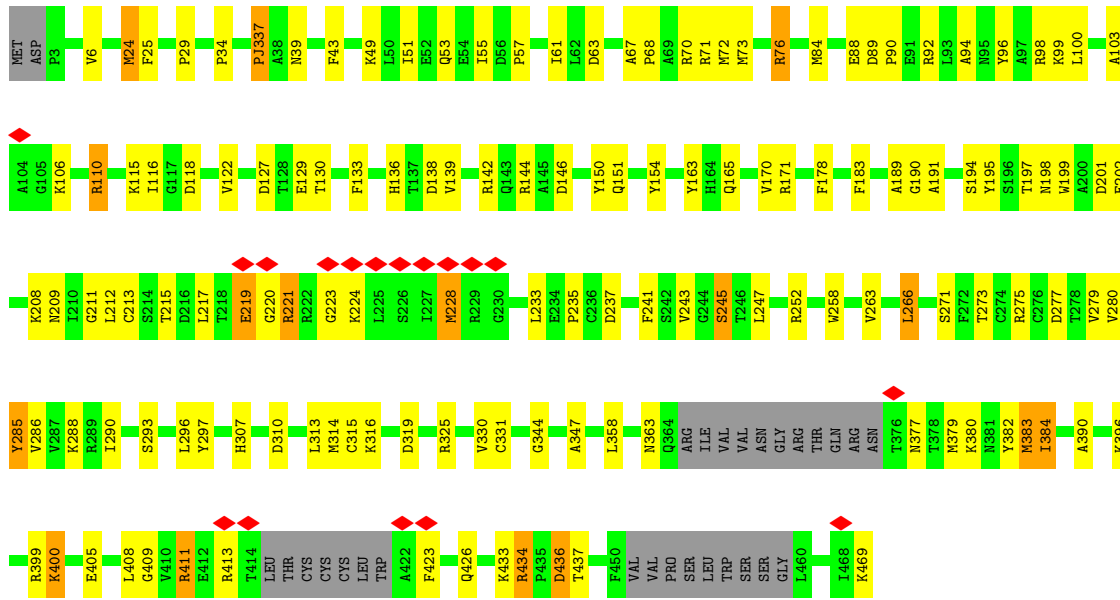


- Molecule 1: Polyprotein P1234

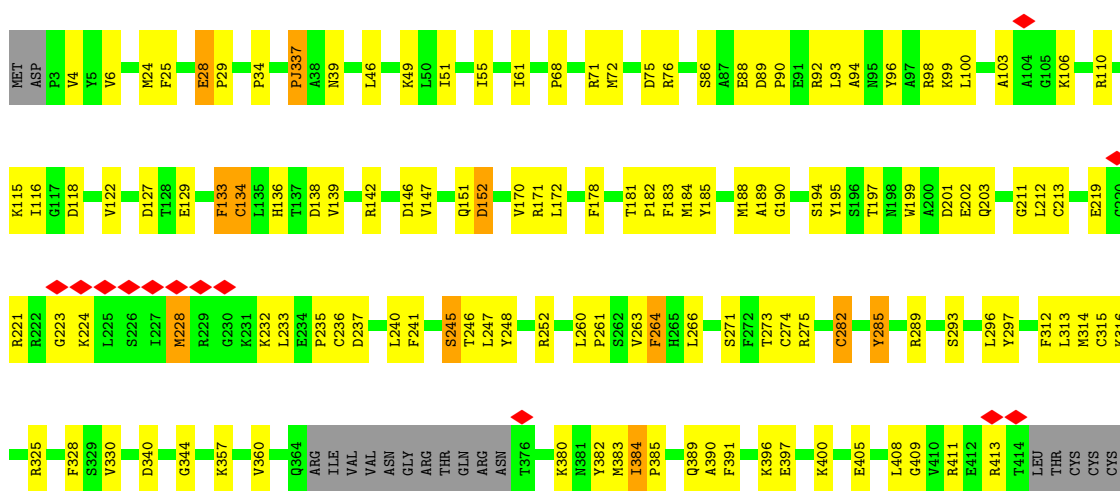


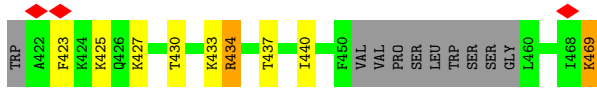


• Molecule 1: Polyprotein P1234

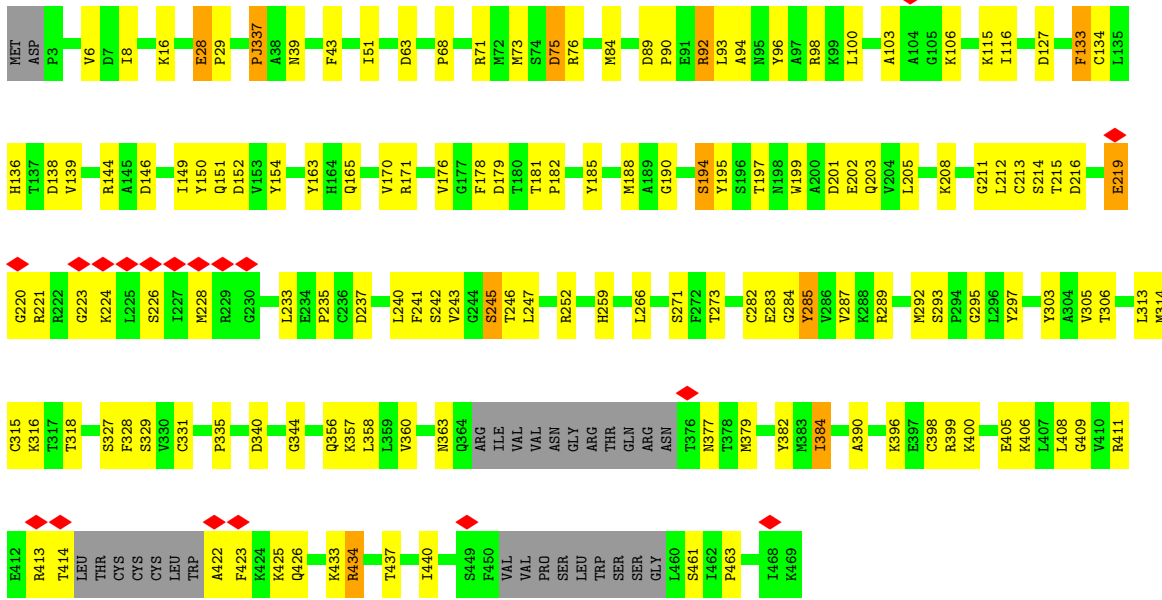


• Molecule 1: Polyprotein P1234

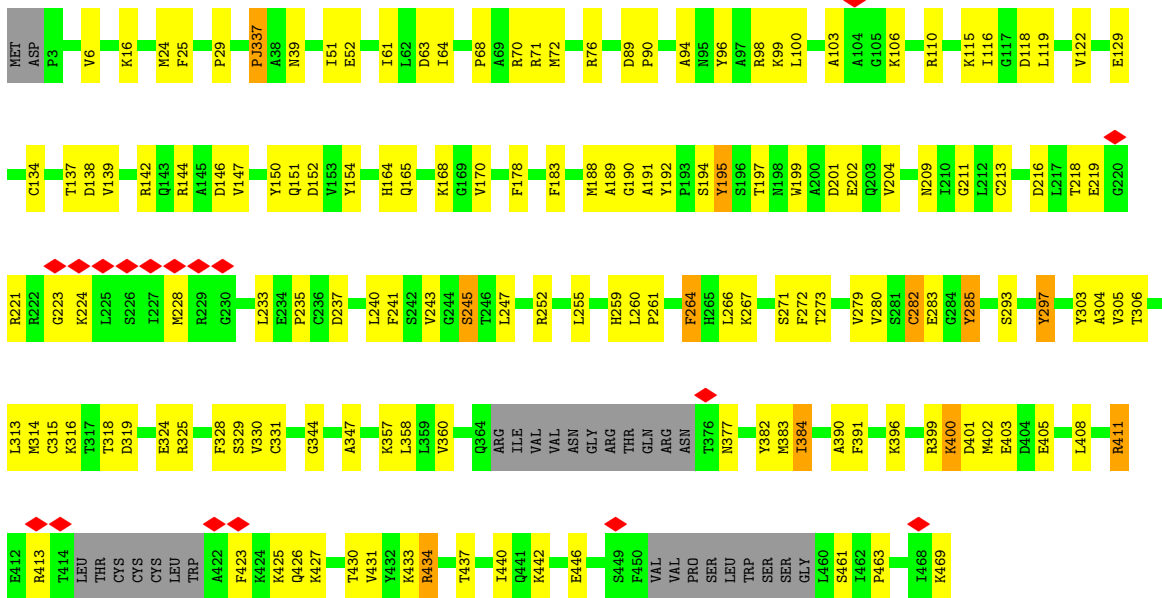




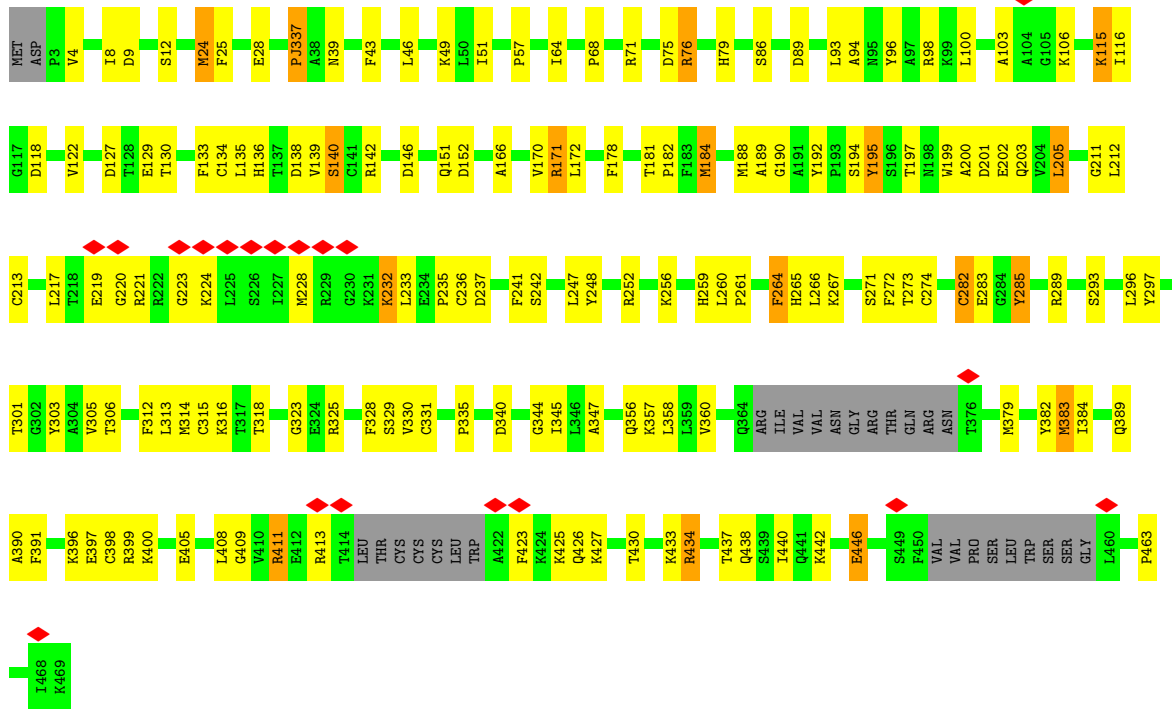
• Molecule 1: Polyprotein P1234



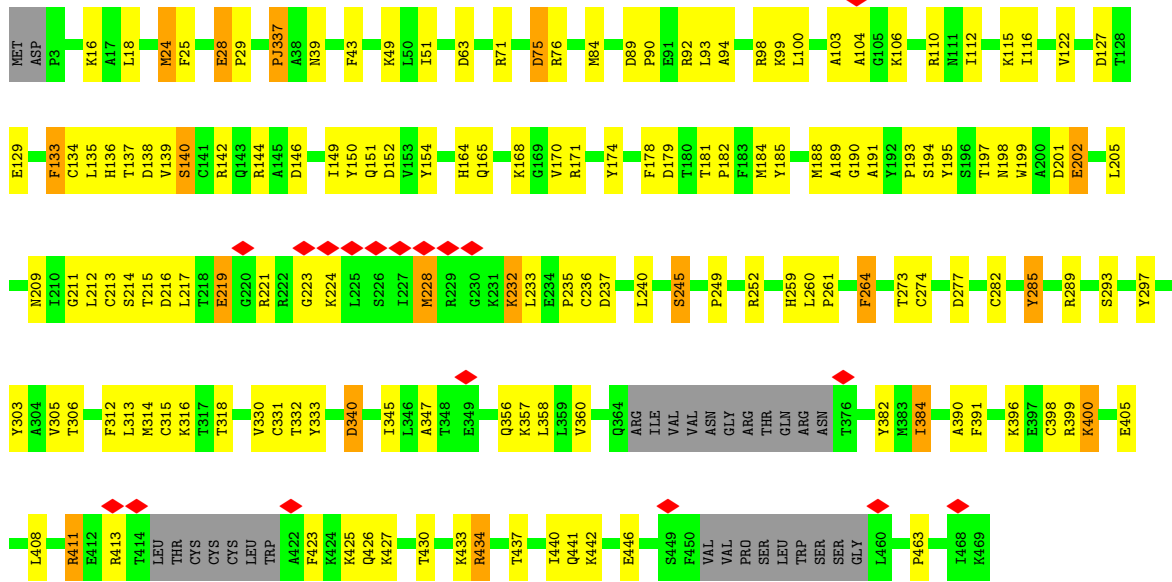
• Molecule 1: Polyprotein P1234



• Molecule 1: Polyprotein P1234

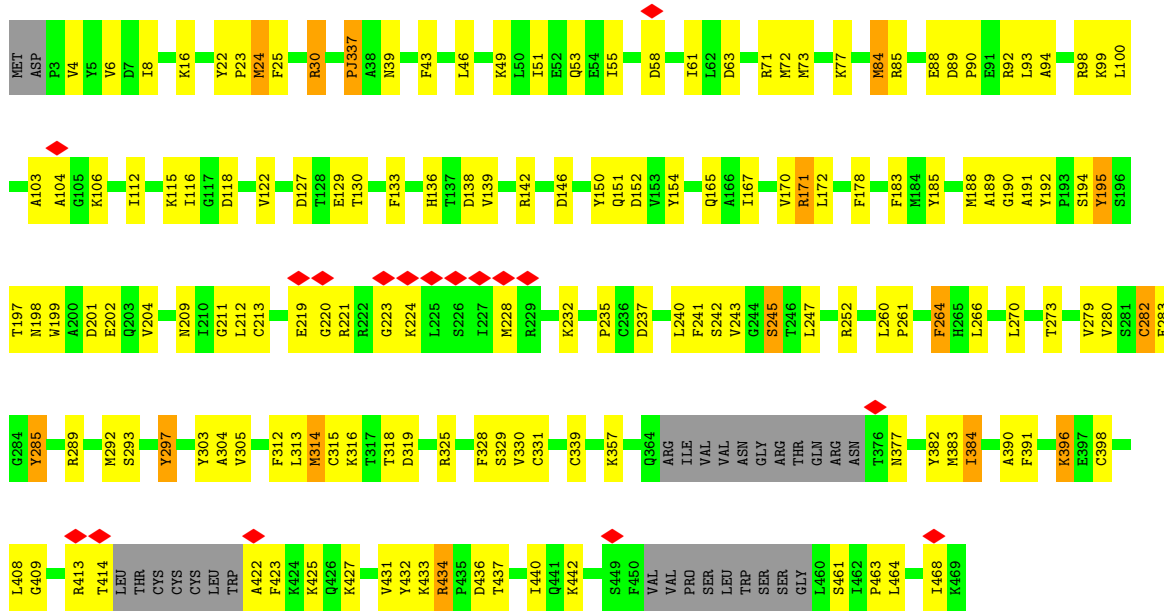


• Molecule 1: Polyprotein P1234

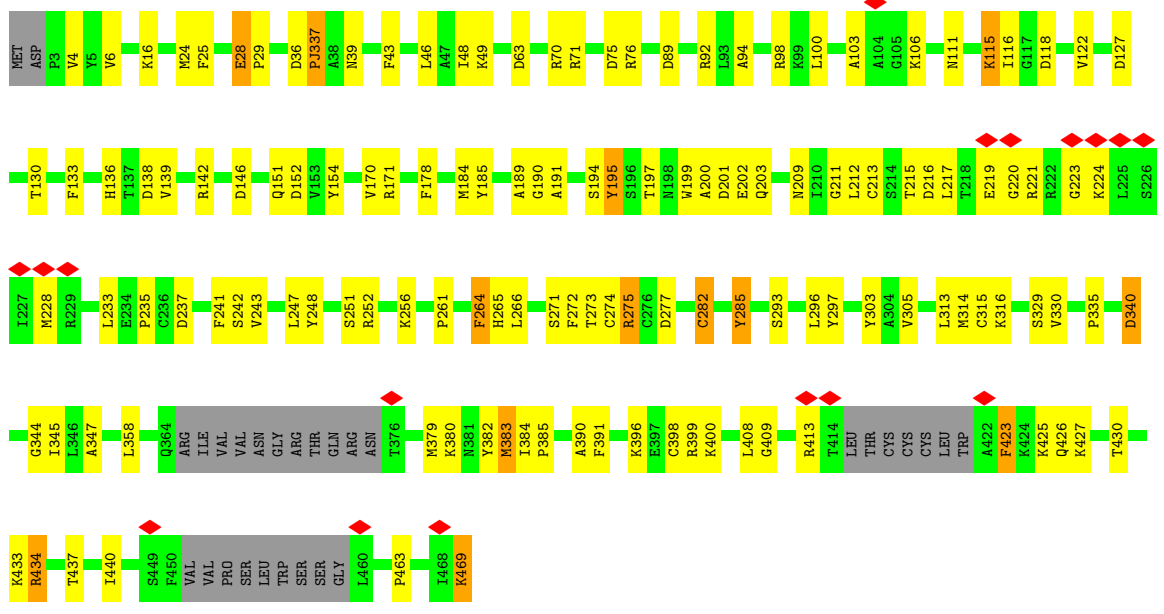


• Molecule 1: Polyprotein P1234

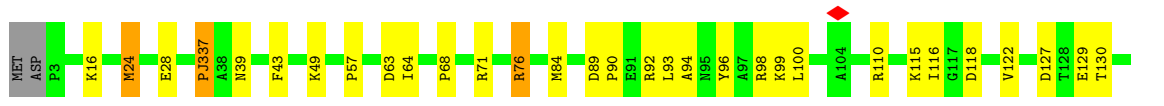


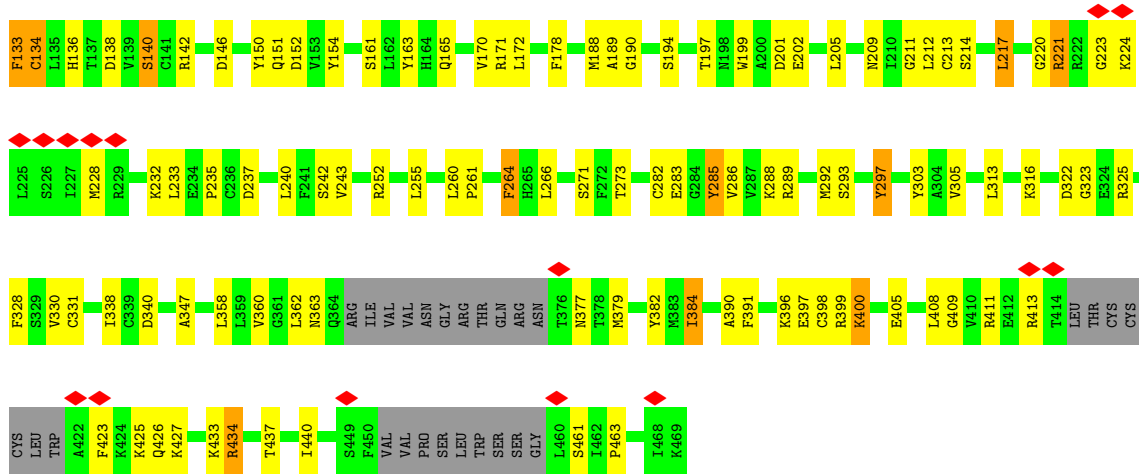


• Molecule 1: Polyprotein P1234

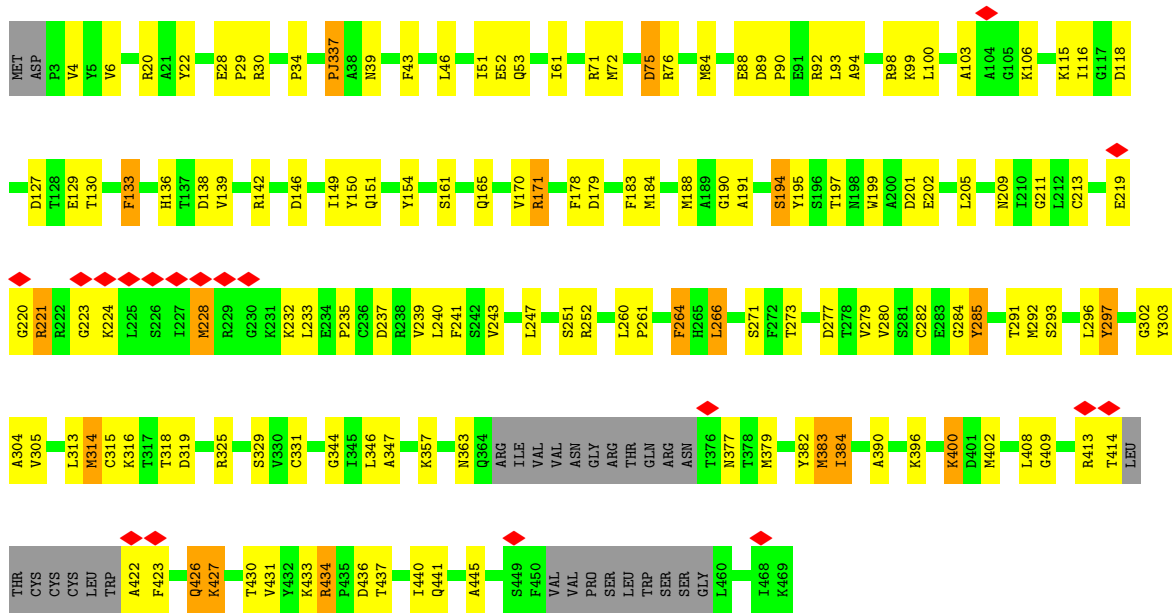


• Molecule 1: Polyprotein P1234





• Molecule 1: Polyprotein P1234



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C12	Depositor
Number of particles used	10758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.830	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.0576	Depositor
Map size (\AA)	307.80002, 307.80002, 307.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8550001, 0.8550001, 0.8550001	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PJ3, SAH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/3475	0.56	0/4705
1	B	0.27	0/3475	0.57	0/4705
1	C	0.27	0/3475	0.56	0/4705
1	D	0.27	0/3475	0.56	0/4705
1	E	0.27	0/3475	0.56	0/4705
1	F	0.26	0/3475	0.55	0/4705
1	G	0.26	0/3475	0.55	0/4705
1	H	0.27	0/3475	0.57	1/4705 (0.0%)
1	I	0.27	0/3475	0.57	0/4705
1	J	0.27	0/3475	0.56	1/4705 (0.0%)
1	K	0.26	0/3475	0.54	0/4705
1	L	0.27	0/3475	0.56	0/4705
All	All	0.27	0/41700	0.56	2/56460 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	2
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	15

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	340	ASP	CB-CG-OD1	5.30	123.07	118.30
1	J	340	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	384	ILE	Peptide
1	B	384	ILE	Peptide
1	B	426	GLN	Peptide
1	C	384	ILE	Peptide
1	D	384	ILE	Peptide
1	E	384	ILE	Peptide
1	F	384	ILE	Peptide
1	G	384	ILE	Peptide
1	G	426	GLN	Peptide
1	H	384	ILE	Peptide
1	I	384	ILE	Peptide
1	J	384	ILE	Peptide
1	K	384	ILE	Peptide
1	L	384	ILE	Peptide
1	L	426	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3441	0	3380	117	0
1	B	3441	0	3380	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3441	0	3380	124	0
1	D	3441	0	3380	117	0
1	E	3441	0	3380	125	0
1	F	3441	0	3380	135	0
1	G	3441	0	3380	131	0
1	H	3441	0	3380	133	0
1	I	3441	0	3380	136	0
1	J	3441	0	3380	112	0
1	K	3441	0	3380	115	0
1	L	3441	0	3380	123	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	26	0	19	2	0
3	B	26	0	19	2	0
3	C	26	0	19	4	0
3	D	26	0	19	2	0
3	E	26	0	19	3	0
3	F	26	0	19	3	0
3	G	26	0	19	2	0
3	H	26	0	19	2	0
3	I	26	0	19	2	0
3	J	26	0	19	2	0
3	K	26	0	19	3	0
3	L	26	0	19	3	0
All	All	41616	0	40788	1249	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 15.

All (1249) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:PJ3:C	1:E:37:PJ3:CA	1.86	1.53
1:L:37:PJ3:C	1:L:37:PJ3:CA	1.86	1.52
1:K:37:PJ3:C	1:K:37:PJ3:CA	1.86	1.52
1:D:37:PJ3:C	1:D:37:PJ3:CA	1.86	1.51
1:A:37:PJ3:C	1:A:37:PJ3:CA	1.86	1.51
1:G:37:PJ3:C	1:G:37:PJ3:CA	1.86	1.51
1:F:37:PJ3:C	1:F:37:PJ3:CA	1.86	1.51
1:B:37:PJ3:CA	1:B:37:PJ3:C	1.86	1.50
1:J:37:PJ3:C	1:J:37:PJ3:CA	1.86	1.50
1:C:37:PJ3:C	1:C:37:PJ3:CA	1.86	1.49
1:H:37:PJ3:C	1:H:37:PJ3:CA	1.86	1.49
1:I:37:PJ3:C	1:I:37:PJ3:CA	1.86	1.48
1:D:37:PJ3:C	1:D:37:PJ3:N	2.35	0.90
1:A:37:PJ3:C	1:A:37:PJ3:N	2.35	0.90
1:A:316:LYS:HE2	1:L:408:LEU:HD21	1.53	0.90
1:B:37:PJ3:C	1:B:37:PJ3:N	2.35	0.89
1:H:37:PJ3:C	1:H:37:PJ3:N	2.35	0.89
1:C:37:PJ3:C	1:C:37:PJ3:N	2.35	0.89
1:J:37:PJ3:C	1:J:37:PJ3:N	2.35	0.88
1:G:37:PJ3:C	1:G:37:PJ3:N	2.35	0.88
1:K:37:PJ3:C	1:K:37:PJ3:N	2.35	0.88
1:I:37:PJ3:C	1:I:37:PJ3:N	2.35	0.88
1:F:37:PJ3:C	1:F:37:PJ3:N	2.35	0.88
1:L:37:PJ3:C	1:L:37:PJ3:N	2.35	0.88
1:E:37:PJ3:C	1:E:37:PJ3:N	2.35	0.88
1:C:221:ARG:HD2	1:C:223:GLY:H	1.38	0.87
1:H:221:ARG:HD2	1:H:223:GLY:H	1.45	0.81
1:B:221:ARG:HD2	1:B:223:GLY:H	1.44	0.80
1:A:325:ARG:NH2	1:L:426:GLN:OE1	2.15	0.80
1:K:427:LYS:NZ	1:L:219:GLU:O	2.14	0.80
1:C:426:GLN:OE1	1:D:325:ARG:NH2	2.15	0.79
1:I:221:ARG:HD2	1:I:223:GLY:H	1.47	0.79
1:A:18:LEU:HD22	1:A:46:LEU:HD12	1.64	0.78
1:H:408:LEU:HB2	1:J:219:GLU:HB3	1.64	0.78
1:H:427:LYS:NZ	1:I:219:GLU:O	2.14	0.77
1:A:221:ARG:HD2	1:A:223:GLY:H	1.49	0.77
1:G:408:LEU:HB2	1:I:219:GLU:HB3	1.65	0.77
1:L:305:VAL:HG22	1:L:440:ILE:HG12	1.66	0.77
1:J:201:ASP:OD1	1:J:202:GLU:N	2.18	0.77
1:I:427:LYS:NZ	1:J:219:GLU:O	2.15	0.77
1:B:409:GLY:HA2	1:C:233:LEU:HB3	1.68	0.76
1:B:24:MET:HE1	1:C:34:PRO:HD3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ARG:HD2	1:D:223:GLY:H	1.51	0.76
1:K:305:VAL:HG22	1:K:440:ILE:HG12	1.66	0.75
1:B:427:LYS:NZ	1:C:219:GLU:O	2.16	0.75
1:F:305:VAL:HG22	1:F:440:ILE:HG12	1.67	0.75
1:C:73:MET:O	1:C:110:ARG:NH2	2.19	0.75
1:I:305:VAL:HG22	1:I:440:ILE:HG12	1.67	0.75
1:E:297:TYR:HD2	1:F:90:PRO:HG3	1.52	0.74
1:L:221:ARG:HD2	1:L:223:GLY:H	1.51	0.74
1:C:201:ASP:OD1	1:C:202:GLU:N	2.21	0.74
1:F:427:LYS:NZ	1:G:219:GLU:O	2.20	0.74
1:D:427:LYS:NZ	1:E:219:GLU:O	2.16	0.74
1:F:408:LEU:HB2	1:H:219:GLU:HB3	1.68	0.74
1:D:297:TYR:HD2	1:E:90:PRO:HG3	1.53	0.73
1:C:408:LEU:HB2	1:E:219:GLU:HB3	1.70	0.73
1:J:184:MET:HG2	1:J:256:LYS:HG3	1.70	0.73
1:D:273:THR:HG21	1:D:297:TYR:H	1.52	0.73
1:H:297:TYR:HD2	1:I:90:PRO:HG3	1.53	0.73
1:F:240:LEU:HD12	1:F:247:LEU:HD11	1.71	0.73
1:A:297:TYR:HD2	1:B:90:PRO:HG3	1.52	0.73
1:A:315:CYS:HB2	1:A:390:ALA:HB2	1.69	0.73
1:G:411:ARG:HH21	1:H:233:LEU:HD12	1.52	0.72
1:A:219:GLU:HB3	1:K:408:LEU:HB2	1.71	0.72
1:L:279:VAL:HG13	1:L:280:VAL:HG23	1.72	0.72
1:G:273:THR:HG21	1:G:297:TYR:H	1.53	0.72
1:F:347:ALA:O	1:F:399:ARG:NH2	2.23	0.71
1:F:426:GLN:OE1	1:G:325:ARG:NH2	2.23	0.71
1:F:279:VAL:HG13	1:F:280:VAL:HG23	1.73	0.71
1:J:315:CYS:HB2	1:J:390:ALA:HB2	1.71	0.71
1:B:201:ASP:OD1	1:B:202:GLU:N	2.23	0.71
1:C:24:MET:HE1	1:D:34:PRO:HD3	1.71	0.71
1:H:426:GLN:OE1	1:I:325:ARG:NH1	2.23	0.71
1:K:221:ARG:HH22	1:K:224:LYS:HB3	1.56	0.71
1:I:279:VAL:HG13	1:I:280:VAL:HG23	1.73	0.71
1:E:201:ASP:OD1	1:E:202:GLU:N	2.24	0.70
1:D:71:ARG:NH1	1:D:151:GLN:OE1	2.24	0.70
1:F:434:ARG:HB3	1:G:382:TYR:HB2	1.73	0.70
1:L:201:ASP:OD1	1:L:202:GLU:N	2.24	0.70
1:A:273:THR:HG21	1:A:297:TYR:H	1.57	0.70
1:G:433:LYS:NZ	1:H:213:CYS:SG	2.64	0.70
1:L:315:CYS:HB2	1:L:390:ALA:HB2	1.72	0.70
1:C:279:VAL:HG13	1:C:280:VAL:HG23	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:434:ARG:HB3	1:J:382:TYR:HB2	1.74	0.69
1:C:434:ARG:HB3	1:D:382:TYR:HB2	1.73	0.69
1:F:315:CYS:HB2	1:F:390:ALA:HB2	1.75	0.69
1:J:221:ARG:HD2	1:J:223:GLY:H	1.57	0.69
1:K:297:TYR:HD2	1:L:90:PRO:HG3	1.58	0.69
1:D:152:ASP:OD2	1:D:285:TYR:OH	2.09	0.69
1:D:433:LYS:NZ	1:E:213:CYS:SG	2.66	0.69
1:F:433:LYS:HA	1:F:433:LYS:HE3	1.75	0.69
1:I:315:CYS:HB2	1:I:390:ALA:HB2	1.73	0.69
1:J:63:ASP:OD2	1:J:71:ARG:NH1	2.25	0.69
1:J:409:GLY:HA2	1:K:233:LEU:HB3	1.74	0.69
1:L:383:MET:O	1:L:383:MET:HG2	1.93	0.69
1:B:197:THR:HB	1:B:243:VAL:HG12	1.76	0.68
1:J:425:LYS:NZ	1:K:322:ASP:O	2.26	0.68
1:A:71:ARG:NH1	1:A:151:GLN:OE1	2.27	0.68
1:K:347:ALA:O	1:K:399:ARG:NH2	2.27	0.68
1:G:195:TYR:OH	1:G:282:CYS:O	2.12	0.68
1:C:297:TYR:HD2	1:D:90:PRO:HG3	1.58	0.68
1:C:347:ALA:O	1:C:399:ARG:NH2	2.25	0.68
1:I:433:LYS:NZ	1:J:213:CYS:SG	2.67	0.68
1:I:437:THR:HG22	1:J:211:GLY:HA2	1.76	0.68
1:H:181:THR:HG21	1:H:306:THR:HG21	1.76	0.68
1:E:408:LEU:HB2	1:G:219:GLU:HB3	1.76	0.67
1:A:433:LYS:NZ	1:B:213:CYS:SG	2.68	0.67
1:D:201:ASP:OD1	1:D:202:GLU:N	2.27	0.67
1:G:25:PHE:HE2	1:G:49:LYS:HB3	1.60	0.67
1:A:347:ALA:O	1:A:399:ARG:NH2	2.26	0.67
1:A:382:TYR:HB2	1:L:434:ARG:HB3	1.75	0.67
1:C:383:MET:HG2	1:C:383:MET:O	1.95	0.67
1:I:260:LEU:HB3	1:I:264:PHE:HE2	1.60	0.67
1:E:181:THR:HG21	1:E:306:THR:HG21	1.75	0.67
1:E:434:ARG:HB3	1:F:382:TYR:HB2	1.76	0.67
1:L:260:LEU:HB3	1:L:264:PHE:HE2	1.59	0.67
1:A:90:PRO:HG3	1:L:297:TYR:HD2	1.58	0.67
1:A:408:LEU:HB2	1:C:219:GLU:HB3	1.77	0.67
1:B:408:LEU:HB2	1:D:219:GLU:HB3	1.75	0.67
1:H:315:CYS:HB2	1:H:390:ALA:HB2	1.75	0.67
1:H:433:LYS:NZ	1:I:213:CYS:SG	2.68	0.66
1:D:408:LEU:HG	1:E:316:LYS:HE3	1.77	0.66
1:A:273:THR:OG1	1:A:293:SER:OG	2.14	0.66
1:C:273:THR:OG1	1:C:293:SER:OG	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:433:LYS:NZ	1:G:213:CYS:SG	2.67	0.66
1:A:213:CYS:SG	1:L:433:LYS:NZ	2.68	0.66
1:K:437:THR:HG22	1:L:211:GLY:HA2	1.75	0.66
1:F:71:ARG:NH1	1:F:151:GLN:OE1	2.29	0.66
1:F:437:THR:HG22	1:G:211:GLY:HA2	1.78	0.66
1:B:263:VAL:HG12	1:B:275:ARG:HG3	1.77	0.66
1:B:273:THR:OG1	1:B:293:SER:OG	2.14	0.66
1:B:297:TYR:HD2	1:C:90:PRO:HG3	1.60	0.66
1:G:383:MET:O	1:G:383:MET:HG2	1.95	0.66
1:C:217:LEU:HD12	1:C:217:LEU:H	1.59	0.66
1:A:233:LEU:HB3	1:L:409:GLY:HA2	1.78	0.66
1:B:181:THR:HG21	1:B:306:THR:HG21	1.77	0.66
1:H:201:ASP:OD1	1:H:202:GLU:N	2.29	0.66
1:C:433:LYS:NZ	1:D:213:CYS:SG	2.69	0.66
1:J:195:TYR:OH	1:J:282:CYS:O	2.14	0.66
1:K:71:ARG:NH1	1:K:151:GLN:OE1	2.28	0.66
1:A:426:GLN:OE1	1:B:325:ARG:NH2	2.28	0.65
1:J:433:LYS:NZ	1:K:213:CYS:SG	2.69	0.65
1:G:200:ALA:HB3	1:G:212:LEU:HD22	1.78	0.65
1:D:469:LYS:HA	1:D:469:LYS:HE2	1.77	0.65
1:H:273:THR:OG1	1:H:293:SER:OG	2.14	0.65
1:F:137:THR:HG22	1:F:139:VAL:H	1.60	0.65
1:H:25:PHE:HE2	1:H:49:LYS:HB3	1.60	0.65
1:J:297:TYR:HD2	1:K:90:PRO:HG3	1.61	0.65
1:B:434:ARG:HB3	1:C:382:TYR:HB2	1.78	0.65
1:A:427:LYS:NZ	1:B:219:GLU:O	2.25	0.65
1:G:315:CYS:HB2	1:G:390:ALA:HB2	1.79	0.65
1:J:273:THR:HG21	1:J:297:TYR:H	1.61	0.65
1:L:71:ARG:NH1	1:L:151:GLN:OE1	2.30	0.65
1:D:408:LEU:HB2	1:F:219:GLU:HB3	1.79	0.65
1:I:195:TYR:OH	1:I:282:CYS:O	2.14	0.65
1:J:408:LEU:HB2	1:L:219:GLU:HB3	1.79	0.64
1:A:434:ARG:HB3	1:B:382:TYR:HB2	1.79	0.64
1:F:411:ARG:HH21	1:G:233:LEU:HD13	1.62	0.64
1:G:188:MET:HG3	1:G:328:PHE:HB2	1.80	0.64
1:J:100:LEU:HD12	1:J:116:ILE:HG12	1.79	0.64
1:G:4:VAL:HG11	1:G:46:LEU:HD11	1.80	0.64
1:H:434:ARG:HB3	1:I:382:TYR:HB2	1.80	0.64
1:I:425:LYS:HG3	1:I:427:LYS:HZ1	1.61	0.64
1:A:195:TYR:OH	1:A:282:CYS:O	2.15	0.64
1:J:398:CYS:SG	1:K:209:ASN:ND2	2.71	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLY:HA2	1:L:427:LYS:NZ	2.13	0.63
1:G:434:ARG:HB3	1:H:382:TYR:HB2	1.80	0.63
1:B:71:ARG:NH1	1:B:151:GLN:OE1	2.31	0.63
1:C:315:CYS:HB2	1:C:390:ALA:HB2	1.78	0.63
1:K:409:GLY:HA2	1:L:233:LEU:HB3	1.79	0.63
1:C:344:GLY:HA3	1:D:360:VAL:HG11	1.79	0.63
1:C:437:THR:HG22	1:D:211:GLY:HA2	1.80	0.63
1:D:437:THR:HG22	1:E:211:GLY:HA2	1.79	0.63
1:I:413:ARG:NH1	1:J:228:MET:O	2.30	0.63
1:H:413:ARG:NH1	1:I:228:MET:O	2.32	0.63
1:J:426:GLN:OE1	1:K:325:ARG:NH2	2.31	0.63
1:D:434:ARG:HB3	1:E:382:TYR:HB2	1.80	0.63
1:F:195:TYR:OH	1:F:282:CYS:O	2.16	0.63
1:G:71:ARG:NH1	1:G:151:GLN:OE1	2.31	0.63
1:G:437:THR:HG22	1:H:211:GLY:HA2	1.81	0.63
1:E:409:GLY:HA2	1:F:233:LEU:HB3	1.81	0.63
1:K:201:ASP:OD1	1:K:202:GLU:N	2.32	0.63
1:A:201:ASP:OD1	1:A:202:GLU:N	2.32	0.62
1:E:305:VAL:HG21	1:F:247:LEU:HB2	1.81	0.62
1:F:150:TYR:OH	1:F:165:GLN:OE1	2.09	0.62
1:F:413:ARG:NH1	1:G:228:MET:O	2.32	0.62
1:G:100:LEU:HD12	1:G:116:ILE:HG12	1.81	0.62
1:G:190:GLY:HA3	1:G:199:TRP:NE1	2.14	0.62
1:B:219:GLU:HB3	1:L:408:LEU:HB2	1.81	0.62
1:B:426:GLN:OE1	1:C:325:ARG:NE	2.32	0.62
1:C:71:ARG:NH1	1:C:151:GLN:OE1	2.32	0.62
1:D:240:LEU:HB3	1:D:247:LEU:HD11	1.81	0.62
1:E:273:THR:OG1	1:E:293:SER:OG	2.14	0.62
1:H:71:ARG:NH1	1:H:151:GLN:OE1	2.32	0.62
1:I:188:MET:HG3	1:I:328:PHE:HB2	1.80	0.62
1:K:24:MET:SD	1:K:24:MET:N	2.66	0.62
1:L:197:THR:HG22	1:L:243:VAL:HG13	1.82	0.62
1:G:413:ARG:NH1	1:H:228:MET:O	2.32	0.62
1:J:469:LYS:HE2	1:J:469:LYS:HA	1.82	0.62
1:A:211:GLY:HA2	1:L:437:THR:HG22	1.80	0.62
1:G:201:ASP:OD1	1:G:202:GLU:N	2.33	0.62
1:J:434:ARG:HB3	1:K:382:TYR:HB2	1.80	0.62
1:C:413:ARG:NH1	1:D:228:MET:O	2.33	0.62
1:H:347:ALA:O	1:H:399:ARG:NH2	2.33	0.62
1:C:263:VAL:HG12	1:C:275:ARG:HG3	1.82	0.61
1:L:273:THR:OG1	1:L:293:SER:OG	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:71:ARG:NH1	1:I:151:GLN:OE1	2.34	0.61
1:F:344:GLY:HA3	1:G:360:VAL:HG11	1.81	0.61
1:K:37:PJ3:C	1:K:37:PJ3:CB	2.78	0.61
1:D:344:GLY:HA3	1:E:360:VAL:HG11	1.82	0.61
1:I:37:PJ3:C	1:I:37:PJ3:CB	2.78	0.61
1:A:437:THR:HG22	1:B:211:GLY:HA2	1.81	0.61
1:I:100:LEU:HD12	1:I:116:ILE:HG12	1.83	0.61
1:A:313:LEU:HD22	1:A:390:ALA:HB1	1.82	0.61
1:H:37:PJ3:C	1:H:37:PJ3:CB	2.77	0.61
1:H:423:PHE:O	1:I:224:LYS:NZ	2.33	0.61
1:J:437:THR:HG22	1:K:211:GLY:HA2	1.82	0.61
1:L:43:PHE:CE1	1:L:285:TYR:HB3	2.36	0.61
1:C:37:PJ3:C	1:C:37:PJ3:CB	2.78	0.60
1:E:437:THR:HG22	1:F:211:GLY:HA2	1.81	0.60
1:B:413:ARG:NH1	1:C:228:MET:O	2.34	0.60
1:G:423:PHE:O	1:H:224:LYS:NZ	2.33	0.60
1:J:37:PJ3:C	1:J:37:PJ3:CB	2.78	0.60
1:K:433:LYS:NZ	1:L:213:CYS:O	2.34	0.60
1:E:205:LEU:HD11	1:E:240:LEU:HD12	1.83	0.60
1:I:273:THR:OG1	1:I:293:SER:OG	2.19	0.60
1:H:37:PJ3:O2'	1:H:285:TYR:OH	2.18	0.60
1:L:100:LEU:HD12	1:L:116:ILE:HG12	1.83	0.60
1:A:413:ARG:NH1	1:B:228:MET:O	2.33	0.60
1:D:37:PJ3:C	1:D:37:PJ3:CB	2.77	0.60
1:D:340:ASP:OD2	1:E:377:ASN:ND2	2.32	0.60
1:E:413:ARG:NH1	1:F:228:MET:O	2.34	0.60
1:F:37:PJ3:C	1:F:37:PJ3:CB	2.77	0.60
1:I:146:ASP:O	1:I:171:ARG:N	2.32	0.60
1:A:423:PHE:O	1:B:224:LYS:NZ	2.33	0.60
1:E:144:ARG:NH1	1:E:144:ARG:HB2	2.17	0.60
1:I:315:CYS:SG	1:I:316:LYS:N	2.74	0.60
1:I:408:LEU:HD21	1:J:316:LYS:HE2	1.83	0.60
1:L:37:PJ3:C	1:L:37:PJ3:CB	2.78	0.60
1:A:340:ASP:OD2	1:B:377:ASN:ND2	2.25	0.60
1:A:360:VAL:HG11	1:L:344:GLY:HA3	1.82	0.60
1:C:408:LEU:HD21	1:D:316:LYS:HE2	1.82	0.60
1:E:37:PJ3:C	1:E:37:PJ3:CB	2.77	0.59
1:D:409:GLY:HA2	1:E:233:LEU:HB3	1.82	0.59
1:F:100:LEU:HD12	1:F:116:ILE:HG12	1.85	0.59
1:A:100:LEU:HD12	1:A:116:ILE:HG12	1.83	0.59
1:E:406:LYS:HE3	1:F:325:ARG:HD2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:HD12	1:C:116:ILE:HG12	1.85	0.59
1:H:146:ASP:HB2	1:H:171:ARG:HH11	1.66	0.59
1:H:261:PRO:HD2	1:H:264:PHE:HD1	1.66	0.59
1:A:344:GLY:HA3	1:B:360:VAL:HG11	1.84	0.59
1:D:423:PHE:O	1:E:224:LYS:NZ	2.35	0.59
1:E:315:CYS:HB2	1:E:390:ALA:HB2	1.85	0.59
1:F:402:MET:SD	1:G:389:GLN:NE2	2.75	0.59
1:K:413:ARG:NH1	1:L:228:MET:O	2.35	0.59
1:A:305:VAL:HG22	1:A:440:ILE:HG12	1.83	0.59
1:E:273:THR:HG1	1:E:293:SER:HG	1.48	0.59
1:G:221:ARG:HD2	1:G:223:GLY:H	1.68	0.59
1:K:100:LEU:HD12	1:K:116:ILE:HG12	1.84	0.59
1:K:146:ASP:O	1:K:171:ARG:N	2.34	0.59
1:B:423:PHE:O	1:C:224:LYS:NZ	2.36	0.59
1:B:24:MET:SD	1:B:24:MET:N	2.75	0.59
1:C:469:LYS:HE2	1:C:469:LYS:HA	1.83	0.59
1:F:273:THR:OG1	1:F:293:SER:OG	2.18	0.59
1:J:313:LEU:HD22	1:J:390:ALA:HB1	1.85	0.59
1:B:37:PJ3:C	1:B:37:PJ3:CB	2.77	0.58
1:H:190:GLY:HA3	1:H:199:TRP:NE1	2.18	0.58
1:A:184:MET:HG2	1:A:256:LYS:HG3	1.84	0.58
1:C:190:GLY:HA3	1:C:199:TRP:NE1	2.19	0.58
1:C:405:GLU:HA	1:D:318:THR:HG21	1.85	0.58
1:B:437:THR:HG22	1:C:211:GLY:HA2	1.84	0.58
1:E:71:ARG:NH1	1:E:151:GLN:OE1	2.36	0.58
1:F:423:PHE:O	1:G:224:LYS:NZ	2.35	0.58
1:G:37:PJ3:C	1:G:37:PJ3:CB	2.78	0.58
1:A:247:LEU:HB2	1:L:305:VAL:HG21	1.84	0.58
1:B:315:CYS:SG	1:B:316:LYS:N	2.77	0.58
1:H:260:LEU:HB3	1:H:264:PHE:HE1	1.69	0.58
1:B:144:ARG:NH1	1:B:144:ARG:HB2	2.19	0.58
1:D:195:TYR:OH	1:D:282:CYS:O	2.17	0.58
1:F:24:MET:HG3	1:F:25:PHE:CD1	2.39	0.58
1:F:305:VAL:HG21	1:G:247:LEU:HB2	1.86	0.58
1:I:436:ASP:OD1	1:J:380:LYS:NZ	2.30	0.58
1:K:340:ASP:OD2	1:L:377:ASN:ND2	2.35	0.58
1:L:261:PRO:HD2	1:L:264:PHE:HD2	1.68	0.58
1:A:228:MET:O	1:L:413:ARG:NH1	2.35	0.58
1:H:437:THR:HG22	1:I:211:GLY:HA2	1.85	0.58
1:K:261:PRO:HD2	1:K:264:PHE:HD2	1.68	0.58
1:A:37:PJ3:C	1:A:37:PJ3:CB	2.78	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:GLY:HA3	1:D:199:TRP:NE1	2.18	0.58
1:H:146:ASP:HB2	1:H:171:ARG:NH1	2.19	0.58
1:B:75:ASP:OD1	1:B:75:ASP:N	2.37	0.58
1:C:423:PHE:O	1:D:224:LYS:NZ	2.36	0.58
1:J:305:VAL:HG22	1:J:440:ILE:HG12	1.84	0.58
1:G:37:PJ3:O2'	1:G:285:TYR:OH	2.22	0.57
1:G:305:VAL:HG22	1:G:440:ILE:HG12	1.86	0.57
1:J:190:GLY:HA3	1:J:199:TRP:NE1	2.20	0.57
1:K:150:TYR:OH	1:K:165:GLN:OE1	2.11	0.57
1:G:347:ALA:O	1:G:399:ARG:NH2	2.38	0.57
1:B:20:ARG:HG3	1:B:20:ARG:HH11	1.69	0.57
1:C:208:LYS:HG3	1:C:215:THR:HG21	1.86	0.57
1:D:115:LYS:H	1:D:115:LYS:HD2	1.70	0.57
1:I:313:LEU:HD22	1:I:390:ALA:HB1	1.85	0.57
1:J:39:ASN:ND2	1:J:194:SER:O	2.36	0.57
1:C:24:MET:SD	1:C:24:MET:N	2.77	0.57
1:C:146:ASP:O	1:C:171:ARG:N	2.32	0.57
1:E:340:ASP:OD2	1:F:377:ASN:ND2	2.36	0.57
1:G:184:MET:HG2	1:G:256:LYS:HG3	1.85	0.57
1:I:4:VAL:HG11	1:I:46:LEU:HD11	1.86	0.57
1:I:24:MET:HE3	1:I:24:MET:H	1.68	0.57
1:J:347:ALA:O	1:J:399:ARG:NH2	2.38	0.57
1:E:150:TYR:OH	1:E:165:GLN:OE1	2.11	0.57
1:K:115:LYS:H	1:K:115:LYS:HD2	1.70	0.57
1:B:279:VAL:HG21	1:B:289:ARG:HD3	1.87	0.57
1:I:39:ASN:ND2	1:I:194:SER:O	2.37	0.57
1:A:409:GLY:HA2	1:B:233:LEU:HB3	1.87	0.57
1:B:63:ASP:OD2	1:B:71:ARG:NE	2.33	0.57
1:H:273:THR:HG21	1:H:297:TYR:H	1.69	0.57
1:J:146:ASP:O	1:J:171:ARG:N	2.36	0.57
1:G:79:HIS:NE2	1:G:134:CYS:HB2	2.19	0.56
1:J:200:ALA:HB3	1:J:212:LEU:HD22	1.87	0.56
1:L:51:ILE:HG13	1:L:149:ILE:HD11	1.87	0.56
1:L:115:LYS:H	1:L:115:LYS:HD2	1.70	0.56
1:B:315:CYS:HB2	1:B:390:ALA:HB2	1.87	0.56
1:L:273:THR:HG1	1:L:293:SER:HG	1.52	0.56
1:A:39:ASN:ND2	1:A:194:SER:O	2.38	0.56
1:B:89:ASP:OD1	3:B:1002:SAH:O3'	2.23	0.56
1:C:313:LEU:HD22	1:C:390:ALA:HB1	1.87	0.56
1:D:100:LEU:HD12	1:D:116:ILE:HG12	1.87	0.56
1:I:43:PHE:CE2	1:I:285:TYR:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:305:VAL:HG21	1:L:247:LEU:HB2	1.87	0.56
1:E:176:VAL:HG12	1:E:287:VAL:HG13	1.87	0.56
1:F:260:LEU:HB3	1:F:264:PHE:HE1	1.69	0.56
1:K:384:ILE:O	1:K:384:ILE:HG13	2.05	0.56
1:G:398:CYS:SG	1:H:209:ASN:ND2	2.79	0.56
1:I:383:MET:O	1:I:383:MET:HG3	2.06	0.56
1:J:89:ASP:OD1	3:J:1002:SAH:O3'	2.21	0.56
1:L:271:SER:HB2	1:L:296:LEU:HD13	1.87	0.56
1:D:39:ASN:ND2	1:D:194:SER:O	2.39	0.56
1:F:469:LYS:HE2	1:F:469:LYS:HA	1.88	0.56
1:K:408:LEU:HD21	1:L:316:LYS:HE2	1.88	0.56
1:K:425:LYS:HG3	1:K:427:LYS:HZ1	1.70	0.56
1:B:436:ASP:OD2	1:C:380:LYS:NZ	2.36	0.56
1:C:144:ARG:HB2	1:C:144:ARG:NH1	2.21	0.56
1:D:413:ARG:NH1	1:E:228:MET:O	2.36	0.56
1:F:64:ILE:HD12	1:F:138:ASP:HB3	1.87	0.56
1:K:423:PHE:O	1:L:224:LYS:NZ	2.38	0.56
1:E:100:LEU:HD12	1:E:116:ILE:HG12	1.88	0.56
1:E:190:GLY:HA3	1:E:199:TRP:NE1	2.21	0.56
1:I:190:GLY:HA3	1:I:199:TRP:NE1	2.21	0.56
1:I:201:ASP:OD1	1:I:202:GLU:N	2.38	0.56
1:C:150:TYR:OH	1:C:165:GLN:OE1	2.10	0.56
1:I:25:PHE:HE2	1:I:49:LYS:HB3	1.70	0.56
1:J:277:ASP:N	1:J:277:ASP:OD1	2.39	0.56
1:A:190:GLY:HA3	1:A:199:TRP:NE1	2.21	0.55
1:C:197:THR:HG22	1:C:243:VAL:HG13	1.88	0.55
1:F:190:GLY:HA3	1:F:199:TRP:NE1	2.21	0.55
1:D:427:LYS:HE3	1:E:220:GLY:HA2	1.89	0.55
1:G:265:HIS:ND1	1:G:273:THR:HG22	2.21	0.55
1:I:150:TYR:OH	1:I:165:GLN:OE1	2.11	0.55
1:D:314:MET:O	1:D:430:THR:HA	2.07	0.55
1:E:240:LEU:HB3	1:E:247:LEU:HD11	1.86	0.55
1:E:423:PHE:O	1:F:224:LYS:NZ	2.39	0.55
1:F:261:PRO:HD2	1:F:264:PHE:HD1	1.72	0.55
1:I:261:PRO:HD2	1:I:264:PHE:HD2	1.70	0.55
1:B:469:LYS:HA	1:B:469:LYS:HE2	1.89	0.55
1:G:260:LEU:HB3	1:G:264:PHE:HE2	1.72	0.55
1:H:100:LEU:HD11	1:H:115:LYS:HB2	1.88	0.55
1:I:305:VAL:HG21	1:J:247:LEU:HB2	1.89	0.55
1:A:316:LYS:NZ	1:A:329:SER:HB3	2.22	0.55
1:B:190:GLY:HA3	1:B:199:TRP:NE1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:LYS:H	1:C:115:LYS:HD2	1.72	0.55
1:H:100:LEU:HD12	1:H:116:ILE:HG12	1.88	0.55
1:K:398:CYS:SG	1:L:209:ASN:ND2	2.80	0.55
1:F:154:TYR:OH	1:F:178:PHE:N	2.38	0.55
1:F:188:MET:HG3	1:F:328:PHE:HB2	1.88	0.55
1:L:118:ASP:HB3	1:L:130:THR:HB	1.88	0.55
1:L:190:GLY:HA3	1:L:199:TRP:NE1	2.21	0.55
1:D:313:LEU:HD22	1:D:390:ALA:HB1	1.88	0.55
1:E:146:ASP:O	1:E:171:ARG:N	2.36	0.55
1:C:195:TYR:HH	1:C:282:CYS:HG	1.55	0.55
1:H:408:LEU:HD21	1:I:316:LYS:HE2	1.89	0.55
1:J:423:PHE:O	1:K:224:LYS:NZ	2.40	0.55
1:D:188:MET:HG3	1:D:328:PHE:HB2	1.89	0.55
1:G:189:ALA:HB3	1:G:330:VAL:HG12	1.88	0.55
1:H:297:TYR:CD2	1:I:90:PRO:HG3	2.40	0.55
1:I:189:ALA:HB3	1:I:330:VAL:HG12	1.89	0.55
1:D:261:PRO:HD2	1:D:264:PHE:HD1	1.72	0.54
1:H:75:ASP:OD1	1:H:75:ASP:N	2.39	0.54
1:J:197:THR:HA	1:J:242:SER:O	2.07	0.54
1:A:197:THR:HG22	1:A:243:VAL:HG13	1.88	0.54
1:B:73:MET:HE2	1:B:73:MET:HA	1.89	0.54
1:B:273:THR:HG21	1:B:297:TYR:H	1.71	0.54
1:B:423:PHE:CE2	1:C:224:LYS:HE2	2.43	0.54
1:G:313:LEU:HD22	1:G:390:ALA:HB1	1.88	0.54
1:A:146:ASP:HA	1:A:170:VAL:HA	1.90	0.54
1:I:423:PHE:O	1:J:224:LYS:NZ	2.39	0.54
1:J:247:LEU:C	1:J:248:TYR:HD1	2.11	0.54
1:B:129:GLU:HG2	1:B:142:ARG:HB3	1.89	0.54
1:C:39:ASN:ND2	1:C:194:SER:O	2.41	0.54
1:E:75:ASP:OD1	1:E:75:ASP:N	2.37	0.54
1:F:201:ASP:OD1	1:F:202:GLU:N	2.40	0.54
1:G:297:TYR:HD2	1:H:90:PRO:HG3	1.72	0.54
1:L:146:ASP:HA	1:L:170:VAL:HA	1.89	0.54
1:B:277:ASP:OD1	1:B:277:ASP:N	2.41	0.54
1:D:315:CYS:HB2	1:D:390:ALA:HB2	1.89	0.54
1:I:146:ASP:HA	1:I:170:VAL:HA	1.89	0.54
1:J:413:ARG:NH1	1:K:228:MET:O	2.40	0.54
1:L:273:THR:HG21	1:L:297:TYR:H	1.72	0.54
1:B:313:LEU:HD22	1:B:390:ALA:HB1	1.90	0.54
1:E:115:LYS:H	1:E:115:LYS:HD2	1.72	0.54
1:A:277:ASP:OD1	1:A:277:ASP:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HD12	1:B:116:ILE:HG12	1.89	0.54
1:E:93:LEU:HD11	1:E:133:PHE:HZ	1.73	0.54
1:K:154:TYR:OH	1:K:178:PHE:N	2.39	0.54
1:H:146:ASP:N	1:H:146:ASP:OD2	2.41	0.53
1:B:100:LEU:HD11	1:B:115:LYS:HB2	1.89	0.53
1:C:6:VAL:HG12	1:C:29:PRO:HA	1.90	0.53
1:D:129:GLU:HG2	1:D:142:ARG:HB3	1.90	0.53
1:E:408:LEU:HD21	1:F:316:LYS:HE2	1.90	0.53
1:F:427:LYS:HE3	1:G:220:GLY:HA2	1.89	0.53
1:I:197:THR:HB	1:I:243:VAL:HG22	1.90	0.53
1:A:115:LYS:HD2	1:A:115:LYS:H	1.74	0.53
1:F:314:MET:O	1:F:430:THR:HA	2.08	0.53
1:H:427:LYS:HE3	1:I:220:GLY:HA2	1.91	0.53
1:I:440:ILE:HD11	1:J:212:LEU:HD11	1.90	0.53
1:B:73:MET:O	1:B:110:ARG:NE	2.33	0.53
1:D:89:ASP:OD1	3:D:1002:SAH:O3'	2.27	0.53
1:G:427:LYS:NZ	1:H:219:GLU:O	2.31	0.53
1:H:127:ASP:OD1	1:H:136:HIS:NE2	2.41	0.53
1:J:37:PJ3:O2'	1:J:285:TYR:OH	2.24	0.53
1:J:118:ASP:O	1:J:122:VAL:HG12	2.08	0.53
1:L:384:ILE:HG13	1:L:384:ILE:O	2.08	0.53
1:A:200:ALA:HB3	1:A:212:LEU:HD22	1.91	0.53
1:B:384:ILE:HG13	1:B:384:ILE:O	2.06	0.53
1:G:89:ASP:OD1	3:G:1002:SAH:O3'	2.23	0.53
1:K:39:ASN:ND2	1:K:194:SER:O	2.42	0.53
1:K:190:GLY:HA3	1:K:199:TRP:NE1	2.24	0.53
1:K:427:LYS:HE3	1:L:220:GLY:HA2	1.91	0.53
1:A:89:ASP:OD1	3:A:1002:SAH:O3'	2.25	0.53
1:E:273:THR:HG21	1:E:297:TYR:H	1.72	0.53
1:G:172:LEU:HD11	1:G:289:ARG:HG2	1.91	0.53
1:H:356:GLN:O	1:H:360:VAL:HG12	2.09	0.53
1:I:118:ASP:O	1:I:122:VAL:HG12	2.09	0.53
1:K:273:THR:HG21	1:K:297:TYR:H	1.74	0.53
1:L:235:PRO:HB3	1:L:252:ARG:HH22	1.73	0.53
1:L:313:LEU:HD22	1:L:390:ALA:HB1	1.89	0.53
1:A:348:THR:HG22	1:B:353:GLU:HG3	1.91	0.53
1:I:273:THR:HG21	1:I:297:TYR:H	1.74	0.53
1:J:70:ARG:HG2	1:J:71:ARG:HG3	1.89	0.53
1:C:88:GLU:OE2	1:C:92:ARG:NH1	2.42	0.53
1:H:43:PHE:CE2	1:H:285:TYR:HB3	2.44	0.53
1:G:118:ASP:O	1:G:122:VAL:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:205:LEU:HD11	1:H:240:LEU:HD12	1.91	0.53
1:D:118:ASP:O	1:D:122:VAL:HG12	2.09	0.52
1:F:37:PJ3:O2'	1:F:285:TYR:OH	2.27	0.52
1:H:305:VAL:HG21	1:I:247:LEU:HB2	1.91	0.52
1:I:37:PJ3:O2'	1:I:285:TYR:OH	2.27	0.52
1:K:363:ASN:HD21	1:K:379:MET:HG2	1.74	0.52
1:B:146:ASP:O	1:B:171:ARG:N	2.37	0.52
1:C:37:PJ3:O2'	1:C:285:TYR:OH	2.27	0.52
1:G:261:PRO:HD2	1:G:264:PHE:HD2	1.74	0.52
1:F:63:ASP:OD2	1:F:71:ARG:NE	2.37	0.52
1:A:100:LEU:HD11	1:A:115:LYS:HB2	1.90	0.52
1:B:185:TYR:HB3	1:B:314:MET:SD	2.50	0.52
1:B:433:LYS:NZ	1:C:213:CYS:O	2.42	0.52
1:G:57:PRO:HA	1:G:76:ARG:HE	1.73	0.52
1:I:100:LEU:HD11	1:I:115:LYS:HB2	1.91	0.52
1:C:273:THR:HG21	1:C:297:TYR:H	1.74	0.52
1:A:37:PJ3:O2'	1:A:285:TYR:OH	2.25	0.52
1:F:115:LYS:H	1:F:115:LYS:HD2	1.74	0.52
1:G:405:GLU:HA	1:H:318:THR:HG21	1.91	0.52
1:D:260:LEU:HB3	1:D:264:PHE:HE1	1.74	0.52
1:G:297:TYR:CD2	1:H:90:PRO:HG3	2.45	0.52
1:I:73:MET:HA	1:I:73:MET:HE2	1.92	0.52
1:K:24:MET:HE1	1:L:34:PRO:HD3	1.92	0.52
1:D:6:VAL:HG12	1:D:29:PRO:HA	1.92	0.52
1:D:146:ASP:O	1:D:171:ARG:N	2.38	0.52
1:D:273:THR:OG1	1:D:293:SER:OG	2.25	0.52
1:E:188:MET:HG3	1:E:328:PHE:HB2	1.92	0.52
1:E:426:GLN:OE1	1:F:325:ARG:NH2	2.40	0.52
1:G:247:LEU:C	1:G:248:TYR:HD1	2.12	0.52
1:L:315:CYS:SG	1:L:316:LYS:N	2.82	0.52
1:D:37:PJ3:O2'	1:D:285:TYR:OH	2.28	0.52
1:F:52:GLU:O	1:F:76:ARG:NH2	2.34	0.52
1:F:197:THR:HG22	1:F:243:VAL:HG23	1.90	0.52
1:I:240:LEU:HD23	1:I:247:LEU:HD11	1.92	0.52
1:J:103:ALA:HA	1:J:106:LYS:HE2	1.92	0.52
1:C:315:CYS:SG	1:C:316:LYS:N	2.83	0.51
1:E:93:LEU:HD11	1:E:133:PHE:CZ	2.46	0.51
1:F:89:ASP:OD1	3:F:1002:SAH:O3'	2.28	0.51
1:J:340:ASP:OD2	1:K:377:ASN:ND2	2.28	0.51
1:G:197:THR:HA	1:G:242:SER:O	2.11	0.51
1:F:118:ASP:O	1:F:122:VAL:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:221:ARG:HD2	1:F:223:GLY:H	1.76	0.51
1:L:89:ASP:OD1	3:L:1002:SAH:O3'	2.28	0.51
1:F:313:LEU:HD22	1:F:390:ALA:HB1	1.92	0.51
1:I:316:LYS:NZ	1:I:329:SER:HB3	2.26	0.51
1:D:237:ASP:O	1:D:252:ARG:N	2.44	0.51
1:D:100:LEU:HD11	1:D:115:LYS:HB2	1.92	0.51
1:B:297:TYR:CD2	1:C:90:PRO:HG3	2.44	0.51
1:C:118:ASP:O	1:C:122:VAL:HG12	2.10	0.51
1:E:237:ASP:O	1:E:252:ARG:N	2.40	0.51
1:I:427:LYS:HE3	1:J:220:GLY:HA2	1.92	0.51
1:G:425:LYS:HG3	1:G:427:LYS:HZ3	1.74	0.51
1:H:146:ASP:HA	1:H:170:VAL:HA	1.93	0.51
1:J:271:SER:HB2	1:J:296:LEU:HD13	1.93	0.51
1:C:178:PHE:HZ	1:C:197:THR:HG21	1.75	0.51
1:D:246:THR:HG22	1:D:248:TYR:HE1	1.74	0.51
1:D:247:LEU:C	1:D:248:TYR:HD1	2.14	0.51
1:E:356:GLN:O	1:E:360:VAL:HG12	2.10	0.51
1:H:89:ASP:OD1	3:H:1002:SAH:O3'	2.26	0.51
1:H:277:ASP:OD1	1:H:277:ASP:N	2.42	0.51
1:A:271:SER:HB2	1:A:296:LEU:HD13	1.93	0.51
1:G:8:ILE:HD12	1:G:9:ASP:H	1.75	0.51
1:L:6:VAL:HG12	1:L:29:PRO:HA	1.92	0.51
1:L:183:PHE:HZ	1:L:241:PHE:CZ	2.29	0.51
1:C:63:ASP:OD2	1:C:71:ARG:NE	2.35	0.50
1:J:344:GLY:HA3	1:K:360:VAL:HG11	1.93	0.50
1:K:237:ASP:O	1:K:252:ARG:N	2.43	0.50
1:K:426:GLN:CD	1:L:325:ARG:HH21	2.15	0.50
1:L:150:TYR:OH	1:L:165:GLN:OE1	2.11	0.50
1:A:189:ALA:HB3	1:A:330:VAL:HG12	1.93	0.50
1:F:273:THR:HG21	1:F:297:TYR:H	1.77	0.50
1:G:266:LEU:O	1:G:271:SER:HA	2.11	0.50
1:J:297:TYR:CD2	1:K:90:PRO:HG3	2.44	0.50
1:L:240:LEU:HB3	1:L:247:LEU:HD11	1.92	0.50
1:A:398:CYS:SG	1:B:209:ASN:ND2	2.84	0.50
1:D:423:PHE:CE2	1:E:224:LYS:HE2	2.46	0.50
1:F:39:ASN:ND2	1:F:194:SER:O	2.44	0.50
1:F:405:GLU:HA	1:G:318:THR:HG21	1.94	0.50
1:G:178:PHE:HD2	1:G:241:PHE:HE2	1.60	0.50
1:H:345:ILE:HG21	1:H:358:LEU:HD13	1.94	0.50
1:K:93:LEU:HD11	1:K:133:PHE:HZ	1.75	0.50
1:B:398:CYS:SG	1:C:209:ASN:ND2	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:GLY:O	1:F:357:LYS:NZ	2.45	0.50
1:I:423:PHE:CE2	1:J:224:LYS:HE2	2.47	0.50
1:J:115:LYS:H	1:J:115:LYS:HD2	1.77	0.50
1:H:154:TYR:OH	1:H:178:PHE:N	2.39	0.50
1:I:115:LYS:H	1:I:115:LYS:HD2	1.76	0.50
1:J:130:THR:OG1	1:J:133:PHE:O	2.25	0.50
1:J:316:LYS:NZ	1:J:329:SER:HB3	2.27	0.50
1:A:127:ASP:OD1	1:A:136:HIS:NE2	2.45	0.50
1:A:224:LYS:HE2	1:L:423:PHE:CE2	2.46	0.50
1:A:240:LEU:HB3	1:A:247:LEU:HD11	1.93	0.50
1:A:315:CYS:SG	1:A:316:LYS:N	2.85	0.50
1:D:146:ASP:HA	1:D:170:VAL:HA	1.93	0.50
1:E:6:VAL:HG12	1:E:8:ILE:H	1.77	0.50
1:E:100:LEU:HD11	1:E:115:LYS:HB2	1.93	0.50
1:J:383:MET:O	1:J:383:MET:HG2	2.11	0.50
1:B:313:LEU:HD11	1:B:391:PHE:CE1	2.47	0.50
1:F:384:ILE:HG13	1:F:384:ILE:O	2.11	0.50
1:G:264:PHE:CE1	1:G:274:CYS:HB2	2.46	0.50
1:H:303:TYR:CE1	1:H:442:LYS:HG3	2.46	0.50
1:I:6:VAL:HG22	1:I:8:ILE:H	1.76	0.50
1:B:151:GLN:HB3	3:B:1002:SAH:HN2	1.76	0.50
1:C:103:ALA:HA	1:C:106:LYS:HE2	1.92	0.50
1:F:129:GLU:HG2	1:F:142:ARG:HB3	1.94	0.50
1:K:89:ASP:OD1	3:K:1002:SAH:O3'	2.25	0.50
1:K:205:LEU:HD11	1:K:240:LEU:HD12	1.94	0.50
1:K:423:PHE:CE2	1:L:224:LYS:HE2	2.47	0.50
1:B:39:ASN:ND2	1:B:194:SER:O	2.45	0.50
1:C:24:MET:HG2	1:C:25:PHE:CD2	2.47	0.50
1:D:127:ASP:OD1	1:D:136:HIS:NE2	2.44	0.50
1:D:384:ILE:HG13	1:D:384:ILE:O	2.11	0.50
1:D:425:LYS:HG3	1:D:427:LYS:HZ1	1.77	0.50
1:K:260:LEU:HB3	1:K:264:PHE:HE2	1.77	0.50
1:E:363:ASN:HD21	1:E:379:MET:HG2	1.77	0.49
1:H:122:VAL:HG21	1:H:135:LEU:HD23	1.92	0.49
1:H:313:LEU:HD22	1:H:390:ALA:HB1	1.94	0.49
1:J:151:GLN:HB3	3:J:1002:SAH:HN2	1.76	0.49
1:L:316:LYS:NZ	1:L:329:SER:HB3	2.28	0.49
1:A:247:LEU:C	1:A:248:TYR:HD1	2.15	0.49
1:B:37:PJ3:O2'	1:B:285:TYR:OH	2.29	0.49
1:C:271:SER:HB2	1:C:296:LEU:HD13	1.93	0.49
1:G:356:GLN:O	1:G:360:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:ALA:HB1	1:H:193:PRO:HD3	1.94	0.49
1:C:195:TYR:OH	1:C:282:CYS:SG	2.68	0.49
1:D:75:ASP:N	1:D:75:ASP:OD1	2.45	0.49
1:E:71:ARG:HG3	1:E:71:ARG:HH11	1.76	0.49
1:E:151:GLN:HB3	3:E:1002:SAH:HN2	1.77	0.49
1:F:103:ALA:HA	1:F:106:LYS:HE2	1.94	0.49
1:J:345:ILE:HG13	1:J:358:LEU:HD13	1.94	0.49
1:A:348:THR:HA	1:A:399:ARG:HH22	1.77	0.49
1:B:303:TYR:CE2	1:B:442:LYS:HG3	2.47	0.49
1:E:344:GLY:HA3	1:F:360:VAL:HG11	1.94	0.49
1:L:39:ASN:ND2	1:L:194:SER:O	2.45	0.49
1:A:405:GLU:HA	1:B:318:THR:HG21	1.93	0.49
1:E:221:ARG:HD2	1:E:223:GLY:H	1.77	0.49
1:E:305:VAL:CG2	1:F:247:LEU:HB2	2.41	0.49
1:E:313:LEU:HD13	1:E:390:ALA:HB3	1.95	0.49
1:H:181:THR:HG22	1:H:259:HIS:CE1	2.47	0.49
1:A:92:ARG:NE	1:A:92:ARG:HA	2.27	0.49
1:C:183:PHE:HZ	1:C:241:PHE:CZ	2.30	0.49
1:E:37:PJ3:O2'	1:E:285:TYR:OH	2.31	0.49
1:E:43:PHE:CE1	1:E:285:TYR:HB3	2.47	0.49
1:E:195:TYR:HE2	1:E:283:GLU:HB3	1.76	0.49
1:B:133:PHE:HD1	1:B:134:CYS:N	2.11	0.49
1:E:133:PHE:HD1	1:E:134:CYS:N	2.10	0.49
1:G:118:ASP:HB3	1:G:130:THR:HB	1.93	0.49
1:H:133:PHE:HD1	1:H:134:CYS:N	2.10	0.49
1:H:179:ASP:OD2	1:H:181:THR:HG23	2.13	0.49
1:B:347:ALA:O	1:B:399:ARG:NH2	2.43	0.49
1:C:129:GLU:HG2	1:C:142:ARG:HB3	1.95	0.49
1:D:271:SER:HB2	1:D:296:LEU:HD13	1.94	0.49
1:H:151:GLN:HB3	3:H:1002:SAH:HN2	1.77	0.49
1:H:305:VAL:CG2	1:I:247:LEU:HB2	2.43	0.49
1:A:431:VAL:HG23	1:B:217:LEU:HD21	1.95	0.49
1:E:245:SER:O	1:E:245:SER:OG	2.29	0.49
1:I:104:ALA:HA	1:I:112:ILE:HG21	1.95	0.49
1:I:431:VAL:HG23	1:J:217:LEU:HD21	1.94	0.49
1:J:316:LYS:HD2	1:K:217:LEU:HD13	1.95	0.49
1:J:408:LEU:HG	1:K:316:LYS:HE3	1.95	0.49
1:A:425:LYS:HG3	1:A:427:LYS:HZ3	1.78	0.48
1:B:205:LEU:HD11	1:B:240:LEU:HD12	1.95	0.48
1:D:172:LEU:HD11	1:D:289:ARG:HG2	1.95	0.48
1:D:245:SER:O	1:D:245:SER:OG	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:PHE:CE2	1:D:274:CYS:HB2	2.47	0.48
1:A:423:PHE:CE2	1:B:224:LYS:HE2	2.49	0.48
1:E:423:PHE:CE2	1:F:224:LYS:HE2	2.48	0.48
1:F:316:LYS:NZ	1:F:329:SER:HB3	2.28	0.48
1:G:271:SER:HB2	1:G:296:LEU:HD13	1.94	0.48
1:G:273:THR:OG1	1:G:293:SER:OG	2.29	0.48
1:I:89:ASP:OD1	3:I:1002:SAH:O3'	2.30	0.48
1:I:151:GLN:HB3	3:I:1002:SAH:HN2	1.77	0.48
1:I:183:PHE:HZ	1:I:241:PHE:CZ	2.31	0.48
1:J:314:MET:O	1:J:430:THR:HA	2.13	0.48
1:L:304:ALA:O	1:L:440:ILE:HA	2.13	0.48
1:B:237:ASP:O	1:B:252:ARG:N	2.44	0.48
1:F:6:VAL:HG12	1:F:29:PRO:HA	1.95	0.48
1:G:100:LEU:HD11	1:G:115:LYS:HB2	1.93	0.48
1:G:314:MET:O	1:G:430:THR:HA	2.13	0.48
1:H:39:ASN:ND2	1:H:194:SER:O	2.46	0.48
1:K:172:LEU:HD11	1:K:289:ARG:HG2	1.95	0.48
1:A:151:GLN:HB3	3:A:1002:SAH:HN2	1.78	0.48
1:B:305:VAL:HG21	1:C:247:LEU:HB2	1.96	0.48
1:C:146:ASP:HA	1:C:170:VAL:HA	1.95	0.48
1:C:384:ILE:O	1:C:384:ILE:HG13	2.13	0.48
1:K:151:GLN:HB3	3:K:1002:SAH:HN2	1.78	0.48
1:B:427:LYS:HE3	1:C:220:GLY:HA2	1.95	0.48
1:B:433:LYS:NZ	1:C:213:CYS:SG	2.87	0.48
1:F:146:ASP:HA	1:F:170:VAL:HA	1.94	0.48
1:K:43:PHE:CE2	1:K:285:TYR:HB3	2.49	0.48
1:F:138:ASP:OD1	1:F:139:VAL:N	2.46	0.48
1:F:201:ASP:HB3	1:F:204:VAL:HG22	1.95	0.48
1:H:185:TYR:HB3	1:H:314:MET:SD	2.54	0.48
1:K:297:TYR:CD2	1:L:90:PRO:HG3	2.44	0.48
1:G:24:MET:HG3	1:G:25:PHE:CD1	2.48	0.48
1:K:133:PHE:HD1	1:K:134:CYS:N	2.10	0.48
1:A:411:ARG:HH21	1:B:233:LEU:HD13	1.78	0.48
1:F:146:ASP:OD2	1:F:147:VAL:HG23	2.13	0.48
1:H:237:ASP:O	1:H:252:ARG:N	2.47	0.48
1:I:427:LYS:HZ2	1:J:219:GLU:C	2.11	0.48
1:A:43:PHE:CE2	1:A:285:TYR:HB3	2.49	0.48
1:B:178:PHE:HZ	1:B:197:THR:HG21	1.78	0.48
1:E:146:ASP:HA	1:E:170:VAL:HA	1.95	0.48
1:E:425:LYS:HD2	1:F:218:THR:OG1	2.14	0.48
1:F:189:ALA:HB3	1:F:330:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:TYR:CE2	1:I:46:LEU:HB3	2.49	0.48
1:I:51:ILE:O	1:I:55:ILE:HG23	2.12	0.48
1:K:197:THR:HG22	1:K:243:VAL:HG13	1.95	0.48
1:C:151:GLN:HB3	3:C:1002:SAH:HN2	1.78	0.48
1:I:103:ALA:HA	1:I:106:LYS:HE2	1.96	0.48
1:K:129:GLU:HG2	1:K:142:ARG:HB3	1.94	0.48
1:C:409:GLY:HA2	1:D:233:LEU:HB3	1.96	0.47
1:F:259:HIS:NE2	1:F:306:THR:OG1	2.47	0.47
1:G:75:ASP:OD1	1:G:75:ASP:N	2.45	0.47
1:G:79:HIS:NE2	1:G:134:CYS:CB	2.77	0.47
1:K:194:SER:HB2	1:K:283:GLU:HG2	1.96	0.47
1:K:313:LEU:HD22	1:K:390:ALA:HB1	1.95	0.47
1:L:195:TYR:OH	1:L:282:CYS:SG	2.72	0.47
1:A:188:MET:HG3	1:A:328:PHE:HB2	1.96	0.47
1:B:340:ASP:OD2	1:C:377:ASN:ND2	2.47	0.47
1:D:182:PRO:HB3	1:D:312:PHE:HZ	1.79	0.47
1:E:266:LEU:O	1:E:271:SER:HA	2.14	0.47
1:E:398:CYS:SG	1:F:209:ASN:ND2	2.87	0.47
1:G:127:ASP:OD1	1:G:136:HIS:NE2	2.46	0.47
1:I:434:ARG:HH12	1:J:385:PRO:HG2	1.79	0.47
1:A:384:ILE:O	1:A:384:ILE:HG13	2.14	0.47
1:I:127:ASP:OD1	1:I:136:HIS:NE2	2.47	0.47
1:J:427:LYS:HD3	1:K:220:GLY:H	1.79	0.47
1:D:266:LEU:O	1:D:271:SER:HA	2.14	0.47
1:F:304:ALA:O	1:F:440:ILE:HA	2.14	0.47
1:G:316:LYS:HZ2	1:G:329:SER:HB3	1.80	0.47
1:H:312:PHE:HB3	1:H:433:LYS:HB2	1.96	0.47
1:H:340:ASP:OD2	1:I:377:ASN:ND2	2.40	0.47
1:A:224:LYS:NZ	1:L:423:PHE:O	2.48	0.47
1:C:237:ASP:O	1:C:252:ARG:N	2.46	0.47
1:G:146:ASP:O	1:G:171:ARG:N	2.41	0.47
1:K:118:ASP:O	1:K:122:VAL:HG12	2.14	0.47
1:K:237:ASP:OD1	1:K:252:ARG:N	2.48	0.47
1:F:303:TYR:HE2	1:F:442:LYS:HE2	1.79	0.47
1:G:115:LYS:H	1:G:115:LYS:HD2	1.78	0.47
1:I:154:TYR:OH	1:I:178:PHE:N	2.37	0.47
1:A:129:GLU:HG2	1:A:142:ARG:HB3	1.97	0.47
1:C:70:ARG:HD2	1:C:71:ARG:NH1	2.30	0.47
1:F:357:LYS:HE2	1:F:357:LYS:HB2	1.60	0.47
1:F:383:MET:O	1:F:383:MET:HG2	2.14	0.47
1:G:357:LYS:HE2	1:G:357:LYS:HB2	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:SER:O	1:H:140:SER:OG	2.32	0.47
1:H:150:TYR:OH	1:H:165:GLN:OE1	2.12	0.47
1:H:427:LYS:HD3	1:H:427:LYS:HA	1.61	0.47
1:L:237:ASP:OD1	1:L:252:ARG:N	2.48	0.47
1:E:303:TYR:HB3	1:E:440:ILE:HG23	1.96	0.47
1:F:100:LEU:HD11	1:F:115:LYS:HB2	1.96	0.47
1:F:266:LEU:O	1:F:271:SER:HA	2.14	0.47
1:J:189:ALA:HB3	1:J:330:VAL:HG12	1.96	0.47
1:B:189:ALA:HB3	1:B:330:VAL:HG12	1.97	0.47
1:C:245:SER:O	1:C:245:SER:OG	2.29	0.47
1:C:423:PHE:CE2	1:D:224:LYS:HE2	2.50	0.47
1:G:129:GLU:HG2	1:G:142:ARG:HB3	1.95	0.47
1:L:154:TYR:OH	1:L:178:PHE:N	2.44	0.47
1:L:277:ASP:OD2	1:L:277:ASP:N	2.47	0.47
1:B:195:TYR:OH	1:B:282:CYS:SG	2.67	0.47
1:C:122:VAL:HG11	1:C:133:PHE:CD2	2.50	0.47
1:H:423:PHE:CE2	1:I:224:LYS:HE2	2.50	0.47
1:I:235:PRO:HB3	1:I:252:ARG:HH22	1.80	0.47
1:J:92:ARG:HA	1:J:92:ARG:NE	2.30	0.47
1:J:273:THR:OG1	1:J:293:SER:OG	2.26	0.47
1:J:423:PHE:CE2	1:K:224:LYS:HE2	2.50	0.47
1:A:247:LEU:HB2	1:L:305:VAL:CG2	2.45	0.46
1:J:75:ASP:OD1	1:J:75:ASP:N	2.47	0.46
1:J:266:LEU:O	1:J:271:SER:HA	2.15	0.46
1:L:103:ALA:HA	1:L:106:LYS:HE2	1.97	0.46
1:B:127:ASP:OD1	1:B:136:HIS:NE2	2.42	0.46
1:B:266:LEU:O	1:B:271:SER:HA	2.14	0.46
1:B:425:LYS:HG3	1:B:427:LYS:HZ1	1.81	0.46
1:D:103:ALA:HA	1:D:106:LYS:HE2	1.96	0.46
1:D:405:GLU:HA	1:E:318:THR:HG21	1.97	0.46
1:H:24:MET:HG3	1:H:25:PHE:CD1	2.50	0.46
1:H:398:CYS:SG	1:I:209:ASN:ND2	2.88	0.46
1:H:405:GLU:HA	1:I:318:THR:HG21	1.96	0.46
1:G:103:ALA:HA	1:G:106:LYS:HE2	1.97	0.46
1:H:129:GLU:HG2	1:H:142:ARG:HB3	1.97	0.46
1:H:316:LYS:HB2	1:H:316:LYS:HE2	1.71	0.46
1:L:88:GLU:OE2	1:L:92:ARG:NH1	2.49	0.46
1:L:408:LEU:HA	1:L:408:LEU:HD23	1.52	0.46
1:A:118:ASP:HB3	1:A:130:THR:HB	1.97	0.46
1:B:401:ASP:HA	1:C:325:ARG:HH11	1.80	0.46
1:E:71:ARG:NH1	1:E:71:ARG:HG3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:ASP:O	1:G:252:ARG:N	2.47	0.46
1:J:28:GLU:OE1	1:J:29:PRO:HD2	2.15	0.46
1:C:127:ASP:OD1	1:C:136:HIS:NE2	2.49	0.46
1:F:151:GLN:HB3	3:F:1002:SAH:HN2	1.81	0.46
1:F:431:VAL:HG23	1:G:217:LEU:HD21	1.97	0.46
1:G:345:ILE:HG13	1:G:358:LEU:HD13	1.97	0.46
1:A:356:GLN:NE2	1:L:347:ALA:HB2	2.30	0.46
1:C:297:TYR:CD2	1:D:90:PRO:HG3	2.46	0.46
1:G:235:PRO:HB3	1:G:252:ARG:NH2	2.31	0.46
1:I:172:LEU:HD11	1:I:289:ARG:HG2	1.97	0.46
1:J:235:PRO:HB3	1:J:252:ARG:HH22	1.81	0.46
1:L:22:TYR:CE2	1:L:46:LEU:HB3	2.51	0.46
1:A:440:ILE:HD11	1:B:212:LEU:HD21	1.98	0.46
1:B:440:ILE:HD12	1:C:212:LEU:HG	1.98	0.46
1:D:133:PHE:HD2	1:D:134:CYS:N	2.13	0.46
1:F:316:LYS:HZ2	1:F:329:SER:HB3	1.80	0.46
1:F:423:PHE:CE2	1:G:224:LYS:HE2	2.51	0.46
1:G:178:PHE:CZ	1:G:197:THR:HG21	2.51	0.46
1:I:235:PRO:HB3	1:I:252:ARG:NH2	2.31	0.46
1:I:312:PHE:HB3	1:I:433:LYS:HB2	1.97	0.46
1:I:427:LYS:HA	1:I:427:LYS:HD3	1.68	0.46
1:K:93:LEU:HD11	1:K:133:PHE:CZ	2.51	0.46
1:K:170:VAL:HG13	1:K:292:MET:HG3	1.98	0.46
1:L:93:LEU:HD11	1:L:133:PHE:CZ	2.51	0.46
1:A:103:ALA:HA	1:A:106:LYS:HE2	1.97	0.46
1:B:25:PHE:HE2	1:B:49:LYS:HB3	1.79	0.46
1:G:57:PRO:HG3	1:G:76:ARG:HH21	1.81	0.46
1:I:237:ASP:OD1	1:I:252:ARG:N	2.49	0.46
1:I:409:GLY:HA2	1:J:233:LEU:HB3	1.98	0.46
1:K:57:PRO:HA	1:K:76:ARG:HE	1.80	0.46
1:L:151:GLN:HB3	3:L:1002:SAH:HN2	1.79	0.46
1:A:24:MET:HG3	1:A:25:PHE:CD1	2.50	0.46
1:B:24:MET:HG2	1:B:25:PHE:CD1	2.51	0.46
1:B:178:PHE:HD1	1:B:241:PHE:HE2	1.64	0.46
1:E:179:ASP:OD1	1:E:181:THR:HG23	2.15	0.46
1:G:316:LYS:NZ	1:G:329:SER:HB3	2.30	0.46
1:I:384:ILE:O	1:I:384:ILE:HG13	2.16	0.46
1:J:25:PHE:HE2	1:J:49:LYS:HB3	1.81	0.46
1:L:4:VAL:HG11	1:L:46:LEU:HD11	1.98	0.46
1:L:150:TYR:OH	1:L:161:SER:OG	2.28	0.46
1:B:140:SER:O	1:B:140:SER:OG	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ILE:N	1:C:61:ILE:HD12	2.31	0.46
1:D:246:THR:HG22	1:D:248:TYR:CE1	2.51	0.46
1:H:313:LEU:HD11	1:H:391:PHE:CE1	2.50	0.46
1:I:61:ILE:HD12	1:I:61:ILE:N	2.31	0.46
1:A:90:PRO:HG3	1:L:297:TYR:CD2	2.46	0.45
1:A:313:LEU:HD11	1:A:391:PHE:CE1	2.51	0.45
1:D:61:ILE:N	1:D:61:ILE:HD12	2.31	0.45
1:D:313:LEU:HD11	1:D:391:PHE:CE1	2.51	0.45
1:G:313:LEU:HD11	1:G:391:PHE:CE1	2.51	0.45
1:E:384:ILE:HG13	1:E:384:ILE:O	2.16	0.45
1:G:427:LYS:HD3	1:G:427:LYS:HA	1.55	0.45
1:A:191:ALA:HB1	1:A:193:PRO:HD3	1.98	0.45
1:E:16:LYS:HA	1:E:16:LYS:HD2	1.60	0.45
1:F:51:ILE:HD13	1:F:51:ILE:HA	1.79	0.45
1:F:245:SER:O	1:F:245:SER:OG	2.32	0.45
1:H:63:ASP:OD2	1:H:71:ARG:NE	2.49	0.45
1:K:235:PRO:HB3	1:K:252:ARG:NH2	2.31	0.45
1:K:434:ARG:N	1:K:437:THR:OG1	2.49	0.45
1:C:89:ASP:OD1	3:C:1002:SAH:O3'	2.29	0.45
1:G:409:GLY:HA2	1:H:233:LEU:HB3	1.98	0.45
1:H:103:ALA:HA	1:H:106:LYS:HE2	1.99	0.45
1:H:245:SER:O	1:H:245:SER:OG	2.33	0.45
1:I:24:MET:H	1:I:24:MET:CE	2.28	0.45
1:I:30:ARG:HE	1:I:30:ARG:HB3	1.59	0.45
1:J:275:ARG:NH1	1:K:92:ARG:HH22	2.15	0.45
1:K:178:PHE:HZ	1:K:197:THR:HG21	1.82	0.45
1:D:28:GLU:OE1	1:D:29:PRO:HD2	2.17	0.45
1:H:104:ALA:HA	1:H:112:ILE:HG21	1.98	0.45
1:H:178:PHE:HZ	1:H:197:THR:HG21	1.81	0.45
1:H:384:ILE:O	1:H:384:ILE:HG13	2.16	0.45
1:I:24:MET:HG2	1:I:25:PHE:CD1	2.51	0.45
1:J:100:LEU:HD11	1:J:115:LYS:HB2	1.97	0.45
1:J:197:THR:HG22	1:J:243:VAL:HG13	1.98	0.45
1:L:61:ILE:HD12	1:L:61:ILE:N	2.31	0.45
1:A:17:ALA:HA	1:A:20:ARG:NH1	2.31	0.45
1:D:51:ILE:O	1:D:55:ILE:HG23	2.17	0.45
1:I:304:ALA:O	1:I:440:ILE:HA	2.16	0.45
1:I:305:VAL:CG2	1:J:247:LEU:HB2	2.46	0.45
1:K:151:GLN:O	3:K:1002:SAH:N	2.49	0.45
1:L:129:GLU:HG2	1:L:142:ARG:HB3	1.98	0.45
1:L:178:PHE:HE1	1:L:285:TYR:CE2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:VAL:HG13	1:E:292:MET:HG3	1.99	0.45
1:F:183:PHE:HZ	1:F:241:PHE:HZ	1.64	0.45
1:H:16:LYS:HD2	1:H:16:LYS:HA	1.68	0.45
1:H:94:ALA:O	1:H:98:ARG:HG3	2.16	0.45
1:B:43:PHE:CE2	1:B:285:TYR:HB3	2.52	0.45
1:B:305:VAL:CG2	1:C:247:LEU:HB2	2.45	0.45
1:D:263:VAL:HG12	1:D:275:ARG:HG2	1.98	0.45
1:E:127:ASP:OD1	1:E:136:HIS:NE2	2.44	0.45
1:E:433:LYS:NZ	1:F:213:CYS:SG	2.89	0.45
1:F:192:TYR:HE1	1:F:199:TRP:HE1	1.64	0.45
1:G:151:GLN:HB3	3:G:1002:SAH:HN2	1.81	0.45
1:K:146:ASP:HA	1:K:170:VAL:HA	1.98	0.45
1:K:235:PRO:HB3	1:K:252:ARG:HH22	1.82	0.45
1:K:427:LYS:HZ2	1:L:219:GLU:C	2.11	0.45
1:E:94:ALA:O	1:E:98:ARG:HG3	2.17	0.45
1:H:195:TYR:CE1	1:H:285:TYR:HD2	2.35	0.45
1:H:260:LEU:HB3	1:H:264:PHE:CE1	2.51	0.45
1:L:184:MET:HB3	1:L:441:GLN:OE1	2.17	0.45
1:C:57:PRO:HA	1:C:76:ARG:HE	1.82	0.45
1:C:190:GLY:HA2	1:C:331:CYS:SG	2.57	0.45
1:F:235:PRO:HB3	1:F:252:ARG:HH22	1.82	0.45
1:G:140:SER:O	1:G:140:SER:OG	2.33	0.45
1:G:190:GLY:HA2	1:G:331:CYS:SG	2.58	0.45
1:J:43:PHE:CE2	1:J:285:TYR:HB3	2.52	0.45
1:K:150:TYR:OH	1:K:161:SER:OG	2.28	0.45
1:B:240:LEU:HB3	1:B:247:LEU:HD11	1.99	0.44
1:E:235:PRO:HB3	1:E:252:ARG:NH2	2.32	0.44
1:G:438:GLN:OE1	1:H:198:ASN:ND2	2.47	0.44
1:J:313:LEU:HD11	1:J:391:PHE:CE1	2.52	0.44
1:K:363:ASN:ND2	1:K:379:MET:HG2	2.33	0.44
1:B:235:PRO:HB3	1:B:252:ARG:HH22	1.82	0.44
1:C:307:HIS:HB3	1:D:245:SER:HB2	1.99	0.44
1:F:70:ARG:HD2	1:F:71:ARG:NH1	2.31	0.44
1:F:399:ARG:HD3	1:F:403:GLU:OE2	2.17	0.44
1:F:411:ARG:NH1	1:G:232:LYS:H	2.15	0.44
1:F:425:LYS:HE2	1:G:323:GLY:HA3	2.00	0.44
1:G:265:HIS:CE1	1:G:273:THR:HG22	2.52	0.44
1:H:440:ILE:HD12	1:I:212:LEU:HG	2.00	0.44
1:I:63:ASP:OD2	1:I:71:ARG:NE	2.47	0.44
1:J:154:TYR:HH	1:J:178:PHE:H	1.53	0.44
1:K:92:ARG:HD3	1:K:92:ARG:HA	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:221:ARG:HH12	1:K:223:GLY:C	2.20	0.44
1:A:178:PHE:HZ	1:A:197:THR:HG21	1.81	0.44
1:C:138:ASP:OD1	1:C:139:VAL:N	2.50	0.44
1:F:237:ASP:O	1:F:252:ARG:N	2.48	0.44
1:F:408:LEU:HD21	1:G:316:LYS:NZ	2.31	0.44
1:I:237:ASP:O	1:I:252:ARG:N	2.47	0.44
1:B:146:ASP:HA	1:B:170:VAL:HA	1.99	0.44
1:B:276:CYS:SG	1:B:288:LYS:HD3	2.57	0.44
1:D:88:GLU:HG2	1:D:92:ARG:HH11	1.82	0.44
1:E:289:ARG:HB3	1:E:289:ARG:NH1	2.33	0.44
1:G:423:PHE:CE2	1:H:224:LYS:HE2	2.52	0.44
1:I:94:ALA:O	1:I:98:ARG:HG3	2.17	0.44
1:A:305:VAL:HG21	1:B:247:LEU:HB2	1.99	0.44
1:C:154:TYR:OH	1:C:178:PHE:N	2.50	0.44
1:D:178:PHE:HD2	1:D:241:PHE:HE2	1.64	0.44
1:D:185:TYR:HB3	1:D:314:MET:SD	2.58	0.44
1:E:73:MET:HE2	1:E:73:MET:HA	1.99	0.44
1:E:103:ALA:HA	1:E:106:LYS:HE2	2.00	0.44
1:E:178:PHE:HD1	1:E:241:PHE:HE2	1.66	0.44
1:G:267:LYS:HE3	1:G:446:GLU:OE1	2.18	0.44
1:H:51:ILE:HD13	1:H:51:ILE:HA	1.79	0.44
1:H:446:GLU:OE1	1:H:446:GLU:HA	2.17	0.44
1:I:303:TYR:CE2	1:I:442:LYS:HE2	2.52	0.44
1:J:127:ASP:OD1	1:J:136:HIS:NE2	2.45	0.44
1:F:235:PRO:HB3	1:F:252:ARG:NH2	2.32	0.44
1:G:94:ALA:O	1:G:98:ARG:HG3	2.18	0.44
1:H:149:ILE:HD13	1:H:149:ILE:HA	1.83	0.44
1:I:130:THR:OG1	1:I:133:PHE:O	2.30	0.44
1:A:413:ARG:HA	1:A:423:PHE:HB3	2.00	0.44
1:B:28:GLU:OE1	1:B:29:PRO:HD2	2.17	0.44
1:B:150:TYR:OH	1:B:165:GLN:OE1	2.12	0.44
1:D:357:LYS:HE2	1:D:357:LYS:HB2	1.80	0.44
1:F:305:VAL:CG2	1:G:247:LEU:HB2	2.47	0.44
1:H:144:ARG:NE	1:H:168:LYS:O	2.42	0.44
1:H:411:ARG:NH1	1:I:232:LYS:H	2.16	0.44
1:L:146:ASP:HB2	1:L:171:ARG:NH1	2.32	0.44
1:B:427:LYS:HA	1:B:427:LYS:HD3	1.68	0.44
1:D:24:MET:HG2	1:D:25:PHE:CD1	2.53	0.44
1:D:25:PHE:HE2	1:D:49:LYS:HB3	1.82	0.44
1:E:181:THR:N	1:E:182:PRO:HD2	2.32	0.44
1:E:433:LYS:NZ	1:F:213:CYS:O	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:ALA:HB1	1:F:383:MET:HE1	1.99	0.44
1:F:425:LYS:HG3	1:F:427:LYS:HZ1	1.83	0.44
1:G:182:PRO:HB3	1:G:312:PHE:HZ	1.83	0.44
1:G:411:ARG:NH1	1:H:232:LYS:H	2.15	0.44
1:I:129:GLU:HG2	1:I:142:ARG:HB3	2.00	0.44
1:J:138:ASP:OD1	1:J:139:VAL:N	2.51	0.44
1:L:296:LEU:HD12	1:L:296:LEU:HA	1.80	0.44
1:E:179:ASP:HB2	1:E:284:GLY:O	2.18	0.44
1:H:137:THR:HG23	1:H:139:VAL:H	1.83	0.44
1:K:16:LYS:HA	1:K:16:LYS:HD2	1.68	0.44
1:L:30:ARG:HE	1:L:30:ARG:HB3	1.58	0.44
1:A:316:LYS:HZ2	1:A:329:SER:HB3	1.81	0.43
1:B:235:PRO:HB3	1:B:252:ARG:NH2	2.33	0.43
1:E:212:LEU:HD12	1:E:212:LEU:HA	1.86	0.43
1:G:51:ILE:HD13	1:G:51:ILE:HA	1.80	0.43
1:I:23:PRO:HD2	1:I:24:MET:CE	2.48	0.43
1:I:414:THR:N	1:I:422:ALA:O	2.39	0.43
1:K:188:MET:HG3	1:K:328:PHE:HB2	2.00	0.43
1:K:189:ALA:HB3	1:K:330:VAL:HG12	2.00	0.43
1:L:433:LYS:HA	1:L:433:LYS:HD2	1.80	0.43
1:A:93:LEU:HD11	1:A:133:PHE:HZ	1.82	0.43
1:B:181:THR:N	1:B:182:PRO:HD2	2.33	0.43
1:C:277:ASP:OD2	1:C:277:ASP:N	2.50	0.43
1:E:399:ARG:HA	1:E:399:ARG:HD3	1.72	0.43
1:H:181:THR:N	1:H:182:PRO:HD2	2.33	0.43
1:I:195:TYR:HB2	1:I:197:THR:HG23	2.00	0.43
1:I:201:ASP:HB3	1:I:204:VAL:HG22	2.00	0.43
1:K:411:ARG:NH1	1:L:232:LYS:H	2.16	0.43
1:A:235:PRO:HB3	1:A:252:ARG:HH22	1.83	0.43
1:A:266:LEU:O	1:A:271:SER:HA	2.18	0.43
1:C:183:PHE:HZ	1:C:241:PHE:HZ	1.64	0.43
1:C:408:LEU:HA	1:C:408:LEU:HD23	1.68	0.43
1:F:144:ARG:NE	1:F:168:LYS:O	2.50	0.43
1:I:408:LEU:HD21	1:J:316:LYS:CE	2.49	0.43
1:L:138:ASP:OD1	1:L:139:VAL:N	2.51	0.43
1:L:239:VAL:HG21	1:L:252:ARG:HE	1.83	0.43
1:F:237:ASP:OD1	1:F:252:ARG:N	2.51	0.43
1:G:43:PHE:CE2	1:G:285:TYR:HB3	2.53	0.43
1:I:357:LYS:HE2	1:I:357:LYS:HB2	1.76	0.43
1:J:6:VAL:HG12	1:J:29:PRO:HA	1.99	0.43
1:K:273:THR:OG1	1:K:293:SER:OG	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD11	1:L:440:ILE:HD11	2.01	0.43
1:B:115:LYS:H	1:B:115:LYS:HD2	1.83	0.43
1:B:118:ASP:O	1:B:122:VAL:HG12	2.18	0.43
1:B:154:TYR:OH	1:B:178:PHE:N	2.46	0.43
1:C:434:ARG:HH12	1:D:385:PRO:HG2	1.84	0.43
1:D:110:ARG:HA	1:D:110:ARG:HD3	1.85	0.43
1:D:235:PRO:HB3	1:D:252:ARG:NH2	2.33	0.43
1:F:183:PHE:N	1:F:183:PHE:CD1	2.86	0.43
1:G:39:ASN:ND2	1:G:194:SER:O	2.51	0.43
1:H:189:ALA:HB3	1:H:330:VAL:HG12	2.00	0.43
1:J:264:PHE:CE1	1:J:274:CYS:HB2	2.54	0.43
1:K:190:GLY:HA2	1:K:331:CYS:SG	2.58	0.43
1:K:286:VAL:HG21	1:K:288:LYS:HZ3	1.84	0.43
1:K:405:GLU:HA	1:L:318:THR:HG21	2.00	0.43
1:B:94:ALA:O	1:B:98:ARG:HG3	2.19	0.43
1:J:235:PRO:HB3	1:J:252:ARG:NH2	2.33	0.43
1:J:425:LYS:NZ	1:K:323:GLY:HA3	2.33	0.43
1:K:68:PRO:HB2	1:K:96:TYR:CG	2.54	0.43
1:K:140:SER:O	1:K:140:SER:OG	2.31	0.43
1:L:237:ASP:O	1:L:252:ARG:N	2.46	0.43
1:C:237:ASP:OD1	1:C:252:ARG:N	2.51	0.43
1:C:411:ARG:NH1	1:D:232:LYS:H	2.16	0.43
1:D:138:ASP:OD1	1:D:139:VAL:N	2.52	0.43
1:E:178:PHE:HZ	1:E:197:THR:HG21	1.84	0.43
1:F:61:ILE:N	1:F:61:ILE:HD12	2.33	0.43
1:H:314:MET:O	1:H:430:THR:HA	2.19	0.43
1:J:237:ASP:O	1:J:252:ARG:N	2.50	0.43
1:K:313:LEU:HD11	1:K:391:PHE:CE1	2.54	0.43
1:A:68:PRO:HB2	1:A:96:TYR:CG	2.54	0.43
1:A:140:SER:O	1:A:140:SER:OG	2.30	0.43
1:B:315:CYS:O	1:B:329:SER:HA	2.19	0.43
1:C:130:THR:OG1	1:C:133:PHE:O	2.29	0.43
1:E:92:ARG:HD3	1:E:92:ARG:HA	1.72	0.43
1:F:400:LYS:HB2	1:F:400:LYS:HE2	1.65	0.43
1:I:93:LEU:HD21	1:I:133:PHE:CZ	2.54	0.43
1:I:433:LYS:HD2	1:I:433:LYS:HA	1.52	0.43
1:J:16:LYS:HA	1:J:16:LYS:HD3	1.71	0.43
1:K:110:ARG:HA	1:K:110:ARG:HD3	1.85	0.43
1:L:94:ALA:O	1:L:98:ARG:HG3	2.18	0.43
1:L:171:ARG:CZ	1:L:171:ARG:HB2	2.48	0.43
1:L:190:GLY:HA2	1:L:331:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:357:LYS:HE2	1:L:357:LYS:HB2	1.76	0.43
1:L:400:LYS:HB2	1:L:400:LYS:HE2	1.62	0.43
1:A:59:SER:HB3	1:A:146:ASP:OD2	2.19	0.43
1:I:245:SER:O	1:I:245:SER:OG	2.28	0.43
1:I:303:TYR:HE2	1:I:442:LYS:HE2	1.83	0.43
1:B:215:THR:OG1	1:B:216:ASP:N	2.52	0.43
1:C:235:PRO:HB3	1:C:252:ARG:NH2	2.34	0.43
1:E:149:ILE:HD13	1:E:149:ILE:HA	1.82	0.43
1:E:181:THR:HG22	1:E:259:HIS:CE1	2.54	0.43
1:E:408:LEU:HA	1:E:408:LEU:HD23	1.60	0.43
1:A:202:GLU:OE2	1:A:238:ARG:NH1	2.52	0.42
1:B:122:VAL:HG21	1:B:135:LEU:HD23	2.00	0.42
1:C:49:LYS:HB2	1:C:49:LYS:HE2	1.90	0.42
1:C:51:ILE:HD13	1:C:51:ILE:HA	1.78	0.42
1:C:286:VAL:HG21	1:C:288:LYS:HZ3	1.84	0.42
1:D:189:ALA:HB3	1:D:330:VAL:HG12	2.01	0.42
1:E:39:ASN:ND2	1:E:194:SER:O	2.52	0.42
1:F:190:GLY:HA2	1:F:331:CYS:SG	2.59	0.42
1:F:401:ASP:OD1	1:G:325:ARG:HD3	2.19	0.42
1:H:215:THR:OG1	1:H:216:ASP:N	2.51	0.42
1:J:4:VAL:HG11	1:J:46:LEU:HD11	2.01	0.42
1:L:127:ASP:OD1	1:L:136:HIS:NE2	2.51	0.42
1:A:191:ALA:HB3	1:A:332:THR:HA	2.00	0.42
1:B:190:GLY:HA2	1:B:331:CYS:SG	2.59	0.42
1:B:408:LEU:HG	1:C:316:LYS:NZ	2.34	0.42
1:F:94:ALA:O	1:F:98:ARG:HG3	2.19	0.42
1:G:235:PRO:HB3	1:G:252:ARG:HH22	1.84	0.42
1:H:235:PRO:HB3	1:H:252:ARG:HH22	1.83	0.42
1:H:400:LYS:O	1:H:400:LYS:HD3	2.18	0.42
1:I:167:ILE:HG12	1:I:270:LEU:HD13	2.00	0.42
1:L:302:GLY:C	1:L:303:TYR:HD1	2.23	0.42
1:L:427:LYS:HB2	1:L:427:LYS:HE2	1.80	0.42
1:A:110:ARG:HD3	1:A:110:ARG:HA	1.83	0.42
1:D:178:PHE:HZ	1:D:197:THR:HG21	1.83	0.42
1:E:335:PRO:HD3	1:E:379:MET:HE3	2.01	0.42
1:G:192:TYR:HB2	1:G:197:THR:HG23	2.01	0.42
1:G:195:TYR:HB2	1:G:197:THR:HG22	2.02	0.42
1:I:261:PRO:HD2	1:I:264:PHE:CD2	2.53	0.42
1:L:75:ASP:OD1	1:L:75:ASP:N	2.50	0.42
1:L:302:GLY:HA2	1:L:445:ALA:HB2	2.00	0.42
1:D:317:THR:HA	1:D:389:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:PHE:HZ	1:F:241:PHE:CZ	2.36	0.42
1:I:190:GLY:HA2	1:I:331:CYS:SG	2.59	0.42
1:I:398:CYS:SG	1:J:209:ASN:ND2	2.91	0.42
1:K:64:ILE:HD12	1:K:138:ASP:HB3	2.01	0.42
1:A:138:ASP:OD1	1:A:139:VAL:N	2.52	0.42
1:A:217:LEU:HD21	1:L:431:VAL:HG23	2.01	0.42
1:B:93:LEU:HD11	1:B:133:PHE:CZ	2.54	0.42
1:B:425:LYS:HG2	1:C:221:ARG:HH21	1.85	0.42
1:I:93:LEU:HD23	1:I:93:LEU:HA	1.86	0.42
1:K:94:ALA:O	1:K:98:ARG:HG3	2.19	0.42
1:L:414:THR:N	1:L:422:ALA:O	2.40	0.42
1:A:51:ILE:O	1:A:55:ILE:HG23	2.20	0.42
1:C:219:GLU:O	1:C:221:ARG:N	2.49	0.42
1:E:89:ASP:OD1	3:E:1002:SAH:O3'	2.32	0.42
1:F:271:SER:C	1:F:272:PHE:HD1	2.23	0.42
1:F:440:ILE:HD12	1:G:205:LEU:HD21	2.00	0.42
1:G:166:ALA:HB1	1:G:272:PHE:CD2	2.54	0.42
1:K:127:ASP:OD1	1:K:136:HIS:NE2	2.46	0.42
1:A:6:VAL:HG12	1:A:29:PRO:HA	2.01	0.42
1:B:25:PHE:CE2	1:B:49:LYS:HB3	2.55	0.42
1:C:100:LEU:HD11	1:C:115:LYS:HB2	2.00	0.42
1:C:363:ASN:HD21	1:C:379:MET:HG2	1.85	0.42
3:C:1002:SAH:HO3'	3:C:1002:SAH:HO2'	1.57	0.42
1:E:215:THR:OG1	1:E:216:ASP:N	2.53	0.42
1:G:303:TYR:CZ	1:G:442:LYS:HE3	2.54	0.42
1:G:335:PRO:HG2	1:G:379:MET:HB3	2.00	0.42
1:H:18:LEU:HD23	1:H:18:LEU:HA	1.85	0.42
1:H:190:GLY:HA2	1:H:331:CYS:SG	2.60	0.42
1:H:235:PRO:HB3	1:H:252:ARG:NH2	2.34	0.42
1:H:261:PRO:HD2	1:H:264:PHE:CD1	2.52	0.42
1:H:264:PHE:CE2	1:H:274:CYS:HB2	2.55	0.42
1:I:396:LYS:HD3	1:I:396:LYS:HA	1.92	0.42
1:J:265:HIS:ND1	1:J:273:THR:HG22	2.35	0.42
1:K:400:LYS:HD3	1:K:400:LYS:HA	1.84	0.42
1:A:51:ILE:HD13	1:A:51:ILE:HA	1.78	0.42
1:C:266:LEU:O	1:C:271:SER:HA	2.19	0.42
1:D:241:PHE:O	1:D:247:LEU:HD12	2.19	0.42
1:E:185:TYR:HB3	1:E:314:MET:SD	2.59	0.42
1:F:194:SER:OG	1:F:283:GLU:HG2	2.20	0.42
1:G:146:ASP:HA	1:G:170:VAL:HA	2.02	0.42
1:J:111:ASN:O	1:J:115:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:217:LEU:HD23	1:K:217:LEU:HA	1.75	0.42
1:A:45:HIS:O	1:A:49:LYS:HG2	2.19	0.42
1:A:94:ALA:O	1:A:98:ARG:HG3	2.19	0.42
1:B:93:LEU:HD11	1:B:133:PHE:HZ	1.84	0.42
1:C:191:ALA:O	1:C:198:ASN:ND2	2.52	0.42
1:F:396:LYS:HD3	1:F:396:LYS:HA	1.88	0.42
1:G:301:THR:HG22	1:H:249:PRO:HG3	2.01	0.42
1:J:178:PHE:HZ	1:J:197:THR:HG21	1.85	0.42
1:J:297:TYR:OH	1:K:461:SER:N	2.52	0.42
1:K:63:ASP:OD2	1:K:71:ARG:NH2	2.47	0.42
1:A:146:ASP:HB2	1:A:171:ARG:NH1	2.35	0.42
1:A:261:PRO:HG2	1:A:445:ALA:HB2	2.01	0.42
1:A:438:GLN:OE1	1:B:198:ASN:ND2	2.51	0.42
1:B:68:PRO:HB2	1:B:96:TYR:CG	2.54	0.42
1:B:396:LYS:HD2	1:B:396:LYS:HA	1.78	0.42
1:F:358:LEU:HD12	1:F:358:LEU:HA	1.88	0.42
1:H:174:TYR:CD2	1:H:289:ARG:HG2	2.55	0.42
1:H:212:LEU:HD12	1:H:212:LEU:HA	1.88	0.42
1:I:303:TYR:HB3	1:I:440:ILE:CG2	2.50	0.42
1:K:118:ASP:HB3	1:K:130:THR:HB	2.01	0.42
1:A:411:ARG:NH1	1:B:232:LYS:H	2.18	0.41
1:D:312:PHE:HB3	1:D:433:LYS:HB2	2.02	0.41
1:E:138:ASP:OD1	1:E:139:VAL:N	2.53	0.41
1:E:188:MET:HB2	1:E:329:SER:O	2.19	0.41
1:H:303:TYR:HB3	1:H:440:ILE:HG23	2.02	0.41
1:H:413:ARG:HA	1:H:423:PHE:HB3	2.01	0.41
1:I:58:ASP:HA	1:I:77:LYS:HZ1	1.85	0.41
1:I:313:LEU:HD11	1:I:391:PHE:CE1	2.54	0.41
1:A:464:LEU:O	1:A:468:ILE:HG12	2.20	0.41
1:C:400:LYS:HD3	1:C:400:LYS:HA	1.86	0.41
1:D:68:PRO:HB2	1:D:96:TYR:CG	2.55	0.41
1:D:146:ASP:OD2	1:D:147:VAL:HG23	2.20	0.41
1:D:235:PRO:HB3	1:D:252:ARG:HH22	1.85	0.41
1:F:139:VAL:HG13	1:F:164:HIS:CE1	2.55	0.41
1:F:357:LYS:O	1:F:360:VAL:HG12	2.20	0.41
1:G:138:ASP:OD1	1:G:139:VAL:N	2.53	0.41
1:G:314:MET:HE3	1:H:217:LEU:HG	2.01	0.41
1:H:408:LEU:HD21	1:I:316:LYS:CE	2.51	0.41
1:H:425:LYS:HG3	1:H:427:LYS:HZ1	1.85	0.41
1:J:184:MET:HA	1:J:256:LYS:HE2	2.01	0.41
1:C:43:PHE:CE1	1:C:285:TYR:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ALA:HB3	1:C:330:VAL:HG12	2.03	0.41
1:C:258:TRP:HZ3	1:C:290:ILE:HD11	1.85	0.41
1:D:212:LEU:HD12	1:D:212:LEU:HA	1.87	0.41
1:E:51:ILE:HA	1:E:51:ILE:HD13	1.80	0.41
1:E:396:LYS:HA	1:E:396:LYS:HD3	1.83	0.41
1:H:28:GLU:OE1	1:H:29:PRO:HD2	2.20	0.41
1:H:191:ALA:HB3	1:H:332:THR:HA	2.01	0.41
1:H:237:ASP:OD1	1:H:252:ARG:N	2.53	0.41
1:I:191:ALA:O	1:I:198:ASN:ND2	2.54	0.41
1:A:25:PHE:HE2	1:A:49:LYS:HB3	1.85	0.41
1:A:130:THR:OG1	1:A:133:PHE:O	2.32	0.41
1:E:208:LYS:HG3	1:E:215:THR:HG21	2.02	0.41
1:E:414:THR:N	1:E:422:ALA:O	2.40	0.41
1:F:151:GLN:O	3:F:1002:SAH:N	2.53	0.41
1:G:68:PRO:HB2	1:G:96:TYR:CG	2.56	0.41
1:G:237:ASP:OD1	1:G:252:ARG:N	2.54	0.41
1:H:289:ARG:NH1	1:H:289:ARG:HB3	2.35	0.41
1:I:23:PRO:HD2	1:I:24:MET:HE1	2.02	0.41
1:I:138:ASP:OD1	1:I:139:VAL:N	2.53	0.41
1:A:425:LYS:HD2	1:B:218:THR:OG1	2.21	0.41
1:B:138:ASP:OD1	1:B:139:VAL:N	2.53	0.41
1:D:427:LYS:HD3	1:D:427:LYS:HA	1.67	0.41
1:E:197:THR:HA	1:E:242:SER:O	2.21	0.41
1:F:267:LYS:HE3	1:F:446:GLU:OE1	2.21	0.41
1:F:313:LEU:HD11	1:F:391:PHE:CE1	2.55	0.41
1:G:194:SER:OG	1:G:283:GLU:HG2	2.20	0.41
1:J:146:ASP:HA	1:J:170:VAL:HA	2.02	0.41
1:A:235:PRO:HB3	1:A:252:ARG:NH2	2.35	0.41
1:B:146:ASP:HB2	1:B:171:ARG:HH11	1.85	0.41
1:B:314:MET:HG3	1:B:331:CYS:HB3	2.03	0.41
1:C:94:ALA:O	1:C:98:ARG:HG3	2.20	0.41
1:C:165:GLN:O	1:C:170:VAL:HG22	2.20	0.41
1:D:93:LEU:HD11	1:D:133:PHE:HZ	1.85	0.41
1:F:24:MET:HG3	1:F:25:PHE:HD1	1.84	0.41
1:H:139:VAL:HG13	1:H:164:HIS:CE1	2.56	0.41
1:H:195:TYR:N	1:H:195:TYR:CD2	2.88	0.41
1:I:84:MET:O	1:I:85:ARG:NE	2.53	0.41
1:I:192:TYR:HB2	1:I:197:THR:O	2.21	0.41
1:I:194:SER:OG	1:I:283:GLU:HG2	2.20	0.41
1:A:237:ASP:O	1:A:252:ARG:N	2.51	0.41
1:D:383:MET:O	1:D:383:MET:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:ARG:NH2	1:E:233:LEU:HD13	2.35	0.41
1:F:110:ARG:HA	1:F:110:ARG:HD3	1.86	0.41
1:F:154:TYR:HD1	1:F:255:LEU:HD13	1.86	0.41
1:J:440:ILE:HD11	1:K:212:LEU:HD21	2.02	0.41
1:K:434:ARG:HB3	1:L:382:TYR:HB2	2.02	0.41
1:L:93:LEU:HD12	1:L:93:LEU:HA	1.77	0.41
1:L:261:PRO:HD2	1:L:264:PHE:CD2	2.51	0.41
1:A:427:LYS:HA	1:A:427:LYS:HD3	1.56	0.41
1:B:104:ALA:HA	1:B:112:ILE:HG21	2.02	0.41
1:C:51:ILE:O	1:C:55:ILE:HG23	2.20	0.41
1:D:94:ALA:O	1:D:98:ARG:HG3	2.21	0.41
1:D:423:PHE:HE1	1:E:226:SER:HB2	1.86	0.41
1:E:235:PRO:HB3	1:E:252:ARG:HH22	1.85	0.41
1:F:425:LYS:HG3	1:F:427:LYS:NZ	2.35	0.41
1:K:99:LYS:HD2	1:K:99:LYS:HA	1.94	0.41
1:L:151:GLN:O	3:L:1002:SAH:N	2.53	0.41
1:L:171:ARG:O	1:L:292:MET:N	2.53	0.41
1:B:184:MET:HB3	1:B:441:GLN:OE1	2.20	0.41
1:B:296:LEU:HD12	1:B:296:LEU:HA	1.86	0.41
1:B:337:THR:O	1:B:341:GLN:OE1	2.39	0.41
1:C:67:ALA:HB3	1:C:70:ARG:NH1	2.36	0.41
1:D:4:VAL:HG11	1:D:46:LEU:HD11	2.01	0.41
1:D:24:MET:HG2	1:D:25:PHE:HD1	1.86	0.41
1:D:181:THR:N	1:D:182:PRO:HD2	2.36	0.41
1:E:6:VAL:HG12	1:E:8:ILE:HG22	2.01	0.41
1:E:151:GLN:O	3:E:1002:SAH:N	2.54	0.41
1:E:190:GLY:HA2	1:E:331:CYS:SG	2.60	0.41
1:F:413:ARG:HA	1:F:423:PHE:HB3	2.02	0.41
1:G:413:ARG:HA	1:G:423:PHE:HB3	2.01	0.41
1:H:179:ASP:OD1	1:H:333:TYR:OH	2.39	0.41
1:H:184:MET:HB3	1:H:441:GLN:OE1	2.21	0.41
1:I:185:TYR:HB3	1:I:314:MET:SD	2.60	0.41
1:I:316:LYS:HZ2	1:I:329:SER:HB3	1.84	0.41
1:J:24:MET:HG2	1:J:25:PHE:CD1	2.56	0.41
1:J:94:ALA:O	1:J:98:ARG:HG3	2.20	0.41
1:J:191:ALA:HB1	1:J:383:MET:HE1	2.03	0.41
1:J:215:THR:OG1	1:J:216:ASP:N	2.54	0.41
1:L:179:ASP:HB2	1:L:284:GLY:O	2.21	0.41
1:L:183:PHE:HZ	1:L:241:PHE:HZ	1.69	0.41
1:A:312:PHE:HB3	1:A:433:LYS:HB2	2.03	0.41
1:B:55:ILE:HD12	1:B:61:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:GLN:O	3:C:1002:SAH:N	2.54	0.41
1:D:151:GLN:O	3:D:1002:SAH:N	2.53	0.41
1:D:427:LYS:HZ2	1:E:219:GLU:C	2.13	0.41
1:G:205:LEU:HD23	1:G:205:LEU:HA	1.94	0.41
1:I:51:ILE:HD13	1:I:51:ILE:HA	1.86	0.41
1:I:197:THR:HA	1:I:242:SER:O	2.21	0.41
1:L:266:LEU:O	1:L:271:SER:HA	2.20	0.41
1:D:232:LYS:HE3	1:D:232:LYS:HB2	1.81	0.40
1:E:28:GLU:OE1	1:E:29:PRO:HD2	2.20	0.40
1:E:154:TYR:OH	1:E:178:PHE:N	2.48	0.40
1:E:243:VAL:HG23	1:E:246:THR:OG1	2.21	0.40
1:F:68:PRO:HB2	1:F:96:TYR:CD1	2.56	0.40
1:G:64:ILE:N	1:G:64:ILE:HD13	2.36	0.40
1:J:48:ILE:HD13	1:J:48:ILE:HA	1.94	0.40
1:J:178:PHE:HD1	1:J:241:PHE:HE1	1.67	0.40
1:K:338:ILE:HD13	1:K:362:LEU:HD22	2.04	0.40
1:L:191:ALA:HB1	1:L:383:MET:SD	2.61	0.40
1:A:190:GLY:HA3	1:A:199:TRP:CE2	2.55	0.40
1:E:181:THR:HG23	1:E:181:THR:H	1.65	0.40
1:E:405:GLU:HA	1:F:318:THR:HG21	2.03	0.40
1:G:259:HIS:HE2	1:G:306:THR:HG1	1.68	0.40
1:G:344:GLY:HA3	1:H:360:VAL:HG11	2.03	0.40
1:H:110:ARG:HA	1:H:110:ARG:HD3	1.84	0.40
1:H:138:ASP:OD1	1:H:139:VAL:N	2.54	0.40
1:I:339:CYS:HG	1:I:432:TYR:HH	1.63	0.40
1:J:237:ASP:OD1	1:J:252:ARG:N	2.54	0.40
1:J:335:PRO:HD3	1:J:379:MET:HE3	2.02	0.40
1:K:154:TYR:CD2	1:K:255:LEU:HD11	2.55	0.40
1:D:183:PHE:HZ	1:D:241:PHE:CE1	2.39	0.40
1:D:440:ILE:HD11	1:E:212:LEU:HD21	2.03	0.40
1:E:68:PRO:HB2	1:E:96:TYR:CG	2.56	0.40
1:E:411:ARG:HB3	1:F:324:GLU:OE2	2.21	0.40
1:G:122:VAL:HG21	1:G:133:PHE:HE1	1.86	0.40
1:G:135:LEU:HD23	1:G:135:LEU:HA	1.83	0.40
1:G:260:LEU:HB3	1:G:264:PHE:CE2	2.54	0.40
1:I:88:GLU:OE2	1:I:92:ARG:NH1	2.54	0.40
1:K:100:LEU:HD11	1:K:115:LYS:HB2	2.03	0.40
1:L:188:MET:HB2	1:L:329:SER:O	2.22	0.40
1:L:346:LEU:HD23	1:L:346:LEU:HA	1.95	0.40
1:L:363:ASN:HD21	1:L:379:MET:HG2	1.86	0.40
1:C:235:PRO:HB3	1:C:252:ARG:HH22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:ASP:OD1	1:D:380:LYS:NZ	2.33	0.40
1:E:63:ASP:OD2	1:E:71:ARG:NH2	2.54	0.40
1:H:93:LEU:HD21	1:H:133:PHE:CZ	2.56	0.40
1:H:115:LYS:H	1:H:115:LYS:HD2	1.87	0.40
1:K:266:LEU:O	1:K:271:SER:HA	2.21	0.40
1:L:314:MET:O	1:L:430:THR:HA	2.21	0.40
1:B:286:VAL:HG21	1:B:288:LYS:HZ2	1.86	0.40
1:C:68:PRO:HB2	1:C:96:TYR:CD1	2.56	0.40
1:C:358:LEU:HD12	1:C:358:LEU:HA	1.96	0.40
1:E:273:THR:HG23	1:E:295:GLY:O	2.21	0.40
1:F:119:LEU:HD23	1:F:119:LEU:HA	1.87	0.40
1:F:413:ARG:HG2	1:F:423:PHE:HB3	2.04	0.40
1:G:181:THR:N	1:G:182:PRO:HD2	2.37	0.40
1:I:464:LEU:O	1:I:468:ILE:HG12	2.22	0.40
1:J:261:PRO:HD2	1:J:264:PHE:HD2	1.86	0.40
1:K:197:THR:HA	1:K:242:SER:O	2.22	0.40
1:K:303:TYR:HB3	1:K:440:ILE:CG2	2.51	0.40
1:L:202:GLU:HA	1:L:205:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/469 (92%)	403 (94%)	28 (6%)	0	100	100
1	B	431/469 (92%)	403 (94%)	28 (6%)	0	100	100
1	C	431/469 (92%)	402 (93%)	29 (7%)	0	100	100
1	D	431/469 (92%)	403 (94%)	28 (6%)	0	100	100
1	E	431/469 (92%)	402 (93%)	29 (7%)	0	100	100
1	F	431/469 (92%)	406 (94%)	25 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	431/469 (92%)	404 (94%)	27 (6%)	0	100	100
1	H	431/469 (92%)	401 (93%)	30 (7%)	0	100	100
1	I	431/469 (92%)	396 (92%)	35 (8%)	0	100	100
1	J	431/469 (92%)	401 (93%)	30 (7%)	0	100	100
1	K	431/469 (92%)	406 (94%)	25 (6%)	0	100	100
1	L	431/469 (92%)	402 (93%)	29 (7%)	0	100	100
All	All	5172/5628 (92%)	4829 (93%)	343 (7%)	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	A	368/405 (91%)	343 (93%)	25 (7%)	16	49
1	B	368/405 (91%)	337 (92%)	31 (8%)	11	39
1	C	368/405 (91%)	344 (94%)	24 (6%)	17	51
1	D	368/405 (91%)	347 (94%)	21 (6%)	20	56
1	E	368/405 (91%)	346 (94%)	22 (6%)	19	54
1	F	368/405 (91%)	350 (95%)	18 (5%)	25	61
1	G	368/405 (91%)	340 (92%)	28 (8%)	13	45
1	H	368/405 (91%)	341 (93%)	27 (7%)	14	46
1	I	368/405 (91%)	345 (94%)	23 (6%)	18	52
1	J	368/405 (91%)	345 (94%)	23 (6%)	18	52
1	K	368/405 (91%)	344 (94%)	24 (6%)	17	51
1	L	368/405 (91%)	339 (92%)	29 (8%)	12	43
All	All	4416/4860 (91%)	4121 (93%)	295 (7%)	20	50

All (295) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	28	GLU
1	A	53	GLN
1	A	72	MET
1	A	76	ARG
1	A	99	LYS
1	A	140	SER
1	A	152	ASP
1	A	174	TYR
1	A	194	SER
1	A	195	TYR
1	A	203	GLN
1	A	232	LYS
1	A	236	CYS
1	A	266	LEU
1	A	282	CYS
1	A	285	TYR
1	A	310	ASP
1	A	314	MET
1	A	357	LYS
1	A	400	LYS
1	A	411	ARG
1	A	423	PHE
1	A	434	ARG
1	A	463	PRO
1	B	24	MET
1	B	72	MET
1	B	75	ASP
1	B	76	ARG
1	B	77	LYS
1	B	99	LYS
1	B	133	PHE
1	B	134	CYS
1	B	140	SER
1	B	152	ASP
1	B	163	TYR
1	B	172	LEU
1	B	194	SER
1	B	202	GLU
1	B	214	SER
1	B	219	GLU
1	B	232	LYS
1	B	236	CYS

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Mol	Chain	Res	Type
1	B	276	CYS
1	B	282	CYS
1	B	285	TYR
1	B	314	MET
1	B	319	ASP
1	B	341	GLN
1	B	358	LEU
1	B	400	LYS
1	B	403	GLU
1	B	423	PHE
1	B	434	ARG
1	B	461	SER
1	B	463	PRO
1	C	24	MET
1	C	53	GLN
1	C	72	MET
1	C	76	ARG
1	C	84	MET
1	C	99	LYS
1	C	110	ARG
1	C	163	TYR
1	C	219	GLU
1	C	221	ARG
1	C	228	MET
1	C	245	SER
1	C	266	LEU
1	C	282	CYS
1	C	285	TYR
1	C	310	ASP
1	C	314	MET
1	C	319	ASP
1	C	383	MET
1	C	396	LYS
1	C	400	LYS
1	C	411	ARG
1	C	434	ARG
1	C	436	ASP
1	D	28	GLU
1	D	72	MET
1	D	76	ARG
1	D	86	SER
1	D	99	LYS

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Mol	Chain	Res	Type
1	D	133	PHE
1	D	134	CYS
1	D	152	ASP
1	D	184	MET
1	D	203	GLN
1	D	228	MET
1	D	236	CYS
1	D	245	SER
1	D	264	PHE
1	D	282	CYS
1	D	285	TYR
1	D	396	LYS
1	D	397	GLU
1	D	400	LYS
1	D	434	ARG
1	D	469	LYS
1	E	28	GLU
1	E	75	ASP
1	E	76	ARG
1	E	84	MET
1	E	92	ARG
1	E	133	PHE
1	E	152	ASP
1	E	163	TYR
1	E	194	SER
1	E	203	GLN
1	E	214	SER
1	E	219	GLU
1	E	245	SER
1	E	282	CYS
1	E	285	TYR
1	E	327	SER
1	E	357	LYS
1	E	358	LEU
1	E	400	LYS
1	E	434	ARG
1	E	461	SER
1	E	463	PRO
1	F	16	LYS
1	F	72	MET
1	F	99	LYS
1	F	134	CYS

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Mol	Chain	Res	Type
1	F	152	ASP
1	F	195	TYR
1	F	216	ASP
1	F	245	SER
1	F	264	PHE
1	F	282	CYS
1	F	285	TYR
1	F	297	TYR
1	F	319	ASP
1	F	400	LYS
1	F	411	ARG
1	F	434	ARG
1	F	461	SER
1	F	463	PRO
1	G	12	SER
1	G	24	MET
1	G	28	GLU
1	G	76	ARG
1	G	86	SER
1	G	93	LEU
1	G	115	LYS
1	G	140	SER
1	G	152	ASP
1	G	171	ARG
1	G	184	MET
1	G	195	TYR
1	G	203	GLN
1	G	205	LEU
1	G	232	LYS
1	G	236	CYS
1	G	264	PHE
1	G	282	CYS
1	G	285	TYR
1	G	340	ASP
1	G	383	MET
1	G	396	LYS
1	G	397	GLU
1	G	400	LYS
1	G	411	ARG
1	G	434	ARG
1	G	446	GLU
1	G	463	PRO

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Mol	Chain	Res	Type
1	H	24	MET
1	H	28	GLU
1	H	75	ASP
1	H	76	ARG
1	H	84	MET
1	H	92	ARG
1	H	99	LYS
1	H	133	PHE
1	H	140	SER
1	H	152	ASP
1	H	188	MET
1	H	202	GLU
1	H	214	SER
1	H	219	GLU
1	H	228	MET
1	H	232	LYS
1	H	236	CYS
1	H	245	SER
1	H	264	PHE
1	H	282	CYS
1	H	285	TYR
1	H	357	LYS
1	H	396	LYS
1	H	400	LYS
1	H	411	ARG
1	H	434	ARG
1	H	463	PRO
1	I	16	LYS
1	I	24	MET
1	I	30	ARG
1	I	53	GLN
1	I	72	MET
1	I	84	MET
1	I	99	LYS
1	I	152	ASP
1	I	171	ARG
1	I	195	TYR
1	I	245	SER
1	I	264	PHE
1	I	266	LEU
1	I	282	CYS
1	I	285	TYR

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Mol	Chain	Res	Type
1	I	292	MET
1	I	297	TYR
1	I	314	MET
1	I	319	ASP
1	I	396	LYS
1	I	434	ARG
1	I	461	SER
1	I	463	PRO
1	J	28	GLU
1	J	36	ASP
1	J	76	ARG
1	J	115	LYS
1	J	142	ARG
1	J	152	ASP
1	J	185	TYR
1	J	195	TYR
1	J	203	GLN
1	J	251	SER
1	J	264	PHE
1	J	272	PHE
1	J	275	ARG
1	J	282	CYS
1	J	285	TYR
1	J	303	TYR
1	J	383	MET
1	J	396	LYS
1	J	400	LYS
1	J	423	PHE
1	J	434	ARG
1	J	463	PRO
1	J	469	LYS
1	K	24	MET
1	K	28	GLU
1	K	49	LYS
1	K	76	ARG
1	K	84	MET
1	K	133	PHE
1	K	134	CYS
1	K	140	SER
1	K	152	ASP
1	K	163	TYR
1	K	214	SER

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Mol	Chain	Res	Type
1	K	217	LEU
1	K	221	ARG
1	K	232	LYS
1	K	264	PHE
1	K	282	CYS
1	K	285	TYR
1	K	297	TYR
1	K	358	LEU
1	K	396	LYS
1	K	397	GLU
1	K	400	LYS
1	K	434	ARG
1	K	463	PRO
1	L	20	ARG
1	L	28	GLU
1	L	52	GLU
1	L	53	GLN
1	L	72	MET
1	L	75	ASP
1	L	76	ARG
1	L	84	MET
1	L	99	LYS
1	L	133	PHE
1	L	171	ARG
1	L	194	SER
1	L	221	ARG
1	L	228	MET
1	L	251	SER
1	L	264	PHE
1	L	266	LEU
1	L	285	TYR
1	L	291	THR
1	L	297	TYR
1	L	314	MET
1	L	319	ASP
1	L	383	MET
1	L	396	LYS
1	L	400	LYS
1	L	402	MET
1	L	427	LYS
1	L	434	ARG
1	L	436	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	389	GLN
1	B	143	GLN
1	C	143	GLN
1	D	389	GLN
1	E	143	GLN
1	E	356	GLN
1	G	356	GLN
1	H	143	GLN
1	I	389	GLN
1	J	143	GLN
1	J	356	GLN
1	J	389	GLN
1	K	143	GLN
1	K	209	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PJ3	E	37	1	32,37,38	4.17	12 (37%)	33,56,58	2.01	9 (27%)
1	PJ3	J	37	1	32,37,38	4.18	14 (43%)	33,56,58	2.03	11 (33%)
1	PJ3	F	37	1	32,37,38	4.17	13 (40%)	33,56,58	2.00	10 (30%)
1	PJ3	K	37	1	32,37,38	4.17	12 (37%)	33,56,58	2.01	9 (27%)
1	PJ3	B	37	1	32,37,38	4.17	12 (37%)	33,56,58	2.00	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PJ3	G	37	1	32,37,38	4.18	14 (43%)	33,56,58	2.02	11 (33%)
1	PJ3	D	37	1	32,37,38	4.19	14 (43%)	33,56,58	2.03	11 (33%)
1	PJ3	I	37	1	32,37,38	4.17	13 (40%)	33,56,58	2.01	10 (30%)
1	PJ3	L	37	1	32,37,38	4.17	13 (40%)	33,56,58	2.00	10 (30%)
1	PJ3	H	37	1	32,37,38	4.16	12 (37%)	33,56,58	2.04	10 (30%)
1	PJ3	A	37	1	32,37,38	4.18	13 (40%)	33,56,58	2.03	11 (33%)
1	PJ3	C	37	1	32,37,38	4.17	13 (40%)	33,56,58	2.01	10 (30%)

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
1	PJ3	E	37	1	-	2/14/50/52	0/4/4/4
1	PJ3	J	37	1	-	2/14/50/52	0/4/4/4
1	PJ3	F	37	1	-	2/14/50/52	0/4/4/4
1	PJ3	K	37	1	-	2/14/50/52	0/4/4/4
1	PJ3	B	37	1	-	2/14/50/52	0/4/4/4
1	PJ3	G	37	1	-	2/14/50/52	0/4/4/4
1	PJ3	D	37	1	-	2/14/50/52	0/4/4/4
1	PJ3	I	37	1	-	2/14/50/52	0/4/4/4
1	PJ3	L	37	1	-	2/14/50/52	0/4/4/4
1	PJ3	H	37	1	-	2/14/50/52	0/4/4/4
1	PJ3	A	37	1	-	2/14/50/52	0/4/4/4
1	PJ3	C	37	1	-	2/14/50/52	0/4/4/4

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	37	PJ3	PA-O5'	16.57	1.73	1.57
1	B	37	PJ3	PA-O5'	16.56	1.73	1.57
1	A	37	PJ3	PA-O5'	16.56	1.73	1.57
1	J	37	PJ3	PA-O5'	16.56	1.73	1.57
1	D	37	PJ3	PA-O5'	16.56	1.73	1.57
1	G	37	PJ3	PA-O5'	16.56	1.73	1.57
1	K	37	PJ3	PA-O5'	16.56	1.73	1.57
1	F	37	PJ3	PA-O5'	16.56	1.73	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	37	PJ3	PA-O5'	16.56	1.73	1.57
1	L	37	PJ3	PA-O5'	16.55	1.73	1.57
1	H	37	PJ3	PA-O5'	16.55	1.73	1.57
1	C	37	PJ3	PA-O5'	16.55	1.73	1.57
1	D	37	PJ3	C5-N7	9.89	1.47	1.35
1	J	37	PJ3	C5-N7	9.86	1.46	1.35
1	G	37	PJ3	C5-N7	9.85	1.46	1.35
1	A	37	PJ3	C5-N7	9.83	1.46	1.35
1	F	37	PJ3	C5-N7	9.77	1.46	1.35
1	I	37	PJ3	C5-N7	9.76	1.46	1.35
1	C	37	PJ3	C5-N7	9.76	1.46	1.35
1	L	37	PJ3	C5-N7	9.75	1.46	1.35
1	H	37	PJ3	C5-N7	9.73	1.46	1.35
1	E	37	PJ3	C5-N7	9.72	1.46	1.35
1	B	37	PJ3	C5-N7	9.72	1.46	1.35
1	K	37	PJ3	C5-N7	9.71	1.46	1.35
1	L	37	PJ3	CA-N	-6.10	1.29	1.48
1	I	37	PJ3	CA-N	-6.10	1.29	1.48
1	C	37	PJ3	CA-N	-6.09	1.29	1.48
1	J	37	PJ3	CA-N	-6.09	1.29	1.48
1	D	37	PJ3	CA-N	-6.09	1.29	1.48
1	A	37	PJ3	CA-N	-6.09	1.29	1.48
1	G	37	PJ3	CA-N	-6.09	1.29	1.48
1	F	37	PJ3	CA-N	-6.09	1.29	1.48
1	H	37	PJ3	CA-N	-6.09	1.29	1.48
1	K	37	PJ3	CA-N	-6.09	1.29	1.48
1	B	37	PJ3	CA-N	-6.08	1.29	1.48
1	E	37	PJ3	CA-N	-6.08	1.29	1.48
1	K	37	PJ3	C8-N9	5.20	1.48	1.46
1	B	37	PJ3	C8-N9	5.18	1.48	1.46
1	E	37	PJ3	C8-N9	5.18	1.48	1.46
1	C	37	PJ3	C8-N9	5.18	1.48	1.46
1	H	37	PJ3	C8-N9	5.18	1.48	1.46
1	L	37	PJ3	C8-N9	5.17	1.48	1.46
1	I	37	PJ3	C8-N9	5.16	1.48	1.46
1	A	37	PJ3	C8-N9	5.16	1.48	1.46
1	F	37	PJ3	C8-N9	5.14	1.48	1.46
1	J	37	PJ3	C8-N9	5.12	1.48	1.46
1	G	37	PJ3	C8-N9	5.11	1.48	1.46
1	D	37	PJ3	C8-N9	5.05	1.48	1.46
1	J	37	PJ3	C6-N1	4.86	1.47	1.38
1	D	37	PJ3	C6-N1	4.85	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	37	PJ3	C6-N1	4.85	1.47	1.38
1	A	37	PJ3	C6-N1	4.85	1.47	1.38
1	B	37	PJ3	C6-N1	4.85	1.47	1.38
1	H	37	PJ3	C6-N1	4.85	1.47	1.38
1	I	37	PJ3	C6-N1	4.84	1.47	1.38
1	L	37	PJ3	C6-N1	4.84	1.47	1.38
1	C	37	PJ3	C6-N1	4.84	1.47	1.38
1	F	37	PJ3	C6-N1	4.84	1.47	1.38
1	E	37	PJ3	C6-N1	4.84	1.47	1.38
1	K	37	PJ3	C6-N1	4.84	1.47	1.38
1	K	37	PJ3	C1'-N9	4.19	1.54	1.46
1	E	37	PJ3	C1'-N9	4.19	1.54	1.46
1	L	37	PJ3	C1'-N9	4.18	1.54	1.46
1	B	37	PJ3	C1'-N9	4.18	1.54	1.46
1	D	37	PJ3	C1'-N9	4.18	1.54	1.46
1	C	37	PJ3	C1'-N9	4.17	1.54	1.46
1	F	37	PJ3	C1'-N9	4.17	1.54	1.46
1	I	37	PJ3	C1'-N9	4.17	1.54	1.46
1	A	37	PJ3	C1'-N9	4.16	1.54	1.46
1	J	37	PJ3	C1'-N9	4.15	1.54	1.46
1	H	37	PJ3	C1'-N9	4.14	1.54	1.46
1	G	37	PJ3	C1'-N9	4.14	1.54	1.46
1	K	37	PJ3	C4-N9	4.09	1.42	1.37
1	E	37	PJ3	C4-N9	4.08	1.42	1.37
1	D	37	PJ3	C4-N9	4.08	1.42	1.37
1	I	37	PJ3	C4-N9	4.08	1.42	1.37
1	B	37	PJ3	C4-N9	4.08	1.42	1.37
1	L	37	PJ3	C4-N9	4.07	1.42	1.37
1	C	37	PJ3	C4-N9	4.07	1.42	1.37
1	H	37	PJ3	C4-N9	4.07	1.42	1.37
1	F	37	PJ3	C4-N9	4.07	1.42	1.37
1	A	37	PJ3	C4-N9	4.06	1.42	1.37
1	G	37	PJ3	C4-N9	4.06	1.42	1.37
1	J	37	PJ3	C4-N9	4.05	1.42	1.37
1	C	37	PJ3	PA-O3A	-3.11	1.48	1.54
1	J	37	PJ3	PA-O3A	-3.11	1.48	1.54
1	A	37	PJ3	PA-O3A	-3.11	1.48	1.54
1	L	37	PJ3	PA-O3A	-3.11	1.48	1.54
1	E	37	PJ3	PA-O3A	-3.10	1.48	1.54
1	K	37	PJ3	PA-O3A	-3.10	1.48	1.54
1	G	37	PJ3	PA-O3A	-3.10	1.48	1.54
1	I	37	PJ3	PA-O3A	-3.10	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	PJ3	PA-O3A	-3.10	1.48	1.54
1	F	37	PJ3	PA-O3A	-3.10	1.48	1.54
1	H	37	PJ3	PA-O3A	-3.10	1.48	1.54
1	D	37	PJ3	PA-O3A	-3.10	1.48	1.54
1	H	37	PJ3	CE1-ND1	2.90	1.40	1.35
1	A	37	PJ3	CE1-ND1	2.90	1.40	1.35
1	F	37	PJ3	CE1-ND1	2.90	1.40	1.35
1	E	37	PJ3	CE1-ND1	2.90	1.40	1.35
1	G	37	PJ3	CE1-ND1	2.90	1.40	1.35
1	L	37	PJ3	CE1-ND1	2.90	1.40	1.35
1	J	37	PJ3	CE1-ND1	2.90	1.40	1.35
1	B	37	PJ3	CE1-ND1	2.90	1.40	1.35
1	D	37	PJ3	CE1-ND1	2.90	1.40	1.35
1	I	37	PJ3	CE1-ND1	2.89	1.40	1.35
1	C	37	PJ3	CE1-ND1	2.89	1.40	1.35
1	K	37	PJ3	CE1-ND1	2.89	1.40	1.35
1	D	37	PJ3	C5'-C4'	2.51	1.59	1.51
1	A	37	PJ3	C5'-C4'	2.51	1.59	1.51
1	J	37	PJ3	C5'-C4'	2.51	1.59	1.51
1	G	37	PJ3	C5'-C4'	2.51	1.59	1.51
1	B	37	PJ3	C5'-C4'	2.51	1.59	1.51
1	K	37	PJ3	C5'-C4'	2.51	1.59	1.51
1	E	37	PJ3	C5'-C4'	2.51	1.59	1.51
1	I	37	PJ3	C5'-C4'	2.51	1.59	1.51
1	D	37	PJ3	C5-C6	2.51	1.50	1.43
1	C	37	PJ3	C5'-C4'	2.51	1.59	1.51
1	F	37	PJ3	C5'-C4'	2.51	1.59	1.51
1	L	37	PJ3	C5'-C4'	2.51	1.59	1.51
1	H	37	PJ3	C5'-C4'	2.50	1.59	1.51
1	C	37	PJ3	CD2-CG	2.30	1.39	1.36
1	A	37	PJ3	CD2-CG	2.29	1.39	1.36
1	G	37	PJ3	CD2-CG	2.29	1.39	1.36
1	J	37	PJ3	CD2-CG	2.29	1.39	1.36
1	K	37	PJ3	CD2-CG	2.29	1.39	1.36
1	L	37	PJ3	CD2-CG	2.29	1.39	1.36
1	F	37	PJ3	CD2-CG	2.28	1.39	1.36
1	B	37	PJ3	CD2-CG	2.28	1.39	1.36
1	D	37	PJ3	CD2-CG	2.28	1.39	1.36
1	I	37	PJ3	CD2-CG	2.28	1.39	1.36
1	H	37	PJ3	CD2-CG	2.28	1.39	1.36
1	E	37	PJ3	CD2-CG	2.27	1.39	1.36
1	D	37	PJ3	C2-N2	2.16	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	37	PJ3	C2-N2	2.16	1.39	1.34
1	A	37	PJ3	C2-N2	2.15	1.39	1.34
1	F	37	PJ3	C2-N2	2.15	1.39	1.34
1	G	37	PJ3	C2-N2	2.15	1.39	1.34
1	I	37	PJ3	C2-N2	2.15	1.39	1.34
1	E	37	PJ3	C2-N2	2.15	1.39	1.34
1	H	37	PJ3	C2-N2	2.15	1.39	1.34
1	C	37	PJ3	C2-N2	2.15	1.39	1.34
1	K	37	PJ3	C2-N2	2.15	1.39	1.34
1	B	37	PJ3	C2-N2	2.15	1.39	1.34
1	L	37	PJ3	C2-N2	2.15	1.39	1.34
1	J	37	PJ3	C5-C6	2.06	1.48	1.43
1	G	37	PJ3	C5-C6	2.02	1.48	1.43
1	J	37	PJ3	C4-N3	2.01	1.39	1.34
1	A	37	PJ3	C4-N3	2.01	1.39	1.34
1	F	37	PJ3	C4-N3	2.00	1.39	1.34
1	D	37	PJ3	C4-N3	2.00	1.39	1.34
1	C	37	PJ3	C4-N3	2.00	1.39	1.34
1	G	37	PJ3	C4-N3	2.00	1.39	1.34
1	I	37	PJ3	C4-N3	2.00	1.39	1.34
1	L	37	PJ3	C4-N3	2.00	1.39	1.34

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	37	PJ3	C5-C4-N9	4.59	112.30	106.35
1	H	37	PJ3	C5-C4-N9	4.58	112.29	106.35
1	H	37	PJ3	O4'-C1'-N9	4.54	115.48	109.30
1	B	37	PJ3	C5-C4-N9	4.52	112.22	106.35
1	E	37	PJ3	C5-C4-N9	4.51	112.21	106.35
1	C	37	PJ3	C5-C4-N9	4.45	112.12	106.35
1	L	37	PJ3	C5-C4-N9	4.43	112.10	106.35
1	J	37	PJ3	C5-C4-N9	4.41	112.07	106.35
1	A	37	PJ3	C5-C4-N9	4.39	112.05	106.35
1	I	37	PJ3	C5-C4-N9	4.39	112.05	106.35
1	D	37	PJ3	C5-C4-N9	4.38	112.04	106.35
1	I	37	PJ3	O4'-C1'-N9	4.38	115.27	109.30
1	F	37	PJ3	C5-C4-N9	4.36	112.01	106.35
1	G	37	PJ3	C5-C4-N9	4.36	112.00	106.35
1	L	37	PJ3	O5'-PA-O1A	-4.36	109.58	115.29
1	H	37	PJ3	O5'-PA-O1A	-4.34	109.61	115.29
1	I	37	PJ3	O5'-PA-O1A	-4.34	109.61	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	37	PJ3	O5'-PA-O1A	-4.34	109.61	115.29
1	A	37	PJ3	O4'-C1'-N9	4.33	115.20	109.30
1	C	37	PJ3	O5'-PA-O1A	-4.32	109.63	115.29
1	K	37	PJ3	O5'-PA-O1A	-4.32	109.63	115.29
1	B	37	PJ3	O5'-PA-O1A	-4.30	109.66	115.29
1	E	37	PJ3	O4'-C1'-N9	4.30	115.15	109.30
1	A	37	PJ3	O5'-PA-O1A	-4.29	109.67	115.29
1	L	37	PJ3	O4'-C1'-N9	4.28	115.13	109.30
1	E	37	PJ3	O5'-PA-O1A	-4.28	109.68	115.29
1	J	37	PJ3	O5'-PA-O1A	-4.28	109.68	115.29
1	G	37	PJ3	O5'-PA-O1A	-4.28	109.68	115.29
1	C	37	PJ3	O4'-C1'-N9	4.28	115.12	109.30
1	J	37	PJ3	O4'-C1'-N9	4.28	115.12	109.30
1	D	37	PJ3	O4'-C1'-N9	4.28	115.12	109.30
1	G	37	PJ3	O4'-C1'-N9	4.27	115.12	109.30
1	B	37	PJ3	O4'-C1'-N9	4.24	115.07	109.30
1	F	37	PJ3	O4'-C1'-N9	4.23	115.06	109.30
1	K	37	PJ3	O4'-C1'-N9	4.23	115.06	109.30
1	D	37	PJ3	O5'-PA-O1A	-4.21	109.78	115.29
1	D	37	PJ3	O6-C6-N1	-4.19	112.09	120.12
1	A	37	PJ3	O6-C6-N1	-4.17	112.12	120.12
1	G	37	PJ3	O6-C6-N1	-4.16	112.14	120.12
1	J	37	PJ3	O6-C6-N1	-4.16	112.15	120.12
1	I	37	PJ3	O6-C6-N1	-4.09	112.28	120.12
1	C	37	PJ3	O6-C6-N1	-4.08	112.29	120.12
1	F	37	PJ3	O6-C6-N1	-4.08	112.29	120.12
1	L	37	PJ3	O6-C6-N1	-4.08	112.29	120.12
1	H	37	PJ3	O6-C6-N1	-4.07	112.32	120.12
1	K	37	PJ3	O6-C6-N1	-4.07	112.32	120.12
1	B	37	PJ3	O6-C6-N1	-4.06	112.33	120.12
1	E	37	PJ3	O6-C6-N1	-4.05	112.35	120.12
1	D	37	PJ3	O6-C6-C5	2.97	134.83	127.54
1	G	37	PJ3	O6-C6-C5	2.89	134.63	127.54
1	J	37	PJ3	O6-C6-C5	2.89	134.62	127.54
1	A	37	PJ3	O6-C6-C5	2.88	134.62	127.54
1	I	37	PJ3	O6-C6-C5	2.84	134.50	127.54
1	F	37	PJ3	O6-C6-C5	2.83	134.49	127.54
1	L	37	PJ3	O6-C6-C5	2.83	134.49	127.54
1	C	37	PJ3	O6-C6-C5	2.82	134.47	127.54
1	B	37	PJ3	O6-C6-C5	2.82	134.46	127.54
1	E	37	PJ3	O6-C6-C5	2.82	134.46	127.54
1	H	37	PJ3	O6-C6-C5	2.82	134.45	127.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	37	PJ3	O6-C6-C5	2.81	134.45	127.54
1	H	37	PJ3	N9-C4-N3	-2.59	121.59	125.47
1	J	37	PJ3	N9-C4-N3	-2.56	121.64	125.47
1	B	37	PJ3	N9-C4-N3	-2.55	121.65	125.47
1	K	37	PJ3	N9-C4-N3	-2.55	121.66	125.47
1	K	37	PJ3	N9-C8-N7	2.53	107.00	103.38
1	D	37	PJ3	N9-C4-N3	-2.49	121.73	125.47
1	A	37	PJ3	N9-C4-N3	-2.49	121.74	125.47
1	G	37	PJ3	N9-C4-N3	-2.49	121.74	125.47
1	E	37	PJ3	N9-C4-N3	-2.49	121.75	125.47
1	J	37	PJ3	N9-C8-N7	2.48	106.92	103.38
1	D	37	PJ3	N9-C8-N7	2.48	106.92	103.38
1	C	37	PJ3	N9-C4-N3	-2.46	121.79	125.47
1	L	37	PJ3	N9-C4-N3	-2.45	121.80	125.47
1	E	37	PJ3	N9-C8-N7	2.45	106.88	103.38
1	C	37	PJ3	N9-C8-N7	2.43	106.86	103.38
1	I	37	PJ3	N9-C4-N3	-2.40	121.87	125.47
1	H	37	PJ3	N9-C8-N7	2.40	106.81	103.38
1	A	37	PJ3	N9-C8-N7	2.39	106.80	103.38
1	F	37	PJ3	N9-C4-N3	-2.39	121.89	125.47
1	K	37	PJ3	C4'-O4'-C1'	2.39	114.74	109.47
1	H	37	PJ3	C3'-C2'-C1'	2.39	105.96	101.43
1	B	37	PJ3	C4'-O4'-C1'	2.38	114.72	109.47
1	L	37	PJ3	N9-C8-N7	2.36	106.75	103.38
1	C	37	PJ3	C4'-O4'-C1'	2.35	114.65	109.47
1	I	37	PJ3	N9-C8-N7	2.33	106.72	103.38
1	I	37	PJ3	C3'-C2'-C1'	2.33	105.85	101.43
1	G	37	PJ3	N9-C8-N7	2.33	106.70	103.38
1	G	37	PJ3	C3'-C2'-C1'	2.32	105.84	101.43
1	A	37	PJ3	C3'-C2'-C1'	2.32	105.84	101.43
1	F	37	PJ3	C4'-O4'-C1'	2.32	114.59	109.47
1	J	37	PJ3	C3'-C2'-C1'	2.32	105.83	101.43
1	E	37	PJ3	C4'-O4'-C1'	2.32	114.59	109.47
1	B	37	PJ3	C3'-C2'-C1'	2.32	105.83	101.43
1	H	37	PJ3	C4'-O4'-C1'	2.32	114.58	109.47
1	F	37	PJ3	N9-C8-N7	2.31	106.69	103.38
1	F	37	PJ3	C3'-C2'-C1'	2.31	105.81	101.43
1	G	37	PJ3	C4'-O4'-C1'	2.30	114.55	109.47
1	E	37	PJ3	C3'-C2'-C1'	2.29	105.78	101.43
1	I	37	PJ3	C4'-O4'-C1'	2.29	114.52	109.47
1	B	37	PJ3	N9-C8-N7	2.28	106.64	103.38
1	C	37	PJ3	C3'-C2'-C1'	2.27	105.74	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	37	PJ3	C4'-O4'-C1'	2.27	114.48	109.47
1	D	37	PJ3	C6-C5-C4	-2.27	117.94	122.62
1	L	37	PJ3	C3'-C2'-C1'	2.26	105.72	101.43
1	K	37	PJ3	C3'-C2'-C1'	2.26	105.72	101.43
1	A	37	PJ3	C4'-O4'-C1'	2.26	114.45	109.47
1	D	37	PJ3	C3'-C2'-C1'	2.25	105.71	101.43
1	J	37	PJ3	C4'-O4'-C1'	2.25	114.44	109.47
1	J	37	PJ3	C6-C5-C4	-2.23	118.03	122.62
1	G	37	PJ3	C6-C5-C4	-2.20	118.08	122.62
1	A	37	PJ3	C6-C5-C4	-2.18	118.12	122.62
1	D	37	PJ3	C4'-O4'-C1'	2.17	114.27	109.47
1	D	37	PJ3	C2-N3-C4	2.10	116.04	112.30
1	C	37	PJ3	C6-C5-C4	-2.04	118.41	122.62
1	F	37	PJ3	C6-C5-C4	-2.04	118.42	122.62
1	I	37	PJ3	C6-C5-C4	-2.04	118.42	122.62
1	L	37	PJ3	C6-C5-C4	-2.04	118.42	122.62
1	A	37	PJ3	C2-N3-C4	2.02	115.90	112.30
1	G	37	PJ3	C2-N3-C4	2.02	115.89	112.30
1	J	37	PJ3	C2-N3-C4	2.02	115.89	112.30
1	B	37	PJ3	C6-C5-C4	-2.01	118.47	122.62
1	H	37	PJ3	C6-C5-C4	-2.00	118.49	122.62

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	37	PJ3	C3'-C4'-C5'-O5'
1	A	37	PJ3	O4'-C4'-C5'-O5'
1	B	37	PJ3	C3'-C4'-C5'-O5'
1	B	37	PJ3	O4'-C4'-C5'-O5'
1	C	37	PJ3	C3'-C4'-C5'-O5'
1	C	37	PJ3	O4'-C4'-C5'-O5'
1	D	37	PJ3	C3'-C4'-C5'-O5'
1	D	37	PJ3	O4'-C4'-C5'-O5'
1	E	37	PJ3	O4'-C4'-C5'-O5'
1	F	37	PJ3	C3'-C4'-C5'-O5'
1	F	37	PJ3	O4'-C4'-C5'-O5'
1	G	37	PJ3	C3'-C4'-C5'-O5'
1	G	37	PJ3	O4'-C4'-C5'-O5'
1	H	37	PJ3	O4'-C4'-C5'-O5'
1	I	37	PJ3	C3'-C4'-C5'-O5'
1	I	37	PJ3	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	J	37	PJ3	C3'-C4'-C5'-O5'
1	J	37	PJ3	O4'-C4'-C5'-O5'
1	K	37	PJ3	O4'-C4'-C5'-O5'
1	L	37	PJ3	C3'-C4'-C5'-O5'
1	L	37	PJ3	O4'-C4'-C5'-O5'
1	E	37	PJ3	C3'-C4'-C5'-O5'
1	H	37	PJ3	C3'-C4'-C5'-O5'
1	K	37	PJ3	C3'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	37	PJ3	4	0
1	J	37	PJ3	4	0
1	F	37	PJ3	4	0
1	K	37	PJ3	3	0
1	B	37	PJ3	4	0
1	G	37	PJ3	4	0
1	D	37	PJ3	4	0
1	I	37	PJ3	4	0
1	L	37	PJ3	3	0
1	H	37	PJ3	4	0
1	A	37	PJ3	4	0
1	C	37	PJ3	4	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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
3	SAH	B	1002	-	24,28,28	1.20	3 (12%)	25,40,40	1.74	5 (20%)
3	SAH	I	1002	-	24,28,28	1.20	3 (12%)	25,40,40	1.75	5 (20%)
3	SAH	A	1002	-	24,28,28	1.20	3 (12%)	25,40,40	1.74	5 (20%)
3	SAH	C	1002	-	24,28,28	1.20	3 (12%)	25,40,40	1.74	5 (20%)
3	SAH	H	1002	-	24,28,28	1.20	3 (12%)	25,40,40	1.74	5 (20%)
3	SAH	J	1002	-	24,28,28	1.20	3 (12%)	25,40,40	1.74	5 (20%)
3	SAH	L	1002	-	24,28,28	1.20	3 (12%)	25,40,40	1.74	5 (20%)
3	SAH	K	1002	-	24,28,28	1.20	3 (12%)	25,40,40	1.74	5 (20%)
3	SAH	D	1002	-	24,28,28	1.20	3 (12%)	25,40,40	1.75	5 (20%)
3	SAH	G	1002	-	24,28,28	1.20	3 (12%)	25,40,40	1.74	5 (20%)
3	SAH	E	1002	-	24,28,28	1.20	3 (12%)	25,40,40	1.75	5 (20%)
3	SAH	F	1002	-	24,28,28	1.20	3 (12%)	25,40,40	1.75	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	B	1002	-	-	1/11/31/31	0/3/3/3
3	SAH	I	1002	-	-	1/11/31/31	0/3/3/3
3	SAH	A	1002	-	-	1/11/31/31	0/3/3/3
3	SAH	C	1002	-	-	2/11/31/31	0/3/3/3
3	SAH	H	1002	-	-	1/11/31/31	0/3/3/3
3	SAH	J	1002	-	-	1/11/31/31	0/3/3/3
3	SAH	L	1002	-	-	2/11/31/31	0/3/3/3
3	SAH	K	1002	-	-	2/11/31/31	0/3/3/3
3	SAH	D	1002	-	-	1/11/31/31	0/3/3/3
3	SAH	G	1002	-	-	1/11/31/31	0/3/3/3
3	SAH	E	1002	-	-	2/11/31/31	0/3/3/3
3	SAH	F	1002	-	-	1/11/31/31	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1002	SAH	C2-N3	3.95	1.38	1.32
3	B	1002	SAH	C2-N3	3.95	1.38	1.32
3	L	1002	SAH	C2-N3	3.94	1.38	1.32
3	K	1002	SAH	C2-N3	3.94	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1002	SAH	C2-N3	3.94	1.38	1.32
3	I	1002	SAH	C2-N3	3.94	1.38	1.32
3	F	1002	SAH	C2-N3	3.94	1.38	1.32
3	C	1002	SAH	C2-N3	3.93	1.38	1.32
3	A	1002	SAH	C2-N3	3.93	1.38	1.32
3	D	1002	SAH	C2-N3	3.93	1.38	1.32
3	J	1002	SAH	C2-N3	3.93	1.38	1.32
3	G	1002	SAH	C2-N3	3.93	1.38	1.32
3	L	1002	SAH	C2-N1	2.43	1.38	1.33
3	B	1002	SAH	C2-N1	2.43	1.38	1.33
3	C	1002	SAH	C2-N1	2.43	1.38	1.33
3	I	1002	SAH	C2-N1	2.43	1.38	1.33
3	F	1002	SAH	C2-N1	2.43	1.38	1.33
3	D	1002	SAH	C2-N1	2.43	1.38	1.33
3	E	1002	SAH	C2-N1	2.43	1.38	1.33
3	A	1002	SAH	C2-N1	2.43	1.38	1.33
3	G	1002	SAH	C2-N1	2.43	1.38	1.33
3	H	1002	SAH	C2-N1	2.42	1.38	1.33
3	K	1002	SAH	C2-N1	2.42	1.38	1.33
3	J	1002	SAH	C2-N1	2.41	1.38	1.33
3	G	1002	SAH	OXT-C	-2.15	1.23	1.30
3	D	1002	SAH	OXT-C	-2.15	1.23	1.30
3	A	1002	SAH	OXT-C	-2.15	1.23	1.30
3	J	1002	SAH	OXT-C	-2.15	1.23	1.30
3	I	1002	SAH	OXT-C	-2.15	1.23	1.30
3	B	1002	SAH	OXT-C	-2.15	1.23	1.30
3	L	1002	SAH	OXT-C	-2.14	1.23	1.30
3	E	1002	SAH	OXT-C	-2.14	1.23	1.30
3	F	1002	SAH	OXT-C	-2.14	1.23	1.30
3	C	1002	SAH	OXT-C	-2.14	1.23	1.30
3	K	1002	SAH	OXT-C	-2.14	1.23	1.30
3	H	1002	SAH	OXT-C	-2.14	1.23	1.30

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1002	SAH	N3-C2-N1	-5.44	120.17	128.68
3	A	1002	SAH	N3-C2-N1	-5.44	120.18	128.68
3	I	1002	SAH	N3-C2-N1	-5.43	120.20	128.68
3	F	1002	SAH	N3-C2-N1	-5.43	120.20	128.68
3	H	1002	SAH	N3-C2-N1	-5.43	120.20	128.68
3	K	1002	SAH	N3-C2-N1	-5.42	120.20	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	SAH	N3-C2-N1	-5.42	120.20	128.68
3	L	1002	SAH	N3-C2-N1	-5.42	120.20	128.68
3	B	1002	SAH	N3-C2-N1	-5.41	120.23	128.68
3	D	1002	SAH	N3-C2-N1	-5.39	120.25	128.68
3	G	1002	SAH	N3-C2-N1	-5.38	120.27	128.68
3	J	1002	SAH	N3-C2-N1	-5.35	120.32	128.68
3	D	1002	SAH	C5'-SD-CG	-4.30	89.36	102.27
3	F	1002	SAH	C5'-SD-CG	-4.25	89.51	102.27
3	I	1002	SAH	C5'-SD-CG	-4.24	89.54	102.27
3	G	1002	SAH	C5'-SD-CG	-4.23	89.56	102.27
3	E	1002	SAH	C5'-SD-CG	-4.23	89.57	102.27
3	C	1002	SAH	C5'-SD-CG	-4.21	89.63	102.27
3	J	1002	SAH	C5'-SD-CG	-4.21	89.64	102.27
3	H	1002	SAH	C5'-SD-CG	-4.20	89.66	102.27
3	L	1002	SAH	C5'-SD-CG	-4.20	89.66	102.27
3	K	1002	SAH	C5'-SD-CG	-4.17	89.75	102.27
3	B	1002	SAH	C5'-SD-CG	-4.17	89.76	102.27
3	A	1002	SAH	C5'-SD-CG	-4.14	89.84	102.27
3	A	1002	SAH	C3'-C2'-C1'	2.76	105.14	100.98
3	A	1002	SAH	OXT-C-O	-2.71	117.93	124.09
3	B	1002	SAH	OXT-C-O	-2.71	117.93	124.09
3	J	1002	SAH	OXT-C-O	-2.71	117.94	124.09
3	K	1002	SAH	OXT-C-O	-2.70	117.95	124.09
3	I	1002	SAH	OXT-C-O	-2.70	117.95	124.09
3	H	1002	SAH	C3'-C2'-C1'	2.70	105.05	100.98
3	C	1002	SAH	OXT-C-O	-2.70	117.96	124.09
3	K	1002	SAH	C3'-C2'-C1'	2.70	105.04	100.98
3	L	1002	SAH	OXT-C-O	-2.70	117.96	124.09
3	E	1002	SAH	OXT-C-O	-2.70	117.97	124.09
3	F	1002	SAH	OXT-C-O	-2.70	117.97	124.09
3	B	1002	SAH	C3'-C2'-C1'	2.69	105.03	100.98
3	H	1002	SAH	OXT-C-O	-2.69	117.98	124.09
3	F	1002	SAH	C3'-C2'-C1'	2.69	105.03	100.98
3	G	1002	SAH	OXT-C-O	-2.68	118.00	124.09
3	D	1002	SAH	C3'-C2'-C1'	2.68	105.01	100.98
3	J	1002	SAH	C3'-C2'-C1'	2.68	105.01	100.98
3	L	1002	SAH	C3'-C2'-C1'	2.66	104.98	100.98
3	D	1002	SAH	OXT-C-O	-2.66	118.06	124.09
3	E	1002	SAH	C3'-C2'-C1'	2.65	104.97	100.98
3	I	1002	SAH	C3'-C2'-C1'	2.65	104.97	100.98
3	G	1002	SAH	C3'-C2'-C1'	2.65	104.97	100.98
3	C	1002	SAH	C3'-C2'-C1'	2.65	104.96	100.98

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	SAH	OXT-C-CA	2.27	121.12	113.38
3	A	1002	SAH	OXT-C-CA	2.27	121.11	113.38
3	K	1002	SAH	OXT-C-CA	2.26	121.09	113.38
3	I	1002	SAH	OXT-C-CA	2.26	121.08	113.38
3	L	1002	SAH	OXT-C-CA	2.26	121.07	113.38
3	C	1002	SAH	OXT-C-CA	2.26	121.07	113.38
3	E	1002	SAH	OXT-C-CA	2.26	121.07	113.38
3	G	1002	SAH	OXT-C-CA	2.25	121.06	113.38
3	J	1002	SAH	OXT-C-CA	2.25	121.06	113.38
3	F	1002	SAH	OXT-C-CA	2.25	121.05	113.38
3	H	1002	SAH	OXT-C-CA	2.25	121.05	113.38
3	D	1002	SAH	OXT-C-CA	2.22	120.93	113.38

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	SAH	CB-CG-SD-C5'
3	D	1002	SAH	CB-CG-SD-C5'
3	G	1002	SAH	CB-CG-SD-C5'
3	J	1002	SAH	CB-CG-SD-C5'
3	B	1002	SAH	CB-CG-SD-C5'
3	F	1002	SAH	CB-CG-SD-C5'
3	C	1002	SAH	CB-CG-SD-C5'
3	H	1002	SAH	CB-CG-SD-C5'
3	I	1002	SAH	CB-CG-SD-C5'
3	L	1002	SAH	CB-CG-SD-C5'
3	K	1002	SAH	CB-CG-SD-C5'
3	E	1002	SAH	CB-CG-SD-C5'
3	C	1002	SAH	OXT-C-CA-N
3	E	1002	SAH	OXT-C-CA-N
3	K	1002	SAH	OXT-C-CA-N
3	L	1002	SAH	OXT-C-CA-N

There are no ring outliers.

12 monomers are involved in 30 short contacts:

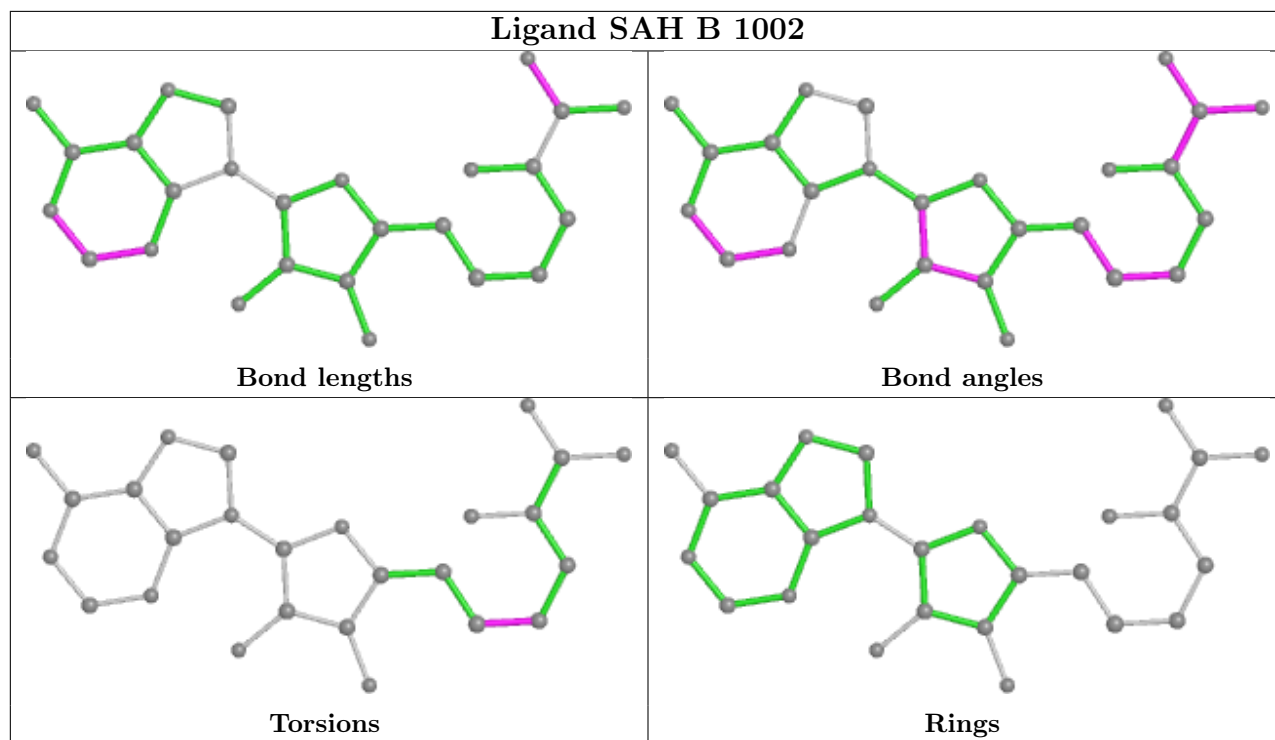
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	SAH	2	0
3	I	1002	SAH	2	0
3	A	1002	SAH	2	0

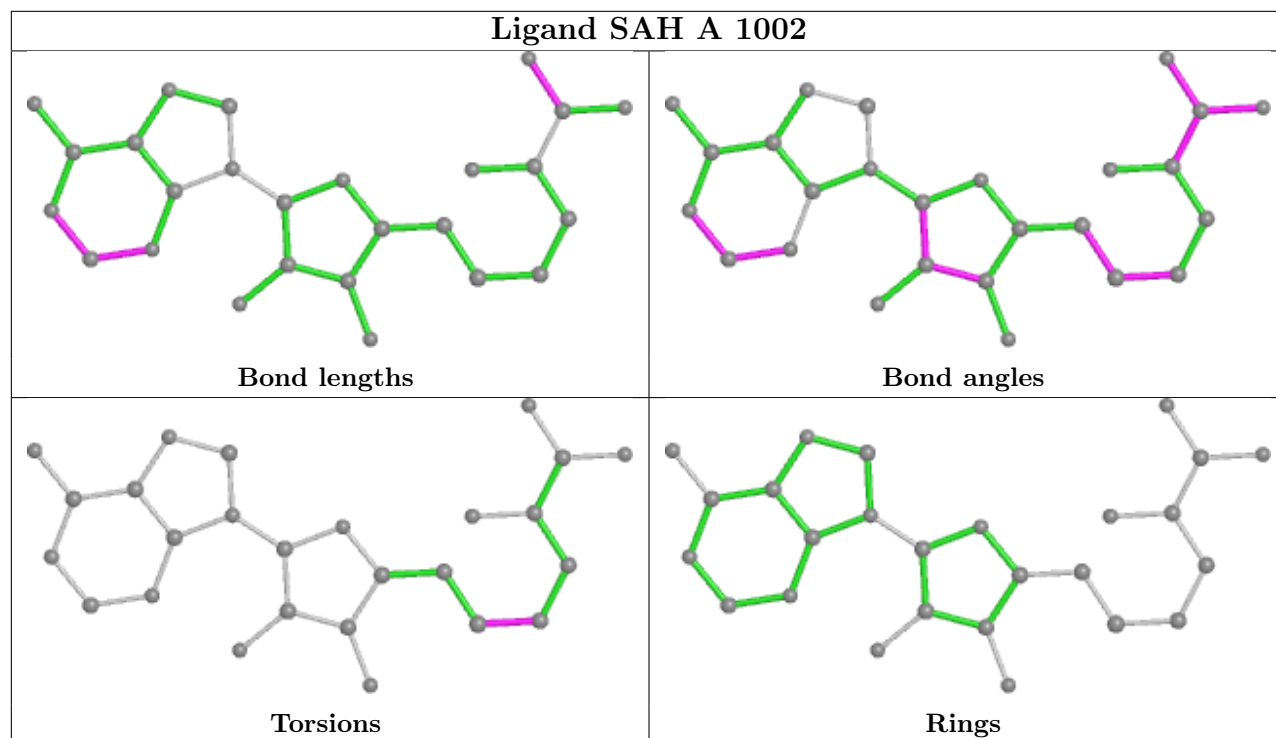
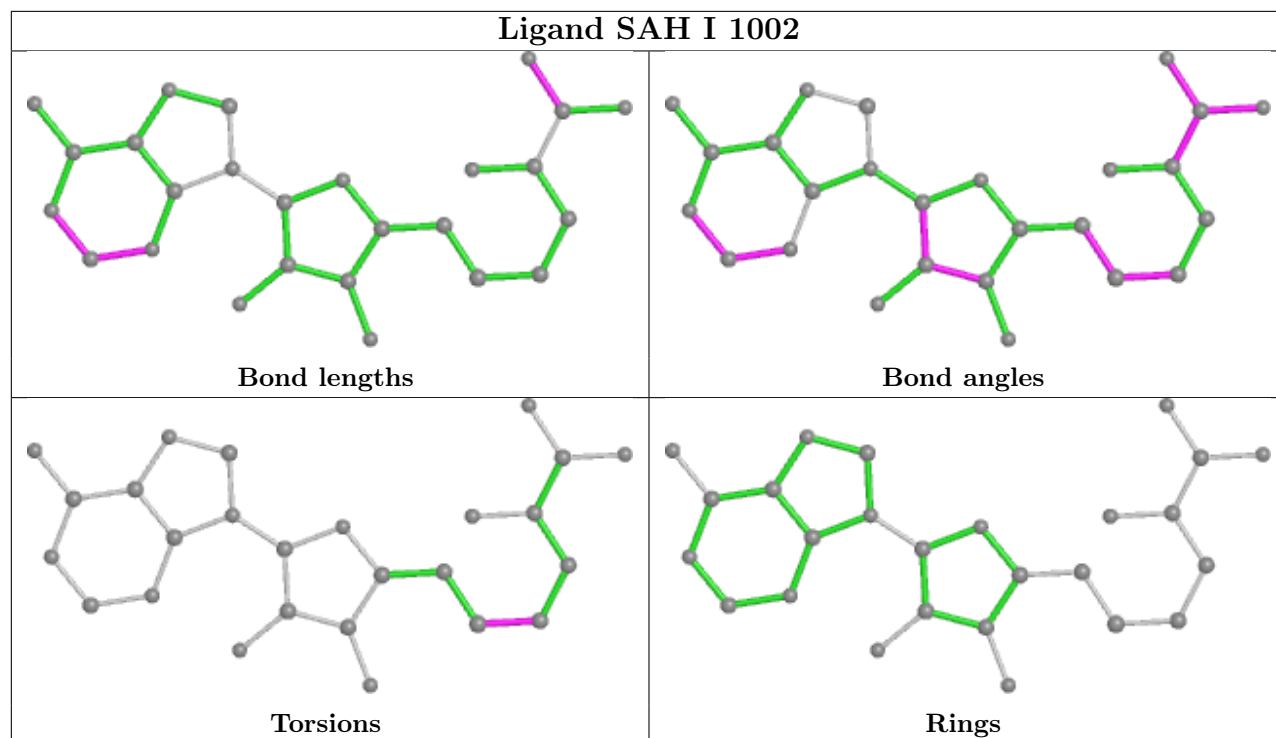
Continued on next page...

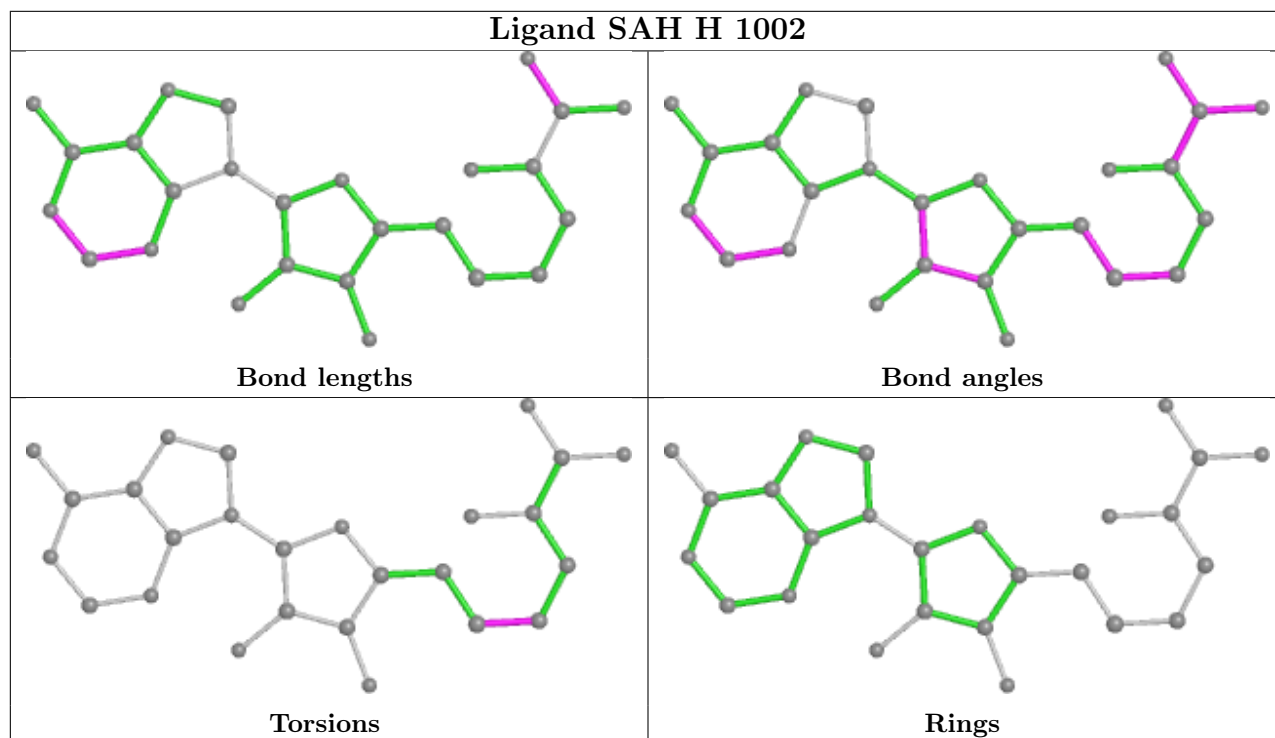
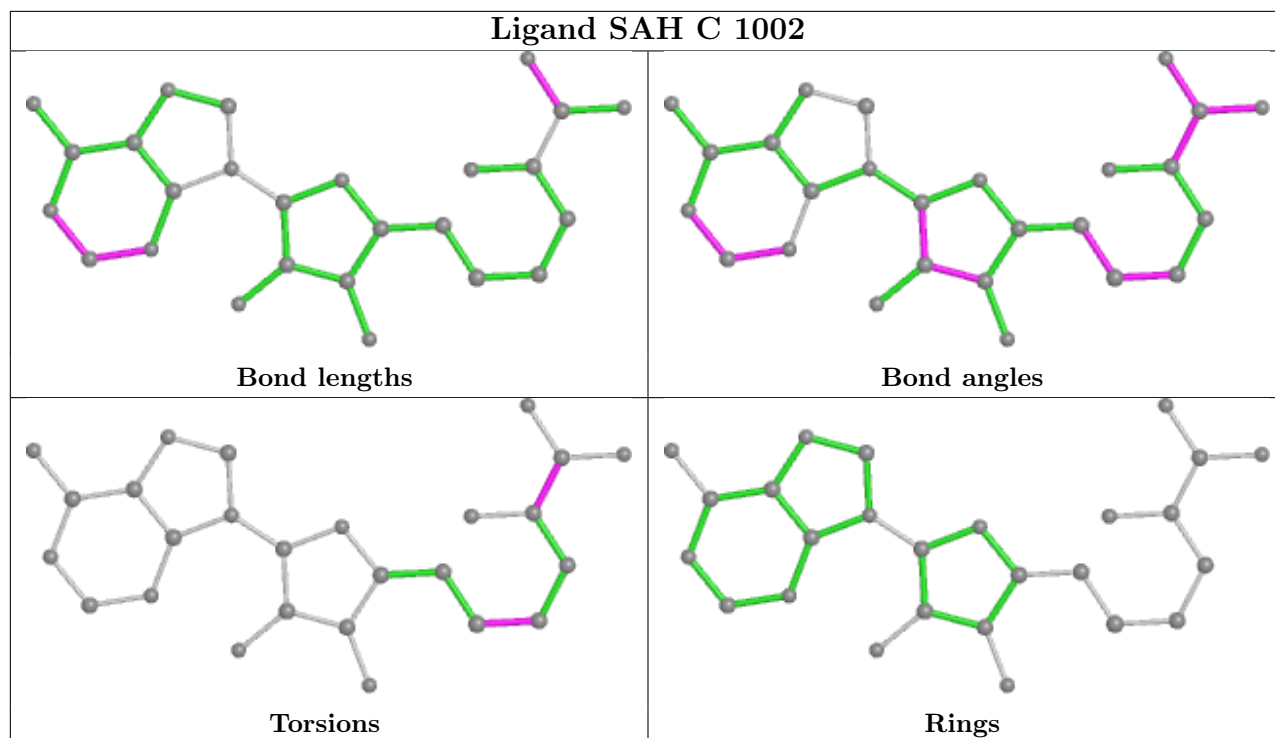
Continued from previous page...

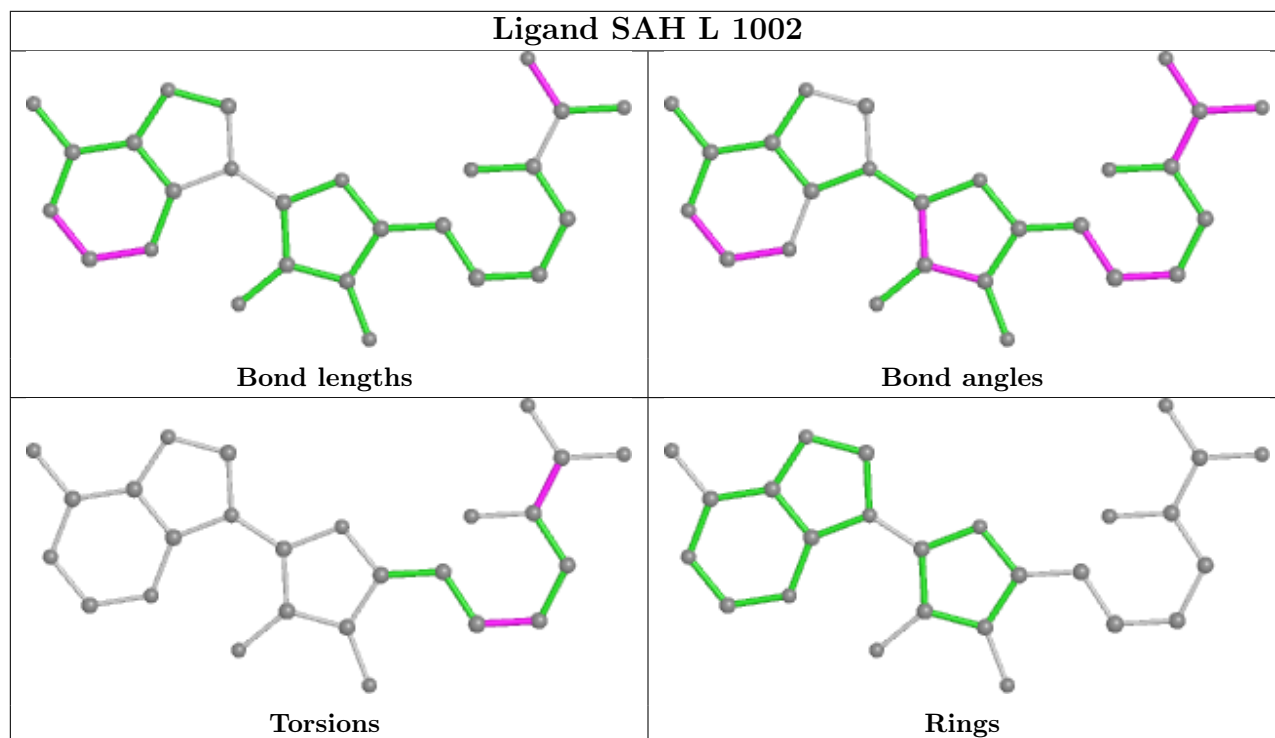
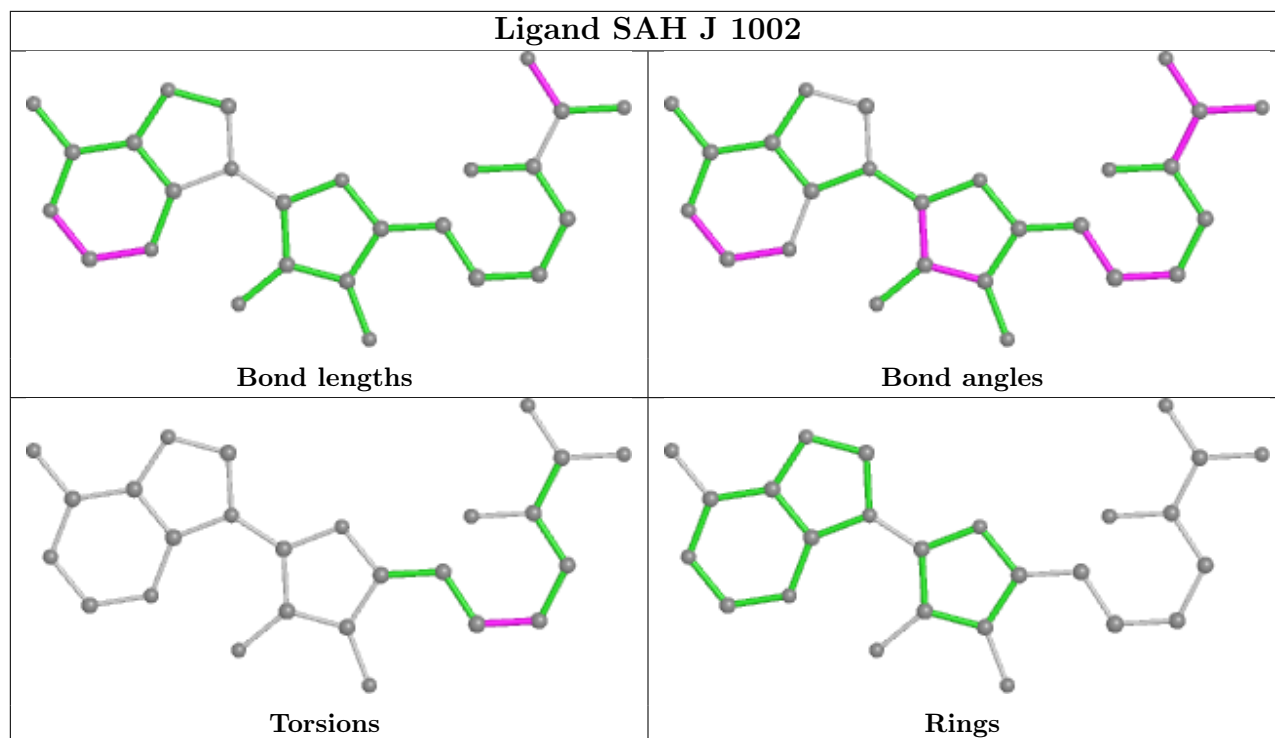
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1002	SAH	4	0
3	H	1002	SAH	2	0
3	J	1002	SAH	2	0
3	L	1002	SAH	3	0
3	K	1002	SAH	3	0
3	D	1002	SAH	2	0
3	G	1002	SAH	2	0
3	E	1002	SAH	3	0
3	F	1002	SAH	3	0

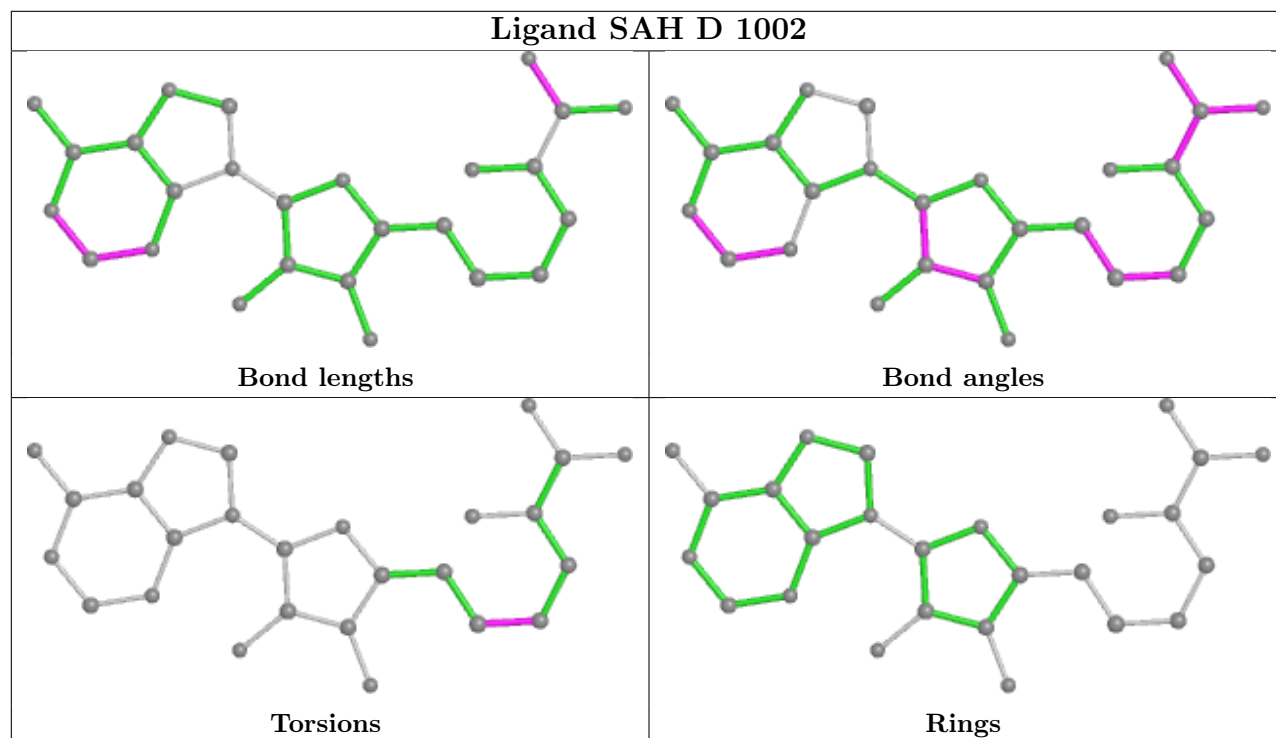
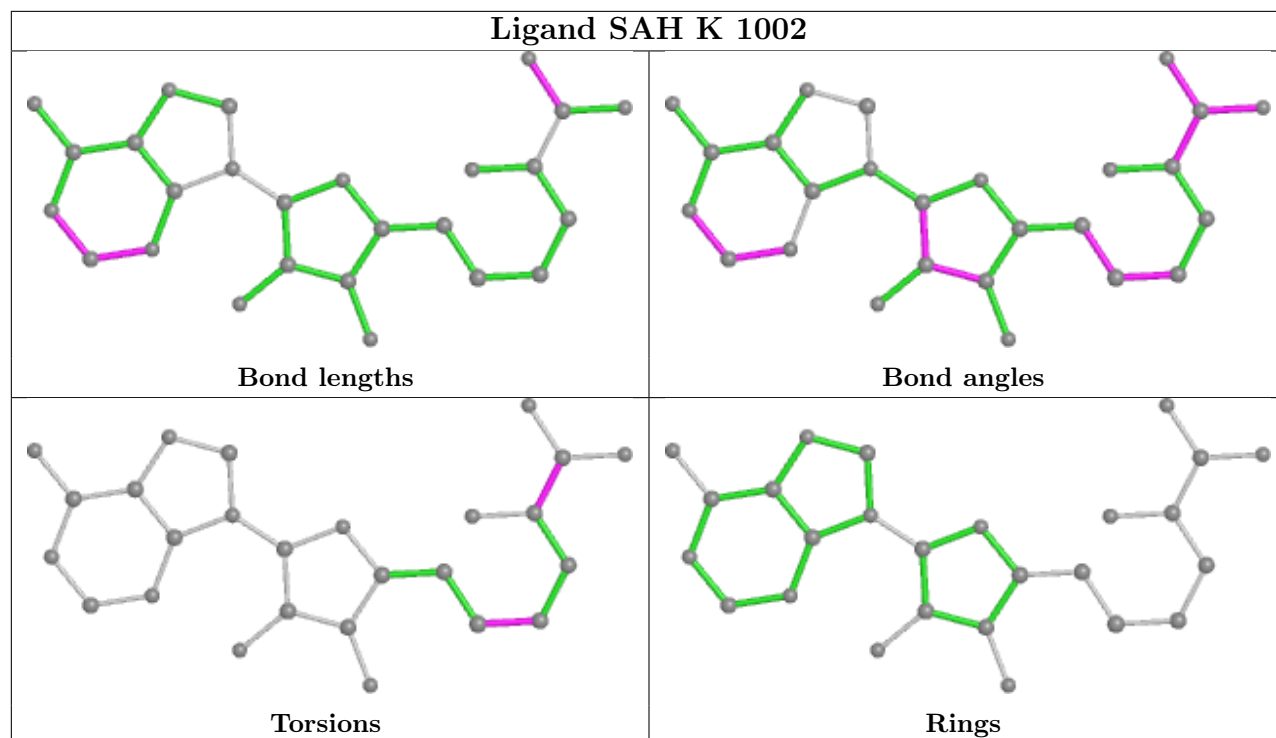
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

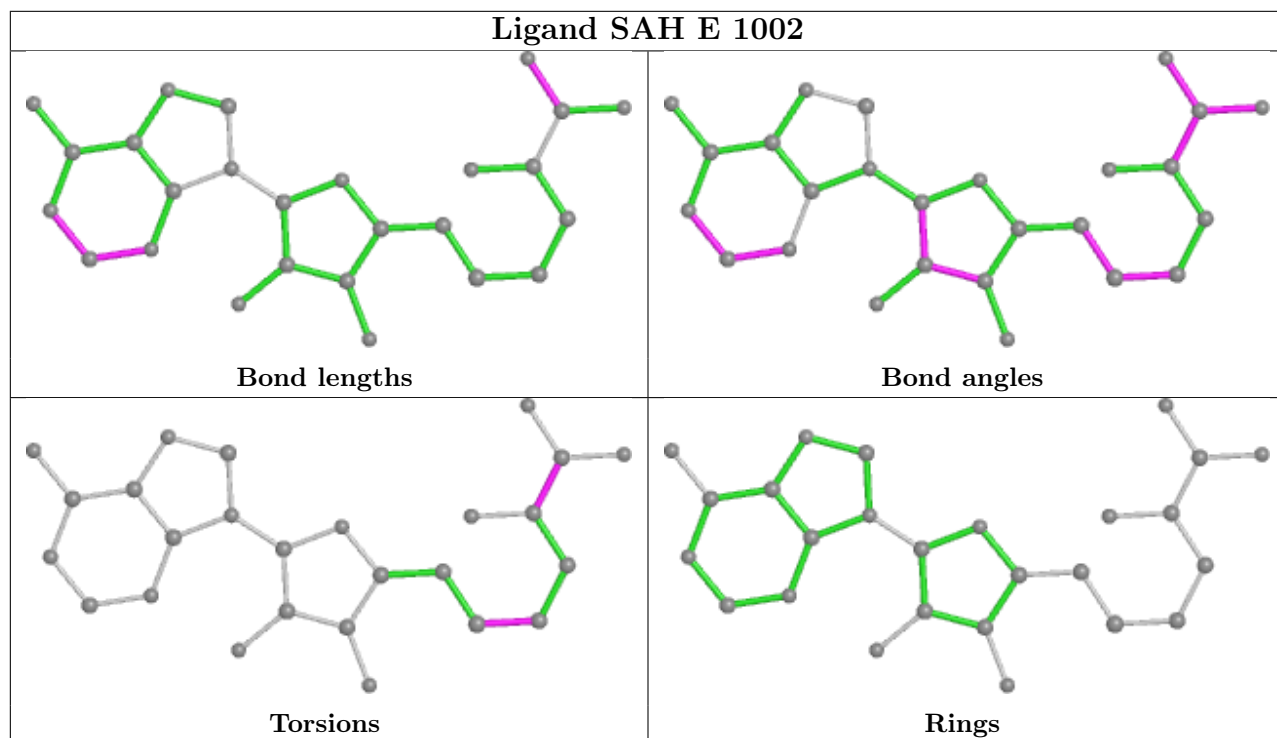
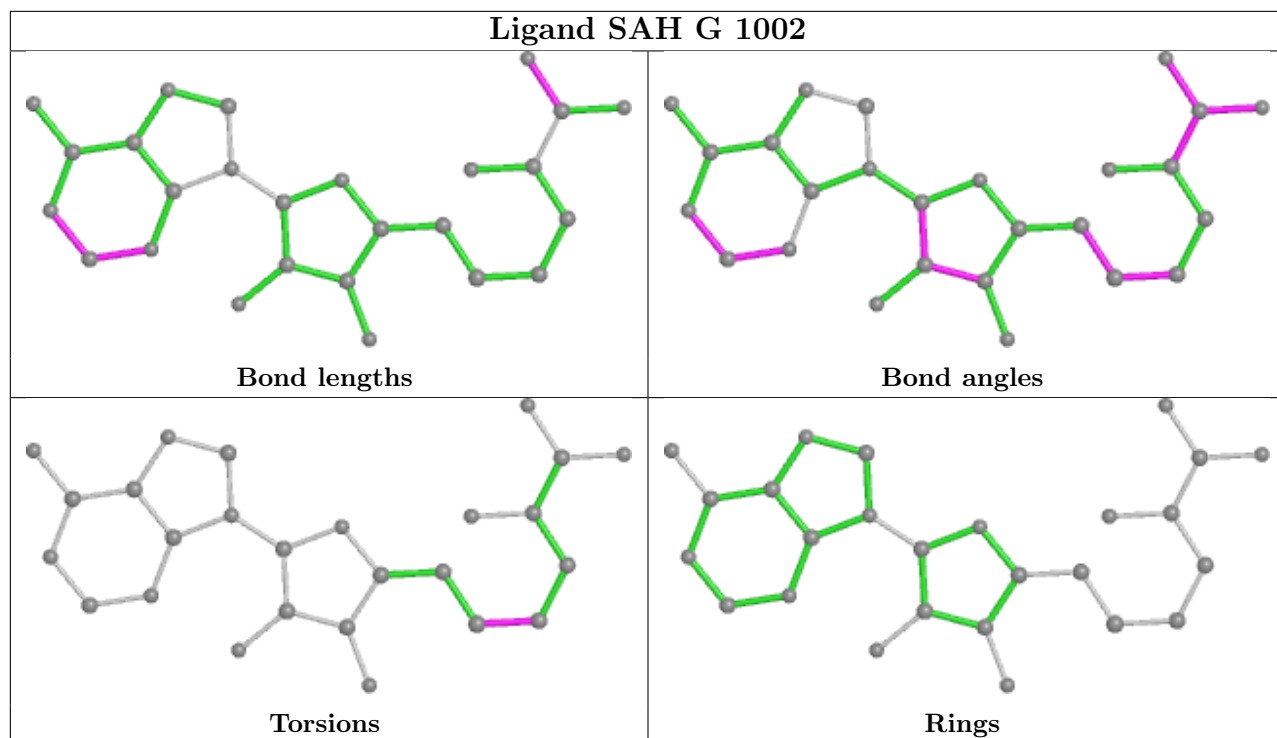


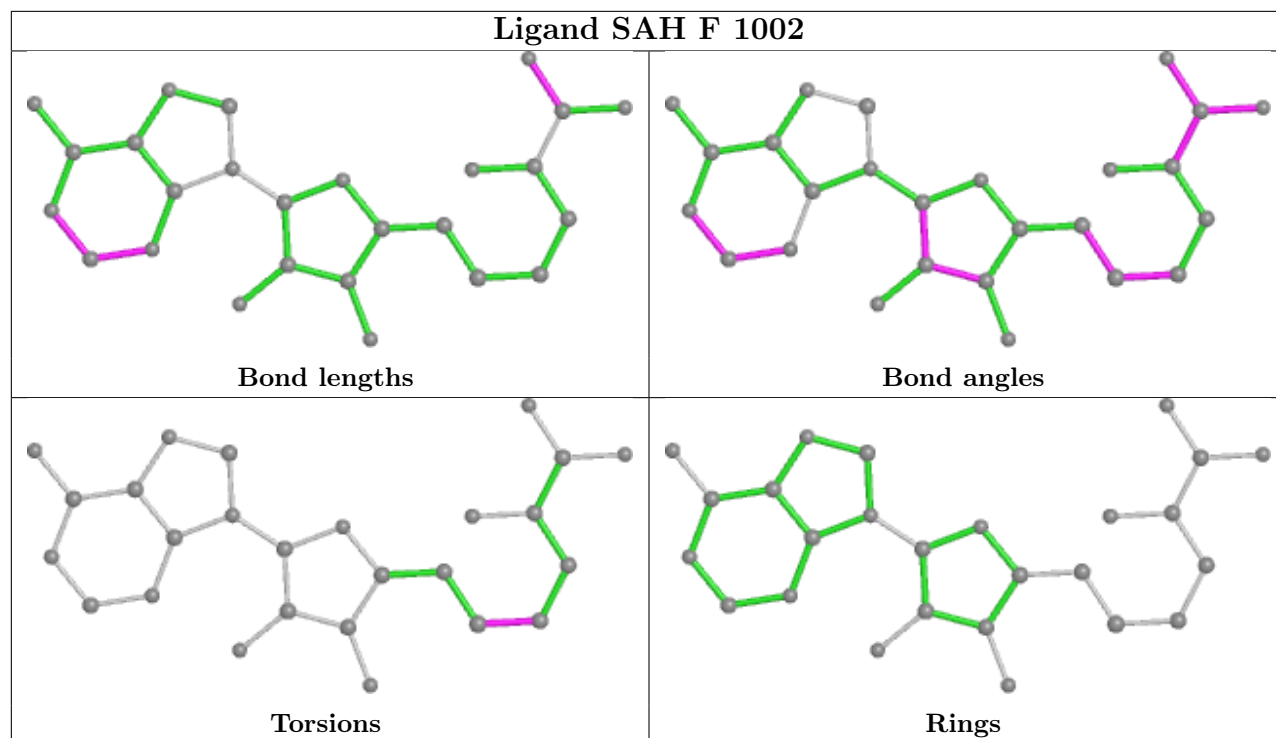












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

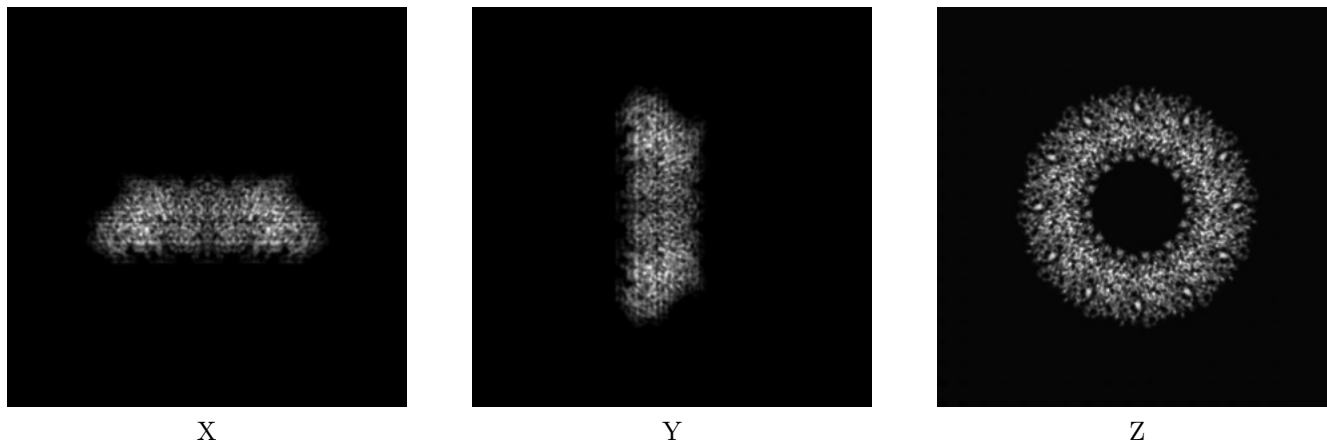
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15578. These allow visual inspection of the internal detail of the map and identification of artifacts.

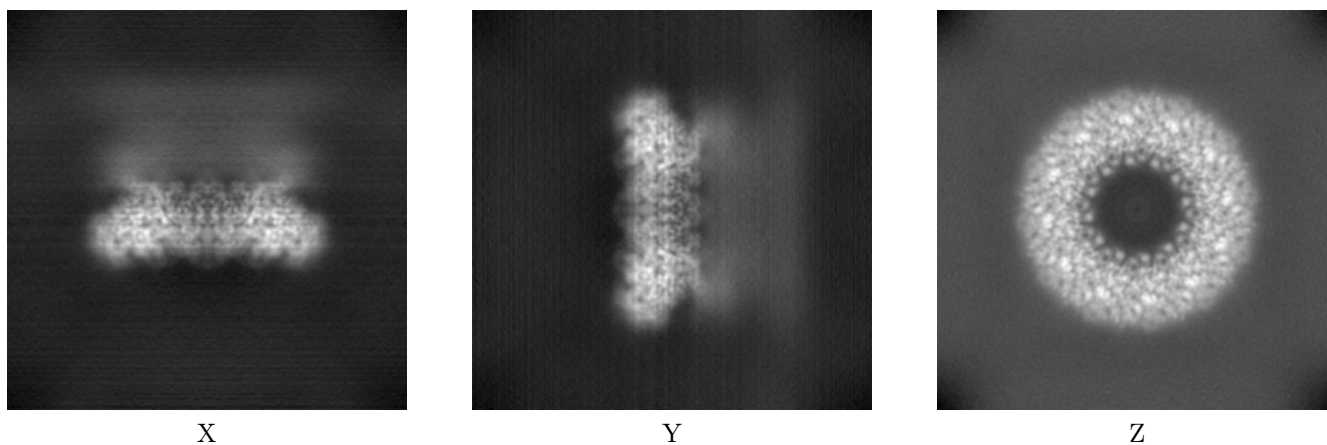
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



6.1.2 Raw map



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

6.2 Central slices [i](#)

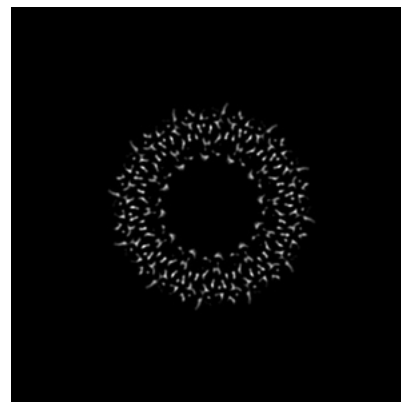
6.2.1 Primary map



X Index: 180

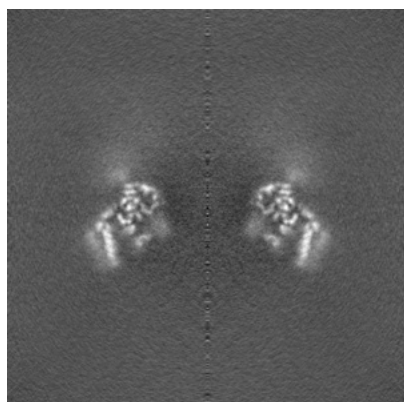


Y Index: 180

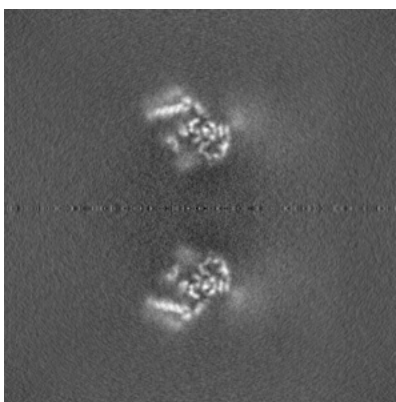


Z Index: 180

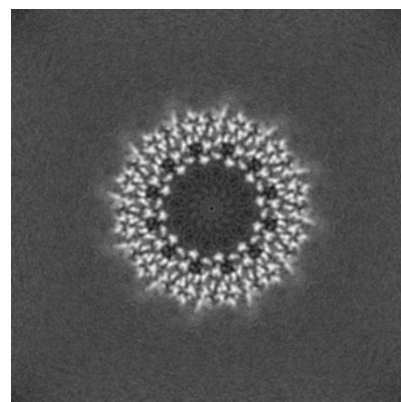
6.2.2 Raw map



X Index: 180



Y Index: 180

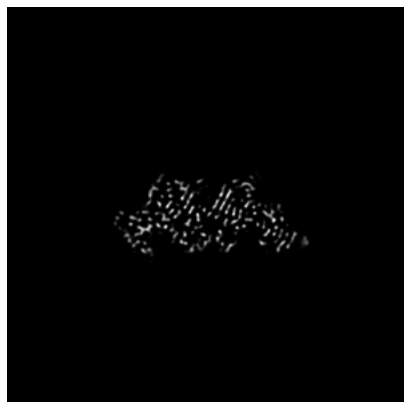


Z Index: 180

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: 119

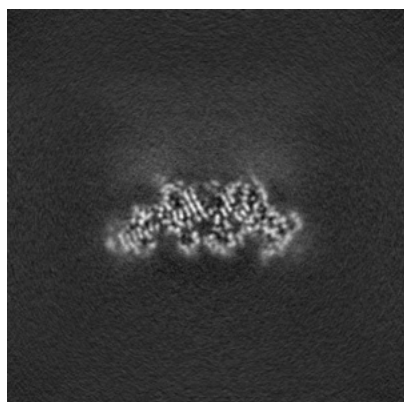


Y Index: 119

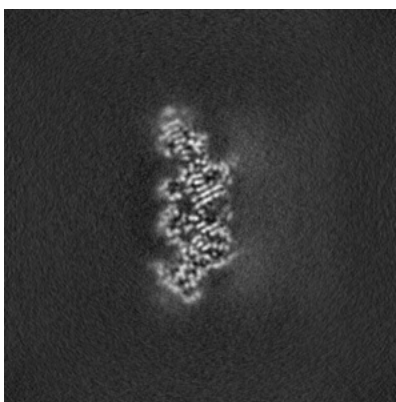


Z Index: 160

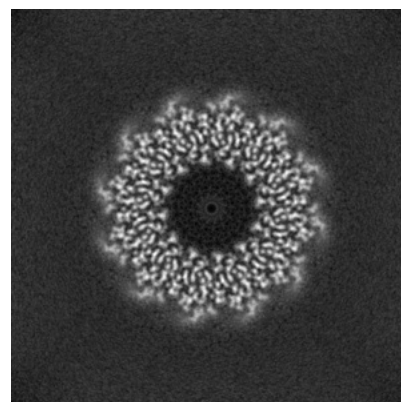
6.3.2 Raw map



X Index: 241



Y Index: 241

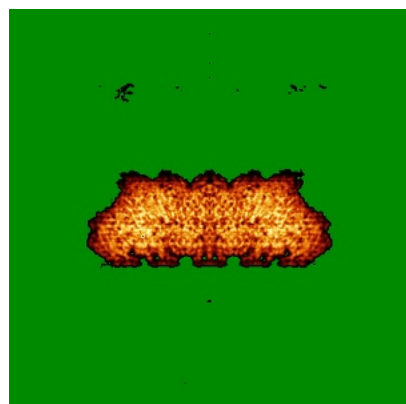


Z Index: 174

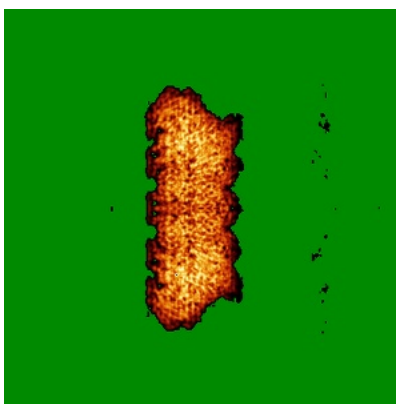
The images above show the largest variance slices of the map in three orthogonal directions.

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

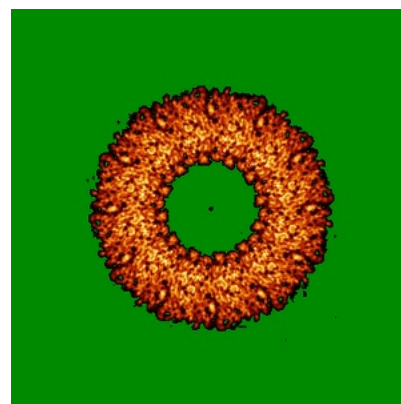
6.4.1 Primary map



X

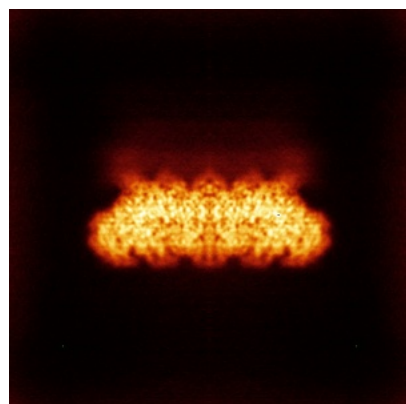


Y

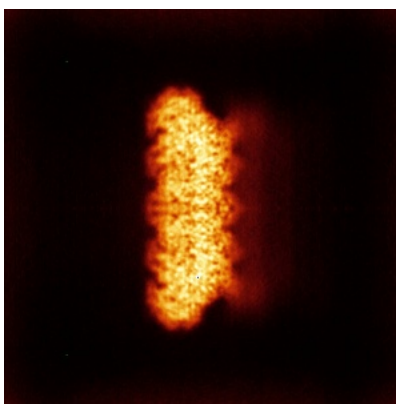


Z

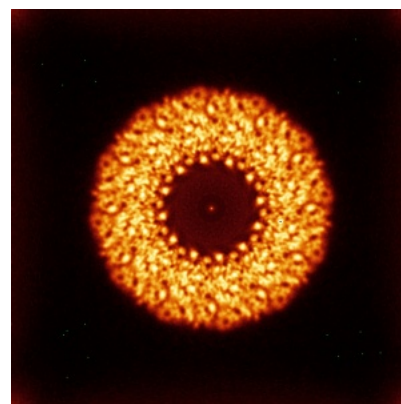
6.4.2 Raw map



X



Y

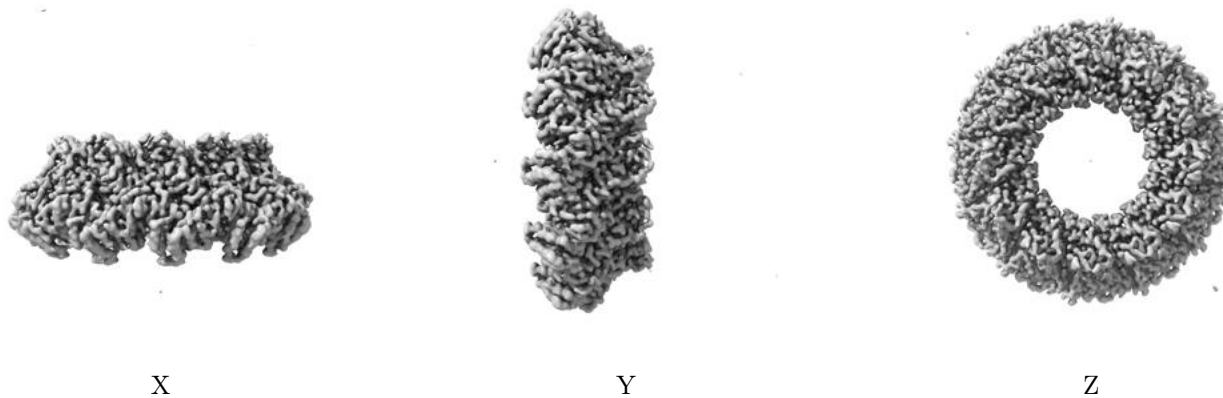


Z

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

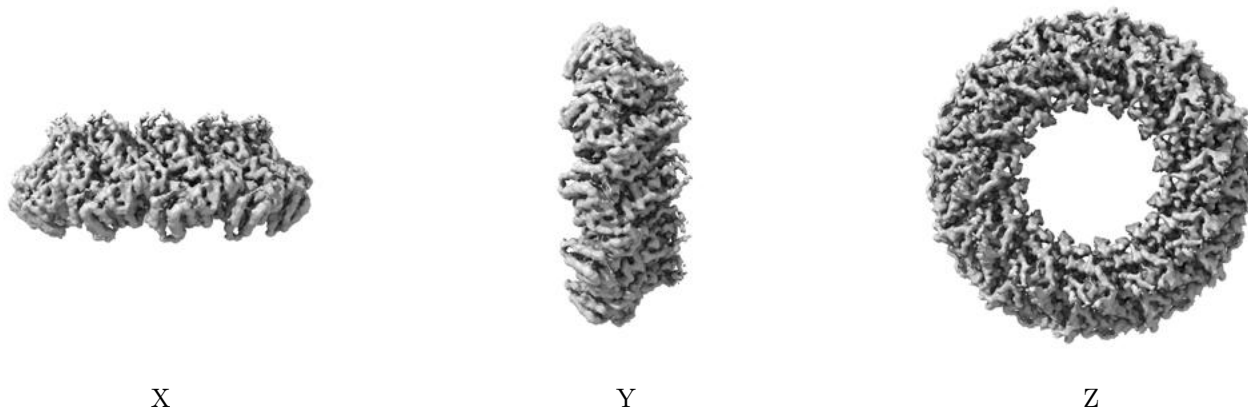
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0576. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

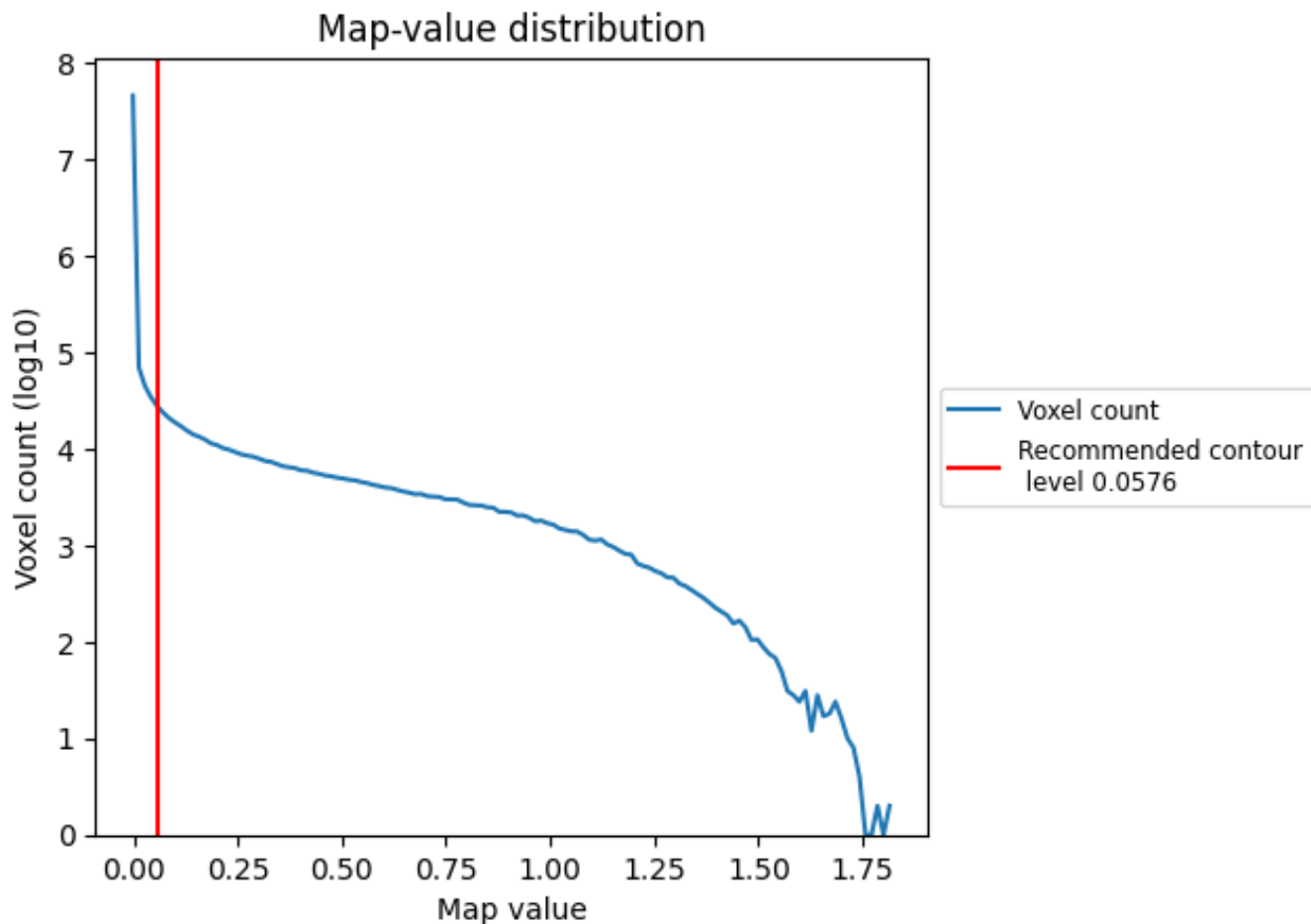
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

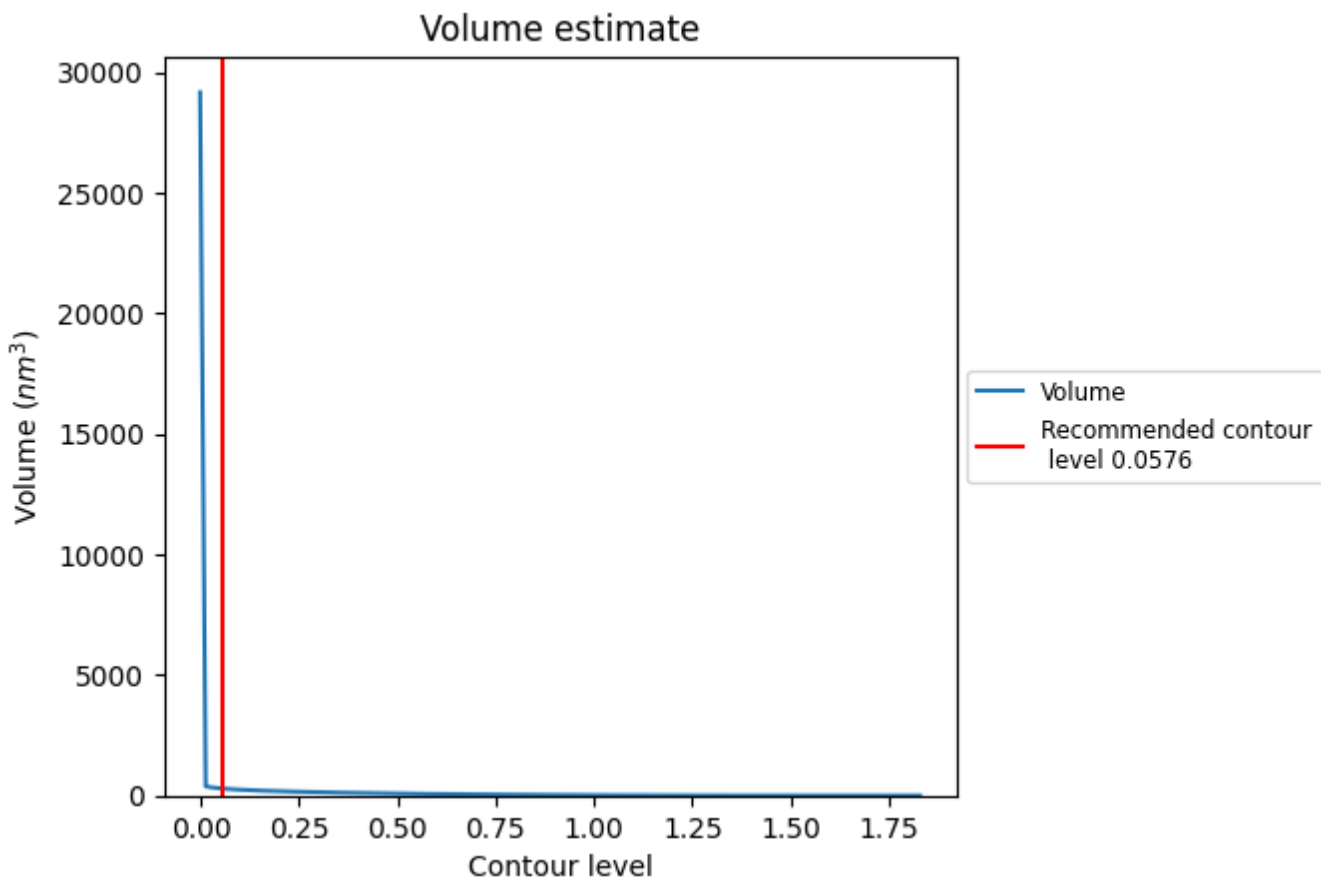
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

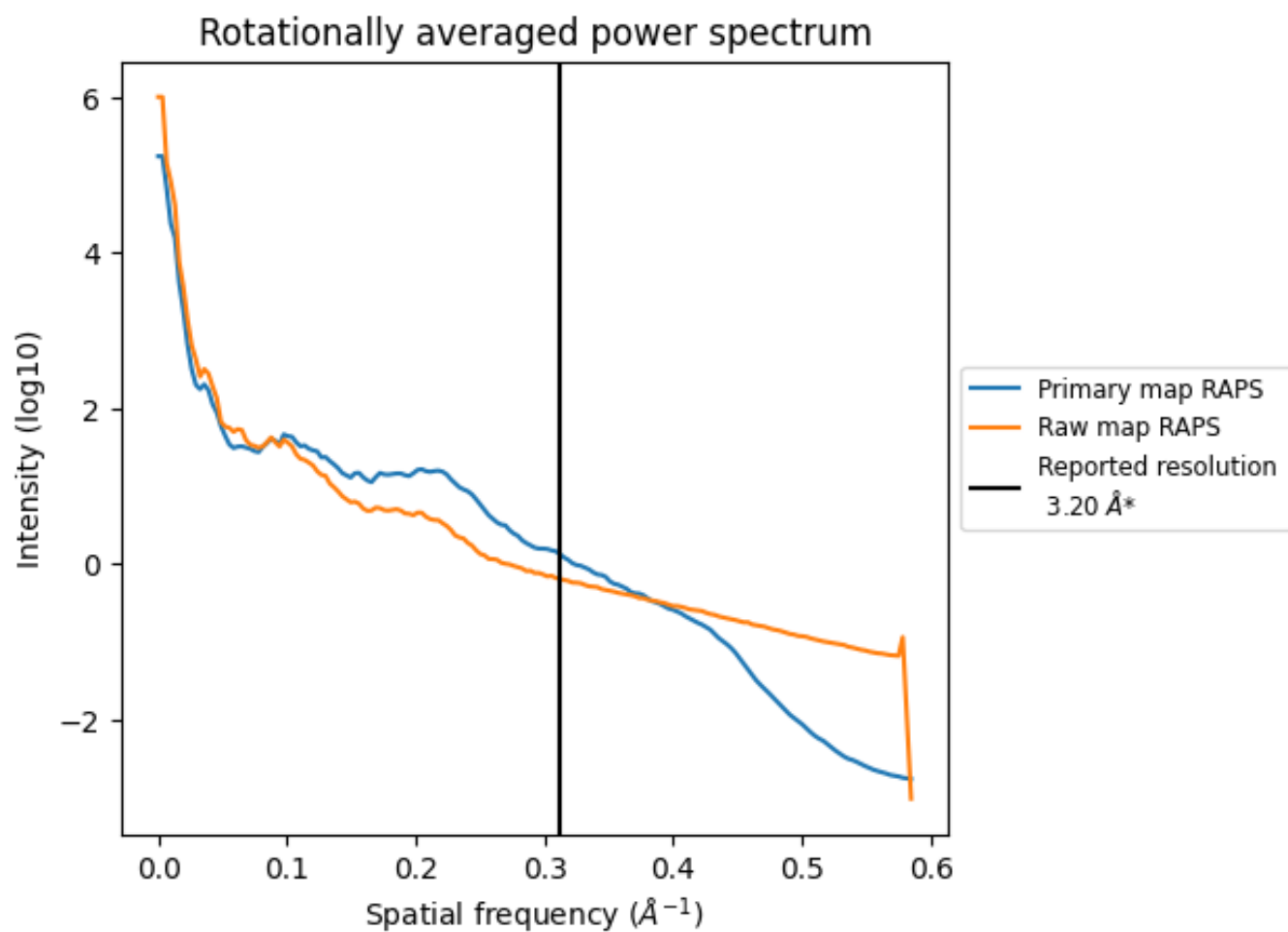
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 288 nm³; this corresponds to an approximate mass of 260 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

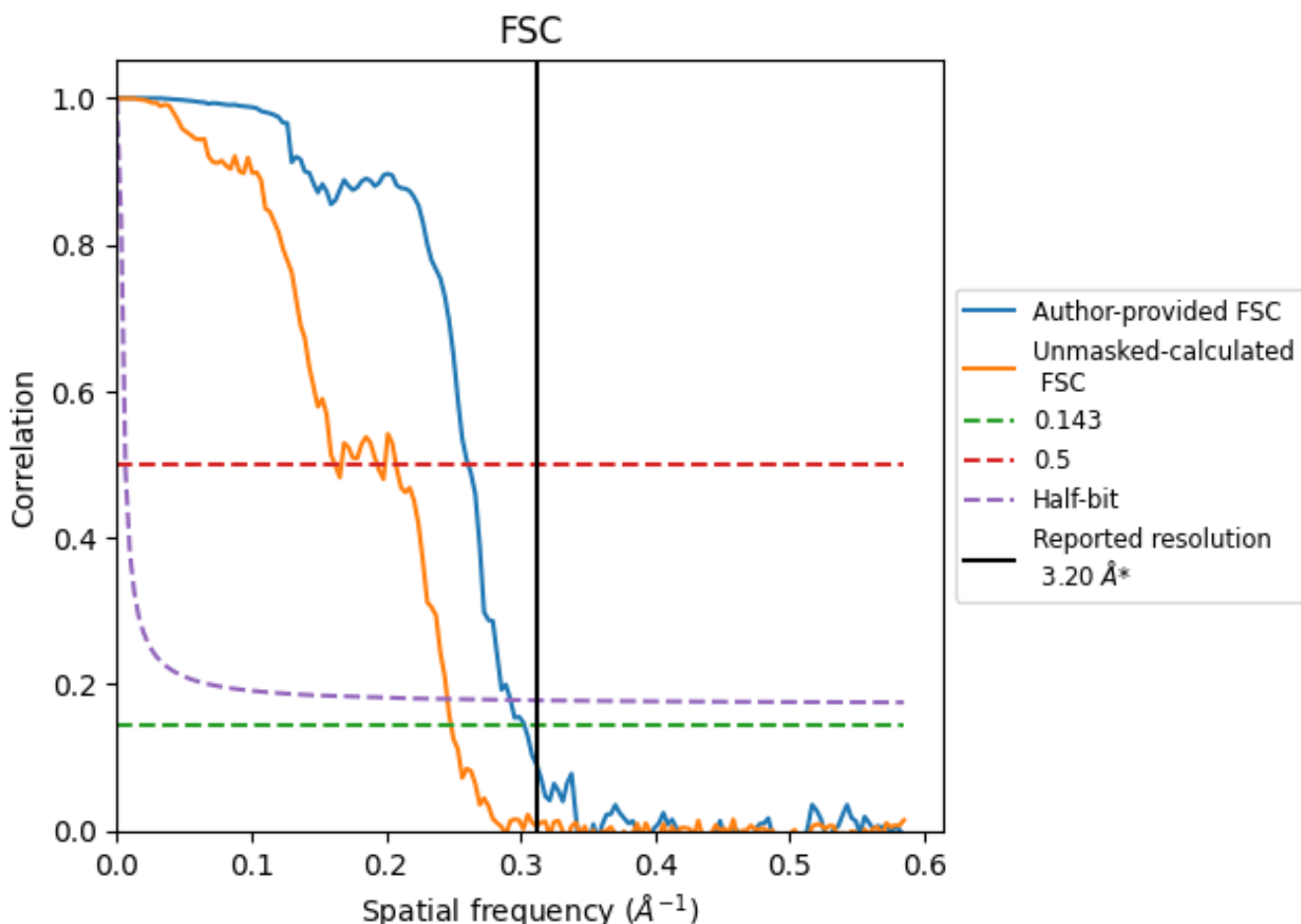


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

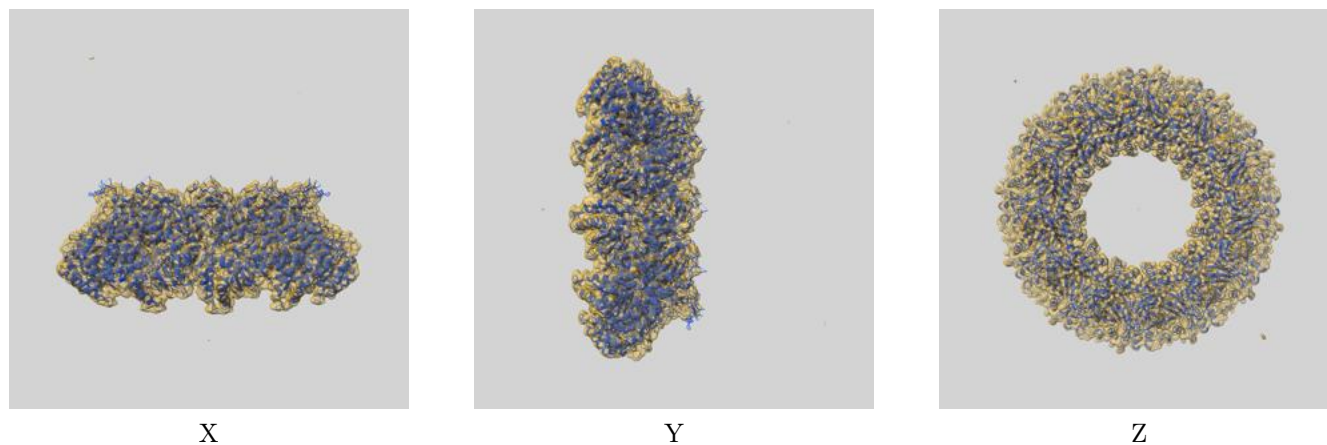
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.30	3.83	3.42
Unmasked-calculated*	4.03	6.17	4.07

*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 4.03 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

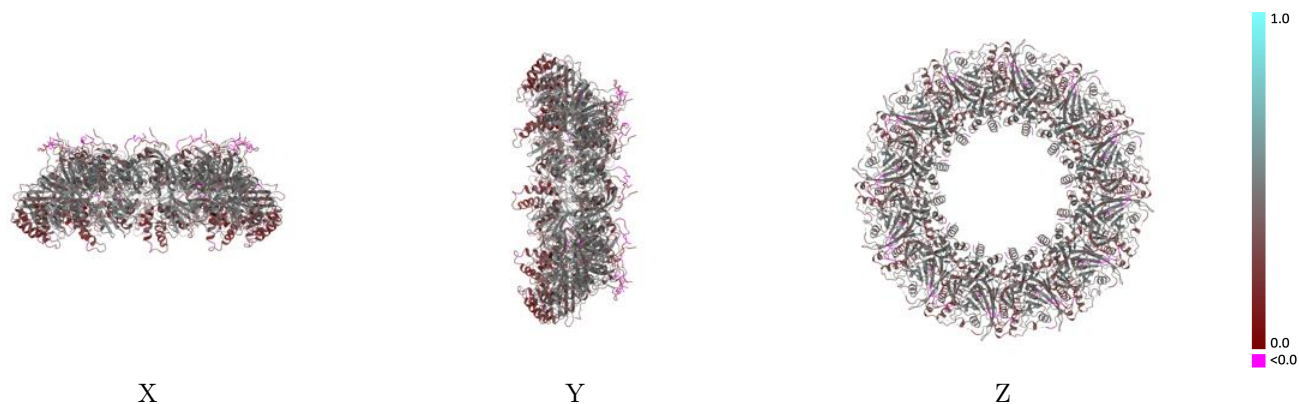
This section contains information regarding the fit between EMDB map EMD-15578 and PDB model 8APX. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



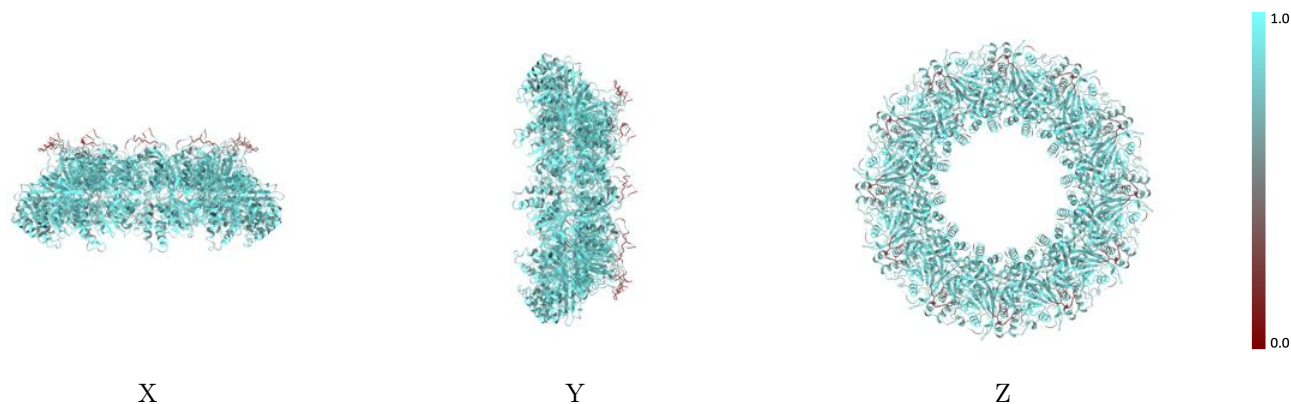
The images above show the 3D surface view of the map at the recommended contour level 0.0576 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



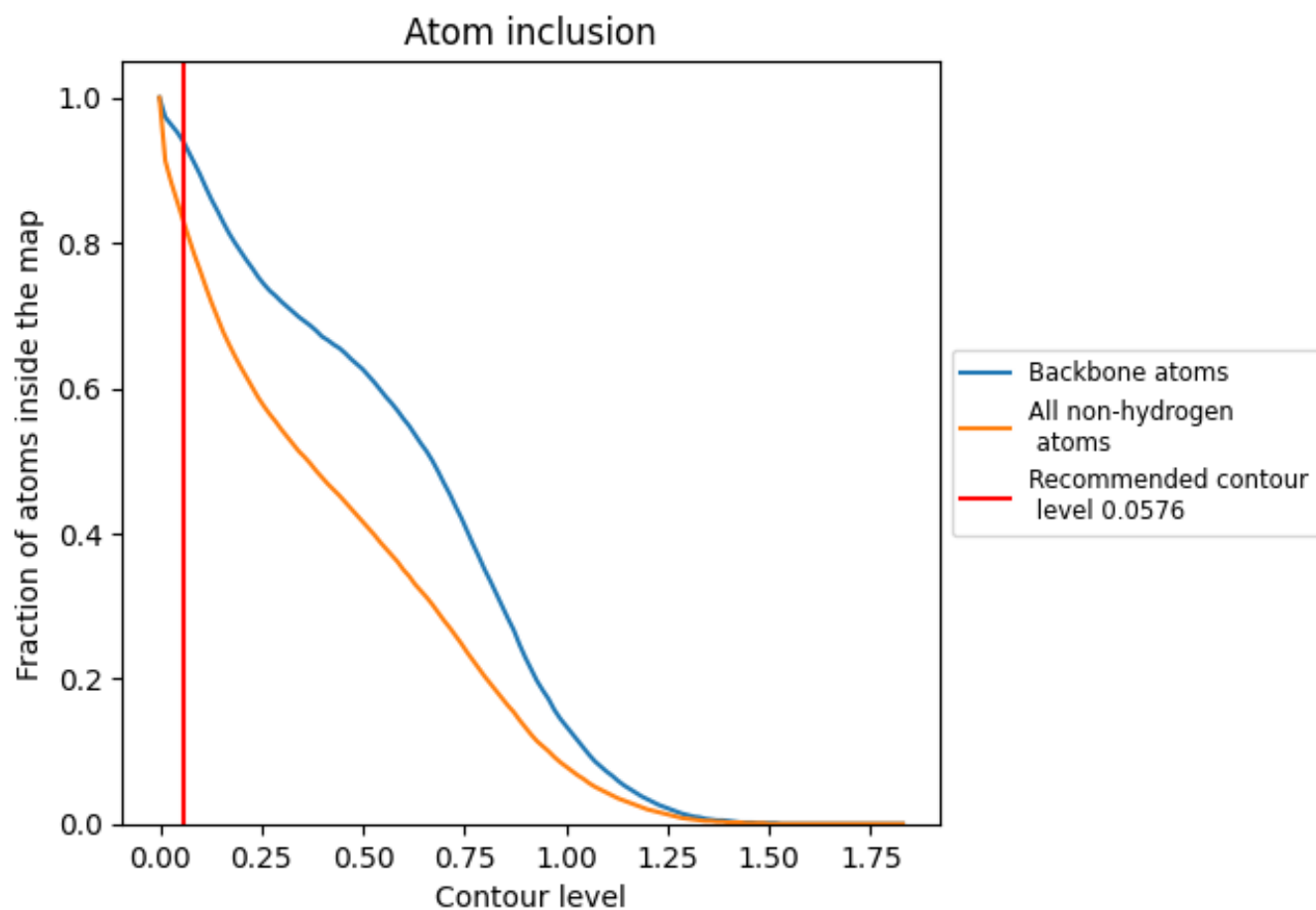
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0576).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0576) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8290	 0.3910
A	 0.8310	 0.3890
B	 0.8340	 0.3930
C	 0.8310	 0.3930
D	 0.8320	 0.3930
E	 0.8270	 0.3900
F	 0.8270	 0.3900
G	 0.8290	 0.3920
H	 0.8270	 0.3920
I	 0.8320	 0.3900
J	 0.8330	 0.3900
K	 0.8260	 0.3910
L	 0.8250	 0.3890

